



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:38 AM UTC

PDB ID : 8YGD / pdb\_00008ygd  
EMDB ID : EMD-39244  
Title : Rhodobacter blasticus RC-LH1 dimer  
Authors : Liu, L.N.; Zhang, Y.Z.; Wang, P.; Christianson, B.M.; Ugurlar, D.  
Deposited on : 2024-02-26  
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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

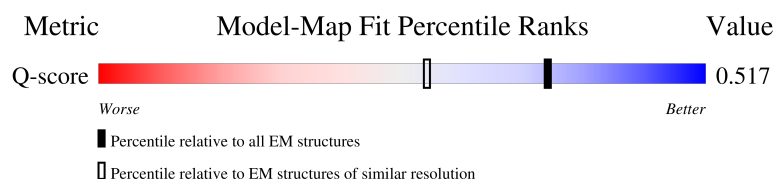
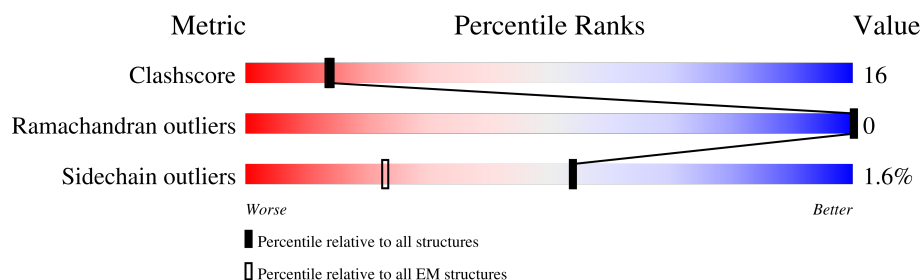
# 1 Overall quality at a glance

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   | 0     | 49     |                  |
| 1   | 2     | 49     |                  |
| 1   | 8     | 49     |                  |
| 1   | B     | 49     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | C     | 49     |                  |
| 1   | E     | 49     |                  |
| 1   | G     | 49     |                  |
| 1   | J     | 49     |                  |
| 1   | N     | 49     |                  |
| 1   | P     | 49     |                  |
| 1   | R     | 49     |                  |
| 1   | T     | 49     |                  |
| 1   | V     | 49     |                  |
| 1   | Z     | 49     |                  |
| 1   | b     | 49     |                  |
| 2   | 1     | 62     |                  |
| 2   | 3     | 62     |                  |
| 2   | 7     | 62     |                  |
| 2   | 9     | 62     |                  |
| 2   | A     | 62     |                  |
| 2   | D     | 62     |                  |
| 2   | F     | 62     |                  |
| 2   | I     | 62     |                  |
| 2   | K     | 62     |                  |
| 2   | O     | 62     |                  |
| 2   | Q     | 62     |                  |
| 2   | S     | 62     |                  |
| 2   | U     | 62     |                  |
| 2   | W     | 62     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | a     | 62     |                  |
| 3   | H     | 256    |                  |
| 4   | L     | 282    |                  |
| 5   | M     | 307    |                  |
| 6   | X     | 75     |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 7   | BCL  | N     | 102 | -         | -        | X       | -                |
| 7   | BCL  | a     | 101 | -         | -        | X       | -                |

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 23255 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 beta chain.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | 0     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 360   | 241 | 56 | 62 | 1 |         |       |
| 1   | 2     | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 319   | 213 | 51 | 54 | 1 |         |       |
| 1   | 8     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 352   | 237 | 55 | 59 | 1 |         |       |
| 1   | B     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 352   | 237 | 55 | 59 | 1 |         |       |
| 1   | C     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 352   | 237 | 55 | 59 | 1 |         |       |
| 1   | E     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 352   | 237 | 55 | 59 | 1 |         |       |
| 1   | G     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 352   | 237 | 55 | 59 | 1 |         |       |
| 1   | J     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 352   | 237 | 55 | 59 | 1 |         |       |
| 1   | N     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 352   | 237 | 55 | 59 | 1 |         |       |
| 1   | P     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 352   | 237 | 55 | 59 | 1 |         |       |
| 1   | R     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 352   | 237 | 55 | 59 | 1 |         |       |
| 1   | T     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 352   | 237 | 55 | 59 | 1 |         |       |
| 1   | V     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 352   | 237 | 55 | 59 | 1 |         |       |
| 1   | Z     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 338   | 228 | 53 | 56 | 1 |         |       |
| 1   | b     | 36       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 300   | 201 | 48 | 50 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | 1     | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 412   | 283 | 65 | 63 | 1 |         |       |
| 2   | 3     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 438   | 298 | 72 | 67 | 1 |         |       |
| 2   | 7     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 379   | 262 | 60 | 55 | 2 |         |       |
| 2   | 9     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 303 | 73 | 68 | 2 |         |       |
| 2   | A     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 303 | 73 | 68 | 2 |         |       |
| 2   | D     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 303 | 73 | 68 | 2 |         |       |
| 2   | F     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 303 | 73 | 68 | 2 |         |       |
| 2   | I     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 303 | 73 | 68 | 2 |         |       |
| 2   | K     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 438   | 298 | 72 | 67 | 1 |         |       |
| 2   | O     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 438   | 298 | 72 | 67 | 1 |         |       |
| 2   | Q     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 438   | 298 | 72 | 67 | 1 |         |       |
| 2   | S     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 438   | 298 | 72 | 67 | 1 |         |       |
| 2   | U     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 438   | 298 | 72 | 67 | 1 |         |       |
| 2   | W     | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 432   | 295 | 71 | 65 | 1 |         |       |
| 2   | a     | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 401   | 274 | 64 | 62 | 1 |         |       |

- Molecule 3 is a protein called Photosynthetic reaction center subunit H.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | H     | 254      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1980  | 1259 | 347 | 366 | 8 |         |       |

- Molecule 4 is a protein called Reaction center protein L chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | L     | 281      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2231  | 1503 | 349 | 370 | 9 |         |       |

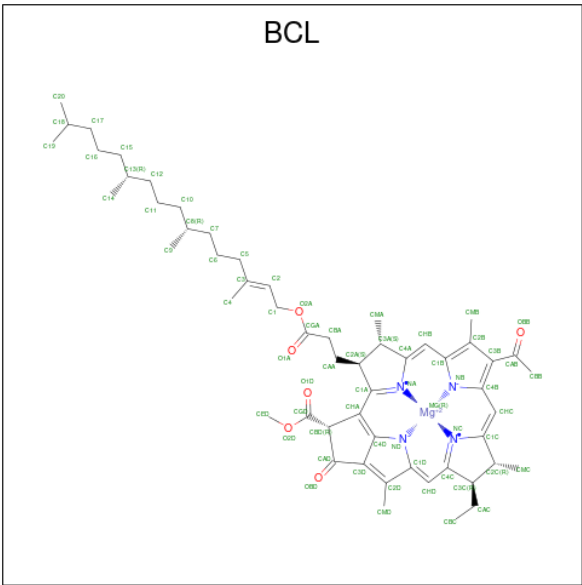
- Molecule 5 is a protein called Reaction center protein M chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | M     | 304      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2432  | 1622 | 394 | 405 | 11 |         |       |

- Molecule 6 is a protein called 1-deoxy-D-xylulose-5-phosphate synthase.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | X     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 451   | 298 | 74 | 77 | 2 |         |       |

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



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 7   | 0     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 7   | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 7   | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 7   | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 7   | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

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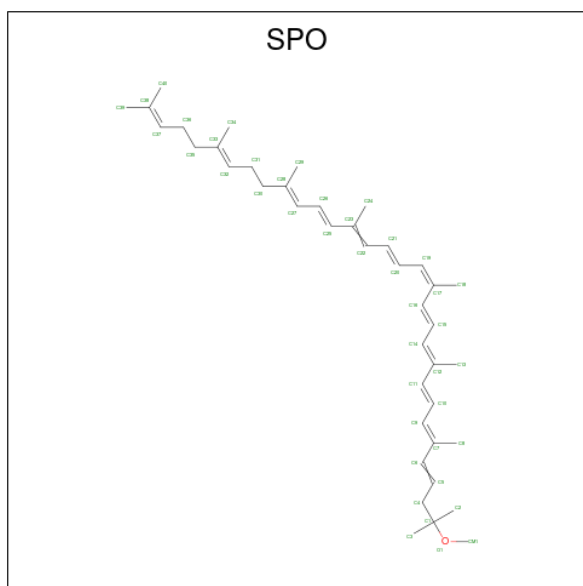
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 7   | 9     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | A     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | B     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | C     | 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   | E     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | F     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | F     | 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   | J     | 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   | L     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | L     | 1        | Total<br>63 | C<br>52 | 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   | N     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | O     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | P     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 7   | Q     | 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   | S     | 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   | T     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | U     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 7   | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 7   | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |

- Molecule 8 is SPHEROIDENE (CCD ID: SPO) (formula:  $C_{41}H_{60}O$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 8   | 0     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | 0     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |

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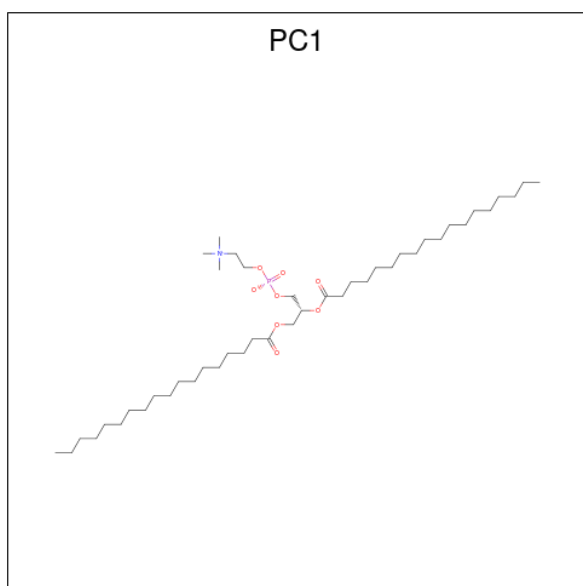
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 8   | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 39    | 38 | 1 |         |
| 8   | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | D     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | D     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | E     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | F     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | I     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | J     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | K     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | M     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | N     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | O     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | P     | 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   | S     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | S     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | T     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | U     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 8   | U     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | W     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |
| 8   | Z     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 41 | 1 |         |

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



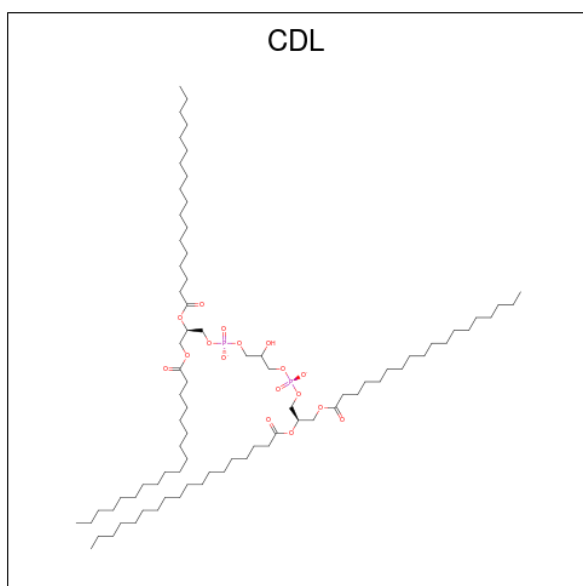
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 9   | 9     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 9   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 32    | 22 | 1 | 8 | 1 |         |
| 9   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 32    | 22 | 1 | 8 | 1 |         |
| 9   | F     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 37    | 27 | 1 | 8 | 1 |         |
| 9   | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 9   | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 9   | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |
| 9   | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |

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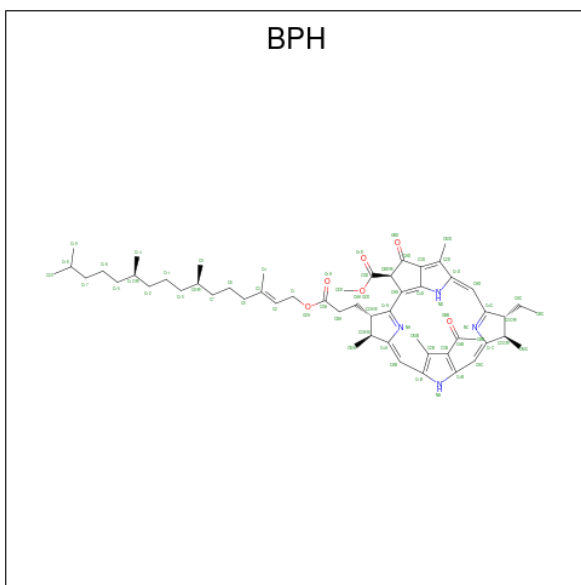
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 9   | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 9   | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 32    | 22 | 1 | 8 | 1 |         |
| 9   | W     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 32    | 22 | 1 | 8 | 1 |         |

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).



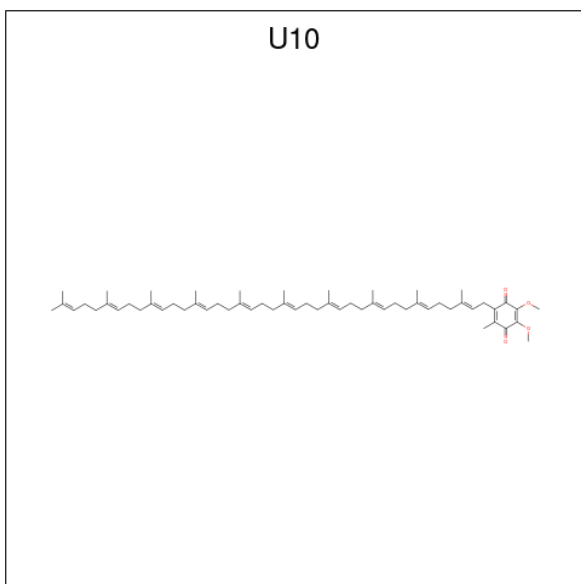
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 10  | F     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 78    | 59 | 17 | 2 |         |
| 10  | M     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 10  | M     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 78    | 59 | 17 | 2 |         |

- Molecule 11 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 11  | L     | 1        | Total | C  | N | O | 0       |
|     |       |          | 62    | 52 | 4 | 6 |         |
| 11  | L     | 1        | Total | C  | N | O | 0       |
|     |       |          | 55    | 45 | 4 | 6 |         |

- Molecule 12 is UBIQUINONE-10 (CCD ID: U10) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 12  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 39 | 4 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 12  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 39 | 4 |         |
| 12  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 44 | 4 |         |
| 12  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 19    | 15 | 4 |         |
| 12  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 38    | 34 | 4 |         |
| 12  | M     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 44 | 4 |         |
| 12  | X     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 44 | 4 |         |

- Molecule 13 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

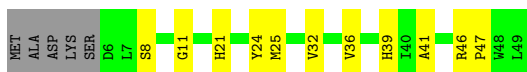
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 13  | M     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

### 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.

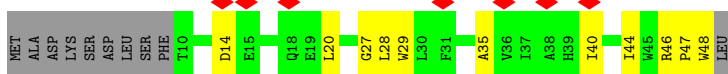
- Molecule 1: Antenna pigment protein beta chain

Chain 0: 



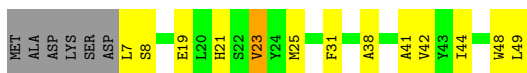
- Molecule 1: Antenna pigment protein beta chain

Chain 2: 



- Molecule 1: Antenna pigment protein beta chain

Chain 8: 



- Molecule 1: Antenna pigment protein beta chain

Chain B: 



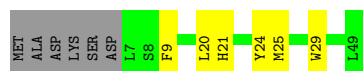
- Molecule 1: Antenna pigment protein beta chain

Chain C: 



- Molecule 1: Antenna pigment protein beta chain

Chain E:  76% 12% 12%



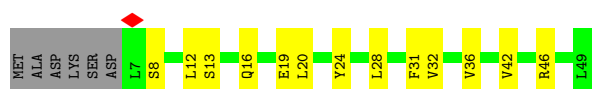
- Molecule 1: Antenna pigment protein beta chain

Chain G:  76% 12% 12%



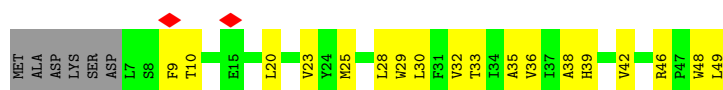
- Molecule 1: Antenna pigment protein beta chain

Chain J:  61% 27% 12%



- Molecule 1: Antenna pigment protein beta chain

Chain N:  51% 37% 12%



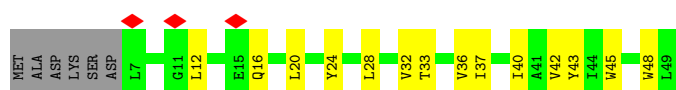
- Molecule 1: Antenna pigment protein beta chain

Chain P:  59% 29% 12%



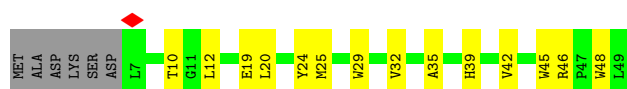
- Molecule 1: Antenna pigment protein beta chain

Chain R:  6% 59% 29% 12%

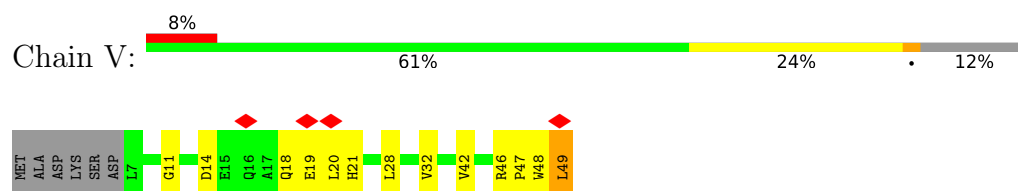


- Molecule 1: Antenna pigment protein beta chain

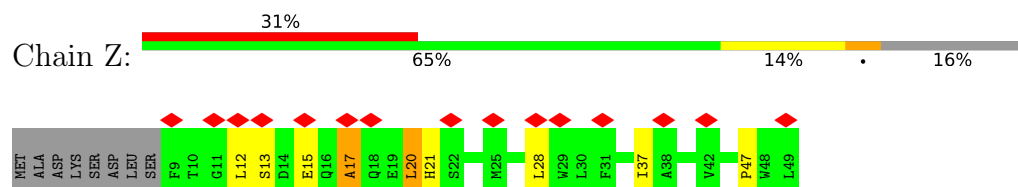
Chain T:  59% 29% 12%



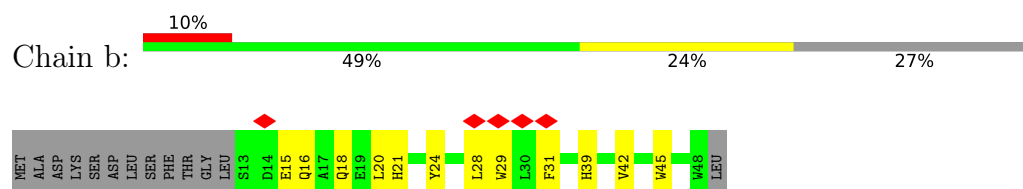
- Molecule 1: Antenna pigment protein beta chain



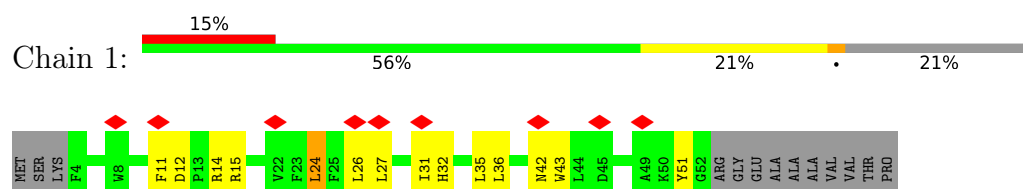
- Molecule 1: Antenna pigment protein beta chain



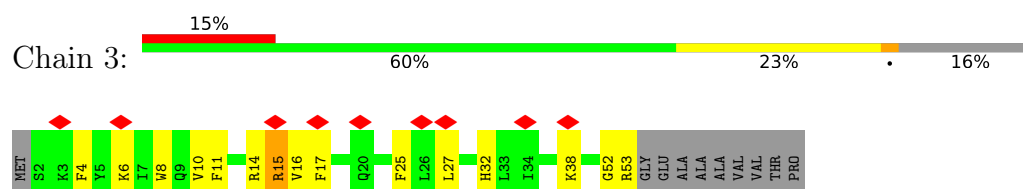
- Molecule 1: Antenna pigment protein beta chain



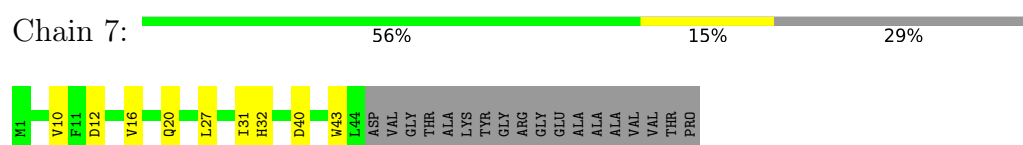
- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain

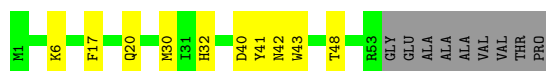


- Molecule 2: Antenna pigment protein alpha chain

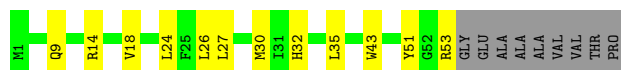


- Molecule 2: Antenna pigment protein alpha chain





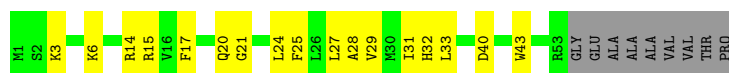
- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain



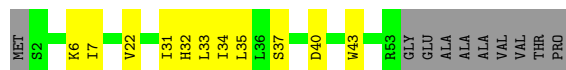
- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain

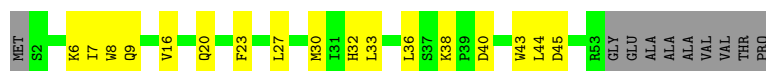


- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain





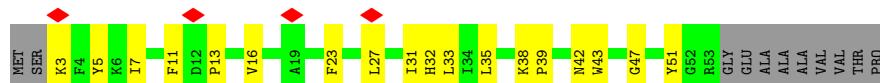
- Molecule 2: Antenna pigment protein alpha chain



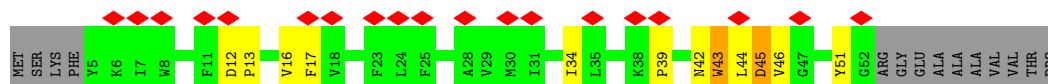
- Molecule 2: Antenna pigment protein alpha chain



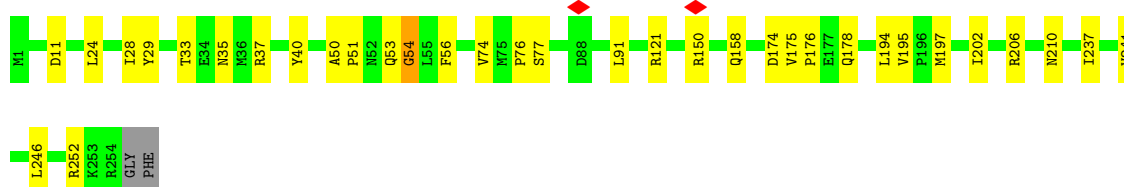
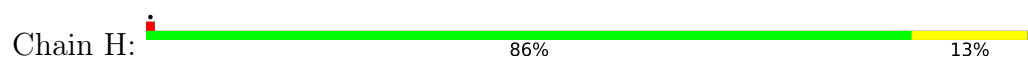
- Molecule 2: Antenna pigment protein alpha chain



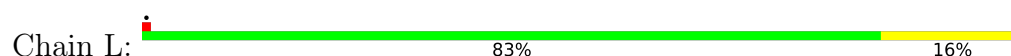
- Molecule 2: Antenna pigment protein alpha chain



- Molecule 3: Photosynthetic reaction center subunit H

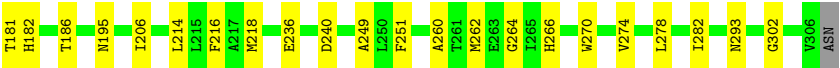
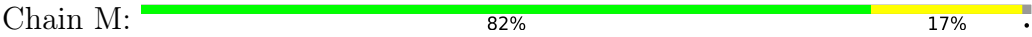


- Molecule 4: Reaction center protein L chain





• Molecule 5: Reaction center protein M chain



• Molecule 6: 1-deoxy-D-xylulose-5-phosphate synthase



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C2                               | Depositor |
| Number of particles used             | 9149                                    | 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 ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 1.177                                   | Depositor |
| Minimum map value                    | -0.768                                  | Depositor |
| Average map value                    | 0.005                                   | Depositor |
| Map value standard deviation         | 0.082                                   | Depositor |
| Recommended contour level            | 0.16                                    | Depositor |
| Map size (Å)                         | 237.824, 237.824, 237.824               | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.929, 0.929, 0.929                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SPO, BPH, BCL, CDL, PC1, FE2, U10

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   | 0     | 0.55         | 0/372         | 0.40        | 0/510         |
| 1   | 2     | 0.79         | 0/330         | 1.16        | 2/453 (0.4%)  |
| 1   | 8     | 0.58         | 0/364         | 0.65        | 1/499 (0.2%)  |
| 1   | B     | 0.57         | 0/364         | 0.52        | 0/499         |
| 1   | C     | 0.79         | 0/364         | 1.04        | 0/499         |
| 1   | E     | 0.73         | 0/364         | 0.59        | 0/499         |
| 1   | G     | 0.65         | 0/364         | 0.56        | 0/499         |
| 1   | J     | 0.54         | 0/364         | 0.56        | 0/499         |
| 1   | N     | 0.44         | 0/364         | 0.70        | 2/499 (0.4%)  |
| 1   | P     | 0.48         | 0/364         | 0.58        | 0/499         |
| 1   | R     | 0.37         | 0/364         | 0.39        | 0/499         |
| 1   | T     | 0.45         | 0/364         | 0.61        | 0/499         |
| 1   | V     | 0.89         | 1/364 (0.3%)  | 1.20        | 1/499 (0.2%)  |
| 1   | Z     | 0.83         | 0/350         | 1.21        | 2/480 (0.4%)  |
| 1   | b     | 0.78         | 0/311         | 1.12        | 1/427 (0.2%)  |
| 2   | 1     | 0.64         | 0/426         | 0.77        | 0/579         |
| 2   | 3     | 0.72         | 0/452         | 1.05        | 1/612 (0.2%)  |
| 2   | 7     | 0.69         | 0/392         | 0.51        | 0/531         |
| 2   | 9     | 0.64         | 0/460         | 0.46        | 0/622         |
| 2   | A     | 0.69         | 0/460         | 0.53        | 0/622         |
| 2   | D     | 0.69         | 0/460         | 0.61        | 0/622         |
| 2   | F     | 0.68         | 0/460         | 0.54        | 0/622         |
| 2   | I     | 0.75         | 0/460         | 0.66        | 0/622         |
| 2   | K     | 0.53         | 0/452         | 0.51        | 0/612         |
| 2   | O     | 0.49         | 0/452         | 0.48        | 0/612         |
| 2   | Q     | 0.46         | 0/452         | 0.45        | 0/612         |
| 2   | S     | 0.56         | 0/452         | 0.71        | 0/612         |
| 2   | U     | 0.55         | 0/452         | 0.68        | 0/612         |
| 2   | W     | 0.83         | 0/446         | 1.04        | 1/604 (0.2%)  |
| 2   | a     | 0.88         | 1/414 (0.2%)  | 1.15        | 2/563 (0.4%)  |
| 3   | H     | 0.66         | 1/2030 (0.0%) | 0.66        | 1/2757 (0.0%) |
| 4   | L     | 0.81         | 0/2317        | 0.75        | 3/3172 (0.1%) |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 5   | M     | 0.82         | 0/2525         | 0.77        | 7/3453 (0.2%)   |
| 6   | X     | 0.67         | 0/463          | 0.80        | 2/636 (0.3%)    |
| All | All   | 0.70         | 3/19392 (0.0%) | 0.74        | 26/26436 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 3   | H     | 0                   | 1                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | a     | 43  | TRP  | C-N   | 6.79  | 1.43        | 1.33     |
| 1   | V     | 19  | GLU  | C-N   | -5.50 | 1.26        | 1.33     |
| 3   | H     | 54  | GLY  | C-O   | -5.19 | 1.17        | 1.23     |

All (26) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | M     | 175 | VAL  | N-CA-C  | 12.19 | 119.12      | 108.63   |
| 1   | Z     | 17  | ALA  | N-CA-C  | -8.16 | 102.38      | 111.28   |
| 4   | L     | 30  | PHE  | N-CA-C  | 7.76  | 121.76      | 110.28   |
| 2   | a     | 43  | TRP  | O-C-N   | 7.70  | 130.28      | 122.12   |
| 1   | N     | 9   | PHE  | N-CA-C  | -7.65 | 102.94      | 111.28   |
| 1   | 8     | 8   | SER  | N-CA-C  | 7.49  | 121.57      | 111.24   |
| 5   | M     | 48  | ILE  | N-CA-C  | -7.31 | 98.39       | 106.21   |
| 1   | b     | 21  | HIS  | N-CA-C  | -7.16 | 103.47      | 111.28   |
| 5   | M     | 302 | GLY  | N-CA-C  | 7.12  | 125.20      | 115.30   |
| 5   | M     | 195 | ASN  | N-CA-C  | -6.41 | 97.82       | 108.34   |
| 1   | N     | 10  | THR  | N-CA-C  | -6.40 | 98.80       | 109.24   |
| 1   | 2     | 46  | ARG  | CA-C-N  | -6.22 | 113.88      | 120.66   |
| 1   | 2     | 46  | ARG  | C-N-CA  | -6.22 | 113.88      | 120.66   |
| 3   | H     | 54  | GLY  | CA-C-O  | -6.16 | 116.90      | 122.57   |
| 6   | X     | 6   | TYR  | N-CA-C  | -6.00 | 102.61      | 110.53   |
| 2   | 3     | 14  | ARG  | N-CA-C  | 5.95  | 117.77      | 111.28   |
| 5   | M     | 20  | GLY  | N-CA-C  | 5.93  | 118.58      | 110.69   |
| 4   | L     | 23  | PHE  | N-CA-C  | 5.93  | 120.46      | 113.23   |
| 4   | L     | 141 | GLY  | N-CA-C  | 5.76  | 123.27      | 115.32   |
| 5   | M     | 266 | HIS  | CB-CA-C | 5.76  | 120.64      | 110.85   |

*Continued on next page...*

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | V     | 11  | GLY  | N-CA-C | -5.71 | 107.22      | 115.27   |
| 5   | M     | 49  | GLY  | N-CA-C | 5.66  | 123.88      | 112.34   |
| 6   | X     | 11  | ASN  | N-CA-C | 5.33  | 118.17      | 110.28   |
| 2   | W     | 42  | ASN  | N-CA-C | -5.20 | 98.84       | 107.99   |
| 1   | Z     | 37  | ILE  | N-CA-C | -5.19 | 105.32      | 110.62   |
| 2   | a     | 39  | PRO  | N-CA-C | -5.18 | 106.33      | 113.53   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | H     | 40  | TYR  | Peptide |

## 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   | 0     | 360   | 0        | 350      | 10      | 0            |
| 1   | 2     | 319   | 0        | 310      | 9       | 0            |
| 1   | 8     | 352   | 0        | 346      | 8       | 0            |
| 1   | B     | 352   | 0        | 346      | 7       | 0            |
| 1   | C     | 352   | 0        | 346      | 9       | 0            |
| 1   | E     | 352   | 0        | 346      | 5       | 0            |
| 1   | G     | 352   | 0        | 346      | 8       | 0            |
| 1   | J     | 352   | 0        | 346      | 15      | 0            |
| 1   | N     | 352   | 0        | 346      | 17      | 0            |
| 1   | P     | 352   | 0        | 346      | 15      | 0            |
| 1   | R     | 352   | 0        | 346      | 13      | 0            |
| 1   | T     | 352   | 0        | 346      | 15      | 0            |
| 1   | V     | 352   | 0        | 346      | 20      | 0            |
| 1   | Z     | 338   | 0        | 330      | 7       | 0            |
| 1   | b     | 300   | 0        | 289      | 7       | 0            |
| 2   | 1     | 412   | 0        | 420      | 16      | 0            |
| 2   | 3     | 438   | 0        | 451      | 16      | 0            |
| 2   | 7     | 379   | 0        | 397      | 8       | 0            |
| 2   | 9     | 446   | 0        | 463      | 14      | 0            |
| 2   | A     | 446   | 0        | 463      | 11      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | D     | 446   | 0        | 463      | 12      | 0            |
| 2   | F     | 446   | 0        | 463      | 20      | 0            |
| 2   | I     | 446   | 0        | 463      | 13      | 0            |
| 2   | K     | 438   | 0        | 451      | 15      | 0            |
| 2   | O     | 438   | 0        | 451      | 10      | 0            |
| 2   | Q     | 438   | 0        | 451      | 17      | 0            |
| 2   | S     | 438   | 0        | 451      | 17      | 0            |
| 2   | U     | 438   | 0        | 451      | 24      | 0            |
| 2   | W     | 432   | 0        | 446      | 20      | 0            |
| 2   | a     | 401   | 0        | 411      | 10      | 0            |
| 3   | H     | 1980  | 0        | 1952     | 23      | 0            |
| 4   | L     | 2231  | 0        | 2169     | 33      | 0            |
| 5   | M     | 2432  | 0        | 2331     | 42      | 0            |
| 6   | X     | 451   | 0        | 461      | 11      | 0            |
| 7   | 0     | 61    | 0        | 61       | 11      | 0            |
| 7   | 1     | 117   | 0        | 112      | 28      | 0            |
| 7   | 3     | 132   | 0        | 148      | 32      | 0            |
| 7   | 7     | 61    | 0        | 61       | 7       | 0            |
| 7   | 8     | 66    | 0        | 74       | 5       | 0            |
| 7   | 9     | 66    | 0        | 74       | 12      | 0            |
| 7   | A     | 66    | 0        | 74       | 11      | 0            |
| 7   | B     | 66    | 0        | 74       | 8       | 0            |
| 7   | C     | 66    | 0        | 74       | 16      | 0            |
| 7   | D     | 66    | 0        | 74       | 4       | 0            |
| 7   | E     | 66    | 0        | 74       | 14      | 0            |
| 7   | F     | 132   | 0        | 148      | 28      | 0            |
| 7   | I     | 66    | 0        | 74       | 8       | 0            |
| 7   | J     | 66    | 0        | 74       | 14      | 0            |
| 7   | K     | 66    | 0        | 74       | 13      | 0            |
| 7   | L     | 195   | 0        | 213      | 21      | 0            |
| 7   | M     | 66    | 0        | 74       | 9       | 0            |
| 7   | N     | 66    | 0        | 74       | 22      | 0            |
| 7   | O     | 66    | 0        | 74       | 12      | 0            |
| 7   | P     | 66    | 0        | 74       | 8       | 0            |
| 7   | Q     | 66    | 0        | 74       | 14      | 0            |
| 7   | R     | 66    | 0        | 74       | 7       | 0            |
| 7   | S     | 66    | 0        | 74       | 8       | 0            |
| 7   | T     | 66    | 0        | 74       | 13      | 0            |
| 7   | U     | 66    | 0        | 74       | 12      | 0            |
| 7   | V     | 66    | 0        | 74       | 7       | 0            |
| 7   | W     | 66    | 0        | 74       | 13      | 0            |
| 7   | a     | 56    | 0        | 51       | 21      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | b     | 61    | 0        | 61       | 4       | 0            |
| 8   | 0     | 84    | 0        | 120      | 10      | 0            |
| 8   | 2     | 126   | 0        | 180      | 24      | 0            |
| 8   | 3     | 42    | 0        | 60       | 1       | 0            |
| 8   | 8     | 39    | 0        | 53       | 0       | 0            |
| 8   | 9     | 42    | 0        | 60       | 9       | 0            |
| 8   | A     | 42    | 0        | 60       | 8       | 0            |
| 8   | D     | 84    | 0        | 120      | 5       | 0            |
| 8   | E     | 42    | 0        | 60       | 4       | 0            |
| 8   | F     | 42    | 0        | 60       | 3       | 0            |
| 8   | I     | 42    | 0        | 60       | 5       | 0            |
| 8   | J     | 42    | 0        | 60       | 11      | 0            |
| 8   | K     | 42    | 0        | 60       | 5       | 0            |
| 8   | M     | 42    | 0        | 60       | 8       | 0            |
| 8   | N     | 42    | 0        | 60       | 9       | 0            |
| 8   | O     | 42    | 0        | 60       | 1       | 0            |
| 8   | P     | 42    | 0        | 60       | 8       | 0            |
| 8   | R     | 84    | 0        | 120      | 9       | 0            |
| 8   | S     | 84    | 0        | 120      | 10      | 0            |
| 8   | T     | 42    | 0        | 60       | 4       | 0            |
| 8   | U     | 84    | 0        | 120      | 12      | 0            |
| 8   | W     | 42    | 0        | 60       | 3       | 0            |
| 8   | Z     | 42    | 0        | 60       | 8       | 0            |
| 9   | 9     | 45    | 0        | 67       | 3       | 0            |
| 9   | A     | 64    | 0        | 76       | 4       | 0            |
| 9   | F     | 37    | 0        | 48       | 5       | 0            |
| 9   | H     | 47    | 0        | 71       | 0       | 0            |
| 9   | L     | 36    | 0        | 46       | 0       | 0            |
| 9   | M     | 152   | 0        | 203      | 5       | 0            |
| 9   | W     | 32    | 0        | 38       | 2       | 0            |
| 10  | F     | 78    | 0        | 106      | 1       | 0            |
| 10  | M     | 178   | 0        | 262      | 5       | 0            |
| 11  | L     | 117   | 0        | 120      | 11      | 0            |
| 12  | L     | 191   | 0        | 237      | 19      | 0            |
| 12  | M     | 48    | 0        | 63       | 4       | 0            |
| 12  | X     | 48    | 0        | 63       | 12      | 0            |
| 13  | M     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 23255 | 0        | 24235    | 747     | 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 16.

All (747) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 7:N:102:BCL:H91  | 7:N:102:BCL:H142  | 1.41                     | 1.02              |
| 7:L:309:BCL:H91  | 12:L:310:U10:H3M1 | 1.44                     | 1.00              |
| 7:3:102:BCL:H101 | 7:3:102:BCL:H143  | 1.43                     | 0.98              |
| 8:Z:101:SPO:H27  | 8:Z:101:SPO:H241  | 1.53                     | 0.91              |
| 1:2:27:GLY:HA3   | 8:2:101:SPO:H26   | 1.54                     | 0.90              |
| 7:a:101:BCL:HED3 | 7:a:101:BCL:H2A   | 1.57                     | 0.85              |
| 7:N:102:BCL:H3A  | 7:N:102:BCL:H11   | 1.58                     | 0.84              |
| 2:D:32:HIS:CE1   | 7:E:101:BCL:HMD1  | 2.14                     | 0.82              |
| 7:K:101:BCL:HMB1 | 7:K:101:BCL:HBB3  | 1.63                     | 0.80              |
| 2:W:33:LEU:HD13  | 9:W:103:PC1:H332  | 1.64                     | 0.80              |
| 2:W:7:ILE:HB     | 8:Z:101:SPO:H343  | 1.63                     | 0.79              |
| 7:O:101:BCL:HBB3 | 7:O:101:BCL:HMB1  | 1.65                     | 0.79              |
| 1:P:38:ALA:O     | 1:P:42:VAL:HG23   | 1.83                     | 0.79              |
| 1:N:32:VAL:O     | 1:N:36:VAL:HG23   | 1.81                     | 0.79              |
| 2:1:32:HIS:CE1   | 7:1:102:BCL:HMD1  | 2.17                     | 0.79              |
| 2:F:32:HIS:CD2   | 7:F:104:BCL:HMD1  | 2.20                     | 0.77              |
| 1:C:12:LEU:HB2   | 1:C:16:GLY:HA2    | 1.67                     | 0.77              |
| 7:N:102:BCL:HMB1 | 7:N:102:BCL:HBB2  | 1.65                     | 0.77              |
| 2:F:32:HIS:NE2   | 7:F:104:BCL:HMD1  | 1.99                     | 0.77              |
| 7:B:101:BCL:HMB1 | 7:B:101:BCL:HBB3  | 1.65                     | 0.76              |
| 12:X:101:U10:H8  | 12:X:101:U10:H1M3 | 1.67                     | 0.76              |
| 7:E:101:BCL:HBB3 | 7:E:101:BCL:HMB1  | 1.66                     | 0.76              |
| 7:F:102:BCL:HMB1 | 7:F:102:BCL:HBB2  | 1.67                     | 0.75              |
| 1:O:41:ALA:HA    | 8:O:103:SPO:C2    | 2.16                     | 0.75              |
| 8:N:101:SPO:H6   | 7:O:101:BCL:HMB2  | 1.68                     | 0.75              |
| 8:A:102:SPO:C13  | 7:F:102:BCL:H2    | 2.17                     | 0.75              |
| 2:A:32:HIS:CE1   | 7:B:101:BCL:HMD1  | 2.21                     | 0.75              |
| 7:O:101:BCL:H43  | 8:O:102:SPO:C29   | 2.16                     | 0.74              |
| 7:1:102:BCL:HBB2 | 7:a:101:BCL:HHC   | 1.70                     | 0.74              |
| 7:O:101:BCL:HBB2 | 7:O:101:BCL:HMB1  | 1.70                     | 0.74              |
| 7:J:102:BCL:H3A  | 7:J:102:BCL:H11   | 1.68                     | 0.73              |
| 8:2:101:SPO:H241 | 8:2:101:SPO:C27   | 2.17                     | 0.73              |
| 7:O:101:BCL:HMD1 | 2:9:32:HIS:CE1    | 2.23                     | 0.73              |
| 8:P:101:SPO:H6   | 7:Q:101:BCL:HMB1  | 1.70                     | 0.73              |
| 8:Z:101:SPO:H241 | 8:Z:101:SPO:C27   | 2.19                     | 0.73              |
| 4:L:154:HIS:O    | 4:L:158:VAL:HG23  | 1.89                     | 0.72              |
| 1:T:32:VAL:HG22  | 7:T:101:BCL:H11   | 1.72                     | 0.72              |
| 2:7:32:HIS:CE1   | 7:8:102:BCL:HMD1  | 2.25                     | 0.72              |
| 7:V:101:BCL:HMB1 | 7:V:101:BCL:HBB2  | 1.71                     | 0.72              |
| 2:7:12:ASP:O     | 2:7:16:VAL:HG23   | 1.89                     | 0.72              |
| 2:S:32:HIS:CE1   | 7:T:101:BCL:HMD1  | 2.24                     | 0.72              |
| 2:a:43:TRP:CD1   | 2:a:44:LEU:HD12   | 2.24                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:Q:6:LYS:NZ      | 1:T:19:GLU:OE1    | 2.22                     | 0.71              |
| 8:9:102:SPO:H182  | 7:A:101:BCL:C9    | 2.20                     | 0.71              |
| 7:3:101:BCL:CHB   | 7:C:101:BCL:HMB3  | 2.19                     | 0.71              |
| 2:F:20:GLN:HE21   | 8:F:105:SPO:H403  | 1.55                     | 0.71              |
| 6:X:25:VAL:CG1    | 12:X:101:U10:H153 | 2.19                     | 0.71              |
| 2:F:6:LYS:HD3     | 8:J:101:SPO:H403  | 1.73                     | 0.70              |
| 2:I:40:ASP:OD1    | 1:J:46:ARG:NH1    | 2.24                     | 0.70              |
| 2:K:43:TRP:CZ2    | 7:K:101:BCL:HHC   | 2.26                     | 0.70              |
| 12:X:101:U10:H1M3 | 12:X:101:U10:C8   | 2.21                     | 0.70              |
| 7:L:309:BCL:CBB   | 7:L:309:BCL:HMB1  | 2.22                     | 0.70              |
| 7:L:301:BCL:CBB   | 7:L:301:BCL:HMB1  | 2.21                     | 0.70              |
| 7:3:101:BCL:HBB1  | 7:C:101:BCL:HMC3  | 1.73                     | 0.69              |
| 5:M:182:HIS:O     | 5:M:186:THR:HG23  | 1.92                     | 0.69              |
| 7:1:101:BCL:OBB   | 7:3:102:BCL:HMC2  | 1.92                     | 0.69              |
| 7:a:101:BCL:CBB   | 7:a:101:BCL:HMB1  | 2.23                     | 0.69              |
| 8:D:103:SPO:H342  | 8:D:103:SPO:H302  | 1.75                     | 0.69              |
| 7:8:102:BCL:CBB   | 7:8:102:BCL:HMB1  | 2.23                     | 0.68              |
| 7:J:102:BCL:H151  | 7:J:102:BCL:H193  | 1.74                     | 0.68              |
| 7:7:101:BCL:H102  | 1:8:31:PHE:HD1    | 1.58                     | 0.68              |
| 7:E:101:BCL:H102  | 7:E:101:BCL:H51   | 1.75                     | 0.68              |
| 8:2:101:SPO:C6    | 7:a:101:BCL:H3A   | 2.24                     | 0.68              |
| 9:A:103:PC1:H121  | 2:D:14:ARG:HB3    | 1.76                     | 0.68              |
| 2:Q:6:LYS:HD3     | 8:S:103:SPO:H393  | 1.76                     | 0.68              |
| 2:Q:32:HIS:CE1    | 7:R:103:BCL:HMD1  | 2.29                     | 0.68              |
| 12:X:101:U10:H302 | 12:X:101:U10:H261 | 1.76                     | 0.68              |
| 12:L:306:U10:H3M2 | 12:L:306:U10:O2   | 1.94                     | 0.68              |
| 8:S:103:SPO:H403  | 1:T:20:LEU:HD13   | 1.76                     | 0.67              |
| 7:T:101:BCL:HBB3  | 7:T:101:BCL:HMB1  | 1.76                     | 0.67              |
| 7:M:403:BCL:CBB   | 7:M:403:BCL:HMB1  | 2.24                     | 0.67              |
| 2:1:12:ASP:HB3    | 2:1:15:ARG:HB2    | 1.75                     | 0.67              |
| 8:P:101:SPO:H393  | 8:P:101:SPO:H341  | 1.77                     | 0.67              |
| 1:V:48:TRP:O      | 2:W:47:GLY:HA3    | 1.94                     | 0.67              |
| 7:W:102:BCL:HAA2  | 7:W:102:BCL:HBD   | 1.75                     | 0.67              |
| 7:0:101:BCL:HMB1  | 7:0:101:BCL:CBB   | 2.24                     | 0.67              |
| 8:S:103:SPO:H16   | 7:T:101:BCL:H43   | 1.77                     | 0.67              |
| 7:L:309:BCL:HMB1  | 7:L:309:BCL:HBB2  | 1.76                     | 0.67              |
| 7:T:101:BCL:HMB1  | 7:T:101:BCL:CBB   | 2.25                     | 0.67              |
| 7:1:101:BCL:HMA3  | 8:2:102:SPO:C22   | 2.25                     | 0.67              |
| 7:N:102:BCL:H41   | 7:N:102:BCL:H71   | 1.77                     | 0.67              |
| 7:Q:101:BCL:H201  | 8:R:101:SPO:H291  | 1.77                     | 0.67              |
| 7:1:102:BCL:H3A   | 7:1:102:BCL:H12   | 1.75                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:2:102:SPO:H21   | 8:2:102:SPO:H181  | 1.76                     | 0.66              |
| 1:0:32:VAL:O      | 1:0:36:VAL:HG23   | 1.95                     | 0.66              |
| 7:L:302:BCL:CBB   | 7:L:302:BCL:HMB1  | 2.25                     | 0.66              |
| 8:J:101:SPO:H6    | 7:K:101:BCL:HMB2  | 1.76                     | 0.66              |
| 7:J:102:BCL:HMB1  | 7:J:102:BCL:CBB   | 2.25                     | 0.66              |
| 7:T:101:BCL:HMC3  | 7:U:101:BCL:HBB1  | 1.78                     | 0.66              |
| 7:3:101:BCL:HBB2  | 8:U:103:SPO:CM1   | 2.25                     | 0.66              |
| 11:L:303:BPH:HBB3 | 11:L:303:BPH:HMB1 | 1.77                     | 0.66              |
| 2:1:24:LEU:HD11   | 8:2:101:SPO:H19   | 1.78                     | 0.66              |
| 7:R:103:BCL:CBB   | 7:R:103:BCL:HMB1  | 2.25                     | 0.66              |
| 7:1:101:BCL:HMB1  | 7:1:101:BCL:HBB3  | 1.78                     | 0.66              |
| 8:W:101:SPO:H11   | 8:W:101:SPO:H81   | 1.78                     | 0.66              |
| 2:9:30:MET:HE1    | 4:L:49:LEU:HD23   | 1.78                     | 0.65              |
| 2:F:24:LEU:HB2    | 7:F:102:BCL:H42   | 1.78                     | 0.65              |
| 7:N:102:BCL:H91   | 7:N:102:BCL:C14   | 2.22                     | 0.65              |
| 2:U:8:TRP:CB      | 1:V:20:LEU:HD23   | 2.27                     | 0.65              |
| 7:0:101:BCL:H43   | 8:0:102:SPO:H293  | 1.78                     | 0.65              |
| 1:2:27:GLY:CA     | 8:2:101:SPO:H26   | 2.27                     | 0.65              |
| 8:U:103:SPO:H82   | 8:U:103:SPO:H42   | 1.78                     | 0.65              |
| 1:J:32:VAL:O      | 1:J:36:VAL:HG23   | 1.97                     | 0.65              |
| 4:L:133:VAL:HG23  | 4:L:134:VAL:HG23  | 1.77                     | 0.65              |
| 7:N:102:BCL:H11   | 7:N:102:BCL:HAA1  | 1.78                     | 0.64              |
| 1:T:35:ALA:O      | 1:T:39:HIS:ND1    | 2.29                     | 0.64              |
| 6:X:25:VAL:HG11   | 12:X:101:U10:H153 | 1.79                     | 0.64              |
| 1:8:48:TRP:O      | 1:8:49:LEU:HD23   | 1.97                     | 0.64              |
| 7:9:101:BCL:HBB2  | 7:9:101:BCL:HMB3  | 1.77                     | 0.64              |
| 2:K:7:ILE:HD13    | 7:O:101:BCL:H172  | 1.78                     | 0.64              |
| 8:A:102:SPO:H6    | 7:F:102:BCL:HMB2  | 1.78                     | 0.64              |
| 7:P:102:BCL:H122  | 7:Q:101:BCL:C19   | 2.27                     | 0.64              |
| 7:R:103:BCL:HMB1  | 7:R:103:BCL:HBB3  | 1.80                     | 0.64              |
| 2:3:27:LEU:HB3    | 7:3:102:BCL:HED2  | 1.79                     | 0.64              |
| 2:A:24:LEU:HB2    | 7:A:101:BCL:H42   | 1.79                     | 0.64              |
| 11:L:311:BPH:H4C2 | 5:M:60:SER:OG     | 1.97                     | 0.63              |
| 7:3:102:BCL:CBB   | 7:3:102:BCL:HMB1  | 2.28                     | 0.63              |
| 7:F:102:BCL:HMB1  | 7:F:102:BCL:CBB   | 2.28                     | 0.63              |
| 12:M:405:U10:H3M3 | 12:M:405:U10:O2   | 1.97                     | 0.63              |
| 2:7:20:GLN:HE21   | 7:9:101:BCL:H122  | 1.63                     | 0.63              |
| 3:H:158:GLN:OE1   | 3:H:206:ARG:NH1   | 2.31                     | 0.63              |
| 7:O:101:BCL:HMB1  | 7:O:101:BCL:CBB   | 2.28                     | 0.63              |
| 3:H:210:ASN:O     | 3:H:252:ARG:NH1   | 2.31                     | 0.63              |
| 7:U:101:BCL:HBB2  | 7:U:101:BCL:HMB3  | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:9:102:SPO:H182  | 7:A:101:BCL:H92   | 1.80                     | 0.62              |
| 7:E:101:BCL:H143  | 7:E:101:BCL:H8    | 1.81                     | 0.62              |
| 2:F:3:LYS:NZ      | 1:J:19:GLU:OE2    | 2.32                     | 0.62              |
| 7:Q:101:BCL:H151  | 8:R:102:SPO:H341  | 1.81                     | 0.62              |
| 7:1:101:BCL:HMB2  | 8:Z:101:SPO:H5    | 1.82                     | 0.61              |
| 7:N:102:BCL:CHB   | 7:O:101:BCL:HMB3  | 2.30                     | 0.61              |
| 2:Q:36:LEU:HD21   | 2:Q:43:TRP:CH2    | 2.35                     | 0.61              |
| 1:R:48:TRP:CZ2    | 7:R:103:BCL:HHC   | 2.35                     | 0.61              |
| 8:2:101:SPO:H133  | 7:a:101:BCL:H43   | 1.81                     | 0.61              |
| 7:3:101:BCL:CBB   | 7:3:101:BCL:HMB1  | 2.31                     | 0.61              |
| 1:C:47:VAL:HG11   | 7:C:101:BCL:HBC1  | 1.82                     | 0.61              |
| 2:F:15:ARG:HG2    | 9:F:103:PC1:H141  | 1.82                     | 0.61              |
| 7:1:102:BCL:HBA2  | 1:2:35:ALA:HB1    | 1.83                     | 0.61              |
| 7:R:103:BCL:HMB3  | 7:S:102:BCL:CHB   | 2.31                     | 0.61              |
| 12:L:304:U10:H102 | 12:L:304:U10:H1M2 | 1.81                     | 0.61              |
| 7:B:101:BCL:HMB1  | 7:B:101:BCL:CBB   | 2.30                     | 0.60              |
| 2:1:43:TRP:CE3    | 7:1:101:BCL:HBC2  | 2.36                     | 0.60              |
| 8:2:101:SPO:H241  | 8:2:101:SPO:H27   | 1.83                     | 0.60              |
| 7:3:101:BCL:H43   | 8:U:103:SPO:H133  | 1.83                     | 0.60              |
| 2:a:46:VAL:HG21   | 1:b:45:TRP:HZ2    | 1.66                     | 0.60              |
| 8:2:102:SPO:H183  | 7:3:102:BCL:HBB2  | 1.83                     | 0.60              |
| 4:L:220:LEU:O     | 5:M:132:ARG:NH2   | 2.34                     | 0.60              |
| 1:V:28:LEU:O      | 1:V:32:VAL:HG23   | 2.01                     | 0.60              |
| 1:8:38:ALA:O      | 1:8:42:VAL:HG23   | 2.01                     | 0.60              |
| 1:N:42:VAL:HG11   | 7:N:102:BCL:HBC1  | 1.82                     | 0.60              |
| 7:Q:101:BCL:HMB3  | 7:Q:101:BCL:CBB   | 2.32                     | 0.60              |
| 2:I:27:LEU:HD12   | 2:I:30:MET:CE     | 2.31                     | 0.60              |
| 5:M:165:PRO:O     | 5:M:169:GLY:N     | 2.35                     | 0.59              |
| 2:3:8:TRP:HE1     | 1:Z:21:HIS:HA     | 1.67                     | 0.59              |
| 1:P:25:MET:HE1    | 7:P:102:BCL:H121  | 1.82                     | 0.59              |
| 2:K:6:LYS:HB3     | 8:P:101:SPO:H392  | 1.84                     | 0.59              |
| 1:R:32:VAL:O      | 1:R:36:VAL:HG23   | 2.03                     | 0.59              |
| 2:S:14:ARG:O      | 2:S:18:VAL:HG23   | 2.01                     | 0.59              |
| 2:F:21:GLY:HA2    | 7:F:102:BCL:H41   | 1.84                     | 0.59              |
| 2:S:8:TRP:O       | 1:T:10:THR:HG21   | 2.03                     | 0.59              |
| 4:L:267:TRP:O     | 4:L:273:TRP:NE1   | 2.33                     | 0.59              |
| 2:U:8:TRP:CG      | 1:V:20:LEU:HD23   | 2.38                     | 0.59              |
| 7:E:101:BCL:HMB1  | 7:E:101:BCL:CBB   | 2.32                     | 0.58              |
| 2:a:46:VAL:HG21   | 1:b:45:TRP:CZ2    | 2.37                     | 0.58              |
| 6:X:6:TYR:O       | 6:X:7:SER:HB2     | 2.03                     | 0.58              |
| 7:E:101:BCL:H41   | 8:F:105:SPO:H26   | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:L:309:BCL:C9    | 12:L:310:U10:H3M1 | 2.27                     | 0.58              |
| 1:O:39:HIS:ND1    | 7:9:101:BCL:HMD1  | 2.19                     | 0.58              |
| 8:N:101:SPO:H182  | 7:O:101:BCL:C9    | 2.34                     | 0.58              |
| 7:8:102:BCL:HMB1  | 7:8:102:BCL:HBB2  | 1.86                     | 0.58              |
| 8:9:102:SPO:H182  | 7:A:101:BCL:H91   | 1.84                     | 0.58              |
| 7:O:101:BCL:H3A   | 7:O:101:BCL:H12   | 1.86                     | 0.58              |
| 7:1:102:BCL:HBB3  | 7:1:102:BCL:HHC   | 1.86                     | 0.58              |
| 1:R:42:VAL:O      | 1:R:45:TRP:N      | 2.37                     | 0.58              |
| 3:H:11:ASP:OD1    | 3:H:11:ASP:N      | 2.38                     | 0.57              |
| 5:M:145:HIS:NE2   | 10:M:407:CDL:OB3  | 2.34                     | 0.57              |
| 2:U:8:TRP:HB3     | 1:V:20:LEU:HD23   | 1.86                     | 0.57              |
| 7:a:101:BCL:H2A   | 7:a:101:BCL:CED   | 2.30                     | 0.57              |
| 7:J:102:BCL:HBB1  | 7:K:101:BCL:HMC3  | 1.87                     | 0.57              |
| 1:N:38:ALA:O      | 1:N:42:VAL:HG23   | 2.05                     | 0.57              |
| 7:B:101:BCL:H43   | 8:E:102:SPO:H293  | 1.87                     | 0.57              |
| 7:C:101:BCL:H3C   | 2:W:35:LEU:HD21   | 1.85                     | 0.57              |
| 2:D:16:VAL:HG21   | 7:F:102:BCL:H142  | 1.86                     | 0.57              |
| 7:F:104:BCL:H51   | 1:G:32:VAL:HG21   | 1.87                     | 0.57              |
| 2:U:24:LEU:HB3    | 7:U:101:BCL:H12   | 1.86                     | 0.57              |
| 8:2:101:SPO:H42   | 7:a:101:BCL:HBA2  | 1.86                     | 0.57              |
| 8:2:101:SPO:HM11  | 7:a:101:BCL:HBB2  | 1.86                     | 0.57              |
| 7:E:101:BCL:H102  | 7:E:101:BCL:C5    | 2.32                     | 0.57              |
| 3:H:174:ASP:O     | 3:H:178:GLN:N     | 2.37                     | 0.57              |
| 7:L:302:BCL:HMB1  | 7:L:302:BCL:HBB2  | 1.86                     | 0.57              |
| 1:O:46:ARG:NH1    | 2:9:40:ASP:OD1    | 2.38                     | 0.56              |
| 2:O:7:ILE:HD11    | 2:O:11:PHE:CE2    | 2.40                     | 0.56              |
| 1:2:47:PRO:HB2    | 2:a:51:TYR:CE2    | 2.40                     | 0.56              |
| 1:E:9:PHE:O       | 2:F:14:ARG:NH2    | 2.38                     | 0.56              |
| 7:F:102:BCL:O2D   | 7:F:102:BCL:HAA2  | 2.05                     | 0.56              |
| 5:M:157:TRP:CE2   | 8:M:406:SPO:H293  | 2.39                     | 0.56              |
| 5:M:130:TRP:O     | 5:M:133:THR:OG1   | 2.24                     | 0.56              |
| 1:C:19:ASP:O      | 1:C:20:GLU:HG3    | 2.05                     | 0.56              |
| 12:L:304:U10:H201 | 12:L:304:U10:H253 | 1.87                     | 0.56              |
| 1:C:26:HIS:O      | 1:C:30:MET:HG2    | 2.05                     | 0.56              |
| 7:B:101:BCL:H43   | 8:E:102:SPO:C29   | 2.35                     | 0.56              |
| 7:J:102:BCL:H2A   | 7:J:102:BCL:O1D   | 2.06                     | 0.56              |
| 5:M:94:SER:HB2    | 5:M:181:THR:HG21  | 1.86                     | 0.56              |
| 1:T:48:TRP:CZ2    | 7:T:101:BCL:HHC   | 2.40                     | 0.56              |
| 4:L:270:LEU:O     | 4:L:274:VAL:HG23  | 2.05                     | 0.56              |
| 5:M:108:ARG:NH2   | 2:Q:45:ASP:OD2    | 2.33                     | 0.56              |
| 1:P:25:MET:HE2    | 7:P:102:BCL:H151  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:Q:20:GLN:HG3    | 7:S:102:BCL:H91   | 1.88                     | 0.56              |
| 7:O:101:BCL:H92   | 8:O:102:SPO:H242  | 1.87                     | 0.56              |
| 7:M:403:BCL:HMB1  | 7:M:403:BCL:HBB2  | 1.88                     | 0.55              |
| 7:1:101:BCL:HMA2  | 8:2:102:SPO:C25   | 2.36                     | 0.55              |
| 3:H:197:MET:HE1   | 3:H:202:ILE:HD11  | 1.87                     | 0.55              |
| 2:9:17:PHE:CE2    | 8:9:102:SPO:H342  | 2.41                     | 0.55              |
| 2:9:17:PHE:CZ     | 8:9:102:SPO:H342  | 2.41                     | 0.55              |
| 4:L:256:TRP:NE1   | 4:L:258:ASP:O     | 2.40                     | 0.55              |
| 7:W:102:BCL:HAA2  | 7:W:102:BCL:CBD   | 2.36                     | 0.55              |
| 2:1:36:LEU:O      | 2:1:42:ASN:ND2    | 2.38                     | 0.55              |
| 7:N:102:BCL:H11   | 7:N:102:BCL:CAA   | 2.35                     | 0.55              |
| 8:U:102:SPO:H402  | 1:V:20:LEU:HA     | 1.88                     | 0.55              |
| 2:a:42:ASN:HB3    | 2:a:45:ASP:HB3    | 1.88                     | 0.55              |
| 2:I:9:GLN:OE1     | 1:J:8:SER:OG      | 2.23                     | 0.55              |
| 4:L:232:ARG:NE    | 5:M:6:ASN:O       | 2.38                     | 0.55              |
| 8:P:101:SPO:H341  | 8:P:101:SPO:C39   | 2.37                     | 0.55              |
| 9:9:103:PC1:H133  | 9:9:103:PC1:O11   | 2.06                     | 0.55              |
| 2:O:38:LYS:HD2    | 2:Q:44:LEU:HD13   | 1.87                     | 0.55              |
| 2:1:35:LEU:CD2    | 7:1:101:BCL:HBC1  | 2.37                     | 0.55              |
| 2:S:27:LEU:HD23   | 7:T:101:BCL:HED3  | 1.89                     | 0.55              |
| 7:3:101:BCL:HMB1  | 7:3:101:BCL:HBB3  | 1.89                     | 0.55              |
| 7:D:102:BCL:CBB   | 7:D:102:BCL:HMB1  | 2.37                     | 0.55              |
| 7:L:302:BCL:HMD2  | 7:M:403:BCL:HBB3  | 1.88                     | 0.55              |
| 2:F:15:ARG:CG     | 9:F:103:PC1:H141  | 2.36                     | 0.55              |
| 7:K:101:BCL:HMD1  | 1:N:39:HIS:ND1    | 2.23                     | 0.55              |
| 4:L:178:ILE:HG12  | 7:L:301:BCL:HMB3  | 1.88                     | 0.54              |
| 12:L:306:U10:H102 | 12:L:306:U10:H1M2 | 1.88                     | 0.54              |
| 7:1:101:BCL:HBB1  | 7:3:102:BCL:HMC3  | 1.89                     | 0.54              |
| 7:I:101:BCL:H143  | 8:I:102:SPO:H341  | 1.88                     | 0.54              |
| 7:W:102:BCL:CBB   | 7:W:102:BCL:HMB1  | 2.37                     | 0.54              |
| 4:L:127:LEU:HD12  | 12:L:306:U10:H301 | 1.89                     | 0.54              |
| 3:H:56:PHE:CD1    | 9:M:401:PC1:H133  | 2.43                     | 0.54              |
| 7:V:101:BCL:HMB1  | 7:V:101:BCL:CBB   | 2.37                     | 0.54              |
| 2:U:13:PRO:CG     | 1:V:20:LEU:HD21   | 2.38                     | 0.54              |
| 7:W:102:BCL:H151  | 7:W:102:BCL:H192  | 1.88                     | 0.54              |
| 7:a:101:BCL:HMB1  | 7:a:101:BCL:HBB2  | 1.88                     | 0.54              |
| 2:7:43:TRP:CZ3    | 7:7:101:BCL:HBC3  | 2.42                     | 0.54              |
| 7:Q:101:BCL:H151  | 8:R:102:SPO:C34   | 2.37                     | 0.54              |
| 8:J:101:SPO:C16   | 7:J:102:BCL:H43   | 2.38                     | 0.54              |
| 7:K:101:BCL:HMB1  | 7:K:101:BCL:CBB   | 2.36                     | 0.54              |
| 8:N:101:SPO:H182  | 7:O:101:BCL:H92   | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:J:102:BCL:HMB1  | 7:J:102:BCL:HBB2  | 1.89                     | 0.54              |
| 2:A:43:TRP:CE3    | 7:A:101:BCL:HBC2  | 2.43                     | 0.54              |
| 11:L:311:BPH:CBB  | 11:L:311:BPH:HMB1 | 2.38                     | 0.54              |
| 7:M:403:BCL:HAA2  | 7:M:403:BCL:HBD   | 1.90                     | 0.54              |
| 7:Q:101:BCL:HMB3  | 7:Q:101:BCL:HBB2  | 1.90                     | 0.54              |
| 7:3:101:BCL:HHB   | 7:C:101:BCL:HMB3  | 1.90                     | 0.53              |
| 9:A:104:PC1:H132  | 9:M:401:PC1:H153  | 1.90                     | 0.53              |
| 3:H:246:LEU:HD23  | 3:H:246:LEU:O     | 2.09                     | 0.53              |
| 1:N:48:TRP:CD1    | 1:N:49:LEU:HG     | 2.44                     | 0.53              |
| 7:N:102:BCL:H11   | 7:N:102:BCL:C3A   | 2.35                     | 0.53              |
| 1:R:28:LEU:HD23   | 1:R:28:LEU:O      | 2.08                     | 0.53              |
| 12:X:101:U10:C8   | 12:X:101:U10:C1M  | 2.86                     | 0.53              |
| 7:C:101:BCL:HHB   | 2:W:35:LEU:HD11   | 1.89                     | 0.53              |
| 8:U:102:SPO:H6    | 7:W:102:BCL:HMB2  | 1.91                     | 0.53              |
| 8:3:103:SPO:H37   | 8:Z:101:SPO:H293  | 1.91                     | 0.53              |
| 7:L:301:BCL:HMB1  | 7:L:301:BCL:HBB3  | 1.89                     | 0.53              |
| 4:L:61:ASN:O      | 4:L:65:ILE:HG13   | 2.08                     | 0.53              |
| 2:F:25:PHE:O      | 2:F:29:VAL:HG23   | 2.09                     | 0.53              |
| 7:3:101:BCL:HBB2  | 8:U:103:SPO:HM13  | 1.90                     | 0.53              |
| 7:A:101:BCL:HMB1  | 7:A:101:BCL:HBB3  | 1.91                     | 0.53              |
| 7:I:101:BCL:CBB   | 7:I:101:BCL:HMB3  | 2.39                     | 0.53              |
| 2:K:32:HIS:CE1    | 7:N:102:BCL:HMD1  | 2.43                     | 0.53              |
| 7:O:101:BCL:H61   | 8:O:102:SPO:H241  | 1.90                     | 0.53              |
| 8:2:101:SPO:H5    | 7:a:101:BCL:HMB2  | 1.89                     | 0.53              |
| 7:3:102:BCL:H72   | 1:Z:28:LEU:HD21   | 1.91                     | 0.53              |
| 7:F:104:BCL:HBB2  | 1:G:48:TRP:HE1    | 1.73                     | 0.53              |
| 7:1:101:BCL:HBB2  | 8:Z:101:SPO:H33   | 1.91                     | 0.52              |
| 1:G:28:LEU:C      | 1:G:28:LEU:HD23   | 2.34                     | 0.52              |
| 11:L:311:BPH:HMB1 | 11:L:311:BPH:HBB2 | 1.91                     | 0.52              |
| 8:D:103:SPO:H132  | 7:I:101:BCL:H2    | 1.92                     | 0.52              |
| 5:M:120:PHE:CD1   | 8:M:406:SPO:H392  | 2.45                     | 0.52              |
| 3:H:24:LEU:O      | 3:H:28:ILE:HG12   | 2.09                     | 0.52              |
| 3:H:37:ARG:HA     | 3:H:76:PRO:HG3    | 1.91                     | 0.52              |
| 2:S:43:TRP:CE3    | 7:S:102:BCL:HBC2  | 2.44                     | 0.52              |
| 2:U:6:LYS:HB3     | 8:U:103:SPO:H402  | 1.91                     | 0.52              |
| 2:A:9:GLN:NE2     | 1:B:14:ASP:OD1    | 2.42                     | 0.52              |
| 2:A:35:LEU:HD13   | 7:A:101:BCL:HBC1  | 1.92                     | 0.52              |
| 2:3:52:GLY:O      | 2:3:53:ARG:C      | 2.53                     | 0.52              |
| 1:E:24:TYR:CE2    | 7:F:102:BCL:H161  | 2.45                     | 0.52              |
| 1:N:28:LEU:C      | 1:N:28:LEU:HD23   | 2.34                     | 0.52              |
| 7:3:102:BCL:HMB1  | 7:3:102:BCL:HBB3  | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:L:301:BCL:H112  | 7:L:302:BCL:HBB2  | 1.92                     | 0.52              |
| 7:A:101:BCL:HMB1  | 7:A:101:BCL:CBB   | 2.40                     | 0.51              |
| 7:L:309:BCL:HBB2  | 7:M:403:BCL:H102  | 1.90                     | 0.51              |
| 9:M:409:PC1:H2C2  | 2:S:29:VAL:HG11   | 1.91                     | 0.51              |
| 1:N:35:ALA:CB     | 7:N:102:BCL:HBA1  | 2.40                     | 0.51              |
| 3:H:29:TYR:O      | 3:H:33:THR:HG23   | 2.11                     | 0.51              |
| 5:M:119:SER:HB3   | 8:M:406:SPO:H342  | 1.93                     | 0.51              |
| 2:Q:20:GLN:NE2    | 1:R:24:TYR:OH     | 2.43                     | 0.51              |
| 1:T:42:VAL:HA     | 1:T:45:TRP:CD1    | 2.45                     | 0.51              |
| 7:3:102:BCL:H101  | 7:3:102:BCL:C14   | 2.18                     | 0.51              |
| 2:D:8:TRP:CH2     | 7:F:102:BCL:H141  | 2.45                     | 0.51              |
| 1:B:35:ALA:O      | 1:B:39:HIS:ND1    | 2.24                     | 0.51              |
| 7:J:102:BCL:C1B   | 7:K:101:BCL:HMB3  | 2.41                     | 0.51              |
| 2:U:5:TYR:HA      | 1:V:21:HIS:HB2    | 1.93                     | 0.51              |
| 2:I:34:ILE:HG23   | 10:M:408:CDL:H112 | 1.92                     | 0.51              |
| 12:M:405:U10:O2   | 12:M:405:U10:C3M  | 2.58                     | 0.51              |
| 7:3:101:BCL:C1B   | 7:C:101:BCL:HMB3  | 2.41                     | 0.51              |
| 1:T:42:VAL:HA     | 1:T:45:TRP:HD1    | 1.75                     | 0.51              |
| 8:M:406:SPO:H391  | 2:O:30:MET:SD     | 2.51                     | 0.51              |
| 1:V:42:VAL:HG23   | 1:V:48:TRP:HZ3    | 1.75                     | 0.51              |
| 2:3:8:TRP:CD1     | 1:Z:20:LEU:HB3    | 2.46                     | 0.51              |
| 12:L:307:U10:C4M  | 12:L:307:U10:H3M3 | 2.41                     | 0.51              |
| 2:U:9:GLN:NE2     | 1:V:14:ASP:HA     | 2.26                     | 0.51              |
| 12:X:101:U10:C23  | 12:X:101:U10:H201 | 2.40                     | 0.51              |
| 7:7:101:BCL:H52   | 6:X:24:MET:SD     | 2.51                     | 0.50              |
| 7:I:101:BCL:HED1  | 1:J:31:PHE:CE1    | 2.46                     | 0.50              |
| 2:W:13:PRO:HA     | 2:W:16:VAL:HG12   | 1.93                     | 0.50              |
| 2:O:34:ILE:O      | 2:O:37:SER:OG     | 2.23                     | 0.50              |
| 1:P:48:TRP:HE1    | 7:P:102:BCL:HBB3  | 1.76                     | 0.50              |
| 8:K:102:SPO:C13   | 1:N:42:VAL:HG22   | 2.41                     | 0.50              |
| 12:L:304:U10:H102 | 12:L:304:U10:C1M  | 2.42                     | 0.50              |
| 2:O:7:ILE:HD11    | 2:O:11:PHE:HE2    | 1.76                     | 0.50              |
| 1:P:28:LEU:O      | 1:P:32:VAL:HG23   | 2.11                     | 0.50              |
| 2:D:7:ILE:HA      | 2:D:10:VAL:HG12   | 1.92                     | 0.50              |
| 1:J:24:TYR:OH     | 7:K:101:BCL:H152  | 2.12                     | 0.50              |
| 4:L:190:LEU:CD2   | 11:L:311:BPH:HMD2 | 2.42                     | 0.50              |
| 2:U:24:LEU:CB     | 7:U:101:BCL:H12   | 2.42                     | 0.50              |
| 7:3:101:BCL:HMB3  | 7:C:101:BCL:CHB   | 2.41                     | 0.50              |
| 1:B:32:VAL:O      | 1:B:36:VAL:HG23   | 2.12                     | 0.50              |
| 1:V:48:TRP:O      | 1:V:49:LEU:C      | 2.55                     | 0.50              |
| 7:1:102:BCL:CHB   | 7:a:101:BCL:HMB3  | 2.42                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:3:101:BCL:HBB1  | 7:C:101:BCL:CMC   | 2.41                     | 0.50              |
| 2:9:40:ASP:OD2    | 2:A:53:ARG:NH1    | 2.45                     | 0.50              |
| 7:L:309:BCL:CBB   | 7:M:403:BCL:H102  | 2.41                     | 0.50              |
| 6:X:25:VAL:HG12   | 12:X:101:U10:H153 | 1.94                     | 0.50              |
| 7:E:101:BCL:H203  | 7:E:101:BCL:H122  | 1.94                     | 0.50              |
| 5:M:260:ALA:N     | 12:M:405:U10:O5   | 2.45                     | 0.50              |
| 1:P:32:VAL:O      | 1:P:36:VAL:HG23   | 2.11                     | 0.50              |
| 2:U:13:PRO:HG3    | 1:V:20:LEU:HD21   | 1.94                     | 0.50              |
| 7:V:101:BCL:CHB   | 7:W:102:BCL:HMB3  | 2.42                     | 0.50              |
| 1:0:39:HIS:CE1    | 7:9:101:BCL:HMD1  | 2.46                     | 0.50              |
| 12:L:307:U10:H3M3 | 12:L:307:U10:O4   | 2.12                     | 0.50              |
| 7:U:101:BCL:H203  | 8:U:102:SPO:H291  | 1.94                     | 0.50              |
| 6:X:14:ILE:O      | 6:X:18:VAL:HG13   | 2.12                     | 0.50              |
| 7:1:102:BCL:HMC3  | 7:a:101:BCL:HBB1  | 1.94                     | 0.49              |
| 8:2:101:SPO:C5    | 7:a:101:BCL:HMB2  | 2.43                     | 0.49              |
| 8:9:102:SPO:H341  | 8:9:102:SPO:C37   | 2.42                     | 0.49              |
| 8:K:102:SPO:H133  | 1:N:42:VAL:HG22   | 1.93                     | 0.49              |
| 8:S:101:SPO:H292  | 7:S:102:BCL:HMA1  | 1.94                     | 0.49              |
| 2:U:23:PHE:CD2    | 7:W:102:BCL:H92   | 2.47                     | 0.49              |
| 3:H:237:ILE:O     | 3:H:241:VAL:HG23  | 2.12                     | 0.49              |
| 2:F:40:ASP:CG     | 2:I:48:THR:HG22   | 2.37                     | 0.49              |
| 7:L:302:BCL:HMD1  | 5:M:206:ILE:HD13  | 1.93                     | 0.49              |
| 7:1:101:BCL:HMB3  | 7:3:102:BCL:C1B   | 2.42                     | 0.49              |
| 4:L:234:GLY:HA3   | 5:M:216:PHE:CE1   | 2.48                     | 0.49              |
| 12:L:310:U10:H4M2 | 12:L:310:U10:O3   | 2.12                     | 0.49              |
| 5:M:278:LEU:O     | 5:M:282:ILE:HG13  | 2.13                     | 0.49              |
| 7:Q:101:BCL:H43   | 8:R:102:SPO:H351  | 1.94                     | 0.49              |
| 2:U:5:TYR:HA      | 1:V:21:HIS:CB     | 2.42                     | 0.49              |
| 2:U:8:TRP:CH2     | 7:W:102:BCL:H161  | 2.48                     | 0.49              |
| 2:1:51:TYR:CD2    | 1:Z:47:PRO:HB2    | 2.48                     | 0.49              |
| 2:I:27:LEU:HD12   | 2:I:30:MET:HE3    | 1.95                     | 0.49              |
| 2:S:43:TRP:HB3    | 7:S:102:BCL:HMC1  | 1.94                     | 0.49              |
| 8:W:101:SPO:H25   | 7:W:102:BCL:H2A   | 1.94                     | 0.49              |
| 2:1:35:LEU:HD23   | 7:1:101:BCL:HBC1  | 1.95                     | 0.49              |
| 1:2:28:LEU:HD13   | 8:2:101:SPO:H183  | 1.95                     | 0.49              |
| 2:O:9:GLN:NE2     | 1:P:8:SER:OG      | 2.46                     | 0.49              |
| 7:0:101:BCL:CAD   | 7:9:101:BCL:HBD   | 2.43                     | 0.49              |
| 2:F:28:ALA:O      | 2:F:32:HIS:HD2    | 1.95                     | 0.49              |
| 7:L:301:BCL:HMB1  | 7:L:301:BCL:HBB2  | 1.93                     | 0.49              |
| 4:L:32:VAL:HG13   | 4:L:32:VAL:O      | 2.12                     | 0.48              |
| 4:L:118:ILE:HB    | 4:L:119:PRO:HD3   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:24:TYR:OH     | 2:9:20:GLN:NE2    | 2.47                     | 0.48              |
| 7:1:102:BCL:HMA3  | 8:2:101:SPO:H9    | 1.96                     | 0.48              |
| 1:N:20:LEU:HB2    | 8:N:101:SPO:H392  | 1.94                     | 0.48              |
| 8:A:102:SPO:C6    | 8:A:102:SPO:H33   | 2.43                     | 0.48              |
| 9:A:103:PC1:H143  | 3:H:53:GLN:H      | 1.77                     | 0.48              |
| 1:G:28:LEU:HD23   | 1:G:28:LEU:O      | 2.13                     | 0.48              |
| 12:X:101:U10:H3M2 | 12:X:101:U10:O2   | 2.13                     | 0.48              |
| 7:0:101:BCL:H43   | 8:0:102:SPO:H292  | 1.95                     | 0.48              |
| 7:1:101:BCL:HHB   | 8:Z:101:SPO:C5    | 2.43                     | 0.48              |
| 1:N:25:MET:O      | 1:N:29:TRP:CD1    | 2.67                     | 0.48              |
| 2:1:14:ARG:HG2    | 2:3:10:VAL:O      | 2.14                     | 0.48              |
| 2:D:7:ILE:CD1     | 8:D:103:SPO:H343  | 2.44                     | 0.48              |
| 7:I:101:BCL:HED1  | 1:J:31:PHE:CD1    | 2.48                     | 0.48              |
| 8:U:102:SPO:H402  | 1:V:20:LEU:CA     | 2.44                     | 0.48              |
| 12:X:101:U10:H261 | 12:X:101:U10:C30  | 2.41                     | 0.48              |
| 7:E:101:BCL:H162  | 7:E:101:BCL:H121  | 1.47                     | 0.48              |
| 12:L:306:U10:H1M2 | 12:L:306:U10:C10  | 2.43                     | 0.48              |
| 5:M:114:MET:HE3   | 9:M:409:PC1:H281  | 1.96                     | 0.48              |
| 2:S:40:ASP:HB2    | 1:T:46:ARG:NH1    | 2.28                     | 0.48              |
| 8:T:102:SPO:H25   | 7:U:101:BCL:H2A   | 1.96                     | 0.48              |
| 1:C:25:LEU:HD21   | 2:W:13:PRO:HG3    | 1.95                     | 0.48              |
| 8:T:102:SPO:H343  | 7:U:101:BCL:H61   | 1.96                     | 0.48              |
| 7:W:102:BCL:HMB1  | 7:W:102:BCL:HBB3  | 1.95                     | 0.48              |
| 1:R:20:LEU:HD12   | 8:R:101:SPO:H341  | 1.95                     | 0.48              |
| 1:b:29:TRP:HZ3    | 7:b:101:BCL:H13   | 1.79                     | 0.48              |
| 2:1:14:ARG:HB3    | 2:3:11:PHE:CE1    | 2.48                     | 0.47              |
| 7:3:101:BCL:HBB3  | 7:C:101:BCL:NB    | 2.29                     | 0.47              |
| 7:I:101:BCL:HAA2  | 7:I:101:BCL:HBD   | 1.95                     | 0.47              |
| 12:L:304:U10:O3   | 12:L:304:U10:H4M3 | 2.14                     | 0.47              |
| 12:L:306:U10:O2   | 12:L:306:U10:C3M  | 2.61                     | 0.47              |
| 8:2:101:SPO:C8    | 8:2:101:SPO:C4    | 2.92                     | 0.47              |
| 3:H:121:ARG:NH2   | 5:M:240:ASP:O     | 2.46                     | 0.47              |
| 5:M:120:PHE:HD1   | 8:M:406:SPO:H392  | 1.79                     | 0.47              |
| 7:T:101:BCL:H91   | 7:T:101:BCL:H142  | 1.96                     | 0.47              |
| 1:b:39:HIS:HA     | 1:b:42:VAL:HG22   | 1.96                     | 0.47              |
| 1:E:29:TRP:CH2    | 7:E:101:BCL:H92   | 2.49                     | 0.47              |
| 2:S:8:TRP:CG      | 1:T:20:LEU:HD23   | 2.50                     | 0.47              |
| 4:L:236:LEU:HD12  | 5:M:43:PHE:CZ     | 2.50                     | 0.47              |
| 2:W:27:LEU:O      | 2:W:31:ILE:HG13   | 2.14                     | 0.47              |
| 6:X:31:ALA:O      | 6:X:35:VAL:HG23   | 2.14                     | 0.47              |
| 7:3:101:BCL:HMB3  | 7:C:101:BCL:C4A   | 2.44                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:9:101:BCL:O1D  | 7:9:101:BCL:H2A  | 2.15                     | 0.47              |
| 8:I:102:SPO:H181 | 8:I:102:SPO:H20  | 1.60                     | 0.47              |
| 2:Q:8:TRP:HZ3    | 2:Q:16:VAL:HG11  | 1.80                     | 0.47              |
| 2:a:43:TRP:CD1   | 2:a:44:LEU:CD1   | 2.95                     | 0.47              |
| 1:C:46:ALA:O     | 1:C:49:ILE:HG12  | 2.15                     | 0.47              |
| 2:D:25:PHE:O     | 2:D:29:VAL:HG23  | 2.15                     | 0.47              |
| 7:F:104:BCL:HBB2 | 7:F:104:BCL:HHC  | 1.97                     | 0.47              |
| 7:F:104:BCL:HHC  | 1:G:48:TRP:CZ2   | 2.50                     | 0.47              |
| 2:I:27:LEU:O     | 2:I:31:ILE:HG13  | 2.15                     | 0.47              |
| 8:2:101:SPO:H82  | 8:2:101:SPO:H41  | 1.97                     | 0.47              |
| 7:M:403:BCL:H2C  | 7:M:403:BCL:HBC2 | 1.39                     | 0.47              |
| 8:J:101:SPO:C9   | 7:K:101:BCL:HHB  | 2.45                     | 0.47              |
| 1:N:48:TRP:O     | 1:N:49:LEU:HD23  | 2.14                     | 0.47              |
| 7:N:102:BCL:HAA1 | 7:N:102:BCL:C1   | 2.44                     | 0.47              |
| 2:Q:7:ILE:HB     | 8:S:103:SPO:H343 | 1.96                     | 0.47              |
| 7:Q:101:BCL:H12  | 8:R:102:SPO:H302 | 1.97                     | 0.47              |
| 7:K:101:BCL:H203 | 7:K:101:BCL:H162 | 1.79                     | 0.46              |
| 4:L:70:PRO:HG3   | 4:L:84:GLY:HA3   | 1.97                     | 0.46              |
| 7:L:301:BCL:CBB  | 7:L:309:BCL:HMD2 | 2.45                     | 0.46              |
| 7:N:102:BCL:HMB1 | 7:N:102:BCL:CBB  | 2.41                     | 0.46              |
| 2:O:12:ASP:OD1   | 2:O:13:PRO:HD2   | 2.15                     | 0.46              |
| 2:S:20:GLN:NE2   | 1:T:24:TYR:OH    | 2.39                     | 0.46              |
| 6:X:51:LEU:HD22  | 2:a:34:ILE:HD11  | 1.96                     | 0.46              |
| 7:1:102:BCL:HBB2 | 7:a:101:BCL:CHC  | 2.44                     | 0.46              |
| 1:8:21:HIS:O     | 1:8:25:MET:HG2   | 2.15                     | 0.46              |
| 2:A:43:TRP:NE1   | 7:A:101:BCL:OBB  | 2.48                     | 0.46              |
| 4:L:178:ILE:HD13 | 7:L:309:BCL:HMD1 | 1.97                     | 0.46              |
| 4:L:234:GLY:HA3  | 5:M:216:PHE:CD1  | 2.50                     | 0.46              |
| 2:I:27:LEU:HA    | 2:I:30:MET:HE2   | 1.97                     | 0.46              |
| 2:A:26:LEU:O     | 2:A:30:MET:HG2   | 2.15                     | 0.46              |
| 7:8:102:BCL:H41  | 7:8:102:BCL:H61  | 1.40                     | 0.46              |
| 8:A:102:SPO:H182 | 7:F:102:BCL:H8   | 1.97                     | 0.46              |
| 7:D:102:BCL:HMB1 | 7:D:102:BCL:HBB3 | 1.97                     | 0.46              |
| 8:2:102:SPO:C18  | 7:3:102:BCL:HBB2 | 2.45                     | 0.46              |
| 2:F:43:TRP:CZ2   | 7:F:102:BCL:HHC  | 2.49                     | 0.46              |
| 2:K:40:ASP:OD2   | 2:O:48:THR:OG1   | 2.28                     | 0.46              |
| 2:1:31:ILE:HG22  | 7:1:102:BCL:HMD3 | 1.98                     | 0.46              |
| 3:H:91:LEU:HD11  | 4:L:9:LYS:HA     | 1.98                     | 0.46              |
| 3:H:150:ARG:HE   | 3:H:202:ILE:HG22 | 1.81                     | 0.46              |
| 7:F:104:BCL:HMB2 | 8:I:102:SPO:H183 | 1.97                     | 0.46              |
| 1:G:9:PHE:HZ     | 1:J:12:LEU:HD11  | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:L:311:BPH:OBB  | 7:M:403:BCL:H11   | 2.16                     | 0.46              |
| 7:Q:101:BCL:O1D   | 7:Q:101:BCL:H2A   | 2.16                     | 0.46              |
| 4:L:190:LEU:HD23  | 11:L:311:BPH:HMD2 | 1.98                     | 0.46              |
| 8:M:406:SPO:H342  | 8:M:406:SPO:H302  | 1.98                     | 0.46              |
| 7:P:102:BCL:HBB2  | 7:Q:101:BCL:HHC   | 1.97                     | 0.46              |
| 7:U:101:BCL:HAA2  | 7:U:101:BCL:HBD   | 1.98                     | 0.46              |
| 7:3:101:BCL:H3A   | 8:U:103:SPO:C9    | 2.46                     | 0.46              |
| 9:9:103:PC1:H133  | 9:9:103:PC1:C1    | 2.46                     | 0.46              |
| 2:K:22:VAL:HG11   | 10:M:407:CDL:H382 | 1.98                     | 0.46              |
| 2:U:24:LEU:HB2    | 7:U:101:BCL:H42   | 1.98                     | 0.46              |
| 12:X:101:U10:H372 | 12:X:101:U10:H351 | 1.78                     | 0.46              |
| 2:a:12:ASP:O      | 2:a:13:PRO:C      | 2.58                     | 0.46              |
| 8:A:102:SPO:CM1   | 2:F:33:LEU:HD21   | 2.46                     | 0.45              |
| 2:K:6:LYS:CB      | 8:P:101:SPO:H392  | 2.45                     | 0.45              |
| 1:N:35:ALA:HB2    | 7:N:102:BCL:HBA1  | 1.98                     | 0.45              |
| 6:X:43:VAL:O      | 6:X:47:LEU:HG     | 2.16                     | 0.45              |
| 7:b:101:BCL:H91   | 7:b:101:BCL:H122  | 1.98                     | 0.45              |
| 3:H:35:ASN:HB3    | 5:M:260:ALA:HA    | 1.98                     | 0.45              |
| 2:Q:27:LEU:HD12   | 2:Q:30:MET:HE2    | 1.99                     | 0.45              |
| 2:7:10:VAL:CG2    | 8:9:102:SPO:H402  | 2.46                     | 0.45              |
| 7:C:101:BCL:HMD1  | 2:W:32:HIS:CE1    | 2.51                     | 0.45              |
| 2:D:15:ARG:NH1    | 3:H:54:GLY:O      | 2.50                     | 0.45              |
| 2:F:33:LEU:HD22   | 10:F:101:CDL:H532 | 1.99                     | 0.45              |
| 8:F:105:SPO:H181  | 1:G:38:ALA:HB1    | 1.97                     | 0.45              |
| 2:I:45:ASP:O      | 2:I:48:THR:OG1    | 2.29                     | 0.45              |
| 7:L:309:BCL:HBC2  | 7:L:309:BCL:CHD   | 2.46                     | 0.45              |
| 2:Q:38:LYS:HB2    | 2:Q:40:ASP:O      | 2.17                     | 0.45              |
| 2:3:6:LYS:C       | 2:3:8:TRP:N       | 2.72                     | 0.45              |
| 12:L:310:U10:H121 | 12:L:310:U10:H101 | 1.83                     | 0.45              |
| 2:1:32:HIS:ND1    | 7:1:102:BCL:HMD1  | 2.32                     | 0.45              |
| 1:8:41:ALA:O      | 1:8:44:ILE:HB     | 2.16                     | 0.45              |
| 3:H:74:VAL:O      | 3:H:77:SER:HB3    | 2.17                     | 0.45              |
| 1:R:12:LEU:HD22   | 1:R:16:GLN:OE1    | 2.15                     | 0.45              |
| 2:W:33:LEU:CD2    | 9:W:103:PC1:H232  | 2.46                     | 0.45              |
| 1:2:47:PRO:HB2    | 2:a:51:TYR:CZ     | 2.51                     | 0.45              |
| 8:2:101:SPO:O1    | 7:a:101:BCL:HMB2  | 2.17                     | 0.45              |
| 2:3:11:PHE:HB3    | 2:3:16:VAL:HG21   | 1.98                     | 0.45              |
| 7:C:101:BCL:H111  | 7:C:101:BCL:H151  | 1.46                     | 0.45              |
| 1:B:38:ALA:O      | 1:B:42:VAL:HG23   | 2.17                     | 0.45              |
| 12:L:308:U10:H102 | 12:L:308:U10:O5   | 2.17                     | 0.45              |
| 1:P:36:VAL:HG12   | 1:P:40:ILE:HD12   | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:41:ALA:CB    | 8:0:103:SPO:H23  | 2.46                     | 0.45              |
| 2:1:36:LEU:HD21  | 2:1:43:TRP:CH2   | 2.51                     | 0.45              |
| 7:D:102:BCL:H61  | 7:D:102:BCL:H102 | 1.66                     | 0.45              |
| 2:K:31:ILE:HG21  | 7:N:102:BCL:C1D  | 2.47                     | 0.45              |
| 2:K:40:ASP:O     | 1:N:46:ARG:NH1   | 2.49                     | 0.45              |
| 8:N:101:SPO:HM13 | 2:O:33:LEU:HD23  | 1.99                     | 0.45              |
| 7:S:102:BCL:CGD  | 7:S:102:BCL:HAA2 | 2.47                     | 0.45              |
| 7:J:102:BCL:H12  | 7:J:102:BCL:HBA1 | 1.35                     | 0.45              |
| 2:K:7:ILE:HD11   | 7:O:101:BCL:H203 | 1.98                     | 0.45              |
| 7:7:101:BCL:CBB  | 7:7:101:BCL:HHC  | 2.47                     | 0.44              |
| 7:J:102:BCL:H71  | 8:K:102:SPO:H241 | 1.99                     | 0.44              |
| 4:L:137:PRO:O    | 4:L:141:GLY:N    | 2.50                     | 0.44              |
| 7:N:102:BCL:H121 | 7:N:102:BCL:H162 | 1.51                     | 0.44              |
| 2:9:43:TRP:CE3   | 7:9:101:BCL:HAC2 | 2.51                     | 0.44              |
| 5:M:119:SER:HB3  | 8:M:406:SPO:H302 | 2.00                     | 0.44              |
| 1:V:47:PRO:HB2   | 2:W:51:TYR:CE2   | 2.52                     | 0.44              |
| 7:7:101:BCL:H102 | 1:8:31:PHE:CD1   | 2.46                     | 0.44              |
| 1:C:13:SER:HA    | 1:Z:12:LEU:HD22  | 2.00                     | 0.44              |
| 1:E:21:HIS:O     | 1:E:25:MET:HG2   | 2.17                     | 0.44              |
| 8:I:102:SPO:H10  | 8:I:102:SPO:H81  | 1.82                     | 0.44              |
| 7:N:102:BCL:H71  | 7:N:102:BCL:C4   | 2.46                     | 0.44              |
| 2:3:17:PHE:HB2   | 2:W:11:PHE:CZ    | 2.53                     | 0.44              |
| 8:T:102:SPO:H10  | 8:T:102:SPO:H81  | 1.90                     | 0.44              |
| 1:b:29:TRP:CZ3   | 7:b:101:BCL:H13  | 2.52                     | 0.44              |
| 7:0:101:BCL:OBD  | 7:9:101:BCL:HBD  | 2.17                     | 0.44              |
| 7:M:403:BCL:HMB1 | 7:M:403:BCL:HBB3 | 1.99                     | 0.44              |
| 8:S:101:SPO:H15  | 8:S:101:SPO:H131 | 1.75                     | 0.44              |
| 7:a:101:BCL:H62  | 7:a:101:BCL:H41  | 1.70                     | 0.44              |
| 7:7:101:BCL:HBC3 | 7:7:101:BCL:H2C  | 1.66                     | 0.44              |
| 7:9:101:BCL:HAA2 | 7:9:101:BCL:CBD  | 2.48                     | 0.44              |
| 7:J:102:BCL:H71  | 8:K:102:SPO:C24  | 2.48                     | 0.44              |
| 4:L:62:PRO:HA    | 4:L:65:ILE:HD12  | 2.00                     | 0.44              |
| 4:L:228:LEU:HD21 | 4:L:232:ARG:NH2  | 2.32                     | 0.44              |
| 1:P:31:PHE:CB    | 8:P:101:SPO:H242 | 2.48                     | 0.44              |
| 7:Q:101:BCL:H201 | 8:R:101:SPO:C29  | 2.47                     | 0.44              |
| 2:K:7:ILE:CD1    | 7:O:101:BCL:H203 | 2.48                     | 0.44              |
| 5:M:214:LEU:HG   | 5:M:218:MET:SD   | 2.58                     | 0.44              |
| 1:R:28:LEU:HD23  | 1:R:28:LEU:C     | 2.42                     | 0.44              |
| 2:W:38:LYS:O     | 2:W:39:PRO:C     | 2.59                     | 0.44              |
| 1:b:15:GLU:HG2   | 1:b:16:GLN:N     | 2.33                     | 0.44              |
| 8:0:102:SPO:H343 | 7:A:101:BCL:H8   | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:17:PHE:N     | 2:F:17:PHE:CD1   | 2.85                     | 0.44              |
| 1:V:49:LEU:HD13  | 1:V:49:LEU:HA    | 1.80                     | 0.44              |
| 7:1:101:BCL:HMB2 | 8:Z:101:SPO:C5   | 2.45                     | 0.44              |
| 2:3:32:HIS:CE1   | 7:3:102:BCL:HMD1 | 2.53                     | 0.44              |
| 7:3:101:BCL:H141 | 7:3:101:BCL:H162 | 1.77                     | 0.44              |
| 2:7:27:LEU:O     | 2:7:31:ILE:HG13  | 2.17                     | 0.44              |
| 9:9:103:PC1:H2   | 9:9:103:PC1:H221 | 1.72                     | 0.44              |
| 7:E:101:BCL:H121 | 7:E:101:BCL:H91  | 1.99                     | 0.44              |
| 5:M:116:PHE:HD2  | 2:Q:33:LEU:HD13  | 1.82                     | 0.44              |
| 2:S:8:TRP:HB3    | 1:T:20:LEU:HD23  | 1.98                     | 0.44              |
| 2:U:7:ILE:HG23   | 2:U:8:TRP:N      | 2.33                     | 0.44              |
| 7:a:101:BCL:HMB1 | 7:a:101:BCL:HBB3 | 1.96                     | 0.44              |
| 7:8:102:BCL:HMB1 | 7:8:102:BCL:HBB3 | 1.98                     | 0.43              |
| 7:J:102:BCL:H3A  | 7:J:102:BCL:C1   | 2.44                     | 0.43              |
| 8:R:101:SPO:C13  | 7:S:102:BCL:H42  | 2.48                     | 0.43              |
| 8:S:103:SPO:C6   | 8:S:103:SPO:H33  | 2.48                     | 0.43              |
| 2:1:36:LEU:HD21  | 2:1:43:TRP:CZ3   | 2.53                     | 0.43              |
| 1:B:32:VAL:HG21  | 7:B:101:BCL:H51  | 2.01                     | 0.43              |
| 2:U:27:LEU:HD23  | 7:V:101:BCL:HED3 | 2.00                     | 0.43              |
| 2:U:32:HIS:CE1   | 7:V:101:BCL:HMD1 | 2.53                     | 0.43              |
| 2:3:15:ARG:HE    | 2:3:15:ARG:HB3   | 1.56                     | 0.43              |
| 2:3:17:PHE:HB2   | 2:W:11:PHE:HZ    | 1.84                     | 0.43              |
| 2:7:40:ASP:OD2   | 2:9:48:THR:OG1   | 2.24                     | 0.43              |
| 7:7:101:BCL:O1D  | 7:7:101:BCL:H2A  | 2.18                     | 0.43              |
| 7:A:101:BCL:HAA2 | 7:A:101:BCL:CGD  | 2.48                     | 0.43              |
| 8:A:102:SPO:H132 | 7:F:102:BCL:H2   | 1.98                     | 0.43              |
| 7:P:102:BCL:H91  | 7:P:102:BCL:H111 | 1.85                     | 0.43              |
| 2:S:5:TYR:OH     | 2:S:6:LYS:NZ     | 2.44                     | 0.43              |
| 7:T:101:BCL:H91  | 7:T:101:BCL:C14  | 2.47                     | 0.43              |
| 2:W:51:TYR:OH    | 8:W:101:SPO:H22A | 2.18                     | 0.43              |
| 4:L:7:GLU:O      | 4:L:11:ARG:HG3   | 2.18                     | 0.43              |
| 5:M:81:PHE:HB3   | 2:U:33:LEU:HD22  | 2.00                     | 0.43              |
| 5:M:270:TRP:O    | 5:M:274:VAL:HG13 | 2.18                     | 0.43              |
| 8:P:101:SPO:C13  | 7:Q:101:BCL:H2   | 2.47                     | 0.43              |
| 7:R:103:BCL:H93  | 7:R:103:BCL:H112 | 1.88                     | 0.43              |
| 2:3:8:TRP:HE1    | 1:Z:21:HIS:CA    | 2.30                     | 0.43              |
| 2:I:7:ILE:HD13   | 8:N:101:SPO:H311 | 1.99                     | 0.43              |
| 7:K:101:BCL:HMA2 | 8:K:102:SPO:C25  | 2.48                     | 0.43              |
| 4:L:136:ARG:HB3  | 4:L:137:PRO:HD3  | 2.00                     | 0.43              |
| 11:L:303:BPH:NB  | 5:M:214:LEU:HD13 | 2.34                     | 0.43              |
| 1:N:23:VAL:HG21  | 8:N:101:SPO:H341 | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:R:20:LEU:HD13   | 8:R:101:SPO:H403  | 1.99                     | 0.43              |
| 1:Z:13:SER:O      | 1:Z:17:ALA:HB2    | 2.19                     | 0.43              |
| 7:a:101:BCL:H3A   | 7:a:101:BCL:HBA1  | 1.62                     | 0.43              |
| 7:E:101:BCL:H203  | 7:E:101:BCL:C12   | 2.48                     | 0.43              |
| 7:S:102:BCL:HHC   | 7:S:102:BCL:HBB2  | 2.00                     | 0.43              |
| 7:T:101:BCL:HMC3  | 7:U:101:BCL:CBB   | 2.46                     | 0.43              |
| 12:X:101:U10:H172 | 12:X:101:U10:H151 | 1.55                     | 0.43              |
| 7:3:101:BCL:HMB3  | 7:C:101:BCL:C1B   | 2.49                     | 0.43              |
| 7:9:101:BCL:H203  | 8:9:102:SPO:H291  | 2.01                     | 0.43              |
| 1:J:13:SER:HB3    | 1:J:16:GLN:HG3    | 2.00                     | 0.43              |
| 2:S:20:GLN:NE2    | 8:S:103:SPO:H22   | 2.34                     | 0.43              |
| 2:W:43:TRP:CE3    | 7:W:102:BCL:HBC2  | 2.53                     | 0.43              |
| 7:I:101:BCL:HMB3  | 7:I:101:BCL:HBB3  | 2.00                     | 0.43              |
| 1:J:20:LEU:CD1    | 8:J:101:SPO:H341  | 2.49                     | 0.43              |
| 4:L:271:PRO:HD2   | 4:L:272:TRP:CE3   | 2.54                     | 0.43              |
| 11:L:303:BPH:OBB  | 11:L:303:BPH:HHC  | 2.19                     | 0.43              |
| 5:M:249:ALA:N     | 12:M:405:U10:H4M2 | 2.34                     | 0.43              |
| 7:N:102:BCL:HBB1  | 7:O:101:BCL:HMC3  | 2.00                     | 0.43              |
| 1:R:36:VAL:HG12   | 1:R:40:ILE:HD12   | 2.00                     | 0.43              |
| 2:9:30:MET:CE     | 4:L:49:LEU:HD23   | 2.48                     | 0.43              |
| 2:9:40:ASP:OD1    | 2:9:41:TYR:N      | 2.48                     | 0.43              |
| 3:H:50:ALA:HB1    | 3:H:51:PRO:HD2    | 2.01                     | 0.43              |
| 8:A:102:SPO:H19   | 2:D:24:LEU:HD21   | 2.01                     | 0.42              |
| 7:J:102:BCL:HMB1  | 7:J:102:BCL:HBB3  | 2.00                     | 0.42              |
| 7:L:301:BCL:HBB3  | 7:L:309:BCL:HMD2  | 2.01                     | 0.42              |
| 7:L:309:BCL:H91   | 12:L:310:U10:C3M  | 2.31                     | 0.42              |
| 5:M:122:MET:SD    | 5:M:157:TRP:NE1   | 2.75                     | 0.42              |
| 1:T:10:THR:HG23   | 1:T:12:LEU:H      | 1.84                     | 0.42              |
| 1:C:23:GLN:HG2    | 2:W:5:TYR:CD1     | 2.54                     | 0.42              |
| 8:J:101:SPO:C6    | 7:K:101:BCL:HHB   | 2.49                     | 0.42              |
| 4:L:194:LEU:HD21  | 4:L:213:GLU:HB3   | 2.01                     | 0.42              |
| 7:b:101:BCL:H2A   | 7:b:101:BCL:HED3  | 2.01                     | 0.42              |
| 2:7:10:VAL:HG22   | 8:9:102:SPO:H402  | 2.02                     | 0.42              |
| 2:A:14:ARG:O      | 2:A:18:VAL:HG23   | 2.19                     | 0.42              |
| 7:a:101:BCL:H51   | 7:a:101:BCL:H8    | 1.64                     | 0.42              |
| 2:1:27:LEU:O      | 2:1:31:ILE:HD12   | 2.20                     | 0.42              |
| 7:E:101:BCL:H142  | 7:E:101:BCL:H112  | 1.86                     | 0.42              |
| 5:M:94:SER:OG     | 5:M:96:ASP:OD1    | 2.36                     | 0.42              |
| 2:Q:43:TRP:CE3    | 7:Q:101:BCL:H2C   | 2.54                     | 0.42              |
| 7:T:101:BCL:H122  | 7:T:101:BCL:H161  | 1.65                     | 0.42              |
| 7:3:101:BCL:CAB   | 8:U:103:SPO:HM11  | 2.50                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:M:119:SER:OG    | 5:M:177:TYR:OH   | 2.26                     | 0.42              |
| 7:O:101:BCL:HED1  | 1:P:31:PHE:CD1   | 2.55                     | 0.42              |
| 2:Q:6:LYS:CD      | 8:S:103:SPO:H393 | 2.49                     | 0.42              |
| 2:U:5:TYR:HB2     | 1:V:18:GLN:HA    | 2.00                     | 0.42              |
| 7:1:102:BCL:HBB3  | 1:2:48:TRP:HE1   | 1.84                     | 0.42              |
| 8:2:101:SPO:H361  | 8:2:101:SPO:H341 | 1.63                     | 0.42              |
| 4:L:109:CYS:HG    | 5:M:251:PHE:HE2  | 1.66                     | 0.42              |
| 5:M:40:LEU:O      | 5:M:43:PHE:N     | 2.51                     | 0.42              |
| 5:M:165:PRO:HB3   | 5:M:170:SER:O    | 2.19                     | 0.42              |
| 9:M:409:PC1:H341  | 2:S:33:LEU:HB3   | 2.01                     | 0.42              |
| 7:1:102:BCL:H93   | 7:1:102:BCL:H61  | 1.82                     | 0.42              |
| 8:2:103:SPO:H42   | 8:2:103:SPO:H83  | 2.01                     | 0.42              |
| 2:9:6:LYS:HB2     | 8:D:101:SPO:H341 | 2.01                     | 0.42              |
| 8:A:102:SPO:H131  | 7:F:102:BCL:H2   | 1.96                     | 0.42              |
| 2:D:19:ALA:HB1    | 9:F:103:PC1:C37  | 2.50                     | 0.42              |
| 8:D:101:SPO:H26   | 8:D:101:SPO:H241 | 1.94                     | 0.42              |
| 2:K:34:ILE:O      | 2:K:37:SER:OG    | 2.30                     | 0.42              |
| 2:S:12:ASP:OD2    | 2:S:14:ARG:HG2   | 2.20                     | 0.42              |
| 2:S:40:ASP:HB2    | 1:T:46:ARG:HH12  | 1.85                     | 0.42              |
| 2:U:5:TYR:HA      | 1:V:21:HIS:CG    | 2.55                     | 0.42              |
| 8:0:102:SPO:H20   | 8:0:102:SPO:H181 | 1.87                     | 0.42              |
| 7:1:101:BCL:H61   | 7:1:101:BCL:H41  | 1.62                     | 0.42              |
| 1:J:20:LEU:HD12   | 8:J:101:SPO:H402 | 2.02                     | 0.42              |
| 11:L:303:BPH:HMB1 | 11:L:303:BPH:CBB | 2.45                     | 0.42              |
| 12:L:307:U10:H33  | 12:L:307:U10:C38 | 2.49                     | 0.42              |
| 8:O:102:SPO:H81   | 1:P:45:TRP:HB2   | 2.02                     | 0.42              |
| 2:W:3:LYS:HA      | 2:W:5:TYR:CE2    | 2.54                     | 0.42              |
| 8:2:101:SPO:H5    | 7:a:101:BCL:CHB  | 2.50                     | 0.42              |
| 1:8:19:GLU:O      | 1:8:23:VAL:HG13  | 2.20                     | 0.42              |
| 1:P:25:MET:O      | 1:P:29:TRP:CD1   | 2.73                     | 0.42              |
| 7:P:102:BCL:H142  | 7:P:102:BCL:H112 | 1.81                     | 0.42              |
| 2:1:11:PHE:O      | 2:1:12:ASP:C     | 2.60                     | 0.42              |
| 2:3:38:LYS:HA     | 2:3:38:LYS:HD3   | 1.80                     | 0.42              |
| 7:C:101:BCL:O1A   | 7:C:101:BCL:H2A  | 2.20                     | 0.42              |
| 7:F:102:BCL:H202  | 7:F:102:BCL:H162 | 1.78                     | 0.42              |
| 1:R:33:THR:O      | 1:R:37:ILE:HG12  | 2.20                     | 0.42              |
| 7:3:101:BCL:CHB   | 8:U:103:SPO:H6   | 2.50                     | 0.41              |
| 1:B:31:PHE:HE2    | 7:B:101:BCL:HBA2 | 1.84                     | 0.41              |
| 2:D:29:VAL:O      | 2:D:33:LEU:HG    | 2.20                     | 0.41              |
| 2:I:20:GLN:NE2    | 8:J:101:SPO:C22  | 2.83                     | 0.41              |
| 7:O:101:BCL:H143  | 7:O:101:BCL:H161 | 1.88                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:U:101:BCL:H72   | 7:U:101:BCL:H112  | 1.83                     | 0.41              |
| 1:0:47:PRO:HB2    | 2:A:51:TYR:CE2    | 2.56                     | 0.41              |
| 2:3:27:LEU:HD12   | 2:3:27:LEU:HA     | 1.79                     | 0.41              |
| 8:E:102:SPO:H183  | 8:E:102:SPO:H14   | 2.02                     | 0.41              |
| 5:M:164:ARG:N     | 5:M:165:PRO:CD    | 2.83                     | 0.41              |
| 5:M:293:ASN:C     | 5:M:293:ASN:OD1   | 2.63                     | 0.41              |
| 1:T:25:MET:O      | 1:T:29:TRP:CD1    | 2.74                     | 0.41              |
| 6:X:6:TYR:O       | 6:X:7:SER:CB      | 2.68                     | 0.41              |
| 1:0:21:HIS:O      | 1:0:25:MET:HG2    | 2.20                     | 0.41              |
| 3:H:175:VAL:HB    | 3:H:176:PRO:HD3   | 2.03                     | 0.41              |
| 2:I:17:PHE:N      | 2:I:17:PHE:CD1    | 2.88                     | 0.41              |
| 4:L:133:VAL:HG23  | 4:L:134:VAL:CG2   | 2.49                     | 0.41              |
| 10:M:408:CDL:H511 | 10:M:408:CDL:HB32 | 2.02                     | 0.41              |
| 8:N:101:SPO:C34   | 8:N:101:SPO:C30   | 2.98                     | 0.41              |
| 2:F:32:HIS:CE1    | 7:F:104:BCL:HMD1  | 2.55                     | 0.41              |
| 1:J:28:LEU:O      | 1:J:32:VAL:HG23   | 2.19                     | 0.41              |
| 3:H:35:ASN:ND2    | 5:M:264:GLY:HA3   | 2.35                     | 0.41              |
| 3:H:121:ARG:NH2   | 5:M:236:GLU:O     | 2.54                     | 0.41              |
| 7:N:102:BCL:H142  | 7:N:102:BCL:H111  | 1.81                     | 0.41              |
| 6:X:9:GLU:HB3     | 6:X:14:ILE:HD11   | 2.01                     | 0.41              |
| 2:a:17:PHE:HZ     | 1:b:24:TYR:HB2    | 1.86                     | 0.41              |
| 1:C:17:LEU:HA     | 1:C:17:LEU:HD23   | 1.78                     | 0.41              |
| 8:E:102:SPO:H14   | 8:E:102:SPO:C18   | 2.51                     | 0.41              |
| 7:F:104:BCL:HBB2  | 1:G:48:TRP:NE1    | 2.35                     | 0.41              |
| 2:Q:9:GLN:NE2     | 1:R:12:LEU:O      | 2.54                     | 0.41              |
| 2:U:7:ILE:O       | 2:U:10:VAL:N      | 2.39                     | 0.41              |
| 1:2:40:ILE:O      | 1:2:44:ILE:HG12   | 2.20                     | 0.41              |
| 7:3:101:BCL:H203  | 2:W:7:ILE:HG21    | 2.01                     | 0.41              |
| 9:F:103:PC1:C37   | 9:F:103:PC1:H331  | 2.51                     | 0.41              |
| 7:F:104:BCL:O1D   | 7:F:104:BCL:H2A   | 2.20                     | 0.41              |
| 1:J:42:VAL:HG11   | 7:J:102:BCL:HBC1  | 2.01                     | 0.41              |
| 2:Q:23:PHE:CE1    | 2:S:25:PHE:CE1    | 3.09                     | 0.41              |
| 8:0:102:SPO:H131  | 1:B:42:VAL:HG22   | 2.02                     | 0.41              |
| 7:1:102:BCL:HMC3  | 7:a:101:BCL:CBB   | 2.50                     | 0.41              |
| 2:3:25:PHE:CE1    | 2:W:23:PHE:HE1    | 2.39                     | 0.41              |
| 9:A:103:PC1:H111  | 9:A:103:PC1:H133  | 1.55                     | 0.41              |
| 7:C:101:BCL:H92   | 7:C:101:BCL:C5    | 2.51                     | 0.41              |
| 7:I:101:BCL:H43   | 8:I:102:SPO:H292  | 2.02                     | 0.41              |
| 1:N:30:LEU:O      | 1:N:33:THR:HG22   | 2.21                     | 0.41              |
| 8:T:102:SPO:H15   | 8:T:102:SPO:H131  | 1.95                     | 0.41              |
| 1:8:48:TRP:CD1    | 1:8:49:LEU:HG     | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:E:101:BCL:H203  | 7:E:101:BCL:H162  | 1.84                     | 0.41              |
| 2:F:29:VAL:O      | 2:F:33:LEU:HG     | 2.20                     | 0.41              |
| 1:J:20:LEU:HD12   | 8:J:101:SPO:C38   | 2.51                     | 0.41              |
| 8:J:101:SPO:H26   | 8:J:101:SPO:H241  | 1.86                     | 0.41              |
| 8:J:101:SPO:HM11  | 2:K:33:LEU:HG     | 2.02                     | 0.41              |
| 4:L:275:ASP:O     | 4:L:276:ILE:C     | 2.63                     | 0.41              |
| 7:L:309:BCL:H92   | 7:L:309:BCL:H62   | 1.88                     | 0.41              |
| 5:M:12:GLN:NE2    | 5:M:41:GLY:HA3    | 2.36                     | 0.41              |
| 5:M:76:TRP:HE1    | 8:M:406:SPO:H32A  | 1.86                     | 0.41              |
| 5:M:148:TRP:HB2   | 5:M:270:TRP:HZ2   | 1.85                     | 0.41              |
| 1:R:42:VAL:O      | 1:R:43:TYR:C      | 2.64                     | 0.41              |
| 2:U:7:ILE:HG21    | 7:W:102:BCL:H172  | 2.02                     | 0.41              |
| 7:V:101:BCL:HHB   | 7:V:101:BCL:HMA1  | 1.94                     | 0.41              |
| 1:O:8:SER:OG      | 1:O:11:GLY:N      | 2.50                     | 0.41              |
| 2:A:27:LEU:HD23   | 7:B:101:BCL:HED3  | 2.03                     | 0.41              |
| 2:D:45:ASP:HA     | 2:D:48:THR:HG22   | 2.03                     | 0.41              |
| 7:F:102:BCL:H71   | 9:F:103:PC1:H261  | 2.02                     | 0.41              |
| 7:F:102:BCL:HBA2  | 7:F:102:BCL:H3A   | 1.88                     | 0.41              |
| 3:H:194:LEU:O     | 3:H:195:VAL:HG23  | 2.21                     | 0.41              |
| 7:K:101:BCL:HMD1  | 1:N:39:HIS:CE1    | 2.56                     | 0.41              |
| 10:M:407:CDL:H722 | 10:M:407:CDL:HB61 | 2.03                     | 0.41              |
| 2:O:46:VAL:HG21   | 1:P:46:ARG:NH1    | 2.36                     | 0.41              |
| 8:S:101:SPO:H10   | 8:S:101:SPO:H81   | 1.91                     | 0.41              |
| 1:V:46:ARG:HA     | 1:V:46:ARG:HD3    | 1.79                     | 0.41              |
| 2:9:40:ASP:C      | 2:9:42:ASN:H      | 2.29                     | 0.40              |
| 2:9:43:TRP:CZ3    | 7:9:101:BCL:HAC2  | 2.56                     | 0.40              |
| 7:F:102:BCL:H93   | 7:F:102:BCL:H112  | 1.91                     | 0.40              |
| 2:I:8:TRP:CG      | 1:J:20:LEU:HD23   | 2.56                     | 0.40              |
| 1:P:31:PHE:HB2    | 8:P:101:SPO:H242  | 2.02                     | 0.40              |
| 2:U:30:MET:O      | 2:U:34:ILE:HG13   | 2.21                     | 0.40              |
| 7:U:101:BCL:HMB3  | 7:U:101:BCL:CBB   | 2.51                     | 0.40              |
| 7:W:102:BCL:H141  | 7:W:102:BCL:H162  | 1.72                     | 0.40              |
| 7:9:101:BCL:HAA2  | 7:9:101:BCL:CGD   | 2.51                     | 0.40              |
| 1:P:42:VAL:HG11   | 7:P:102:BCL:HBC1  | 2.03                     | 0.40              |
| 7:T:101:BCL:H91   | 7:T:101:BCL:H121  | 2.03                     | 0.40              |
| 7:3:102:BCL:H71   | 7:3:102:BCL:H112  | 1.84                     | 0.40              |
| 4:L:79:ALA:HB1    | 4:L:80:PRO:HD2    | 2.03                     | 0.40              |
| 11:L:303:BPH:CBB  | 11:L:303:BPH:CMB  | 3.00                     | 0.40              |
| 12:L:306:U10:H102 | 12:L:306:U10:C1M  | 2.51                     | 0.40              |
| 8:N:101:SPO:H26   | 8:N:101:SPO:H241  | 1.91                     | 0.40              |
| 7:R:103:BCL:H112  | 7:R:103:BCL:H142  | 1.83                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:25:MET:O     | 1:E:29:TRP:CD1   | 2.74                     | 0.40              |
| 2:U:8:TRP:HE1    | 1:V:21:HIS:HA    | 1.87                     | 0.40              |
| 1:2:29:TRP:CE3   | 1:2:29:TRP:HA    | 2.57                     | 0.40              |
| 7:D:102:BCL:H203 | 7:D:102:BCL:H162 | 1.98                     | 0.40              |
| 2:F:27:LEU:O     | 2:F:31:ILE:HG13  | 2.22                     | 0.40              |
| 2:K:31:ILE:HG22  | 7:N:102:BCL:HMD3 | 2.02                     | 0.40              |
| 2:K:35:LEU:HD11  | 7:N:102:BCL:HHD  | 2.04                     | 0.40              |
| 7:V:101:BCL:H141 | 7:V:101:BCL:H162 | 1.90                     | 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   | 0     | 42/49 (86%) | 40 (95%)  | 2 (5%)  | 0        | 100         | 100 |
| 1   | 2     | 37/49 (76%) | 35 (95%)  | 2 (5%)  | 0        | 100         | 100 |
| 1   | 8     | 41/49 (84%) | 40 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 1   | B     | 41/49 (84%) | 40 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 1   | C     | 41/49 (84%) | 38 (93%)  | 3 (7%)  | 0        | 100         | 100 |
| 1   | E     | 41/49 (84%) | 41 (100%) | 0       | 0        | 100         | 100 |
| 1   | G     | 41/49 (84%) | 41 (100%) | 0       | 0        | 100         | 100 |
| 1   | J     | 41/49 (84%) | 40 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 1   | N     | 41/49 (84%) | 40 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 1   | P     | 41/49 (84%) | 40 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 1   | R     | 41/49 (84%) | 41 (100%) | 0       | 0        | 100         | 100 |
| 1   | T     | 41/49 (84%) | 40 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 1   | V     | 41/49 (84%) | 40 (98%)  | 1 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | Z     | 39/49 (80%)     | 37 (95%)   | 2 (5%)  | 0        | 100         | 100 |
| 1   | b     | 34/49 (69%)     | 34 (100%)  | 0       | 0        | 100         | 100 |
| 2   | 1     | 47/62 (76%)     | 46 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 2   | 3     | 50/62 (81%)     | 49 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 2   | 7     | 42/62 (68%)     | 41 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 2   | 9     | 51/62 (82%)     | 50 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 2   | A     | 51/62 (82%)     | 49 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 2   | D     | 51/62 (82%)     | 49 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 2   | F     | 51/62 (82%)     | 49 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 2   | I     | 51/62 (82%)     | 50 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 2   | K     | 50/62 (81%)     | 48 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 2   | O     | 50/62 (81%)     | 47 (94%)   | 3 (6%)  | 0        | 100         | 100 |
| 2   | Q     | 50/62 (81%)     | 46 (92%)   | 4 (8%)  | 0        | 100         | 100 |
| 2   | S     | 50/62 (81%)     | 46 (92%)   | 4 (8%)  | 0        | 100         | 100 |
| 2   | U     | 50/62 (81%)     | 49 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 2   | W     | 49/62 (79%)     | 48 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 2   | a     | 46/62 (74%)     | 46 (100%)  | 0       | 0        | 100         | 100 |
| 3   | H     | 252/256 (98%)   | 235 (93%)  | 17 (7%) | 0        | 100         | 100 |
| 4   | L     | 279/282 (99%)   | 262 (94%)  | 17 (6%) | 0        | 100         | 100 |
| 5   | M     | 302/307 (98%)   | 291 (96%)  | 11 (4%) | 0        | 100         | 100 |
| 6   | X     | 58/75 (77%)     | 55 (95%)   | 3 (5%)  | 0        | 100         | 100 |
| All | All   | 2233/2585 (86%) | 2143 (96%) | 90 (4%) | 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   | 0     | 38/42 (90%)    | 38 (100%)  | 0        | 100         | 100 |
| 1   | 2     | 33/42 (79%)    | 31 (94%)   | 2 (6%)   | 17          | 35  |
| 1   | 8     | 37/42 (88%)    | 35 (95%)   | 2 (5%)   | 20          | 42  |
| 1   | B     | 37/42 (88%)    | 37 (100%)  | 0        | 100         | 100 |
| 1   | C     | 37/42 (88%)    | 34 (92%)   | 3 (8%)   | 11          | 24  |
| 1   | E     | 37/42 (88%)    | 36 (97%)   | 1 (3%)   | 39          | 63  |
| 1   | G     | 37/42 (88%)    | 36 (97%)   | 1 (3%)   | 39          | 63  |
| 1   | J     | 37/42 (88%)    | 37 (100%)  | 0        | 100         | 100 |
| 1   | N     | 37/42 (88%)    | 37 (100%)  | 0        | 100         | 100 |
| 1   | P     | 37/42 (88%)    | 36 (97%)   | 1 (3%)   | 39          | 63  |
| 1   | R     | 37/42 (88%)    | 37 (100%)  | 0        | 100         | 100 |
| 1   | T     | 37/42 (88%)    | 37 (100%)  | 0        | 100         | 100 |
| 1   | V     | 37/42 (88%)    | 36 (97%)   | 1 (3%)   | 39          | 63  |
| 1   | Z     | 35/42 (83%)    | 33 (94%)   | 2 (6%)   | 18          | 39  |
| 1   | b     | 31/42 (74%)    | 27 (87%)   | 4 (13%)  | 4           | 8   |
| 2   | 1     | 43/52 (83%)    | 41 (95%)   | 2 (5%)   | 23          | 47  |
| 2   | 3     | 46/52 (88%)    | 44 (96%)   | 2 (4%)   | 26          | 50  |
| 2   | 7     | 41/52 (79%)    | 41 (100%)  | 0        | 100         | 100 |
| 2   | 9     | 47/52 (90%)    | 47 (100%)  | 0        | 100         | 100 |
| 2   | A     | 47/52 (90%)    | 47 (100%)  | 0        | 100         | 100 |
| 2   | D     | 47/52 (90%)    | 47 (100%)  | 0        | 100         | 100 |
| 2   | F     | 47/52 (90%)    | 47 (100%)  | 0        | 100         | 100 |
| 2   | I     | 47/52 (90%)    | 46 (98%)   | 1 (2%)   | 47          | 70  |
| 2   | K     | 46/52 (88%)    | 46 (100%)  | 0        | 100         | 100 |
| 2   | O     | 46/52 (88%)    | 46 (100%)  | 0        | 100         | 100 |
| 2   | Q     | 46/52 (88%)    | 46 (100%)  | 0        | 100         | 100 |
| 2   | S     | 46/52 (88%)    | 44 (96%)   | 2 (4%)   | 26          | 50  |
| 2   | U     | 46/52 (88%)    | 46 (100%)  | 0        | 100         | 100 |
| 2   | W     | 45/52 (86%)    | 45 (100%)  | 0        | 100         | 100 |
| 2   | a     | 42/52 (81%)    | 40 (95%)   | 2 (5%)   | 23          | 46  |
| 3   | H     | 207/208 (100%) | 207 (100%) | 0        | 100         | 100 |
| 4   | L     | 223/224 (100%) | 220 (99%)  | 3 (1%)   | 61          | 79  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 5   | M     | 237/239 (99%)   | 235 (99%)  | 2 (1%)   | 73          | 86  |
| 6   | X     | 47/59 (80%)     | 47 (100%)  | 0        | 100         | 100 |
| All | All   | 1940/2140 (91%) | 1909 (98%) | 31 (2%)  | 54          | 76  |

All (31) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1     | 24  | LEU  |
| 2   | 1     | 26  | LEU  |
| 1   | 2     | 14  | ASP  |
| 1   | 2     | 20  | LEU  |
| 2   | 3     | 4   | PHE  |
| 2   | 3     | 15  | ARG  |
| 1   | 8     | 7   | LEU  |
| 1   | 8     | 23  | VAL  |
| 1   | C     | 18  | SER  |
| 1   | C     | 35  | LEU  |
| 1   | C     | 54  | LEU  |
| 1   | E     | 20  | LEU  |
| 1   | G     | 42  | VAL  |
| 2   | I     | 46  | VAL  |
| 4   | L     | 224 | SER  |
| 4   | L     | 248 | CYS  |
| 4   | L     | 252 | THR  |
| 5   | M     | 175 | VAL  |
| 5   | M     | 262 | MET  |
| 1   | P     | 12  | LEU  |
| 2   | S     | 40  | ASP  |
| 2   | S     | 53  | ARG  |
| 1   | V     | 49  | LEU  |
| 1   | Z     | 15  | GLU  |
| 1   | Z     | 20  | LEU  |
| 2   | a     | 16  | VAL  |
| 2   | a     | 45  | ASP  |
| 1   | b     | 18  | GLN  |
| 1   | b     | 20  | LEU  |
| 1   | b     | 28  | LEU  |
| 1   | b     | 31  | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 18  | GLN  |
| 2   | 7     | 9   | GLN  |
| 2   | 7     | 20  | GLN  |
| 2   | 9     | 20  | GLN  |
| 1   | C     | 23  | GLN  |
| 2   | F     | 9   | GLN  |
| 2   | F     | 20  | GLN  |
| 2   | F     | 32  | HIS  |
| 3   | H     | 32  | GLN  |
| 3   | H     | 132 | HIS  |
| 2   | O     | 32  | HIS  |
| 2   | Q     | 9   | GLN  |
| 1   | R     | 18  | GLN  |
| 2   | U     | 20  | GLN  |
| 1   | V     | 21  | HIS  |
| 1   | Z     | 16  | GLN  |
| 1   | b     | 39  | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 1 is monoatomic - leaving 86 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  | U     | 101 | -    | 69,74,74     | 0.57 | 1 (1%)   | 79,115,115  | 1.08 | 9 (11%)  |
| 8   | SPO  | D     | 101 | -    | 41,41,41     | 0.27 | 0        | 47,50,50    | 0.33 | 0        |
| 8   | SPO  | R     | 102 | -    | 41,41,41     | 0.85 | 0        | 47,50,50    | 1.90 | 12 (25%) |
| 7   | BCL  | R     | 103 | -    | 69,74,74     | 0.65 | 2 (2%)   | 79,115,115  | 1.12 | 12 (15%) |
| 7   | BCL  | B     | 101 | -    | 69,74,74     | 0.74 | 2 (2%)   | 79,115,115  | 1.18 | 11 (13%) |
| 8   | SPO  | M     | 406 | -    | 41,41,41     | 0.36 | 0        | 47,50,50    | 0.32 | 0        |
| 8   | SPO  | 2     | 102 | -    | 41,41,41     | 0.95 | 2 (4%)   | 47,50,50    | 2.17 | 16 (34%) |
| 8   | SPO  | Z     | 101 | -    | 41,41,41     | 0.21 | 0        | 47,50,50    | 0.55 | 0        |
| 9   | PC1  | L     | 305 | -    | 35,35,53     | 0.35 | 0        | 41,43,61    | 0.37 | 0        |
| 8   | SPO  | 2     | 101 | -    | 41,41,41     | 0.25 | 0        | 47,50,50    | 0.91 | 3 (6%)   |
| 8   | SPO  | R     | 101 | -    | 41,41,41     | 0.21 | 0        | 47,50,50    | 0.31 | 0        |
| 8   | SPO  | 0     | 102 | -    | 41,41,41     | 0.95 | 2 (4%)   | 47,50,50    | 2.41 | 13 (27%) |
| 7   | BCL  | N     | 102 | -    | 69,74,74     | 0.58 | 0        | 79,115,115  | 1.12 | 12 (15%) |
| 8   | SPO  | P     | 101 | -    | 41,41,41     | 0.22 | 0        | 47,50,50    | 0.45 | 0        |
| 8   | SPO  | W     | 101 | -    | 41,41,41     | 0.97 | 2 (4%)   | 47,50,50    | 1.71 | 12 (25%) |
| 7   | BCL  | b     | 101 | -    | 64,69,74     | 0.50 | 0        | 73,109,115  | 1.49 | 15 (20%) |
| 7   | BCL  | V     | 101 | -    | 69,74,74     | 0.55 | 1 (1%)   | 79,115,115  | 1.11 | 11 (13%) |
| 7   | BCL  | D     | 102 | -    | 69,74,74     | 0.66 | 1 (1%)   | 79,115,115  | 1.10 | 11 (13%) |
| 8   | SPO  | A     | 102 | -    | 41,41,41     | 0.36 | 0        | 47,50,50    | 0.40 | 0        |
| 12  | U10  | L     | 306 | -    | 43,43,63     | 0.21 | 0        | 54,55,79    | 0.54 | 1 (1%)   |
| 11  | BPH  | L     | 303 | -    | 56,67,70     | 1.44 | 6 (10%)  | 55,97,101   | 1.12 | 6 (10%)  |
| 8   | SPO  | J     | 101 | -    | 41,41,41     | 0.26 | 0        | 47,50,50    | 0.45 | 0        |
| 9   | PC1  | F     | 103 | -    | 36,36,53     | 0.35 | 0        | 42,44,61    | 0.36 | 0        |
| 8   | SPO  | S     | 103 | -    | 41,41,41     | 0.27 | 0        | 47,50,50    | 0.69 | 1 (2%)   |
| 7   | BCL  | 9     | 101 | -    | 69,74,74     | 0.60 | 1 (1%)   | 79,115,115  | 1.12 | 10 (12%) |
| 8   | SPO  | 3     | 103 | -    | 41,41,41     | 0.95 | 2 (4%)   | 47,50,50    | 1.92 | 15 (31%) |
| 7   | BCL  | a     | 101 | -    | 59,64,74     | 0.63 | 1 (1%)   | 67,103,115  | 1.21 | 10 (14%) |
| 7   | BCL  | M     | 403 | -    | 69,74,74     | 0.65 | 1 (1%)   | 79,115,115  | 1.13 | 10 (12%) |
| 8   | SPO  | 0     | 103 | -    | 41,41,41     | 0.68 | 0        | 47,50,50    | 2.67 | 17 (36%) |
| 10  | CDL  | M     | 407 | -    | 99,99,99     | 0.32 | 0        | 105,111,111 | 0.44 | 0        |
| 12  | U10  | L     | 304 | -    | 43,43,63     | 0.23 | 0        | 54,55,79    | 0.54 | 1 (1%)   |
| 7   | BCL  | F     | 102 | -    | 69,74,74     | 0.59 | 1 (1%)   | 79,115,115  | 1.07 | 9 (11%)  |
| 7   | BCL  | W     | 102 | -    | 69,74,74     | 0.53 | 0        | 79,115,115  | 1.11 | 12 (15%) |
| 9   | PC1  | H     | 301 | -    | 46,46,53     | 1.00 | 2 (4%)   | 52,54,61    | 1.01 | 2 (3%)   |
| 10  | CDL  | F     | 101 | -    | 77,77,99     | 1.06 | 4 (5%)   | 83,89,111   | 1.06 | 7 (8%)   |
| 12  | U10  | X     | 101 | -    | 48,48,63     | 0.28 | 0        | 60,61,79    | 0.78 | 2 (3%)   |
| 7   | BCL  | J     | 102 | -    | 69,74,74     | 0.73 | 4 (5%)   | 79,115,115  | 1.16 | 12 (15%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 7   | BCL  | 0     | 101 | -    | 64,69,74     | 0.71 | 2 (3%)   | 73,109,115  | 1.24 | 12 (16%) |
| 9   | PC1  | M     | 401 | -    | 39,39,53     | 0.34 | 0        | 45,47,61    | 0.34 | 0        |
| 7   | BCL  | K     | 101 | -    | 69,74,74     | 0.68 | 1 (1%)   | 79,115,115  | 1.11 | 13 (16%) |
| 9   | PC1  | 9     | 103 | -    | 44,44,53     | 0.33 | 0        | 50,52,61    | 0.51 | 0        |
| 7   | BCL  | 1     | 101 | -    | 59,64,74     | 0.66 | 1 (1%)   | 67,103,115  | 1.16 | 12 (17%) |
| 9   | PC1  | M     | 402 | -    | 34,34,53     | 1.15 | 2 (5%)   | 40,42,61    | 1.01 | 2 (5%)   |
| 9   | PC1  | M     | 409 | -    | 44,44,53     | 0.31 | 0        | 50,52,61    | 0.40 | 0        |
| 7   | BCL  | L     | 301 | -    | 69,74,74     | 0.69 | 2 (2%)   | 79,115,115  | 1.18 | 12 (15%) |
| 8   | SPO  | I     | 102 | -    | 41,41,41     | 1.13 | 3 (7%)   | 47,50,50    | 2.29 | 15 (31%) |
| 12  | U10  | M     | 405 | -    | 48,48,63     | 0.32 | 0        | 60,61,79    | 0.58 | 1 (1%)   |
| 8   | SPO  | S     | 101 | -    | 41,41,41     | 0.98 | 1 (2%)   | 47,50,50    | 2.31 | 18 (38%) |
| 7   | BCL  | I     | 101 | -    | 69,74,74     | 0.59 | 1 (1%)   | 79,115,115  | 1.13 | 9 (11%)  |
| 7   | BCL  | 8     | 102 | -    | 69,74,74     | 0.62 | 2 (2%)   | 79,115,115  | 1.10 | 10 (12%) |
| 9   | PC1  | A     | 103 | -    | 31,31,53     | 1.25 | 2 (6%)   | 37,39,61    | 1.34 | 5 (13%)  |
| 7   | BCL  | 7     | 101 | -    | 64,69,74     | 0.64 | 2 (3%)   | 73,109,115  | 1.20 | 10 (13%) |
| 8   | SPO  | O     | 102 | -    | 41,41,41     | 0.93 | 2 (4%)   | 47,50,50    | 1.66 | 10 (21%) |
| 10  | CDL  | M     | 408 | -    | 77,77,99     | 0.34 | 0        | 83,89,111   | 0.42 | 0        |
| 12  | U10  | L     | 307 | -    | 48,48,63     | 0.23 | 0        | 60,61,79    | 0.60 | 1 (1%)   |
| 8   | SPO  | F     | 105 | -    | 41,41,41     | 0.80 | 1 (2%)   | 47,50,50    | 1.61 | 7 (14%)  |
| 7   | BCL  | P     | 102 | -    | 69,74,74     | 0.63 | 2 (2%)   | 79,115,115  | 1.09 | 12 (15%) |
| 7   | BCL  | O     | 101 | -    | 69,74,74     | 0.66 | 1 (1%)   | 79,115,115  | 1.05 | 10 (12%) |
| 8   | SPO  | N     | 101 | -    | 41,41,41     | 0.28 | 0        | 47,50,50    | 0.39 | 0        |
| 12  | U10  | L     | 308 | -    | 19,19,63     | 0.32 | 0        | 24,26,79    | 0.76 | 1 (4%)   |
| 7   | BCL  | 3     | 102 | -    | 69,74,74     | 0.62 | 2 (2%)   | 79,115,115  | 1.14 | 12 (15%) |
| 7   | BCL  | F     | 104 | -    | 69,74,74     | 0.73 | 3 (4%)   | 79,115,115  | 1.17 | 11 (13%) |
| 8   | SPO  | 9     | 102 | -    | 41,41,41     | 0.37 | 0        | 47,50,50    | 0.51 | 0        |
| 12  | U10  | L     | 310 | -    | 38,38,63     | 0.20 | 0        | 48,49,79    | 0.51 | 1 (2%)   |
| 7   | BCL  | L     | 309 | -    | 69,74,74     | 0.70 | 2 (2%)   | 79,115,115  | 1.10 | 8 (10%)  |
| 8   | SPO  | D     | 103 | -    | 41,41,41     | 0.22 | 0        | 47,50,50    | 0.52 | 0        |
| 11  | BPH  | L     | 311 | -    | 49,60,70     | 1.51 | 6 (12%)  | 47,89,101   | 1.17 | 6 (12%)  |
| 7   | BCL  | 3     | 101 | -    | 69,74,74     | 0.53 | 1 (1%)   | 79,115,115  | 1.18 | 13 (16%) |
| 7   | BCL  | 1     | 102 | -    | 64,69,74     | 0.64 | 1 (1%)   | 73,109,115  | 1.10 | 10 (13%) |
| 8   | SPO  | 8     | 101 | -    | 38,38,41     | 0.40 | 0        | 42,46,50    | 0.59 | 1 (2%)   |
| 7   | BCL  | A     | 101 | -    | 69,74,74     | 0.62 | 1 (1%)   | 79,115,115  | 1.06 | 8 (10%)  |
| 7   | BCL  | C     | 101 | -    | 69,74,74     | 0.63 | 3 (4%)   | 79,115,115  | 1.09 | 10 (12%) |
| 7   | BCL  | S     | 102 | -    | 69,74,74     | 0.54 | 1 (1%)   | 79,115,115  | 1.13 | 11 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | PC1  | A     | 104 | -    | 31,31,53     | 0.38 | 0        | 37,39,61    | 0.41 | 0        |
| 8   | SPO  | 2     | 103 | -    | 41,41,41     | 0.88 | 1 (2%)   | 47,50,50    | 2.05 | 17 (36%) |
| 7   | BCL  | T     | 101 | -    | 69,74,74     | 0.61 | 2 (2%)   | 79,115,115  | 1.19 | 12 (15%) |
| 7   | BCL  | E     | 101 | -    | 69,74,74     | 0.67 | 2 (2%)   | 79,115,115  | 1.11 | 10 (12%) |
| 7   | BCL  | Q     | 101 | -    | 69,74,74     | 0.61 | 1 (1%)   | 79,115,115  | 1.07 | 8 (10%)  |
| 8   | SPO  | E     | 102 | -    | 41,41,41     | 1.03 | 3 (7%)   | 47,50,50    | 2.15 | 17 (36%) |
| 9   | PC1  | W     | 103 | -    | 31,31,53     | 0.36 | 0        | 37,39,61    | 0.50 | 0        |
| 8   | SPO  | T     | 102 | -    | 41,41,41     | 0.81 | 0        | 47,50,50    | 1.76 | 10 (21%) |
| 7   | BCL  | L     | 302 | -    | 66,71,74     | 0.68 | 2 (3%)   | 75,111,115  | 1.17 | 11 (14%) |
| 8   | SPO  | K     | 102 | -    | 41,41,41     | 1.02 | 2 (4%)   | 47,50,50    | 2.63 | 17 (36%) |
| 9   | PC1  | M     | 410 | -    | 31,31,53     | 0.36 | 0        | 37,39,61    | 0.35 | 0        |
| 8   | SPO  | U     | 102 | -    | 41,41,41     | 0.15 | 0        | 47,50,50    | 0.30 | 0        |
| 8   | SPO  | U     | 103 | -    | 41,41,41     | 0.20 | 0        | 47,50,50    | 0.45 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings |
|-----|------|-------|-----|------|---------|---------------|-------|
| 7   | BCL  | U     | 101 | -    | -       | 16/41/137/137 | -     |
| 8   | SPO  | D     | 101 | -    | -       | 6/47/47/47    | -     |
| 8   | SPO  | R     | 102 | -    | -       | 11/47/47/47   | -     |
| 7   | BCL  | R     | 103 | -    | -       | 24/41/137/137 | -     |
| 7   | BCL  | B     | 101 | -    | -       | 17/41/137/137 | -     |
| 8   | SPO  | M     | 406 | -    | -       | 9/47/47/47    | -     |
| 8   | SPO  | 2     | 102 | -    | -       | 7/47/47/47    | -     |
| 8   | SPO  | Z     | 101 | -    | -       | 11/47/47/47   | -     |
| 9   | PC1  | L     | 305 | -    | -       | 13/39/39/57   | -     |
| 8   | SPO  | 2     | 101 | -    | -       | 12/47/47/47   | -     |
| 8   | SPO  | R     | 101 | -    | -       | 4/47/47/47    | -     |
| 8   | SPO  | 0     | 102 | -    | -       | 15/47/47/47   | -     |
| 7   | BCL  | N     | 102 | -    | -       | 16/41/137/137 | -     |
| 8   | SPO  | P     | 101 | -    | -       | 4/47/47/47    | -     |
| 8   | SPO  | W     | 101 | -    | -       | 7/47/47/47    | -     |
| 7   | BCL  | b     | 101 | -    | -       | 22/35/131/137 | -     |
| 7   | BCL  | V     | 101 | -    | -       | 17/41/137/137 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 7   | BCL  | D     | 102 | -    | -       | 15/41/137/137  | -       |
| 8   | SPO  | A     | 102 | -    | -       | 8/47/47/47     | -       |
| 12  | U10  | L     | 306 | -    | -       | 14/39/63/87    | 0/1/1/1 |
| 11  | BPH  | L     | 303 | -    | -       | 6/34/102/105   | 0/5/6/6 |
| 8   | SPO  | J     | 101 | -    | -       | 6/47/47/47     | -       |
| 9   | PC1  | F     | 103 | -    | -       | 13/40/40/57    | -       |
| 8   | SPO  | S     | 103 | -    | -       | 17/47/47/47    | -       |
| 7   | BCL  | 9     | 101 | -    | -       | 19/41/137/137  | -       |
| 8   | SPO  | 3     | 103 | -    | -       | 11/47/47/47    | -       |
| 7   | BCL  | a     | 101 | -    | -       | 13/29/125/137  | -       |
| 7   | BCL  | M     | 403 | -    | -       | 17/41/137/137  | -       |
| 8   | SPO  | 0     | 103 | -    | -       | 15/47/47/47    | -       |
| 10  | CDL  | M     | 407 | -    | -       | 38/110/110/110 | -       |
| 12  | U10  | L     | 304 | -    | -       | 11/39/63/87    | 0/1/1/1 |
| 7   | BCL  | F     | 102 | -    | -       | 23/41/137/137  | -       |
| 7   | BCL  | W     | 102 | -    | -       | 17/41/137/137  | -       |
| 9   | PC1  | H     | 301 | -    | -       | 18/50/50/57    | -       |
| 10  | CDL  | F     | 101 | -    | -       | 32/88/88/110   | -       |
| 12  | U10  | X     | 101 | -    | -       | 18/45/69/87    | 0/1/1/1 |
| 7   | BCL  | J     | 102 | -    | -       | 21/41/137/137  | -       |
| 7   | BCL  | 0     | 101 | -    | -       | 15/35/131/137  | -       |
| 9   | PC1  | M     | 401 | -    | -       | 10/43/43/57    | -       |
| 7   | BCL  | K     | 101 | -    | -       | 13/41/137/137  | -       |
| 9   | PC1  | 9     | 103 | -    | -       | 20/48/48/57    | -       |
| 7   | BCL  | 1     | 101 | -    | -       | 9/29/125/137   | -       |
| 9   | PC1  | M     | 402 | -    | -       | 14/38/38/57    | -       |
| 9   | PC1  | M     | 409 | -    | -       | 10/48/48/57    | -       |
| 7   | BCL  | L     | 301 | -    | -       | 4/41/137/137   | -       |
| 8   | SPO  | I     | 102 | -    | -       | 5/47/47/47     | -       |
| 12  | U10  | M     | 405 | -    | -       | 5/45/69/87     | 0/1/1/1 |
| 8   | SPO  | S     | 101 | -    | -       | 6/47/47/47     | -       |
| 7   | BCL  | I     | 101 | -    | -       | 11/41/137/137  | -       |
| 7   | BCL  | 8     | 102 | -    | -       | 20/41/137/137  | -       |
| 9   | PC1  | A     | 103 | -    | -       | 8/35/35/57     | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 7   | BCL  | 7     | 101 | -    | -       | 8/35/131/137  | -       |
| 8   | SPO  | O     | 102 | -    | -       | 4/47/47/47    | -       |
| 10  | CDL  | M     | 408 | -    | -       | 18/88/88/110  | -       |
| 12  | U10  | L     | 307 | -    | -       | 12/45/69/87   | 0/1/1/1 |
| 8   | SPO  | F     | 105 | -    | -       | 3/47/47/47    | -       |
| 7   | BCL  | P     | 102 | -    | -       | 20/41/137/137 | -       |
| 7   | BCL  | O     | 101 | -    | -       | 14/41/137/137 | -       |
| 8   | SPO  | N     | 101 | -    | -       | 4/47/47/47    | -       |
| 12  | U10  | L     | 308 | -    | -       | 1/11/35/87    | 0/1/1/1 |
| 7   | BCL  | 3     | 102 | -    | -       | 16/41/137/137 | -       |
| 7   | BCL  | F     | 104 | -    | -       | 22/41/137/137 | -       |
| 8   | SPO  | 9     | 102 | -    | -       | 6/47/47/47    | -       |
| 12  | U10  | L     | 310 | -    | -       | 10/33/57/87   | 0/1/1/1 |
| 7   | BCL  | L     | 309 | -    | -       | 18/41/137/137 | -       |
| 8   | SPO  | D     | 103 | -    | -       | 14/47/47/47   | -       |
| 11  | BPH  | L     | 311 | -    | -       | 5/25/93/105   | 0/5/6/6 |
| 7   | BCL  | 3     | 101 | -    | -       | 17/41/137/137 | -       |
| 7   | BCL  | 1     | 102 | -    | -       | 20/35/131/137 | -       |
| 8   | SPO  | 8     | 101 | -    | -       | 6/44/44/47    | -       |
| 7   | BCL  | A     | 101 | -    | -       | 11/41/137/137 | -       |
| 7   | BCL  | C     | 101 | -    | -       | 24/41/137/137 | -       |
| 7   | BCL  | S     | 102 | -    | -       | 10/41/137/137 | -       |
| 9   | PC1  | A     | 104 | -    | -       | 10/35/35/57   | -       |
| 8   | SPO  | 2     | 103 | -    | -       | 11/47/47/47   | -       |
| 7   | BCL  | T     | 101 | -    | -       | 15/41/137/137 | -       |
| 7   | BCL  | E     | 101 | -    | -       | 25/41/137/137 | -       |
| 7   | BCL  | Q     | 101 | -    | -       | 15/41/137/137 | -       |
| 8   | SPO  | E     | 102 | -    | -       | 10/47/47/47   | -       |
| 9   | PC1  | W     | 103 | -    | -       | 15/35/35/57   | -       |
| 8   | SPO  | T     | 102 | -    | -       | 3/47/47/47    | -       |
| 7   | BCL  | L     | 302 | -    | -       | 9/38/134/137  | -       |
| 8   | SPO  | K     | 102 | -    | -       | 11/47/47/47   | -       |
| 9   | PC1  | M     | 410 | -    | -       | 7/35/35/57    | -       |
| 8   | SPO  | U     | 102 | -    | -       | 5/47/47/47    | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 8   | SPO  | U     | 103 | -    | -       | 9/47/47/47 | -     |

All (93) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | L     | 303 | BPH  | C1D-C2D | 5.81  | 1.45        | 1.39     |
| 11  | L     | 311 | BPH  | C3A-C2A | -5.78 | 1.49        | 1.54     |
| 11  | L     | 311 | BPH  | C1D-C2D | 5.48  | 1.45        | 1.39     |
| 11  | L     | 303 | BPH  | C3A-C2A | -5.05 | 1.50        | 1.54     |
| 10  | F     | 101 | CDL  | OB8-CB7 | 4.42  | 1.46        | 1.33     |
| 9   | A     | 103 | PC1  | O21-C21 | 4.38  | 1.46        | 1.34     |
| 9   | H     | 301 | PC1  | O21-C21 | 4.31  | 1.46        | 1.34     |
| 10  | F     | 101 | CDL  | OA6-CA5 | 4.31  | 1.46        | 1.34     |
| 9   | M     | 402 | PC1  | O21-C21 | 4.30  | 1.46        | 1.34     |
| 10  | F     | 101 | CDL  | OA8-CA7 | 4.26  | 1.45        | 1.33     |
| 9   | M     | 402 | PC1  | O31-C31 | 4.23  | 1.45        | 1.33     |
| 9   | A     | 103 | PC1  | O31-C31 | 4.02  | 1.45        | 1.33     |
| 11  | L     | 303 | BPH  | C2C-C3C | -3.98 | 1.51        | 1.54     |
| 9   | H     | 301 | PC1  | O31-C31 | 3.95  | 1.44        | 1.33     |
| 10  | F     | 101 | CDL  | OB6-CB5 | 3.89  | 1.45        | 1.34     |
| 11  | L     | 311 | BPH  | C3B-C4B | -3.79 | 1.35        | 1.41     |
| 7   | B     | 101 | BCL  | MG-NA   | -3.32 | 1.98        | 2.06     |
| 8   | I     | 102 | SPO  | C16-C17 | 3.11  | 1.52        | 1.46     |
| 11  | L     | 303 | BPH  | C3B-C4B | -3.11 | 1.36        | 1.41     |
| 7   | F     | 104 | BCL  | C1D-C2D | -3.10 | 1.39        | 1.45     |
| 7   | L     | 301 | BCL  | C1D-C2D | -2.99 | 1.39        | 1.45     |
| 7   | E     | 101 | BCL  | C1D-C2D | -2.97 | 1.39        | 1.45     |
| 7   | B     | 101 | BCL  | C1D-C2D | -2.88 | 1.39        | 1.45     |
| 7   | L     | 309 | BCL  | C1D-C2D | -2.87 | 1.39        | 1.45     |
| 7   | J     | 102 | BCL  | C1D-C2D | -2.81 | 1.39        | 1.45     |
| 7   | O     | 101 | BCL  | C1D-C2D | -2.80 | 1.39        | 1.45     |
| 7   | R     | 103 | BCL  | MG-NA   | -2.75 | 1.99        | 2.06     |
| 7   | D     | 102 | BCL  | C1D-C2D | -2.71 | 1.40        | 1.45     |
| 7   | 0     | 101 | BCL  | MG-NA   | -2.69 | 1.99        | 2.06     |
| 7   | J     | 102 | BCL  | MG-NA   | -2.68 | 1.99        | 2.06     |
| 7   | K     | 101 | BCL  | C1D-C2D | -2.68 | 1.40        | 1.45     |
| 11  | L     | 303 | BPH  | C4D-CHA | -2.66 | 1.35        | 1.39     |
| 7   | 1     | 102 | BCL  | C1D-C2D | -2.65 | 1.40        | 1.45     |
| 11  | L     | 311 | BPH  | C2C-C3C | -2.64 | 1.52        | 1.54     |
| 8   | I     | 102 | SPO  | C11-C12 | 2.64  | 1.51        | 1.46     |
| 7   | E     | 101 | BCL  | MG-NA   | -2.59 | 2.00        | 2.06     |
| 7   | L     | 309 | BCL  | MG-NA   | -2.55 | 2.00        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | 0     | 101 | BCL  | C1D-C2D | -2.49 | 1.40        | 1.45     |
| 7   | 7     | 101 | BCL  | C1D-C2D | -2.48 | 1.40        | 1.45     |
| 7   | C     | 101 | BCL  | MG-NA   | -2.48 | 2.00        | 2.06     |
| 7   | M     | 403 | BCL  | C1D-C2D | -2.43 | 1.40        | 1.45     |
| 7   | V     | 101 | BCL  | C1D-C2D | -2.42 | 1.40        | 1.45     |
| 7   | 8     | 102 | BCL  | MG-NA   | -2.41 | 2.00        | 2.06     |
| 8   | S     | 101 | SPO  | C25-C23 | 2.41  | 1.51        | 1.46     |
| 7   | F     | 104 | BCL  | MG-NA   | -2.41 | 2.00        | 2.06     |
| 7   | R     | 103 | BCL  | C1D-C2D | -2.40 | 1.40        | 1.45     |
| 8   | K     | 102 | SPO  | C25-C23 | 2.37  | 1.51        | 1.46     |
| 7   | L     | 301 | BCL  | MG-NA   | -2.36 | 2.00        | 2.06     |
| 7   | 8     | 102 | BCL  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 7   | L     | 302 | BCL  | MG-NA   | -2.32 | 2.00        | 2.06     |
| 7   | P     | 102 | BCL  | MG-NA   | -2.30 | 2.00        | 2.06     |
| 7   | C     | 101 | BCL  | C1D-C2D | -2.29 | 1.40        | 1.45     |
| 7   | T     | 101 | BCL  | MG-NA   | -2.29 | 2.00        | 2.06     |
| 7   | I     | 101 | BCL  | MG-NA   | -2.28 | 2.00        | 2.06     |
| 8   | 3     | 103 | SPO  | C11-C12 | 2.27  | 1.50        | 1.46     |
| 8   | 0     | 102 | SPO  | C15-C14 | 2.24  | 1.50        | 1.43     |
| 7   | 9     | 101 | BCL  | C1D-C2D | -2.23 | 1.40        | 1.45     |
| 8   | 2     | 102 | SPO  | C6-C7   | 2.23  | 1.50        | 1.46     |
| 11  | L     | 311 | BPH  | C4D-CHA | -2.23 | 1.36        | 1.39     |
| 7   | a     | 101 | BCL  | C1B-NB  | -2.23 | 1.34        | 1.37     |
| 8   | 2     | 103 | SPO  | C11-C12 | 2.21  | 1.50        | 1.46     |
| 7   | Q     | 101 | BCL  | C1D-C2D | -2.20 | 1.41        | 1.45     |
| 11  | L     | 303 | BPH  | C3B-C2B | 2.20  | 1.43        | 1.39     |
| 8   | E     | 102 | SPO  | C16-C17 | 2.19  | 1.50        | 1.46     |
| 7   | T     | 101 | BCL  | C1D-C2D | -2.18 | 1.41        | 1.45     |
| 8   | 3     | 103 | SPO  | C16-C17 | 2.18  | 1.50        | 1.46     |
| 7   | J     | 102 | BCL  | C1B-NB  | -2.17 | 1.35        | 1.37     |
| 7   | U     | 101 | BCL  | C1D-C2D | -2.17 | 1.41        | 1.45     |
| 7   | 3     | 102 | BCL  | MG-NA   | -2.16 | 2.01        | 2.06     |
| 8   | W     | 101 | SPO  | C25-C23 | 2.16  | 1.50        | 1.46     |
| 7   | 3     | 102 | BCL  | C1D-C2D | -2.16 | 1.41        | 1.45     |
| 7   | L     | 302 | BCL  | C1D-C2D | -2.15 | 1.41        | 1.45     |
| 8   | O     | 102 | SPO  | C25-C23 | 2.13  | 1.50        | 1.46     |
| 8   | 2     | 102 | SPO  | C16-C17 | 2.11  | 1.50        | 1.46     |
| 8   | O     | 102 | SPO  | C6-C7   | 2.11  | 1.50        | 1.46     |
| 8   | E     | 102 | SPO  | C25-C23 | 2.09  | 1.50        | 1.46     |
| 8   | E     | 102 | SPO  | C15-C14 | 2.08  | 1.49        | 1.43     |
| 7   | P     | 102 | BCL  | C1D-C2D | -2.08 | 1.41        | 1.45     |
| 7   | 3     | 101 | BCL  | C1D-C2D | -2.07 | 1.41        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | S     | 102 | BCL  | C1D-C2D | -2.06 | 1.41        | 1.45     |
| 7   | F     | 104 | BCL  | C1B-NB  | -2.06 | 1.35        | 1.37     |
| 7   | 7     | 101 | BCL  | MG-NA   | -2.05 | 2.01        | 2.06     |
| 7   | 1     | 101 | BCL  | C1D-C2D | -2.05 | 1.41        | 1.45     |
| 8   | K     | 102 | SPO  | C15-C14 | 2.04  | 1.49        | 1.43     |
| 7   | J     | 102 | BCL  | C1D-ND  | -2.04 | 1.35        | 1.37     |
| 8   | 0     | 102 | SPO  | C6-C7   | 2.04  | 1.50        | 1.46     |
| 8   | W     | 101 | SPO  | C11-C12 | 2.04  | 1.50        | 1.46     |
| 7   | F     | 102 | BCL  | C1D-C2D | -2.03 | 1.41        | 1.45     |
| 7   | A     | 101 | BCL  | C1D-C2D | -2.03 | 1.41        | 1.45     |
| 7   | C     | 101 | BCL  | C3C-C4C | 2.02  | 1.54        | 1.51     |
| 11  | L     | 311 | BPH  | C3B-C2B | 2.02  | 1.43        | 1.39     |
| 8   | I     | 102 | SPO  | C20-C19 | 2.01  | 1.49        | 1.43     |
| 8   | F     | 105 | SPO  | C25-C23 | 2.01  | 1.50        | 1.46     |

All (605) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | 0     | 103 | SPO  | C20-C19-C17 | -8.91 | 114.78      | 127.28   |
| 8   | K     | 102 | SPO  | C8-C7-C9    | -7.95 | 109.93      | 122.82   |
| 8   | 0     | 103 | SPO  | C20-C21-C22 | -6.91 | 109.38      | 123.52   |
| 8   | K     | 102 | SPO  | C10-C9-C7   | 6.63  | 136.58      | 127.28   |
| 8   | I     | 102 | SPO  | C29-C28-C30 | 6.39  | 126.32      | 115.23   |
| 8   | S     | 101 | SPO  | C21-C22-C23 | 5.97  | 135.65      | 127.28   |
| 8   | 0     | 103 | SPO  | C10-C11-C12 | -5.85 | 110.33      | 126.36   |
| 8   | 0     | 102 | SPO  | C21-C20-C19 | 5.60  | 134.97      | 123.52   |
| 8   | 2     | 103 | SPO  | C8-C7-C9    | -5.31 | 114.21      | 122.82   |
| 8   | 0     | 102 | SPO  | C5-C6-C7    | 5.19  | 133.73      | 125.89   |
| 8   | 2     | 103 | SPO  | C13-C12-C14 | -5.14 | 114.49      | 122.82   |
| 8   | 0     | 102 | SPO  | C20-C21-C22 | 5.10  | 133.96      | 123.52   |
| 8   | E     | 102 | SPO  | C21-C20-C19 | 5.07  | 133.90      | 123.52   |
| 8   | S     | 101 | SPO  | C24-C23-C25 | 4.96  | 125.67      | 118.09   |
| 8   | 0     | 102 | SPO  | C8-C7-C6    | -4.92 | 110.58      | 118.09   |
| 8   | K     | 102 | SPO  | C4-C5-C6    | 4.87  | 131.75      | 124.91   |
| 8   | 0     | 102 | SPO  | C21-C22-C23 | -4.84 | 120.50      | 127.28   |
| 8   | S     | 101 | SPO  | C20-C21-C22 | 4.78  | 133.31      | 123.52   |
| 8   | R     | 102 | SPO  | C29-C28-C30 | 4.74  | 123.45      | 115.23   |
| 8   | 2     | 102 | SPO  | C4-C5-C6    | 4.72  | 131.54      | 124.91   |
| 8   | T     | 102 | SPO  | C4-C5-C6    | -4.66 | 118.37      | 124.91   |
| 8   | 0     | 102 | SPO  | C6-C7-C9    | 4.63  | 126.28      | 119.01   |
| 11  | L     | 303 | BPH  | C1C-C2C-C3C | -4.55 | 98.50       | 102.84   |
| 8   | 0     | 102 | SPO  | C29-C28-C30 | 4.54  | 123.11      | 115.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | K     | 102 | SPO  | C6-C7-C9    | 4.48  | 126.05      | 119.01   |
| 8   | T     | 102 | SPO  | C13-C12-C11 | 4.45  | 124.89      | 118.09   |
| 8   | 2     | 102 | SPO  | C20-C19-C17 | 4.44  | 133.50      | 127.28   |
| 8   | O     | 102 | SPO  | C29-C28-C30 | 4.41  | 122.88      | 115.23   |
| 8   | K     | 102 | SPO  | C20-C21-C22 | 4.39  | 132.50      | 123.52   |
| 8   | S     | 101 | SPO  | C26-C27-C28 | 4.38  | 133.86      | 127.69   |
| 10  | F     | 101 | CDL  | OA6-CA5-C11 | 4.38  | 120.96      | 111.48   |
| 8   | K     | 102 | SPO  | C21-C20-C19 | 4.38  | 132.48      | 123.52   |
| 8   | I     | 102 | SPO  | C21-C22-C23 | -4.36 | 121.16      | 127.28   |
| 8   | 2     | 102 | SPO  | C24-C23-C25 | 4.36  | 124.75      | 118.09   |
| 8   | 0     | 102 | SPO  | C4-C5-C6    | 4.35  | 131.03      | 124.91   |
| 8   | I     | 102 | SPO  | C21-C20-C19 | 4.34  | 132.40      | 123.52   |
| 9   | H     | 301 | PC1  | O21-C21-C22 | 4.32  | 120.83      | 111.48   |
| 8   | F     | 105 | SPO  | C29-C28-C30 | 4.30  | 122.70      | 115.23   |
| 8   | S     | 101 | SPO  | C4-C5-C6    | -4.29 | 118.89      | 124.91   |
| 8   | E     | 102 | SPO  | C20-C21-C22 | 4.28  | 132.27      | 123.52   |
| 8   | I     | 102 | SPO  | C18-C17-C19 | -4.27 | 115.89      | 122.82   |
| 8   | O     | 102 | SPO  | C24-C23-C25 | 4.25  | 124.57      | 118.09   |
| 8   | W     | 101 | SPO  | C10-C9-C7   | 4.22  | 133.20      | 127.28   |
| 9   | A     | 103 | PC1  | O21-C21-C22 | 4.19  | 120.54      | 111.48   |
| 8   | K     | 102 | SPO  | C26-C27-C28 | -4.16 | 121.83      | 127.69   |
| 8   | 2     | 102 | SPO  | C5-C6-C7    | 4.16  | 132.18      | 125.89   |
| 8   | I     | 102 | SPO  | C15-C14-C12 | -4.14 | 121.47      | 127.28   |
| 8   | F     | 105 | SPO  | C4-C5-C6    | -4.13 | 119.11      | 124.91   |
| 8   | E     | 102 | SPO  | C8-C7-C9    | -4.05 | 116.25      | 122.82   |
| 7   | L     | 301 | BCL  | C3D-C4D-ND  | -4.03 | 103.43      | 109.99   |
| 8   | R     | 102 | SPO  | C24-C23-C25 | 4.03  | 124.24      | 118.09   |
| 7   | b     | 101 | BCL  | C1D-CHD-C4C | -3.97 | 117.05      | 126.62   |
| 8   | I     | 102 | SPO  | C20-C19-C17 | -3.96 | 121.73      | 127.28   |
| 7   | b     | 101 | BCL  | CMA-C3A-C4A | -3.93 | 101.21      | 111.77   |
| 8   | S     | 101 | SPO  | C21-C20-C19 | -3.92 | 115.49      | 123.52   |
| 8   | 0     | 103 | SPO  | C24-C23-C25 | 3.87  | 124.00      | 118.09   |
| 8   | 2     | 102 | SPO  | C18-C17-C16 | 3.87  | 124.00      | 118.09   |
| 8   | E     | 102 | SPO  | C21-C22-C23 | -3.85 | 121.88      | 127.28   |
| 8   | 0     | 102 | SPO  | C20-C19-C17 | -3.85 | 121.88      | 127.28   |
| 8   | E     | 102 | SPO  | C5-C6-C7    | 3.85  | 131.71      | 125.89   |
| 8   | F     | 105 | SPO  | C24-C23-C25 | 3.82  | 123.93      | 118.09   |
| 8   | K     | 102 | SPO  | C8-C7-C6    | 3.80  | 123.89      | 118.09   |
| 8   | I     | 102 | SPO  | C10-C9-C7   | -3.79 | 121.96      | 127.28   |
| 8   | W     | 101 | SPO  | C24-C23-C25 | 3.77  | 123.85      | 118.09   |
| 8   | 2     | 102 | SPO  | C21-C20-C19 | 3.72  | 131.13      | 123.52   |
| 8   | R     | 102 | SPO  | C4-C5-C6    | -3.71 | 119.70      | 124.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | W     | 101 | SPO  | C8-C7-C6    | 3.69  | 123.72      | 118.09   |
| 8   | E     | 102 | SPO  | C29-C28-C30 | 3.68  | 121.61      | 115.23   |
| 9   | A     | 103 | PC1  | C11-C12-N   | -3.68 | 104.02      | 115.82   |
| 8   | K     | 102 | SPO  | C21-C22-C23 | -3.64 | 122.18      | 127.28   |
| 8   | 0     | 103 | SPO  | C5-C6-C7    | -3.63 | 120.40      | 125.89   |
| 7   | 0     | 101 | BCL  | C1D-ND-C4D  | 3.63  | 108.86      | 106.31   |
| 8   | I     | 102 | SPO  | C20-C21-C22 | 3.63  | 130.94      | 123.52   |
| 9   | M     | 402 | PC1  | O21-C21-C22 | 3.61  | 119.29      | 111.48   |
| 12  | X     | 101 | U10  | C7-C6-C5    | -3.60 | 114.33      | 118.52   |
| 8   | S     | 101 | SPO  | C25-C23-C22 | -3.57 | 113.39      | 119.01   |
| 8   | I     | 102 | SPO  | C18-C17-C16 | 3.54  | 123.50      | 118.09   |
| 8   | K     | 102 | SPO  | C5-C6-C7    | 3.54  | 131.24      | 125.89   |
| 10  | F     | 101 | CDL  | OB6-CB5-C51 | 3.52  | 119.10      | 111.48   |
| 7   | b     | 101 | BCL  | C2C-C3C-C4C | -3.52 | 96.06       | 101.34   |
| 11  | L     | 311 | BPH  | CMA-C3A-C4A | -3.52 | 107.03      | 114.61   |
| 8   | 3     | 103 | SPO  | C11-C12-C14 | 3.51  | 124.53      | 119.01   |
| 8   | E     | 102 | SPO  | C26-C27-C28 | -3.51 | 122.75      | 127.69   |
| 7   | F     | 104 | BCL  | C2A-C3A-C4A | -3.49 | 96.23       | 101.87   |
| 8   | T     | 102 | SPO  | C24-C23-C25 | 3.49  | 123.42      | 118.09   |
| 7   | I     | 101 | BCL  | CMA-C3A-C4A | -3.48 | 102.42      | 111.77   |
| 8   | 2     | 103 | SPO  | C21-C20-C19 | -3.47 | 116.42      | 123.52   |
| 8   | 3     | 103 | SPO  | C14-C15-C16 | 3.46  | 133.24      | 123.20   |
| 8   | R     | 102 | SPO  | C11-C12-C14 | 3.43  | 124.41      | 119.01   |
| 8   | 3     | 103 | SPO  | C13-C12-C14 | -3.42 | 117.28      | 122.82   |
| 8   | O     | 102 | SPO  | C5-C6-C7    | 3.41  | 131.05      | 125.89   |
| 7   | M     | 403 | BCL  | C4D-CHA-C1A | 3.41  | 125.31      | 121.24   |
| 8   | 3     | 103 | SPO  | C8-C7-C9    | -3.41 | 117.29      | 122.82   |
| 8   | K     | 102 | SPO  | C9-C10-C11  | 3.41  | 133.07      | 123.20   |
| 8   | T     | 102 | SPO  | C8-C7-C6    | 3.40  | 123.29      | 118.09   |
| 8   | O     | 102 | SPO  | C8-C7-C6    | 3.40  | 123.29      | 118.09   |
| 8   | E     | 102 | SPO  | C20-C19-C17 | -3.40 | 122.52      | 127.28   |
| 8   | 3     | 103 | SPO  | C6-C7-C9    | 3.38  | 124.32      | 119.01   |
| 7   | L     | 302 | BCL  | CHC-C1C-NC  | 3.38  | 129.27      | 124.40   |
| 7   | b     | 101 | BCL  | CGD-CBD-CAD | 3.37  | 121.77      | 110.85   |
| 8   | 3     | 103 | SPO  | C26-C27-C28 | -3.37 | 122.94      | 127.69   |
| 7   | 7     | 101 | BCL  | C4D-CHA-C1A | 3.37  | 125.26      | 121.24   |
| 8   | 2     | 102 | SPO  | C26-C27-C28 | -3.36 | 122.96      | 127.69   |
| 8   | S     | 101 | SPO  | C8-C7-C6    | 3.36  | 123.22      | 118.09   |
| 7   | S     | 102 | BCL  | C1D-ND-C4D  | 3.36  | 108.67      | 106.31   |
| 7   | N     | 102 | BCL  | C4D-CHA-C1A | 3.36  | 125.25      | 121.24   |
| 8   | 0     | 103 | SPO  | C26-C27-C28 | -3.35 | 122.97      | 127.69   |
| 8   | 3     | 103 | SPO  | C21-C22-C23 | -3.33 | 122.60      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | 0     | 103 | SPO  | C34-C33-C35 | 3.33  | 121.01      | 115.23   |
| 8   | W     | 101 | SPO  | C9-C10-C11  | 3.32  | 132.82      | 123.20   |
| 7   | 3     | 102 | BCL  | C2A-C3A-C4A | -3.29 | 96.55       | 101.87   |
| 8   | W     | 101 | SPO  | C4-C5-C6    | -3.28 | 120.31      | 124.91   |
| 8   | 2     | 103 | SPO  | C13-C12-C11 | 3.28  | 123.09      | 118.09   |
| 7   | P     | 102 | BCL  | C4D-CHA-C1A | 3.27  | 125.14      | 121.24   |
| 10  | F     | 101 | CDL  | OA8-CA7-C31 | 3.25  | 121.76      | 111.83   |
| 8   | 3     | 103 | SPO  | C18-C17-C19 | -3.25 | 117.55      | 122.82   |
| 7   | 0     | 101 | BCL  | CMA-C3A-C4A | -3.24 | 103.05      | 111.77   |
| 7   | B     | 101 | BCL  | C2A-C3A-C4A | -3.23 | 96.65       | 101.87   |
| 8   | R     | 102 | SPO  | C15-C14-C12 | -3.23 | 122.75      | 127.28   |
| 7   | L     | 309 | BCL  | C1D-ND-C4D  | 3.23  | 108.58      | 106.31   |
| 8   | E     | 102 | SPO  | C13-C12-C11 | 3.23  | 123.02      | 118.09   |
| 8   | W     | 101 | SPO  | C6-C7-C9    | -3.23 | 113.94      | 119.01   |
| 7   | 3     | 102 | BCL  | CHC-C1C-NC  | 3.22  | 129.04      | 124.40   |
| 7   | 9     | 101 | BCL  | C4D-CHA-C1A | 3.21  | 125.07      | 121.24   |
| 8   | 2     | 102 | SPO  | C16-C17-C19 | -3.21 | 113.96      | 119.01   |
| 8   | K     | 102 | SPO  | C31-C32-C33 | -3.20 | 120.30      | 127.62   |
| 7   | I     | 101 | BCL  | C1D-ND-C4D  | 3.19  | 108.55      | 106.31   |
| 7   | U     | 101 | BCL  | C4D-CHA-C1A | 3.19  | 125.05      | 121.24   |
| 7   | J     | 102 | BCL  | C3D-C4D-ND  | -3.18 | 104.81      | 109.99   |
| 7   | Q     | 101 | BCL  | C4D-CHA-C1A | 3.18  | 125.03      | 121.24   |
| 11  | L     | 311 | BPH  | C4D-CHA-CBD | 3.18  | 109.98      | 108.45   |
| 7   | B     | 101 | BCL  | CHC-C1C-NC  | 3.17  | 128.98      | 124.40   |
| 8   | R     | 102 | SPO  | C34-C33-C35 | 3.17  | 120.73      | 115.23   |
| 8   | 2     | 102 | SPO  | C8-C7-C6    | 3.16  | 122.92      | 118.09   |
| 8   | 2     | 102 | SPO  | C20-C21-C22 | -3.15 | 117.07      | 123.52   |
| 7   | a     | 101 | BCL  | C4D-CHA-C1A | 3.14  | 124.99      | 121.24   |
| 7   | L     | 302 | BCL  | C1D-ND-C4D  | 3.14  | 108.51      | 106.31   |
| 8   | K     | 102 | SPO  | C20-C19-C17 | -3.13 | 122.89      | 127.28   |
| 8   | E     | 102 | SPO  | C34-C33-C35 | 3.13  | 120.66      | 115.23   |
| 7   | J     | 102 | BCL  | C4D-CHA-C1A | 3.12  | 124.97      | 121.24   |
| 7   | I     | 101 | BCL  | C4D-CHA-C1A | 3.12  | 124.97      | 121.24   |
| 8   | I     | 102 | SPO  | C14-C15-C16 | 3.12  | 132.23      | 123.20   |
| 7   | W     | 102 | BCL  | CHC-C1C-NC  | 3.12  | 128.90      | 124.40   |
| 8   | 2     | 102 | SPO  | C6-C7-C9    | -3.11 | 114.11      | 119.01   |
| 7   | F     | 104 | BCL  | C4D-CHA-C1A | 3.11  | 124.95      | 121.24   |
| 7   | b     | 101 | BCL  | C1C-NC-C4C  | -3.11 | 105.26      | 106.68   |
| 8   | S     | 101 | SPO  | C13-C12-C11 | 3.11  | 122.83      | 118.09   |
| 7   | E     | 101 | BCL  | C4D-CHA-C1A | 3.10  | 124.95      | 121.24   |
| 7   | b     | 101 | BCL  | CHC-C1C-NC  | 3.10  | 128.88      | 124.40   |
| 7   | L     | 309 | BCL  | CHC-C1C-NC  | 3.09  | 128.86      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | M     | 403 | BCL  | CHC-C1C-NC  | 3.09  | 128.86      | 124.40   |
| 8   | 0     | 102 | SPO  | C14-C15-C16 | 3.08  | 132.13      | 123.20   |
| 7   | 3     | 101 | BCL  | C4D-CHA-C1A | 3.08  | 124.91      | 121.24   |
| 7   | B     | 101 | BCL  | C1D-CHD-C4C | -3.07 | 119.21      | 126.62   |
| 7   | 9     | 101 | BCL  | CMA-C3A-C4A | -3.07 | 103.52      | 111.77   |
| 7   | a     | 101 | BCL  | CHC-C4B-NB  | -3.07 | 119.44      | 124.05   |
| 8   | 2     | 103 | SPO  | C16-C17-C19 | -3.07 | 114.18      | 119.01   |
| 8   | 0     | 103 | SPO  | C8-C7-C6    | 3.07  | 122.77      | 118.09   |
| 7   | 3     | 101 | BCL  | C3D-C4D-ND  | -3.06 | 105.02      | 109.99   |
| 8   | 0     | 103 | SPO  | C15-C16-C17 | -3.05 | 117.99      | 126.36   |
| 7   | T     | 101 | BCL  | C2A-C3A-C4A | -3.05 | 96.94       | 101.87   |
| 7   | 9     | 101 | BCL  | CHC-C1C-NC  | 3.05  | 128.80      | 124.40   |
| 7   | b     | 101 | BCL  | CHA-C1A-NA  | -3.05 | 119.49      | 126.39   |
| 7   | J     | 102 | BCL  | CHC-C1C-NC  | 3.05  | 128.80      | 124.40   |
| 8   | R     | 102 | SPO  | C13-C12-C11 | -3.04 | 113.44      | 118.09   |
| 8   | 0     | 103 | SPO  | C10-C9-C7   | -3.04 | 123.02      | 127.28   |
| 7   | 3     | 101 | BCL  | CHC-C1C-NC  | 3.02  | 128.76      | 124.40   |
| 7   | D     | 102 | BCL  | C4D-CHA-C1A | 3.02  | 124.85      | 121.24   |
| 8   | 3     | 103 | SPO  | C15-C16-C17 | 3.02  | 134.65      | 126.36   |
| 7   | C     | 101 | BCL  | C4D-CHA-C1A | 3.02  | 124.84      | 121.24   |
| 7   | 0     | 101 | BCL  | C2A-C3A-C4A | -3.02 | 97.00       | 101.87   |
| 7   | F     | 102 | BCL  | CMA-C3A-C4A | -3.01 | 103.67      | 111.77   |
| 7   | 1     | 102 | BCL  | C4D-CHA-C1A | 3.01  | 124.84      | 121.24   |
| 8   | 2     | 103 | SPO  | C4-C5-C6    | 3.01  | 129.14      | 124.91   |
| 8   | S     | 101 | SPO  | C16-C17-C19 | -3.01 | 114.28      | 119.01   |
| 8   | 0     | 103 | SPO  | C31-C32-C33 | -3.01 | 120.74      | 127.62   |
| 7   | W     | 102 | BCL  | C2C-C3C-C4C | -3.00 | 96.84       | 101.34   |
| 8   | 0     | 103 | SPO  | C27-C26-C25 | -3.00 | 114.52      | 123.20   |
| 12  | X     | 101 | U10  | C8-C7-C6    | 2.99  | 119.45      | 112.08   |
| 8   | 0     | 102 | SPO  | C31-C32-C33 | -2.99 | 120.78      | 127.62   |
| 8   | R     | 102 | SPO  | C20-C21-C22 | -2.99 | 117.40      | 123.52   |
| 7   | O     | 101 | BCL  | C4D-CHA-C1A | 2.98  | 124.80      | 121.24   |
| 8   | 2     | 103 | SPO  | C5-C6-C7    | 2.97  | 130.39      | 125.89   |
| 7   | K     | 101 | BCL  | C4D-CHA-C1A | 2.97  | 124.79      | 121.24   |
| 8   | 0     | 102 | SPO  | C26-C27-C28 | -2.96 | 123.53      | 127.69   |
| 7   | 7     | 101 | BCL  | CMA-C3A-C4A | -2.96 | 103.83      | 111.77   |
| 7   | 7     | 101 | BCL  | C1D-CHD-C4C | -2.96 | 119.49      | 126.62   |
| 7   | S     | 102 | BCL  | CHC-C4B-NB  | -2.95 | 119.63      | 124.05   |
| 7   | L     | 301 | BCL  | CMA-C3A-C4A | -2.94 | 103.86      | 111.77   |
| 7   | S     | 102 | BCL  | CHC-C1C-NC  | 2.94  | 128.65      | 124.40   |
| 7   | P     | 102 | BCL  | CMA-C3A-C4A | -2.94 | 103.86      | 111.77   |
| 7   | T     | 101 | BCL  | C4D-CHA-C1A | 2.94  | 124.75      | 121.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | W     | 101 | SPO  | C34-C33-C35 | 2.93  | 120.32      | 115.23   |
| 8   | 2     | 103 | SPO  | C8-C7-C6    | 2.93  | 122.56      | 118.09   |
| 8   | I     | 102 | SPO  | C4-C5-C6    | -2.93 | 120.80      | 124.91   |
| 7   | E     | 101 | BCL  | CHC-C4B-NB  | -2.92 | 119.67      | 124.05   |
| 7   | A     | 101 | BCL  | C4D-CHA-C1A | 2.92  | 124.72      | 121.24   |
| 7   | W     | 102 | BCL  | C4D-CHA-C1A | 2.91  | 124.72      | 121.24   |
| 7   | D     | 102 | BCL  | C1D-ND-C4D  | 2.91  | 108.36      | 106.31   |
| 7   | 1     | 102 | BCL  | CMA-C3A-C4A | -2.91 | 103.95      | 111.77   |
| 8   | 0     | 103 | SPO  | C18-C17-C19 | -2.91 | 118.10      | 122.82   |
| 7   | C     | 101 | BCL  | CMA-C3A-C4A | -2.91 | 103.96      | 111.77   |
| 8   | S     | 101 | SPO  | C15-C14-C12 | -2.89 | 123.22      | 127.28   |
| 7   | 0     | 101 | BCL  | C4D-CHA-C1A | 2.89  | 124.69      | 121.24   |
| 7   | R     | 103 | BCL  | CMA-C3A-C4A | -2.88 | 104.02      | 111.77   |
| 8   | S     | 101 | SPO  | C18-C17-C16 | 2.88  | 122.49      | 118.09   |
| 7   | 8     | 102 | BCL  | C4D-CHA-C1A | 2.88  | 124.68      | 121.24   |
| 8   | 0     | 103 | SPO  | C40-C38-C39 | 2.87  | 121.20      | 114.59   |
| 7   | 9     | 101 | BCL  | CHC-C4B-NB  | -2.87 | 119.74      | 124.05   |
| 7   | C     | 101 | BCL  | CHC-C4B-NB  | -2.87 | 119.74      | 124.05   |
| 7   | R     | 103 | BCL  | C2A-C3A-C4A | -2.87 | 97.23       | 101.87   |
| 7   | T     | 101 | BCL  | C1D-CHD-C4C | -2.86 | 119.72      | 126.62   |
| 7   | Q     | 101 | BCL  | CHC-C4B-NB  | -2.86 | 119.77      | 124.05   |
| 7   | S     | 102 | BCL  | C4D-CHA-C1A | 2.85  | 124.64      | 121.24   |
| 7   | 8     | 102 | BCL  | CMA-C3A-C4A | -2.85 | 104.11      | 111.77   |
| 8   | 3     | 103 | SPO  | C4-C5-C6    | -2.85 | 120.91      | 124.91   |
| 8   | S     | 101 | SPO  | C14-C15-C16 | 2.85  | 131.46      | 123.20   |
| 7   | 1     | 101 | BCL  | C4D-CHA-C1A | 2.85  | 124.64      | 121.24   |
| 7   | W     | 102 | BCL  | CMA-C3A-C4A | -2.85 | 104.12      | 111.77   |
| 8   | K     | 102 | SPO  | C14-C15-C16 | 2.84  | 131.44      | 123.20   |
| 7   | L     | 309 | BCL  | CMA-C3A-C4A | -2.84 | 104.14      | 111.77   |
| 7   | A     | 101 | BCL  | CHC-C4B-NB  | -2.84 | 119.79      | 124.05   |
| 7   | N     | 102 | BCL  | CMA-C3A-C4A | -2.84 | 104.15      | 111.77   |
| 7   | F     | 104 | BCL  | CHC-C4B-NB  | -2.83 | 119.80      | 124.05   |
| 7   | R     | 103 | BCL  | CHC-C4B-NB  | -2.83 | 119.80      | 124.05   |
| 8   | 2     | 103 | SPO  | C24-C23-C25 | 2.82  | 122.40      | 118.09   |
| 8   | 2     | 103 | SPO  | C21-C22-C23 | -2.82 | 123.32      | 127.28   |
| 7   | P     | 102 | BCL  | CHC-C4B-NB  | -2.82 | 119.82      | 124.05   |
| 9   | A     | 103 | PC1  | O31-C31-C32 | 2.82  | 120.42      | 111.83   |
| 7   | J     | 102 | BCL  | CMA-C3A-C4A | -2.81 | 104.22      | 111.77   |
| 7   | 7     | 101 | BCL  | CHC-C1C-NC  | 2.81  | 128.45      | 124.40   |
| 7   | J     | 102 | BCL  | CHC-C4B-NB  | -2.80 | 119.85      | 124.05   |
| 8   | T     | 102 | SPO  | C29-C28-C30 | 2.80  | 120.08      | 115.23   |
| 7   | U     | 101 | BCL  | CHC-C1C-NC  | 2.80  | 128.44      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | K     | 101 | BCL  | CHC-C4B-NB  | -2.79 | 119.86      | 124.05   |
| 7   | F     | 102 | BCL  | CHC-C1C-NC  | 2.79  | 128.43      | 124.40   |
| 8   | T     | 102 | SPO  | C11-C12-C14 | -2.79 | 114.62      | 119.01   |
| 8   | 3     | 103 | SPO  | C21-C20-C19 | 2.79  | 129.23      | 123.52   |
| 8   | 3     | 103 | SPO  | C24-C23-C25 | 2.79  | 122.35      | 118.09   |
| 7   | T     | 101 | BCL  | CMA-C3A-C4A | -2.79 | 104.28      | 111.77   |
| 10  | F     | 101 | CDL  | OB8-CB7-C71 | 2.79  | 120.33      | 111.83   |
| 7   | N     | 102 | BCL  | CHC-C1C-NC  | 2.78  | 128.42      | 124.40   |
| 7   | F     | 102 | BCL  | C4D-CHA-C1A | 2.78  | 124.56      | 121.24   |
| 7   | V     | 101 | BCL  | C4D-CHA-C1A | 2.77  | 124.55      | 121.24   |
| 8   | 2     | 101 | SPO  | C21-C20-C19 | 2.77  | 129.19      | 123.52   |
| 7   | U     | 101 | BCL  | CMA-C3A-C4A | -2.77 | 104.33      | 111.77   |
| 7   | T     | 101 | BCL  | CHC-C4B-NB  | -2.77 | 119.90      | 124.05   |
| 7   | U     | 101 | BCL  | CHC-C4B-NB  | -2.77 | 119.90      | 124.05   |
| 8   | R     | 102 | SPO  | C8-C7-C6    | -2.77 | 113.86      | 118.09   |
| 7   | V     | 101 | BCL  | CHC-C4B-NB  | -2.77 | 119.90      | 124.05   |
| 7   | L     | 301 | BCL  | C4D-CHA-C1A | 2.76  | 124.54      | 121.24   |
| 7   | T     | 101 | BCL  | CHC-C1C-NC  | 2.76  | 128.38      | 124.40   |
| 7   | K     | 101 | BCL  | CMA-C3A-C4A | -2.76 | 104.35      | 111.77   |
| 7   | I     | 101 | BCL  | CHC-C4B-NB  | -2.76 | 119.91      | 124.05   |
| 7   | I     | 101 | BCL  | CHC-C1C-NC  | 2.75  | 128.37      | 124.40   |
| 7   | N     | 102 | BCL  | CHC-C4B-NB  | -2.75 | 119.92      | 124.05   |
| 7   | 7     | 101 | BCL  | CHC-C4B-NB  | -2.75 | 119.92      | 124.05   |
| 7   | B     | 101 | BCL  | CMA-C3A-C4A | -2.75 | 104.38      | 111.77   |
| 7   | E     | 101 | BCL  | C1D-CHD-C4C | -2.75 | 119.99      | 126.62   |
| 8   | R     | 102 | SPO  | C6-C7-C9    | 2.75  | 123.33      | 119.01   |
| 7   | F     | 102 | BCL  | CHC-C4B-NB  | -2.75 | 119.93      | 124.05   |
| 7   | 0     | 101 | BCL  | CHC-C4B-NB  | -2.75 | 119.93      | 124.05   |
| 7   | N     | 102 | BCL  | C1-C2-C3    | -2.74 | 121.72      | 126.20   |
| 7   | V     | 101 | BCL  | C1D-CHD-C4C | -2.73 | 120.03      | 126.62   |
| 7   | B     | 101 | BCL  | CHC-C4B-NB  | -2.72 | 119.96      | 124.05   |
| 7   | L     | 301 | BCL  | CHC-C4B-NB  | -2.72 | 119.96      | 124.05   |
| 7   | M     | 403 | BCL  | CHC-C4B-NB  | -2.72 | 119.97      | 124.05   |
| 11  | L     | 303 | BPH  | CMA-C3A-C4A | -2.72 | 108.75      | 114.61   |
| 8   | O     | 102 | SPO  | C20-C21-C22 | -2.72 | 117.96      | 123.52   |
| 7   | R     | 103 | BCL  | C4D-CHA-C1A | 2.71  | 124.48      | 121.24   |
| 7   | 3     | 102 | BCL  | CHC-C4B-NB  | -2.71 | 119.98      | 124.05   |
| 7   | A     | 101 | BCL  | C1D-ND-C4D  | 2.71  | 108.21      | 106.31   |
| 7   | 3     | 102 | BCL  | CMA-C3A-C4A | -2.70 | 104.51      | 111.77   |
| 7   | D     | 102 | BCL  | CHC-C4B-NB  | -2.70 | 120.00      | 124.05   |
| 7   | F     | 104 | BCL  | CMA-C3A-C4A | -2.70 | 104.53      | 111.77   |
| 8   | 0     | 103 | SPO  | C29-C28-C30 | 2.69  | 119.91      | 115.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | 3     | 101 | BCL  | CHC-C4B-NB  | -2.69 | 120.01      | 124.05   |
| 7   | M     | 403 | BCL  | C3C-C4C-CHD | -2.69 | 117.71      | 123.39   |
| 7   | L     | 302 | BCL  | CHC-C4B-NB  | -2.69 | 120.02      | 124.05   |
| 7   | E     | 101 | BCL  | C2A-C3A-C4A | -2.68 | 97.54       | 101.87   |
| 7   | b     | 101 | BCL  | C4D-CHA-C1A | 2.68  | 124.44      | 121.24   |
| 8   | 2     | 102 | SPO  | C9-C10-C11  | 2.68  | 130.95      | 123.20   |
| 7   | L     | 309 | BCL  | C4D-CHA-C1A | 2.67  | 124.43      | 121.24   |
| 7   | 1     | 102 | BCL  | CHC-C4B-NB  | -2.67 | 120.04      | 124.05   |
| 8   | E     | 102 | SPO  | C14-C15-C16 | 2.67  | 130.94      | 123.20   |
| 11  | L     | 311 | BPH  | C2D-C1D-ND  | -2.67 | 107.50      | 109.43   |
| 8   | F     | 105 | SPO  | C11-C12-C14 | -2.67 | 114.81      | 119.01   |
| 7   | 1     | 101 | BCL  | CHC-C4B-NB  | -2.67 | 120.05      | 124.05   |
| 8   | 2     | 103 | SPO  | C6-C7-C9    | 2.67  | 123.20      | 119.01   |
| 7   | J     | 102 | BCL  | C3D-C2D-C1D | -2.67 | 102.19      | 105.83   |
| 7   | 8     | 102 | BCL  | C2A-C3A-C4A | -2.66 | 97.57       | 101.87   |
| 7   | b     | 101 | BCL  | C3D-C2D-C1D | -2.66 | 102.21      | 105.83   |
| 7   | L     | 309 | BCL  | CHC-C4B-NB  | -2.65 | 120.07      | 124.05   |
| 7   | C     | 101 | BCL  | CHC-C1C-NC  | 2.65  | 128.23      | 124.40   |
| 7   | S     | 102 | BCL  | CMA-C3A-C4A | -2.65 | 104.65      | 111.77   |
| 7   | A     | 101 | BCL  | C3C-C4C-CHD | -2.65 | 117.81      | 123.39   |
| 7   | L     | 301 | BCL  | C3D-C2D-C1D | -2.65 | 102.22      | 105.83   |
| 7   | M     | 403 | BCL  | CMA-C3A-C4A | -2.64 | 104.67      | 111.77   |
| 7   | J     | 102 | BCL  | C2A-C3A-C4A | -2.64 | 97.60       | 101.87   |
| 11  | L     | 311 | BPH  | C2B-C1B-NB  | -2.64 | 107.52      | 109.43   |
| 7   | 0     | 101 | BCL  | CHC-C1C-NC  | 2.64  | 128.21      | 124.40   |
| 8   | 2     | 103 | SPO  | C14-C15-C16 | -2.63 | 115.57      | 123.20   |
| 7   | K     | 101 | BCL  | C1D-CHD-C4C | -2.63 | 120.27      | 126.62   |
| 7   | A     | 101 | BCL  | CMA-C3A-C4A | -2.63 | 104.71      | 111.77   |
| 7   | a     | 101 | BCL  | CHC-C1C-NC  | 2.62  | 128.19      | 124.40   |
| 7   | F     | 102 | BCL  | C1D-ND-C4D  | 2.62  | 108.15      | 106.31   |
| 7   | F     | 104 | BCL  | C3D-C4D-ND  | -2.62 | 105.72      | 109.99   |
| 7   | 8     | 102 | BCL  | CHC-C4B-NB  | -2.62 | 120.12      | 124.05   |
| 7   | P     | 102 | BCL  | C3D-C2D-C1D | -2.61 | 102.27      | 105.83   |
| 7   | N     | 102 | BCL  | CMD-C2D-C1D | 2.61  | 129.32      | 124.73   |
| 7   | D     | 102 | BCL  | C3C-C4C-CHD | -2.61 | 117.89      | 123.39   |
| 11  | L     | 303 | BPH  | C2D-C1D-ND  | -2.61 | 107.55      | 109.43   |
| 7   | L     | 301 | BCL  | CMD-C2D-C1D | 2.60  | 129.31      | 124.73   |
| 7   | D     | 102 | BCL  | CHC-C1C-NC  | 2.60  | 128.16      | 124.40   |
| 8   | I     | 102 | SPO  | C29-C28-C27 | -2.60 | 111.27      | 122.50   |
| 11  | L     | 303 | BPH  | C2B-C1B-NB  | -2.60 | 107.55      | 109.43   |
| 7   | 1     | 101 | BCL  | CHC-C1C-NC  | 2.59  | 128.14      | 124.40   |
| 7   | O     | 101 | BCL  | CMA-C3A-C4A | -2.58 | 104.83      | 111.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | K     | 101 | BCL  | C1C-NC-C4C  | -2.58 | 105.50      | 106.68   |
| 7   | F     | 104 | BCL  | CHC-C1C-NC  | 2.58  | 128.12      | 124.40   |
| 7   | O     | 101 | BCL  | CHC-C1C-NC  | 2.58  | 128.12      | 124.40   |
| 7   | D     | 102 | BCL  | CMA-C3A-C4A | -2.58 | 104.85      | 111.77   |
| 7   | A     | 101 | BCL  | CHC-C1C-NC  | 2.58  | 128.12      | 124.40   |
| 7   | 1     | 101 | BCL  | CMA-C3A-C4A | -2.58 | 104.85      | 111.77   |
| 7   | Q     | 101 | BCL  | CMA-C3A-C4A | -2.57 | 104.87      | 111.77   |
| 7   | b     | 101 | BCL  | CHC-C4B-NB  | -2.56 | 120.21      | 124.05   |
| 7   | W     | 102 | BCL  | C1C-NC-C4C  | -2.55 | 105.52      | 106.68   |
| 12  | L     | 306 | U10  | C7-C6-C5    | -2.55 | 115.56      | 118.52   |
| 7   | B     | 101 | BCL  | C4D-CHA-C1A | 2.54  | 124.28      | 121.24   |
| 8   | E     | 102 | SPO  | C4-C5-C6    | 2.54  | 128.48      | 124.91   |
| 7   | 1     | 101 | BCL  | CHA-C1A-NA  | -2.54 | 120.65      | 126.39   |
| 7   | E     | 101 | BCL  | CMA-C3A-C4A | -2.53 | 104.97      | 111.77   |
| 7   | C     | 101 | BCL  | C2A-C3A-C4A | -2.53 | 97.79       | 101.87   |
| 7   | a     | 101 | BCL  | CMA-C3A-C4A | -2.53 | 104.98      | 111.77   |
| 7   | 1     | 102 | BCL  | C3D-C4D-ND  | -2.52 | 105.88      | 109.99   |
| 8   | S     | 103 | SPO  | C14-C15-C16 | 2.52  | 130.51      | 123.20   |
| 7   | a     | 101 | BCL  | CMD-C2D-C1D | 2.52  | 129.17      | 124.73   |
| 8   | 3     | 103 | SPO  | C20-C21-C22 | 2.52  | 128.68      | 123.52   |
| 7   | T     | 101 | BCL  | C3D-C4D-ND  | -2.52 | 105.89      | 109.99   |
| 7   | L     | 302 | BCL  | CMA-C3A-C4A | -2.52 | 105.01      | 111.77   |
| 7   | a     | 101 | BCL  | C3D-C2D-C1D | -2.51 | 102.40      | 105.83   |
| 12  | L     | 304 | U10  | C7-C6-C5    | -2.51 | 115.60      | 118.52   |
| 7   | W     | 102 | BCL  | CHC-C4B-NB  | -2.51 | 120.28      | 124.05   |
| 7   | N     | 102 | BCL  | C3D-C2D-C1D | -2.51 | 102.41      | 105.83   |
| 7   | 3     | 102 | BCL  | C4D-CHA-C1A | 2.50  | 124.23      | 121.24   |
| 8   | E     | 102 | SPO  | C8-C7-C6    | 2.50  | 121.91      | 118.09   |
| 7   | V     | 101 | BCL  | CHC-C1C-NC  | 2.50  | 128.00      | 124.40   |
| 10  | F     | 101 | CDL  | OA6-CA5-OA7 | -2.50 | 117.87      | 123.70   |
| 7   | E     | 101 | BCL  | CHC-C1C-NC  | 2.49  | 128.00      | 124.40   |
| 7   | O     | 101 | BCL  | CHC-C4B-NB  | -2.49 | 120.31      | 124.05   |
| 8   | O     | 102 | SPO  | C31-C32-C33 | -2.49 | 121.93      | 127.62   |
| 7   | O     | 101 | BCL  | C1D-CHD-C4C | -2.49 | 120.62      | 126.62   |
| 8   | 2     | 102 | SPO  | C25-C23-C22 | -2.49 | 115.10      | 119.01   |
| 8   | R     | 102 | SPO  | C25-C23-C22 | -2.48 | 115.10      | 119.01   |
| 7   | 1     | 102 | BCL  | C1D-CHD-C4C | -2.48 | 120.63      | 126.62   |
| 7   | V     | 101 | BCL  | C3D-C4D-ND  | -2.47 | 105.96      | 109.99   |
| 7   | T     | 101 | BCL  | CHA-C1A-NA  | -2.47 | 120.80      | 126.39   |
| 7   | R     | 103 | BCL  | C3D-C4D-ND  | -2.47 | 105.97      | 109.99   |
| 7   | b     | 101 | BCL  | C3D-C4D-ND  | -2.47 | 105.97      | 109.99   |
| 7   | N     | 102 | BCL  | C3D-C4D-ND  | -2.47 | 105.97      | 109.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | I     | 101 | BCL  | C1D-CHD-C4C | -2.47 | 120.67      | 126.62   |
| 12  | L     | 308 | U10  | C7-C6-C5    | -2.47 | 115.65      | 118.52   |
| 7   | 3     | 101 | BCL  | C3D-C2D-C1D | -2.46 | 102.47      | 105.83   |
| 8   | R     | 102 | SPO  | C34-C33-C32 | -2.45 | 117.33      | 123.63   |
| 7   | V     | 101 | BCL  | CMA-C3A-C4A | -2.45 | 105.20      | 111.77   |
| 8   | O     | 102 | SPO  | C4-C5-C6    | 2.45  | 128.35      | 124.91   |
| 8   | O     | 102 | SPO  | C6-C7-C9    | -2.44 | 115.17      | 119.01   |
| 7   | 8     | 102 | BCL  | CHC-C1C-NC  | 2.44  | 127.92      | 124.40   |
| 7   | L     | 302 | BCL  | CGD-CBD-CAD | -2.44 | 102.94      | 110.85   |
| 8   | E     | 102 | SPO  | C24-C23-C22 | -2.44 | 118.87      | 122.82   |
| 7   | b     | 101 | BCL  | CMD-C2D-C1D | 2.43  | 129.01      | 124.73   |
| 7   | 3     | 101 | BCL  | CMA-C3A-C4A | -2.43 | 105.23      | 111.77   |
| 7   | P     | 102 | BCL  | CMD-C2D-C1D | 2.43  | 129.00      | 124.73   |
| 7   | 1     | 102 | BCL  | CHC-C1C-NC  | 2.42  | 127.90      | 124.40   |
| 8   | 0     | 103 | SPO  | C11-C12-C14 | -2.42 | 115.21      | 119.01   |
| 7   | L     | 301 | BCL  | C1D-ND-C4D  | 2.41  | 108.01      | 106.31   |
| 7   | 7     | 101 | BCL  | C3D-C4D-ND  | -2.41 | 106.06      | 109.99   |
| 8   | 0     | 102 | SPO  | C34-C33-C35 | 2.41  | 119.41      | 115.23   |
| 7   | U     | 101 | BCL  | C3C-C4C-CHD | -2.40 | 118.32      | 123.39   |
| 7   | L     | 302 | BCL  | CHA-C1A-NA  | -2.40 | 120.95      | 126.39   |
| 7   | 0     | 101 | BCL  | C1D-CHD-C4C | -2.40 | 120.82      | 126.62   |
| 12  | L     | 307 | U10  | C7-C6-C5    | -2.40 | 115.73      | 118.52   |
| 8   | W     | 101 | SPO  | C24-C23-C22 | -2.40 | 118.93      | 122.82   |
| 7   | P     | 102 | BCL  | CHC-C1C-NC  | 2.40  | 127.86      | 124.40   |
| 8   | F     | 105 | SPO  | C21-C20-C19 | -2.39 | 118.62      | 123.52   |
| 7   | 3     | 101 | BCL  | CHB-C1B-NB  | -2.39 | 120.46      | 124.05   |
| 7   | L     | 301 | BCL  | CHA-C1A-NA  | -2.38 | 120.99      | 126.39   |
| 8   | 3     | 103 | SPO  | C15-C14-C12 | -2.38 | 123.94      | 127.28   |
| 7   | Q     | 101 | BCL  | CHA-C1A-NA  | -2.38 | 121.01      | 126.39   |
| 7   | a     | 101 | BCL  | CHB-C1B-NB  | -2.38 | 120.48      | 124.05   |
| 7   | 1     | 102 | BCL  | C1C-NC-C4C  | -2.37 | 105.60      | 106.68   |
| 7   | 7     | 101 | BCL  | C3D-C2D-C1D | -2.37 | 102.59      | 105.83   |
| 7   | 0     | 101 | BCL  | CHA-C1A-NA  | -2.37 | 121.02      | 126.39   |
| 8   | K     | 102 | SPO  | C40-C38-C39 | 2.37  | 120.04      | 114.59   |
| 8   | 2     | 102 | SPO  | C11-C12-C14 | -2.37 | 115.29      | 119.01   |
| 7   | F     | 104 | BCL  | CHA-C1A-NA  | -2.36 | 121.04      | 126.39   |
| 7   | 7     | 101 | BCL  | CMD-C2D-C1D | 2.36  | 128.88      | 124.73   |
| 7   | 9     | 101 | BCL  | CHA-C1A-NA  | -2.36 | 121.06      | 126.39   |
| 7   | 9     | 101 | BCL  | C3C-C4C-CHD | -2.35 | 118.43      | 123.39   |
| 7   | T     | 101 | BCL  | C3D-C2D-C1D | -2.35 | 102.62      | 105.83   |
| 8   | S     | 101 | SPO  | C15-C16-C17 | 2.35  | 132.82      | 126.36   |
| 8   | E     | 102 | SPO  | C11-C12-C14 | -2.35 | 115.31      | 119.01   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | 0     | 103 | SPO  | C25-C23-C22 | -2.35 | 115.31      | 119.01   |
| 7   | 3     | 101 | BCL  | CMD-C2D-C1D | 2.35  | 128.86      | 124.73   |
| 7   | L     | 301 | BCL  | CHC-C1C-NC  | 2.35  | 127.79      | 124.40   |
| 7   | 3     | 101 | BCL  | C2C-C3C-C4C | -2.35 | 97.83       | 101.34   |
| 7   | J     | 102 | BCL  | C1D-CHD-C4C | -2.34 | 120.98      | 126.62   |
| 7   | K     | 101 | BCL  | CHC-C1C-NC  | 2.34  | 127.77      | 124.40   |
| 7   | K     | 101 | BCL  | CHA-C1A-NA  | -2.33 | 121.10      | 126.39   |
| 7   | O     | 101 | BCL  | C3D-C2D-C1D | -2.33 | 102.65      | 105.83   |
| 7   | 7     | 101 | BCL  | C2C-C3C-C4C | -2.33 | 97.85       | 101.34   |
| 7   | 8     | 102 | BCL  | C1-C2-C3    | -2.33 | 122.38      | 126.20   |
| 9   | M     | 402 | PC1  | O31-C31-C32 | 2.32  | 118.92      | 111.83   |
| 7   | V     | 101 | BCL  | CHA-C1A-NA  | -2.32 | 121.13      | 126.39   |
| 8   | T     | 102 | SPO  | C21-C20-C19 | -2.32 | 118.77      | 123.52   |
| 7   | W     | 102 | BCL  | C1D-CHD-C4C | -2.32 | 121.02      | 126.62   |
| 8   | 2     | 102 | SPO  | C13-C12-C11 | 2.32  | 121.63      | 118.09   |
| 8   | W     | 101 | SPO  | C34-C33-C32 | -2.32 | 117.67      | 123.63   |
| 7   | D     | 102 | BCL  | CHA-C1A-NA  | -2.31 | 121.16      | 126.39   |
| 7   | M     | 403 | BCL  | C3D-C2D-C1D | -2.31 | 102.68      | 105.83   |
| 7   | 1     | 101 | BCL  | C3D-C2D-C1D | -2.30 | 102.69      | 105.83   |
| 7   | Q     | 101 | BCL  | CHC-C1C-NC  | 2.30  | 127.72      | 124.40   |
| 8   | E     | 102 | SPO  | C35-C33-C32 | -2.30 | 116.00      | 121.17   |
| 7   | D     | 102 | BCL  | C3D-C4D-ND  | -2.30 | 106.25      | 109.99   |
| 7   | 8     | 102 | BCL  | C3D-C2D-C1D | -2.29 | 102.70      | 105.83   |
| 7   | O     | 101 | BCL  | C3D-C4D-ND  | -2.29 | 106.26      | 109.99   |
| 7   | B     | 101 | BCL  | C2C-C3C-C4C | -2.29 | 97.91       | 101.34   |
| 7   | J     | 102 | BCL  | CMD-C2D-C1D | 2.29  | 128.76      | 124.73   |
| 7   | R     | 103 | BCL  | CHC-C1C-NC  | 2.29  | 127.70      | 124.40   |
| 8   | 2     | 103 | SPO  | C9-C10-C11  | 2.29  | 129.82      | 123.20   |
| 7   | 3     | 102 | BCL  | CHA-C1A-NA  | -2.28 | 121.22      | 126.39   |
| 8   | 2     | 103 | SPO  | C26-C27-C28 | -2.28 | 124.48      | 127.69   |
| 7   | K     | 101 | BCL  | C3D-C2D-C1D | -2.28 | 102.72      | 105.83   |
| 7   | V     | 101 | BCL  | CHB-C1B-NB  | -2.28 | 120.63      | 124.05   |
| 7   | V     | 101 | BCL  | C3D-C2D-C1D | -2.28 | 102.72      | 105.83   |
| 7   | S     | 102 | BCL  | CHA-C1A-NA  | -2.27 | 121.25      | 126.39   |
| 7   | K     | 101 | BCL  | C2A-C3A-C4A | -2.27 | 98.20       | 101.87   |
| 7   | 8     | 102 | BCL  | C1D-CHD-C4C | -2.27 | 121.15      | 126.62   |
| 7   | 3     | 101 | BCL  | CHA-C1A-NA  | -2.27 | 121.26      | 126.39   |
| 7   | R     | 103 | BCL  | C3D-C2D-C1D | -2.25 | 102.75      | 105.83   |
| 12  | L     | 310 | U10  | C7-C6-C5    | -2.25 | 115.90      | 118.52   |
| 7   | 9     | 101 | BCL  | CMD-C2D-C1D | 2.25  | 128.69      | 124.73   |
| 7   | 9     | 101 | BCL  | C3D-C2D-C1D | -2.25 | 102.76      | 105.83   |
| 7   | 1     | 102 | BCL  | C3D-C2D-C1D | -2.25 | 102.76      | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | S     | 101 | SPO  | C13-C12-C14 | -2.24 | 119.18      | 122.82   |
| 7   | A     | 101 | BCL  | CHA-C1A-NA  | -2.24 | 121.31      | 126.39   |
| 7   | Q     | 101 | BCL  | C3C-C4C-CHD | -2.24 | 118.68      | 123.39   |
| 7   | 8     | 102 | BCL  | C3C-C4C-CHD | -2.24 | 118.68      | 123.39   |
| 7   | b     | 101 | BCL  | CHB-C1B-NB  | -2.24 | 120.70      | 124.05   |
| 8   | 2     | 101 | SPO  | C20-C21-C22 | 2.23  | 128.09      | 123.52   |
| 7   | 7     | 101 | BCL  | CHA-C1A-NA  | -2.23 | 121.34      | 126.39   |
| 7   | 3     | 101 | BCL  | C1D-CHD-C4C | -2.23 | 121.24      | 126.62   |
| 7   | 1     | 101 | BCL  | C2A-C3A-C4A | -2.23 | 98.26       | 101.87   |
| 7   | S     | 102 | BCL  | CHB-C1B-NB  | -2.23 | 120.70      | 124.05   |
| 7   | 3     | 102 | BCL  | C3D-C2D-C1D | -2.23 | 102.79      | 105.83   |
| 7   | O     | 101 | BCL  | CHA-C1A-NA  | -2.23 | 121.35      | 126.39   |
| 7   | A     | 101 | BCL  | CMD-C2D-C1D | 2.22  | 128.64      | 124.73   |
| 7   | M     | 403 | BCL  | CMD-C2D-C1D | 2.22  | 128.64      | 124.73   |
| 7   | V     | 101 | BCL  | C1-C2-C3    | -2.22 | 122.56      | 126.20   |
| 7   | 1     | 101 | BCL  | CMD-C2D-C1D | 2.22  | 128.64      | 124.73   |
| 7   | L     | 309 | BCL  | C3C-C4C-CHD | -2.22 | 118.71      | 123.39   |
| 7   | J     | 102 | BCL  | CHB-C1B-NB  | -2.22 | 120.72      | 124.05   |
| 7   | a     | 101 | BCL  | C2A-C3A-C4A | -2.22 | 98.29       | 101.87   |
| 7   | C     | 101 | BCL  | CHB-C1B-NB  | -2.21 | 120.73      | 124.05   |
| 8   | W     | 101 | SPO  | C20-C21-C22 | -2.21 | 119.00      | 123.52   |
| 7   | U     | 101 | BCL  | CHA-C1A-NA  | -2.21 | 121.39      | 126.39   |
| 7   | 3     | 102 | BCL  | C3D-C4D-ND  | -2.21 | 106.40      | 109.99   |
| 7   | S     | 102 | BCL  | C3C-C4C-CHD | -2.21 | 118.74      | 123.39   |
| 9   | A     | 103 | PC1  | O12-P-O14   | 2.21  | 122.70      | 112.44   |
| 7   | B     | 101 | BCL  | C1C-NC-C4C  | -2.20 | 105.67      | 106.68   |
| 7   | b     | 101 | BCL  | C2A-C1A-CHA | 2.20  | 127.69      | 123.87   |
| 7   | L     | 309 | BCL  | CHA-C1A-NA  | -2.20 | 121.41      | 126.39   |
| 7   | 3     | 101 | BCL  | C2A-C3A-C4A | -2.20 | 98.32       | 101.87   |
| 8   | 8     | 101 | SPO  | C26-C27-C28 | -2.20 | 124.60      | 127.69   |
| 8   | K     | 102 | SPO  | C39-C38-C37 | -2.19 | 116.08      | 122.66   |
| 7   | T     | 101 | BCL  | CHB-C1B-NB  | -2.19 | 120.77      | 124.05   |
| 8   | O     | 102 | SPO  | C25-C23-C22 | -2.19 | 115.57      | 119.01   |
| 7   | 3     | 102 | BCL  | CHB-C1B-NB  | -2.19 | 120.77      | 124.05   |
| 7   | T     | 101 | BCL  | C1-C2-C3    | -2.19 | 122.62      | 126.20   |
| 8   | S     | 101 | SPO  | C10-C9-C7   | -2.18 | 124.22      | 127.28   |
| 7   | 3     | 101 | BCL  | C1D-ND-C4D  | 2.18  | 107.84      | 106.31   |
| 7   | 3     | 102 | BCL  | C1D-ND-C4D  | 2.18  | 107.84      | 106.31   |
| 7   | L     | 301 | BCL  | C1D-CHD-C4C | -2.18 | 121.36      | 126.62   |
| 7   | U     | 101 | BCL  | CHB-C1B-NB  | -2.18 | 120.78      | 124.05   |
| 7   | B     | 101 | BCL  | CHA-C1A-NA  | -2.18 | 121.46      | 126.39   |
| 7   | I     | 101 | BCL  | CHA-C1A-NA  | -2.18 | 121.46      | 126.39   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | 9     | 101 | BCL  | CHB-C1B-NB  | -2.18 | 120.78      | 124.05   |
| 7   | 8     | 102 | BCL  | CMD-C2D-C1D | 2.17  | 128.56      | 124.73   |
| 8   | O     | 102 | SPO  | C34-C33-C35 | 2.17  | 119.00      | 115.23   |
| 7   | F     | 104 | BCL  | C1D-CHD-C4C | -2.17 | 121.38      | 126.62   |
| 7   | T     | 101 | BCL  | CMD-C2D-C1D | 2.17  | 128.55      | 124.73   |
| 7   | Q     | 101 | BCL  | C3D-C2D-C1D | -2.17 | 102.87      | 105.83   |
| 8   | 2     | 103 | SPO  | C11-C12-C14 | 2.17  | 122.42      | 119.01   |
| 7   | E     | 101 | BCL  | CHB-C1B-NB  | -2.17 | 120.80      | 124.05   |
| 7   | E     | 101 | BCL  | C3D-C4D-ND  | -2.17 | 106.47      | 109.99   |
| 7   | L     | 302 | BCL  | CMD-C2D-C1D | 2.17  | 128.54      | 124.73   |
| 7   | M     | 403 | BCL  | CHA-C1A-NA  | -2.16 | 121.50      | 126.39   |
| 7   | N     | 102 | BCL  | C3C-C4C-CHD | -2.16 | 118.83      | 123.39   |
| 7   | P     | 102 | BCL  | C1D-CHD-C4C | -2.16 | 121.41      | 126.62   |
| 7   | Q     | 101 | BCL  | CMD-C2D-C1D | 2.16  | 128.53      | 124.73   |
| 7   | O     | 101 | BCL  | CMD-C2D-C1D | 2.16  | 128.53      | 124.73   |
| 7   | J     | 102 | BCL  | C3C-C4C-CHD | -2.16 | 118.85      | 123.39   |
| 8   | F     | 105 | SPO  | C24-C23-C22 | -2.15 | 119.33      | 122.82   |
| 7   | F     | 104 | BCL  | C3D-C2D-C1D | -2.15 | 102.90      | 105.83   |
| 7   | J     | 102 | BCL  | CHA-C1A-NA  | -2.15 | 121.53      | 126.39   |
| 7   | I     | 101 | BCL  | CMD-C2D-C1D | 2.15  | 128.51      | 124.73   |
| 8   | K     | 102 | SPO  | C15-C16-C17 | 2.15  | 132.25      | 126.36   |
| 7   | W     | 102 | BCL  | CMD-C2D-C1D | 2.15  | 128.51      | 124.73   |
| 7   | E     | 101 | BCL  | CHA-C1A-NA  | -2.14 | 121.54      | 126.39   |
| 8   | 2     | 101 | SPO  | C5-C6-C7    | 2.14  | 129.13      | 125.89   |
| 7   | P     | 102 | BCL  | C3D-C4D-ND  | -2.14 | 106.50      | 109.99   |
| 7   | P     | 102 | BCL  | C3C-C4C-CHD | -2.14 | 118.88      | 123.39   |
| 7   | 3     | 102 | BCL  | CMD-C2D-C1D | 2.14  | 128.50      | 124.73   |
| 11  | L     | 311 | BPH  | OBD-CAD-CBD | -2.14 | 122.69      | 125.82   |
| 8   | W     | 101 | SPO  | C13-C12-C11 | 2.14  | 121.36      | 118.09   |
| 7   | C     | 101 | BCL  | CHA-C1A-NA  | -2.14 | 121.55      | 126.39   |
| 7   | C     | 101 | BCL  | C3D-C4D-ND  | -2.14 | 106.51      | 109.99   |
| 11  | L     | 311 | BPH  | CMD-C2D-C3D | 2.13  | 128.95      | 124.68   |
| 7   | 3     | 102 | BCL  | C3C-C4C-CHD | -2.13 | 118.90      | 123.39   |
| 7   | D     | 102 | BCL  | C3D-C2D-C1D | -2.13 | 102.92      | 105.83   |
| 7   | R     | 103 | BCL  | CHB-C1B-NB  | -2.13 | 120.86      | 124.05   |
| 7   | R     | 103 | BCL  | CHA-C1A-NA  | -2.13 | 121.58      | 126.39   |
| 7   | R     | 103 | BCL  | CMD-C2D-C1D | 2.12  | 128.47      | 124.73   |
| 7   | P     | 102 | BCL  | CHA-C1A-NA  | -2.12 | 121.58      | 126.39   |
| 7   | D     | 102 | BCL  | CMD-C2D-C1D | 2.12  | 128.47      | 124.73   |
| 12  | M     | 405 | U10  | C7-C6-C5    | -2.12 | 116.05      | 118.52   |
| 7   | N     | 102 | BCL  | CHA-C1A-NA  | -2.12 | 121.58      | 126.39   |
| 7   | F     | 102 | BCL  | CHB-C1B-NB  | -2.12 | 120.87      | 124.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | B     | 101 | BCL  | CHB-C1B-NB  | -2.12 | 120.87      | 124.05   |
| 7   | L     | 309 | BCL  | C2A-C3A-C4A | -2.12 | 98.44       | 101.87   |
| 9   | A     | 103 | PC1  | O31-C31-O32 | -2.12 | 118.33      | 123.63   |
| 7   | U     | 101 | BCL  | C3D-C2D-C1D | -2.12 | 102.94      | 105.83   |
| 7   | 0     | 101 | BCL  | CHB-C1B-NB  | -2.11 | 120.88      | 124.05   |
| 7   | F     | 102 | BCL  | C3C-C4C-CHD | -2.11 | 118.94      | 123.39   |
| 8   | S     | 101 | SPO  | C27-C26-C25 | 2.11  | 129.32      | 123.20   |
| 8   | 3     | 103 | SPO  | C31-C32-C33 | -2.11 | 122.79      | 127.62   |
| 8   | 2     | 103 | SPO  | C18-C17-C16 | 2.11  | 121.31      | 118.09   |
| 7   | a     | 101 | BCL  | CHA-C1A-NA  | -2.11 | 121.61      | 126.39   |
| 7   | 1     | 102 | BCL  | CHB-C1B-NB  | -2.11 | 120.88      | 124.05   |
| 7   | F     | 104 | BCL  | CHB-C1B-NB  | -2.11 | 120.88      | 124.05   |
| 7   | K     | 101 | BCL  | C3D-C4D-ND  | -2.11 | 106.56      | 109.99   |
| 8   | 2     | 103 | SPO  | C34-C33-C35 | 2.10  | 118.88      | 115.23   |
| 8   | I     | 102 | SPO  | C13-C12-C14 | -2.10 | 119.41      | 122.82   |
| 7   | 1     | 102 | BCL  | CHA-C1A-NA  | -2.10 | 121.64      | 126.39   |
| 7   | B     | 101 | BCL  | C3D-C2D-C1D | -2.10 | 102.97      | 105.83   |
| 7   | N     | 102 | BCL  | CHB-C1B-NB  | -2.10 | 120.91      | 124.05   |
| 7   | L     | 302 | BCL  | C4D-CHA-C1A | 2.10  | 123.74      | 121.24   |
| 7   | 9     | 101 | BCL  | C1D-CHD-C4C | -2.09 | 121.57      | 126.62   |
| 7   | K     | 101 | BCL  | CMD-C2D-C1D | 2.09  | 128.41      | 124.73   |
| 7   | W     | 102 | BCL  | CHA-C1A-NA  | -2.09 | 121.65      | 126.39   |
| 10  | F     | 101 | CDL  | CB6-OB8-CB7 | 2.09  | 124.77      | 117.12   |
| 8   | T     | 102 | SPO  | C40-C38-C39 | 2.08  | 119.39      | 114.59   |
| 7   | I     | 101 | BCL  | CHB-C1B-NB  | -2.08 | 120.92      | 124.05   |
| 7   | K     | 101 | BCL  | C1D-ND-C4D  | 2.08  | 107.77      | 106.31   |
| 7   | L     | 302 | BCL  | C3C-C4C-CHD | -2.08 | 119.00      | 123.39   |
| 7   | W     | 102 | BCL  | C1-C2-C3    | -2.08 | 122.79      | 126.20   |
| 7   | K     | 101 | BCL  | CHB-C1B-NB  | -2.08 | 120.93      | 124.05   |
| 8   | I     | 102 | SPO  | C24-C23-C25 | 2.08  | 121.26      | 118.09   |
| 7   | P     | 102 | BCL  | C1-C2-C3    | -2.07 | 122.80      | 126.20   |
| 7   | E     | 101 | BCL  | C3D-C2D-C1D | -2.07 | 103.00      | 105.83   |
| 8   | E     | 102 | SPO  | C24-C23-C25 | 2.07  | 121.26      | 118.09   |
| 9   | H     | 301 | PC1  | C3-O31-C31  | 2.07  | 124.69      | 117.12   |
| 8   | T     | 102 | SPO  | C10-C9-C7   | -2.07 | 124.37      | 127.28   |
| 7   | L     | 302 | BCL  | CHB-C1B-NB  | -2.07 | 120.94      | 124.05   |
| 7   | C     | 101 | BCL  | C1D-ND-C4D  | 2.07  | 107.76      | 106.31   |
| 10  | F     | 101 | CDL  | OA8-CA7-OA9 | -2.07 | 118.45      | 123.63   |
| 11  | L     | 303 | BPH  | C3D-C4D-ND  | 2.07  | 110.36      | 107.71   |
| 7   | 1     | 101 | BCL  | CHB-C1B-NB  | -2.07 | 120.95      | 124.05   |
| 7   | N     | 102 | BCL  | C1D-CHD-C4C | -2.07 | 121.64      | 126.62   |
| 7   | S     | 102 | BCL  | CMD-C2D-C1D | 2.06  | 128.36      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | P     | 102 | BCL  | CHB-C1B-NB  | -2.06 | 120.96      | 124.05   |
| 7   | 1     | 101 | BCL  | C3C-C4C-CHD | -2.05 | 119.06      | 123.39   |
| 7   | S     | 102 | BCL  | C2C-C3C-C4C | -2.05 | 98.26       | 101.34   |
| 7   | 1     | 101 | BCL  | C3D-C4D-ND  | -2.05 | 106.65      | 109.99   |
| 7   | F     | 104 | BCL  | C3C-C4C-CHD | -2.05 | 119.07      | 123.39   |
| 8   | T     | 102 | SPO  | C31-C32-C33 | -2.05 | 122.93      | 127.62   |
| 7   | W     | 102 | BCL  | C3D-C2D-C1D | -2.05 | 103.04      | 105.83   |
| 7   | R     | 103 | BCL  | C1D-ND-C4D  | 2.05  | 107.75      | 106.31   |
| 7   | U     | 101 | BCL  | CMD-C2D-C1D | 2.04  | 128.32      | 124.73   |
| 8   | W     | 101 | SPO  | C26-C27-C28 | -2.04 | 124.82      | 127.69   |
| 8   | F     | 105 | SPO  | C31-C32-C33 | -2.04 | 122.96      | 127.62   |
| 7   | R     | 103 | BCL  | C1D-CHD-C4C | -2.04 | 121.70      | 126.62   |
| 7   | 0     | 101 | BCL  | CMD-C2D-C1D | 2.04  | 128.31      | 124.73   |
| 7   | L     | 301 | BCL  | CHB-C1B-NB  | -2.03 | 121.00      | 124.05   |
| 7   | F     | 102 | BCL  | C1D-CHD-C4C | -2.03 | 121.72      | 126.62   |
| 7   | V     | 101 | BCL  | CMD-C2D-C1D | 2.03  | 128.31      | 124.73   |
| 7   | C     | 101 | BCL  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 8   | S     | 101 | SPO  | C34-C33-C35 | 2.03  | 118.75      | 115.23   |
| 8   | I     | 102 | SPO  | C27-C26-C25 | -2.03 | 117.32      | 123.20   |
| 7   | D     | 102 | BCL  | CHB-C1B-NB  | -2.02 | 121.01      | 124.05   |
| 7   | W     | 102 | BCL  | CHB-C1B-NB  | -2.02 | 121.01      | 124.05   |
| 7   | M     | 403 | BCL  | CHB-C1B-NB  | -2.02 | 121.01      | 124.05   |
| 8   | 2     | 102 | SPO  | C10-C11-C12 | 2.02  | 131.91      | 126.36   |
| 7   | F     | 102 | BCL  | CHA-C1A-NA  | -2.02 | 121.81      | 126.39   |
| 7   | 0     | 101 | BCL  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 7   | b     | 101 | BCL  | C2A-C3A-C4A | -2.02 | 98.60       | 101.87   |
| 7   | M     | 403 | BCL  | C1D-CHD-C4C | -2.02 | 121.75      | 126.62   |
| 7   | 0     | 101 | BCL  | C2C-C3C-C4C | -2.02 | 98.32       | 101.34   |
| 7   | 1     | 101 | BCL  | C1D-CHD-C4C | -2.02 | 121.76      | 126.62   |
| 7   | a     | 101 | BCL  | C1D-ND-C4D  | 2.02  | 107.73      | 106.31   |
| 7   | L     | 302 | BCL  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 11  | L     | 303 | BPH  | CMD-C2D-C3D | 2.01  | 128.70      | 124.68   |
| 7   | O     | 101 | BCL  | C1C-NC-C4C  | -2.01 | 105.76      | 106.68   |
| 7   | L     | 301 | BCL  | C3C-C4C-CHD | -2.00 | 119.17      | 123.39   |
| 7   | S     | 102 | BCL  | C1-C2-C3    | -2.00 | 122.92      | 126.20   |

There are no chirality outliers.

All (1101) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | 1     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 7   | 1     | 101 | BCL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | 1     | 101 | BCL  | C1-C2-C3-C4     |
| 7   | 1     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 7   | 1     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 7   | 1     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 7   | 1     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 7   | 1     | 102 | BCL  | C1-C2-C3-C4     |
| 7   | 1     | 102 | BCL  | C1-C2-C3-C5     |
| 7   | 3     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 7   | 3     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 7   | 3     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 7   | 3     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 7   | 3     | 102 | BCL  | C1-C2-C3-C5     |
| 7   | 3     | 102 | BCL  | C2-C3-C5-C6     |
| 7   | 3     | 102 | BCL  | C4-C3-C5-C6     |
| 7   | 3     | 102 | BCL  | C14-C13-C15-C16 |
| 7   | 8     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 7   | 9     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 7   | 9     | 101 | BCL  | C14-C13-C15-C16 |
| 7   | C     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 7   | C     | 101 | BCL  | C1-C2-C3-C4     |
| 7   | D     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 7   | D     | 102 | BCL  | CBD-CGD-O2D-CED |
| 7   | E     | 101 | BCL  | C1-C2-C3-C5     |
| 7   | F     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 7   | F     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 7   | F     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 7   | F     | 102 | BCL  | C11-C10-C8-C9   |
| 7   | F     | 104 | BCL  | C1A-C2A-CAA-CBA |
| 7   | F     | 104 | BCL  | C3A-C2A-CAA-CBA |
| 7   | F     | 104 | BCL  | C2B-C3B-CAB-OBB |
| 7   | F     | 104 | BCL  | C2B-C3B-CAB-CBB |
| 7   | F     | 104 | BCL  | C4B-C3B-CAB-CBB |
| 7   | F     | 104 | BCL  | C2C-C3C-CAC-CBC |
| 7   | J     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 7   | J     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 7   | J     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 7   | K     | 101 | BCL  | C1-C2-C3-C5     |
| 7   | L     | 302 | BCL  | C4C-C3C-CAC-CBC |
| 7   | L     | 309 | BCL  | C4C-C3C-CAC-CBC |
| 7   | L     | 309 | BCL  | CHA-CBD-CGD-O1D |
| 7   | L     | 309 | BCL  | CHA-CBD-CGD-O2D |
| 7   | L     | 309 | BCL  | C1-C2-C3-C4     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | L     | 309 | BCL  | C1-C2-C3-C5     |
| 7   | M     | 403 | BCL  | C2C-C3C-CAC-CBC |
| 7   | M     | 403 | BCL  | C4C-C3C-CAC-CBC |
| 7   | M     | 403 | BCL  | C2-C3-C5-C6     |
| 7   | M     | 403 | BCL  | C4-C3-C5-C6     |
| 7   | N     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 7   | P     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 7   | P     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 7   | P     | 102 | BCL  | C11-C10-C8-C9   |
| 7   | P     | 102 | BCL  | C11-C12-C13-C14 |
| 7   | Q     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 7   | Q     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 7   | Q     | 101 | BCL  | C14-C13-C15-C16 |
| 7   | R     | 103 | BCL  | C1A-C2A-CAA-CBA |
| 7   | R     | 103 | BCL  | C2C-C3C-CAC-CBC |
| 7   | S     | 102 | BCL  | CHA-CBD-CGD-O1D |
| 7   | S     | 102 | BCL  | CHA-CBD-CGD-O2D |
| 7   | U     | 101 | BCL  | CBD-CGD-O2D-CED |
| 7   | U     | 101 | BCL  | C1-C2-C3-C5     |
| 7   | a     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 7   | a     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 7   | a     | 101 | BCL  | C1-C2-C3-C4     |
| 7   | a     | 101 | BCL  | C1-C2-C3-C5     |
| 7   | b     | 101 | BCL  | C2B-C3B-CAB-OB  |
| 7   | b     | 101 | BCL  | C4B-C3B-CAB-OB  |
| 7   | b     | 101 | BCL  | C1-C2-C3-C4     |
| 8   | 0     | 102 | SPO  | O1-C1-C4-C5     |
| 8   | 0     | 102 | SPO  | C10-C11-C12-C14 |
| 8   | 0     | 103 | SPO  | C5-C6-C7-C8     |
| 8   | 0     | 103 | SPO  | C5-C6-C7-C9     |
| 8   | 0     | 103 | SPO  | C12-C14-C15-C16 |
| 8   | 0     | 103 | SPO  | C17-C19-C20-C21 |
| 8   | 0     | 103 | SPO  | C27-C28-C30-C31 |
| 8   | 0     | 103 | SPO  | C29-C28-C30-C31 |
| 8   | 2     | 101 | SPO  | C1-C4-C5-C6     |
| 8   | 2     | 101 | SPO  | C17-C19-C20-C21 |
| 8   | 2     | 102 | SPO  | O1-C1-C4-C5     |
| 8   | 2     | 102 | SPO  | C2-C1-C4-C5     |
| 8   | 2     | 102 | SPO  | C3-C1-C4-C5     |
| 8   | 3     | 103 | SPO  | O1-C1-C4-C5     |
| 8   | A     | 102 | SPO  | C3-C1-O1-CM1    |
| 8   | A     | 102 | SPO  | C4-C1-O1-CM1    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | D     | 101 | SPO  | C2-C1-O1-CM1    |
| 8   | D     | 101 | SPO  | C4-C1-O1-CM1    |
| 8   | D     | 103 | SPO  | O1-C1-C4-C5     |
| 8   | D     | 103 | SPO  | C3-C1-C4-C5     |
| 8   | D     | 103 | SPO  | C30-C31-C32-C33 |
| 8   | E     | 102 | SPO  | C1-C4-C5-C6     |
| 8   | F     | 105 | SPO  | C1-C4-C5-C6     |
| 8   | J     | 101 | SPO  | C1-C4-C5-C6     |
| 8   | J     | 101 | SPO  | C32-C33-C35-C36 |
| 8   | J     | 101 | SPO  | C34-C33-C35-C36 |
| 8   | K     | 102 | SPO  | O1-C1-C4-C5     |
| 8   | K     | 102 | SPO  | C2-C1-C4-C5     |
| 8   | K     | 102 | SPO  | C3-C1-C4-C5     |
| 8   | N     | 101 | SPO  | C30-C31-C32-C33 |
| 8   | O     | 102 | SPO  | C1-C4-C5-C6     |
| 8   | R     | 102 | SPO  | C1-C4-C5-C6     |
| 8   | S     | 101 | SPO  | C1-C4-C5-C6     |
| 8   | S     | 103 | SPO  | C4-C1-O1-CM1    |
| 8   | T     | 102 | SPO  | C1-C4-C5-C6     |
| 8   | U     | 103 | SPO  | C5-C6-C7-C9     |
| 8   | Z     | 101 | SPO  | C3-C1-O1-CM1    |
| 8   | Z     | 101 | SPO  | C4-C1-O1-CM1    |
| 9   | 9     | 103 | PC1  | C11-O13-P-O14   |
| 9   | 9     | 103 | PC1  | C11-O13-P-O11   |
| 9   | 9     | 103 | PC1  | O13-C11-C12-N   |
| 9   | 9     | 103 | PC1  | C2-C1-O11-P     |
| 9   | 9     | 103 | PC1  | O22-C21-O21-C2  |
| 9   | 9     | 103 | PC1  | C22-C21-O21-C2  |
| 9   | A     | 103 | PC1  | C1-O11-P-O14    |
| 9   | A     | 103 | PC1  | C1-O11-P-O13    |
| 9   | A     | 103 | PC1  | O13-C11-C12-N   |
| 9   | A     | 104 | PC1  | C11-O13-P-O12   |
| 9   | A     | 104 | PC1  | C1-O11-P-O12    |
| 9   | A     | 104 | PC1  | C1-O11-P-O13    |
| 9   | F     | 103 | PC1  | C1-O11-P-O14    |
| 9   | F     | 103 | PC1  | C1-O11-P-O13    |
| 9   | H     | 301 | PC1  | C11-O13-P-O12   |
| 9   | H     | 301 | PC1  | C11-O13-P-O14   |
| 9   | H     | 301 | PC1  | C11-O13-P-O11   |
| 9   | H     | 301 | PC1  | O13-C11-C12-N   |
| 9   | L     | 305 | PC1  | C11-O13-P-O12   |
| 9   | L     | 305 | PC1  | C11-O13-P-O14   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | L     | 305 | PC1  | C11-O13-P-O11   |
| 9   | L     | 305 | PC1  | C1-O11-P-O14    |
| 9   | L     | 305 | PC1  | O21-C2-C3-O31   |
| 9   | M     | 401 | PC1  | C11-O13-P-O12   |
| 9   | M     | 401 | PC1  | C11-O13-P-O11   |
| 9   | M     | 401 | PC1  | C2-C1-O11-P     |
| 9   | M     | 401 | PC1  | O32-C31-O31-C3  |
| 9   | M     | 401 | PC1  | C32-C31-O31-C3  |
| 9   | M     | 402 | PC1  | C11-O13-P-O11   |
| 9   | M     | 402 | PC1  | C1-O11-P-O12    |
| 9   | M     | 402 | PC1  | C1-O11-P-O14    |
| 9   | M     | 402 | PC1  | C1-O11-P-O13    |
| 9   | M     | 409 | PC1  | C1-O11-P-O14    |
| 9   | M     | 410 | PC1  | C1-O11-P-O14    |
| 9   | M     | 410 | PC1  | O21-C2-C3-O31   |
| 9   | W     | 103 | PC1  | C11-O13-P-O12   |
| 9   | W     | 103 | PC1  | C11-O13-P-O11   |
| 9   | W     | 103 | PC1  | C1-O11-P-O12    |
| 10  | F     | 101 | CDL  | CA2-OA2-PA1-OA3 |
| 10  | F     | 101 | CDL  | CA3-OA5-PA1-OA4 |
| 10  | F     | 101 | CDL  | OA7-CA5-OA6-CA4 |
| 10  | F     | 101 | CDL  | C11-CA5-OA6-CA4 |
| 10  | F     | 101 | CDL  | CB2-OB2-PB2-OB4 |
| 10  | F     | 101 | CDL  | CB2-OB2-PB2-OB5 |
| 10  | F     | 101 | CDL  | CB3-OB5-PB2-OB3 |
| 10  | F     | 101 | CDL  | C51-CB5-OB6-CB4 |
| 10  | M     | 407 | CDL  | CA2-OA2-PA1-OA4 |
| 10  | M     | 407 | CDL  | CA2-OA2-PA1-OA5 |
| 10  | M     | 407 | CDL  | OA7-CA5-OA6-CA4 |
| 10  | M     | 407 | CDL  | C11-CA5-OA6-CA4 |
| 10  | M     | 407 | CDL  | OB9-CB7-OB8-CB6 |
| 10  | M     | 407 | CDL  | C71-CB7-OB8-CB6 |
| 10  | M     | 408 | CDL  | OB7-CB5-OB6-CB4 |
| 10  | M     | 408 | CDL  | C51-CB5-OB6-CB4 |
| 12  | L     | 304 | U10  | C31-C32-C33-C34 |
| 12  | L     | 306 | U10  | C24-C26-C27-C28 |
| 12  | L     | 310 | U10  | C14-C16-C17-C18 |
| 12  | X     | 101 | U10  | C1-C6-C7-C8     |
| 12  | X     | 101 | U10  | C5-C6-C7-C8     |
| 12  | X     | 101 | U10  | C26-C27-C28-C29 |
| 12  | X     | 101 | U10  | C29-C31-C32-C33 |
| 7   | 1     | 101 | BCL  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | F     | 102 | BCL  | CBD-CGD-O2D-CED |
| 7   | a     | 101 | BCL  | CBD-CGD-O2D-CED |
| 7   | 1     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 9   | H     | 301 | PC1  | C2-C3-O31-C31   |
| 7   | F     | 102 | BCL  | O1D-CGD-O2D-CED |
| 7   | 1     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 7   | C     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 7   | N     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 7   | N     | 102 | BCL  | C15-C16-C17-C18 |
| 7   | D     | 102 | BCL  | O1D-CGD-O2D-CED |
| 7   | U     | 101 | BCL  | O1D-CGD-O2D-CED |
| 9   | A     | 103 | PC1  | O22-C21-O21-C2  |
| 10  | F     | 101 | CDL  | OB7-CB5-OB6-CB4 |
| 7   | 0     | 101 | BCL  | C3-C5-C6-C7     |
| 7   | 3     | 101 | BCL  | C3-C5-C6-C7     |
| 7   | F     | 102 | BCL  | C3-C5-C6-C7     |
| 7   | F     | 104 | BCL  | C3-C5-C6-C7     |
| 7   | L     | 309 | BCL  | C3-C5-C6-C7     |
| 7   | S     | 102 | BCL  | C3-C5-C6-C7     |
| 7   | N     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 7   | M     | 403 | BCL  | CBD-CGD-O2D-CED |
| 7   | b     | 101 | BCL  | CBD-CGD-O2D-CED |
| 7   | 1     | 101 | BCL  | C4-C3-C5-C6     |
| 7   | R     | 103 | BCL  | C4-C3-C5-C6     |
| 7   | T     | 101 | BCL  | C4-C3-C5-C6     |
| 8   | 0     | 102 | SPO  | C29-C28-C30-C31 |
| 8   | 9     | 102 | SPO  | C34-C33-C35-C36 |
| 8   | E     | 102 | SPO  | C29-C28-C30-C31 |
| 8   | I     | 102 | SPO  | C29-C28-C30-C31 |
| 8   | R     | 102 | SPO  | C29-C28-C30-C31 |
| 8   | W     | 101 | SPO  | C34-C33-C35-C36 |
| 12  | L     | 306 | U10  | C20-C19-C21-C22 |
| 12  | L     | 307 | U10  | C30-C29-C31-C32 |
| 12  | L     | 310 | U10  | C12-C11-C9-C10  |
| 12  | L     | 310 | U10  | C20-C19-C21-C22 |
| 12  | X     | 101 | U10  | C15-C14-C16-C17 |
| 7   | R     | 103 | BCL  | C2-C3-C5-C6     |
| 7   | T     | 101 | BCL  | C2-C3-C5-C6     |
| 8   | 0     | 102 | SPO  | C27-C28-C30-C31 |
| 8   | E     | 102 | SPO  | C27-C28-C30-C31 |
| 8   | M     | 406 | SPO  | C27-C28-C30-C31 |
| 8   | R     | 102 | SPO  | C27-C28-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | L     | 306 | U10  | C18-C19-C21-C22 |
| 12  | L     | 307 | U10  | C28-C29-C31-C32 |
| 12  | L     | 310 | U10  | C12-C11-C9-C8   |
| 7   | C     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 7   | V     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 7   | 7     | 101 | BCL  | C3-C5-C6-C7     |
| 7   | D     | 102 | BCL  | C3-C5-C6-C7     |
| 7   | Q     | 101 | BCL  | C3-C5-C6-C7     |
| 7   | 1     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 7   | C     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 8   | 0     | 103 | SPO  | C11-C10-C9-C7   |
| 8   | 2     | 102 | SPO  | C17-C19-C20-C21 |
| 8   | K     | 102 | SPO  | C11-C10-C9-C7   |
| 8   | S     | 101 | SPO  | C20-C21-C22-C23 |
| 8   | S     | 101 | SPO  | C25-C26-C27-C28 |
| 8   | W     | 101 | SPO  | C11-C10-C9-C7   |
| 7   | U     | 101 | BCL  | C3-C5-C6-C7     |
| 7   | b     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 7   | 1     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 7   | F     | 104 | BCL  | CBD-CGD-O2D-CED |
| 9   | A     | 103 | PC1  | C22-C21-O21-C2  |
| 7   | a     | 101 | BCL  | O1D-CGD-O2D-CED |
| 7   | R     | 103 | BCL  | CBD-CGD-O2D-CED |
| 7   | 8     | 102 | BCL  | C4-C3-C5-C6     |
| 7   | L     | 309 | BCL  | C4-C3-C5-C6     |
| 8   | 2     | 101 | SPO  | C34-C33-C35-C36 |
| 8   | E     | 102 | SPO  | C34-C33-C35-C36 |
| 8   | F     | 105 | SPO  | C29-C28-C30-C31 |
| 8   | M     | 406 | SPO  | C29-C28-C30-C31 |
| 12  | X     | 101 | U10  | C12-C11-C9-C10  |
| 12  | X     | 101 | U10  | C20-C19-C21-C22 |
| 7   | 1     | 101 | BCL  | C2-C3-C5-C6     |
| 7   | 8     | 102 | BCL  | C2-C3-C5-C6     |
| 8   | 2     | 101 | SPO  | C32-C33-C35-C36 |
| 8   | E     | 102 | SPO  | C32-C33-C35-C36 |
| 8   | F     | 105 | SPO  | C27-C28-C30-C31 |
| 8   | I     | 102 | SPO  | C27-C28-C30-C31 |
| 8   | R     | 102 | SPO  | C32-C33-C35-C36 |
| 8   | W     | 101 | SPO  | C32-C33-C35-C36 |
| 12  | L     | 304 | U10  | C12-C11-C9-C8   |
| 12  | X     | 101 | U10  | C12-C11-C9-C8   |
| 12  | X     | 101 | U10  | C13-C14-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | X     | 101 | U10  | C18-C19-C21-C22 |
| 8   | 0     | 102 | SPO  | C33-C35-C36-C37 |
| 8   | 0     | 103 | SPO  | C28-C30-C31-C32 |
| 8   | 2     | 101 | SPO  | C33-C35-C36-C37 |
| 8   | 2     | 103 | SPO  | C28-C30-C31-C32 |
| 8   | 3     | 103 | SPO  | C28-C30-C31-C32 |
| 8   | A     | 102 | SPO  | C28-C30-C31-C32 |
| 8   | A     | 102 | SPO  | C33-C35-C36-C37 |
| 8   | J     | 101 | SPO  | C28-C30-C31-C32 |
| 8   | J     | 101 | SPO  | C33-C35-C36-C37 |
| 8   | K     | 102 | SPO  | C33-C35-C36-C37 |
| 8   | N     | 101 | SPO  | C33-C35-C36-C37 |
| 8   | P     | 101 | SPO  | C33-C35-C36-C37 |
| 8   | R     | 101 | SPO  | C33-C35-C36-C37 |
| 8   | S     | 101 | SPO  | C28-C30-C31-C32 |
| 8   | S     | 103 | SPO  | C33-C35-C36-C37 |
| 8   | T     | 102 | SPO  | C28-C30-C31-C32 |
| 8   | U     | 103 | SPO  | C33-C35-C36-C37 |
| 12  | L     | 304 | U10  | C14-C16-C17-C18 |
| 12  | L     | 304 | U10  | C19-C21-C22-C23 |
| 12  | L     | 304 | U10  | C29-C31-C32-C33 |
| 12  | L     | 306 | U10  | C19-C21-C22-C23 |
| 12  | L     | 307 | U10  | C9-C11-C12-C13  |
| 12  | L     | 307 | U10  | C14-C16-C17-C18 |
| 12  | L     | 307 | U10  | C24-C26-C27-C28 |
| 12  | L     | 307 | U10  | C29-C31-C32-C33 |
| 12  | L     | 310 | U10  | C19-C21-C22-C23 |
| 12  | L     | 310 | U10  | C24-C26-C27-C28 |
| 12  | X     | 101 | U10  | C14-C16-C17-C18 |
| 12  | X     | 101 | U10  | C24-C26-C27-C28 |
| 7   | b     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 7   | 3     | 102 | BCL  | C10-C11-C12-C13 |
| 7   | B     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 9   | W     | 103 | PC1  | C11-C12-N-C15   |
| 8   | O     | 102 | SPO  | C29-C28-C30-C31 |
| 8   | R     | 102 | SPO  | C34-C33-C35-C36 |
| 12  | L     | 304 | U10  | C12-C11-C9-C10  |
| 12  | X     | 101 | U10  | C35-C34-C36-C37 |
| 7   | L     | 309 | BCL  | C2-C3-C5-C6     |
| 8   | 9     | 102 | SPO  | C32-C33-C35-C36 |
| 8   | O     | 102 | SPO  | C27-C28-C30-C31 |
| 12  | L     | 310 | U10  | C18-C19-C21-C22 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | X     | 101 | U10  | C33-C34-C36-C37 |
| 7   | 8     | 102 | BCL  | C3-C5-C6-C7     |
| 7   | 0     | 101 | BCL  | C6-C7-C8-C9     |
| 7   | 1     | 102 | BCL  | C6-C7-C8-C9     |
| 7   | 3     | 101 | BCL  | C11-C12-C13-C14 |
| 7   | 8     | 102 | BCL  | C11-C10-C8-C9   |
| 7   | 9     | 101 | BCL  | C11-C12-C13-C14 |
| 7   | B     | 101 | BCL  | C6-C7-C8-C9     |
| 7   | C     | 101 | BCL  | C11-C10-C8-C9   |
| 7   | C     | 101 | BCL  | C14-C13-C15-C16 |
| 7   | J     | 102 | BCL  | C6-C7-C8-C9     |
| 7   | K     | 101 | BCL  | C14-C13-C15-C16 |
| 7   | N     | 102 | BCL  | C6-C7-C8-C9     |
| 7   | N     | 102 | BCL  | C11-C12-C13-C14 |
| 7   | P     | 102 | BCL  | C14-C13-C15-C16 |
| 7   | R     | 103 | BCL  | C11-C10-C8-C9   |
| 7   | V     | 101 | BCL  | C11-C10-C8-C9   |
| 7   | V     | 101 | BCL  | C14-C13-C15-C16 |
| 7   | W     | 102 | BCL  | C11-C12-C13-C14 |
| 7   | W     | 102 | BCL  | C14-C13-C15-C16 |
| 10  | M     | 408 | CDL  | O1-C1-CB2-OB2   |
| 7   | M     | 403 | BCL  | O1D-CGD-O2D-CED |
| 8   | 0     | 103 | SPO  | C10-C11-C12-C13 |
| 8   | 0     | 103 | SPO  | C24-C23-C25-C26 |
| 8   | R     | 102 | SPO  | C5-C6-C7-C8     |
| 8   | U     | 103 | SPO  | C5-C6-C7-C8     |
| 8   | Z     | 101 | SPO  | C5-C6-C7-C8     |
| 8   | 0     | 102 | SPO  | C5-C6-C7-C9     |
| 8   | 0     | 103 | SPO  | C10-C11-C12-C14 |
| 8   | 0     | 103 | SPO  | C22-C23-C25-C26 |
| 8   | R     | 102 | SPO  | C5-C6-C7-C9     |
| 8   | S     | 103 | SPO  | C15-C16-C17-C19 |
| 8   | Z     | 101 | SPO  | C5-C6-C7-C9     |
| 7   | N     | 102 | BCL  | C5-C6-C7-C8     |
| 10  | F     | 101 | CDL  | C31-CA7-OA8-CA6 |
| 7   | b     | 101 | BCL  | O1D-CGD-O2D-CED |
| 7   | P     | 102 | BCL  | C10-C11-C12-C13 |
| 7   | Q     | 101 | BCL  | C15-C16-C17-C18 |
| 7   | S     | 102 | BCL  | C15-C16-C17-C18 |
| 7   | W     | 102 | BCL  | C10-C11-C12-C13 |
| 7   | C     | 101 | BCL  | CBD-CGD-O2D-CED |
| 7   | J     | 102 | BCL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | 3     | 101 | BCL  | C11-C10-C8-C7   |
| 7   | C     | 101 | BCL  | C11-C12-C13-C15 |
| 7   | E     | 101 | BCL  | C12-C13-C15-C16 |
| 7   | F     | 104 | BCL  | C6-C7-C8-C10    |
| 7   | I     | 101 | BCL  | C11-C12-C13-C15 |
| 7   | L     | 309 | BCL  | C11-C10-C8-C7   |
| 7   | N     | 102 | BCL  | C12-C13-C15-C16 |
| 7   | R     | 103 | BCL  | C5-C6-C7-C8     |
| 8   | 2     | 101 | SPO  | C12-C14-C15-C16 |
| 8   | D     | 103 | SPO  | C33-C35-C36-C37 |
| 8   | K     | 102 | SPO  | C28-C30-C31-C32 |
| 8   | P     | 101 | SPO  | C28-C30-C31-C32 |
| 8   | T     | 102 | SPO  | C33-C35-C36-C37 |
| 8   | Z     | 101 | SPO  | C33-C35-C36-C37 |
| 12  | L     | 304 | U10  | C24-C26-C27-C28 |
| 12  | L     | 306 | U10  | C9-C11-C12-C13  |
| 12  | L     | 306 | U10  | C29-C31-C32-C33 |
| 12  | M     | 405 | U10  | C34-C36-C37-C38 |
| 7   | 3     | 102 | BCL  | C13-C15-C16-C17 |
| 7   | I     | 101 | BCL  | C15-C16-C17-C18 |
| 7   | K     | 101 | BCL  | C8-C10-C11-C12  |
| 7   | a     | 101 | BCL  | C5-C6-C7-C8     |
| 9   | W     | 103 | PC1  | C11-C12-N-C14   |
| 9   | 9     | 103 | PC1  | C31-C32-C33-C34 |
| 7   | 3     | 102 | BCL  | C8-C10-C11-C12  |
| 7   | T     | 101 | BCL  | C10-C11-C12-C13 |
| 7   | W     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 7   | a     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 7   | 9     | 101 | BCL  | C5-C6-C7-C8     |
| 7   | C     | 101 | BCL  | C10-C11-C12-C13 |
| 7   | E     | 101 | BCL  | C8-C10-C11-C12  |
| 7   | E     | 101 | BCL  | C10-C11-C12-C13 |
| 7   | E     | 101 | BCL  | C15-C16-C17-C18 |
| 7   | J     | 102 | BCL  | C8-C10-C11-C12  |
| 7   | L     | 309 | BCL  | C8-C10-C11-C12  |
| 7   | V     | 101 | BCL  | C5-C6-C7-C8     |
| 9   | M     | 410 | PC1  | C31-C32-C33-C34 |
| 7   | L     | 302 | BCL  | C3-C5-C6-C7     |
| 7   | 3     | 101 | BCL  | C13-C15-C16-C17 |
| 7   | E     | 101 | BCL  | C13-C15-C16-C17 |
| 7   | P     | 102 | BCL  | C8-C10-C11-C12  |
| 7   | R     | 103 | BCL  | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | 1     | 102 | BCL  | C5-C6-C7-C8     |
| 7   | 1     | 102 | BCL  | C8-C10-C11-C12  |
| 7   | Q     | 101 | BCL  | C5-C6-C7-C8     |
| 7   | V     | 101 | BCL  | C8-C10-C11-C12  |
| 7   | B     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 7   | W     | 102 | BCL  | CBD-CGD-O2D-CED |
| 7   | M     | 403 | BCL  | C10-C11-C12-C13 |
| 8   | 0     | 103 | SPO  | C25-C26-C27-C28 |
| 8   | S     | 103 | SPO  | C12-C14-C15-C16 |
| 7   | K     | 101 | BCL  | C15-C16-C17-C18 |
| 9   | M     | 401 | PC1  | C21-C22-C23-C24 |
| 7   | 1     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 7   | b     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 7   | R     | 103 | BCL  | CBA-CGA-O2A-C1  |
| 7   | D     | 102 | BCL  | C8-C10-C11-C12  |
| 7   | F     | 104 | BCL  | C13-C15-C16-C17 |
| 7   | J     | 102 | BCL  | C13-C15-C16-C17 |
| 7   | F     | 104 | BCL  | O1D-CGD-O2D-CED |
| 7   | 1     | 102 | BCL  | C10-C11-C12-C13 |
| 7   | A     | 101 | BCL  | C5-C6-C7-C8     |
| 7   | b     | 101 | BCL  | C5-C6-C7-C8     |
| 7   | O     | 101 | BCL  | C15-C16-C17-C18 |
| 7   | F     | 102 | BCL  | C10-C11-C12-C13 |
| 7   | F     | 104 | BCL  | C4B-C3B-CAB-OB  |
| 8   | W     | 101 | SPO  | C28-C30-C31-C32 |
| 7   | E     | 101 | BCL  | C16-C17-C18-C19 |
| 7   | O     | 101 | BCL  | C16-C17-C18-C20 |
| 10  | F     | 101 | CDL  | OA9-CA7-OA8-CA6 |
| 7   | A     | 101 | BCL  | C8-C10-C11-C12  |
| 7   | U     | 101 | BCL  | C10-C11-C12-C13 |
| 8   | 0     | 102 | SPO  | C5-C6-C7-C8     |
| 8   | D     | 103 | SPO  | C5-C6-C7-C8     |
| 8   | R     | 102 | SPO  | C10-C11-C12-C13 |
| 8   | S     | 103 | SPO  | C15-C16-C17-C18 |
| 8   | U     | 103 | SPO  | C10-C11-C12-C13 |
| 10  | F     | 101 | CDL  | CA4-CA3-OA5-PA1 |
| 8   | D     | 103 | SPO  | C5-C6-C7-C9     |
| 8   | R     | 102 | SPO  | C10-C11-C12-C14 |
| 7   | 8     | 102 | BCL  | C2A-CAA-CBA-CGA |
| 7   | J     | 102 | BCL  | O2A-C1-C2-C3    |
| 10  | F     | 101 | CDL  | CB3-CB4-OB6-CB5 |
| 7   | 1     | 102 | BCL  | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | 9     | 101 | BCL  | C16-C17-C18-C19 |
| 7   | a     | 101 | BCL  | C6-C7-C8-C9     |
| 7   | R     | 103 | BCL  | O1D-CGD-O2D-CED |
| 7   | B     | 101 | BCL  | C3-C5-C6-C7     |
| 8   | S     | 103 | SPO  | C11-C12-C14-C15 |
| 8   | S     | 103 | SPO  | C16-C17-C19-C20 |
| 7   | N     | 102 | BCL  | C10-C11-C12-C13 |
| 9   | W     | 103 | PC1  | C11-C12-N-C13   |
| 7   | E     | 101 | BCL  | C2-C1-O2A-CGA   |
| 7   | M     | 403 | BCL  | C2-C1-O2A-CGA   |
| 7   | 0     | 101 | BCL  | C11-C12-C13-C14 |
| 7   | B     | 101 | BCL  | C16-C17-C18-C20 |
| 7   | T     | 101 | BCL  | C16-C17-C18-C19 |
| 10  | F     | 101 | CDL  | C38-C39-C40-C41 |
| 10  | M     | 408 | CDL  | C83-C84-C85-C86 |
| 7   | 0     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 10  | F     | 101 | CDL  | C40-C41-C42-C43 |
| 9   | H     | 301 | PC1  | C2C-C2D-C2E-C2F |
| 10  | F     | 101 | CDL  | C79-C80-C81-C82 |
| 7   | 0     | 101 | BCL  | C11-C12-C13-C15 |
| 7   | B     | 101 | BCL  | C16-C17-C18-C19 |
| 7   | F     | 102 | BCL  | C16-C17-C18-C19 |
| 7   | F     | 104 | BCL  | C16-C17-C18-C19 |
| 7   | O     | 101 | BCL  | C16-C17-C18-C19 |
| 7   | P     | 102 | BCL  | C16-C17-C18-C19 |
| 7   | T     | 101 | BCL  | C16-C17-C18-C20 |
| 11  | L     | 311 | BPH  | C6-C7-C8-C9     |
| 7   | 1     | 102 | BCL  | C6-C7-C8-C10    |
| 7   | U     | 101 | BCL  | C15-C16-C17-C18 |
| 9   | 9     | 103 | PC1  | C2A-C2B-C2C-C2D |
| 7   | R     | 103 | BCL  | O1A-CGA-O2A-C1  |
| 7   | 0     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 7   | 3     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 7   | E     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 7   | N     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 7   | P     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 7   | R     | 103 | BCL  | C3A-C2A-CAA-CBA |
| 7   | T     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 7   | K     | 101 | BCL  | C13-C15-C16-C17 |
| 7   | O     | 101 | BCL  | C8-C10-C11-C12  |
| 7   | E     | 101 | BCL  | C16-C17-C18-C20 |
| 7   | F     | 104 | BCL  | C16-C17-C18-C20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | V     | 101 | BCL  | C16-C17-C18-C19 |
| 7   | a     | 101 | BCL  | C6-C7-C8-C10    |
| 7   | 7     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 7   | E     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 7   | L     | 302 | BCL  | C13-C15-C16-C17 |
| 10  | M     | 407 | CDL  | CA5-C11-C12-C13 |
| 9   | H     | 301 | PC1  | C22-C23-C24-C25 |
| 10  | M     | 407 | CDL  | C34-C35-C36-C37 |
| 10  | M     | 407 | CDL  | C21-C22-C23-C24 |
| 12  | M     | 405 | U10  | C4-C3-O3-C3M    |
| 7   | 1     | 102 | BCL  | C11-C12-C13-C14 |
| 7   | 9     | 101 | BCL  | C16-C17-C18-C20 |
| 10  | M     | 407 | CDL  | CB5-C51-C52-C53 |
| 10  | M     | 408 | CDL  | C36-C37-C38-C39 |
| 7   | D     | 102 | BCL  | C15-C16-C17-C18 |
| 10  | M     | 408 | CDL  | C32-C33-C34-C35 |
| 7   | 0     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 10  | M     | 407 | CDL  | C71-C72-C73-C74 |
| 10  | M     | 407 | CDL  | C62-C63-C64-C65 |
| 7   | I     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 7   | L     | 302 | BCL  | C6-C7-C8-C9     |
| 7   | B     | 101 | BCL  | C8-C10-C11-C12  |
| 7   | L     | 309 | BCL  | C15-C16-C17-C18 |
| 7   | W     | 102 | BCL  | C8-C10-C11-C12  |
| 7   | N     | 102 | BCL  | C13-C15-C16-C17 |
| 10  | M     | 408 | CDL  | C71-C72-C73-C74 |
| 7   | C     | 101 | BCL  | C16-C17-C18-C20 |
| 7   | 9     | 101 | BCL  | C8-C10-C11-C12  |
| 9   | H     | 301 | PC1  | C29-C2A-C2B-C2C |
| 7   | F     | 104 | BCL  | C10-C11-C12-C13 |
| 8   | 0     | 102 | SPO  | C10-C11-C12-C13 |
| 8   | I     | 102 | SPO  | C1-C4-C5-C6     |
| 8   | K     | 102 | SPO  | C1-C4-C5-C6     |
| 8   | N     | 101 | SPO  | C1-C4-C5-C6     |
| 7   | I     | 101 | BCL  | C16-C17-C18-C19 |
| 9   | 9     | 103 | PC1  | C2E-C2F-C2G-C2H |
| 7   | E     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 7   | 7     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 8   | S     | 101 | SPO  | C33-C35-C36-C37 |
| 7   | L     | 302 | BCL  | C8-C10-C11-C12  |
| 7   | S     | 102 | BCL  | C16-C17-C18-C19 |
| 10  | M     | 408 | CDL  | C75-C76-C77-C78 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | L     | 305 | PC1  | C31-C32-C33-C34 |
| 7   | F     | 102 | BCL  | C13-C15-C16-C17 |
| 7   | O     | 101 | BCL  | C13-C15-C16-C17 |
| 9   | W     | 103 | PC1  | O21-C2-C3-O31   |
| 10  | M     | 407 | CDL  | C54-C55-C56-C57 |
| 9   | A     | 104 | PC1  | C21-C22-C23-C24 |
| 10  | M     | 407 | CDL  | C72-C73-C74-C75 |
| 7   | 9     | 101 | BCL  | C15-C16-C17-C18 |
| 8   | U     | 102 | SPO  | C30-C31-C32-C33 |
| 7   | F     | 104 | BCL  | C4-C3-C5-C6     |
| 7   | T     | 101 | BCL  | CBD-CGD-O2D-CED |
| 7   | F     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 9   | A     | 103 | PC1  | C22-C23-C24-C25 |
| 7   | F     | 102 | BCL  | C16-C17-C18-C20 |
| 7   | I     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 7   | E     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 7   | N     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 7   | T     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 7   | U     | 101 | BCL  | C8-C10-C11-C12  |
| 10  | F     | 101 | CDL  | OA5-CA3-CA4-CA6 |
| 7   | 8     | 102 | BCL  | C11-C10-C8-C7   |
| 7   | 8     | 102 | BCL  | C11-C12-C13-C15 |
| 7   | 9     | 101 | BCL  | C11-C10-C8-C7   |
| 7   | D     | 102 | BCL  | C11-C12-C13-C15 |
| 7   | E     | 101 | BCL  | C6-C7-C8-C10    |
| 7   | R     | 103 | BCL  | C11-C10-C8-C7   |
| 7   | R     | 103 | BCL  | C12-C13-C15-C16 |
| 7   | S     | 102 | BCL  | C11-C10-C8-C7   |
| 7   | V     | 101 | BCL  | C11-C12-C13-C15 |
| 7   | 3     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 7   | 9     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 7   | C     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 7   | F     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 7   | J     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 7   | N     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 7   | P     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 7   | V     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 8   | 0     | 102 | SPO  | C2-C1-C4-C5     |
| 8   | 2     | 101 | SPO  | C2-C1-C4-C5     |
| 8   | 3     | 103 | SPO  | C2-C1-C4-C5     |
| 8   | 3     | 103 | SPO  | C3-C1-C4-C5     |
| 8   | D     | 103 | SPO  | C2-C1-C4-C5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | L     | 309 | BCL  | C5-C6-C7-C8     |
| 9   | M     | 409 | PC1  | C27-C28-C29-C2A |
| 7   | F     | 104 | BCL  | C2-C3-C5-C6     |
| 7   | W     | 102 | BCL  | C2-C3-C5-C6     |
| 10  | M     | 407 | CDL  | C19-C20-C21-C22 |
| 10  | M     | 407 | CDL  | C41-C42-C43-C44 |
| 7   | 3     | 101 | BCL  | C5-C6-C7-C8     |
| 7   | b     | 101 | BCL  | C4B-C3B-CAB-CBB |
| 7   | 8     | 102 | BCL  | C11-C12-C13-C14 |
| 7   | 9     | 101 | BCL  | C11-C10-C8-C9   |
| 7   | E     | 101 | BCL  | C11-C12-C13-C14 |
| 7   | F     | 104 | BCL  | C6-C7-C8-C9     |
| 7   | I     | 101 | BCL  | C6-C7-C8-C9     |
| 7   | S     | 102 | BCL  | C11-C10-C8-C9   |
| 7   | V     | 101 | BCL  | C11-C12-C13-C14 |
| 11  | L     | 303 | BPH  | C11-C10-C8-C9   |
| 9   | H     | 301 | PC1  | C32-C31-O31-C3  |
| 8   | 0     | 102 | SPO  | C4-C1-O1-CM1    |
| 8   | 2     | 103 | SPO  | C4-C1-O1-CM1    |
| 8   | U     | 102 | SPO  | C4-C1-O1-CM1    |
| 8   | W     | 101 | SPO  | C4-C1-O1-CM1    |
| 7   | R     | 103 | BCL  | C15-C16-C17-C18 |
| 7   | C     | 101 | BCL  | O1D-CGD-O2D-CED |
| 7   | J     | 102 | BCL  | C16-C17-C18-C20 |
| 7   | J     | 102 | BCL  | O1D-CGD-O2D-CED |
| 7   | C     | 101 | BCL  | C3-C5-C6-C7     |
| 9   | A     | 103 | PC1  | C21-C22-C23-C24 |
| 7   | P     | 102 | BCL  | C4-C3-C5-C6     |
| 7   | W     | 102 | BCL  | C4-C3-C5-C6     |
| 7   | P     | 102 | BCL  | C2-C3-C5-C6     |
| 7   | B     | 101 | BCL  | C10-C11-C12-C13 |
| 7   | L     | 309 | BCL  | C10-C11-C12-C13 |
| 7   | F     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 9   | H     | 301 | PC1  | O32-C31-O31-C3  |
| 7   | 3     | 101 | BCL  | O2A-C1-C2-C3    |
| 10  | M     | 407 | CDL  | C51-C52-C53-C54 |
| 10  | M     | 407 | CDL  | C61-C62-C63-C64 |
| 9   | M     | 409 | PC1  | O11-C1-C2-O21   |
| 10  | M     | 408 | CDL  | C51-C52-C53-C54 |
| 7   | W     | 102 | BCL  | O1D-CGD-O2D-CED |
| 7   | a     | 101 | BCL  | C4-C3-C5-C6     |
| 7   | A     | 101 | BCL  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | M     | 407 | CDL  | C16-C17-C18-C19 |
| 9   | L     | 305 | PC1  | O31-C31-C32-C33 |
| 8   | 9     | 102 | SPO  | C28-C30-C31-C32 |
| 8   | M     | 406 | SPO  | C28-C30-C31-C32 |
| 7   | D     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 8   | 0     | 102 | SPO  | C2-C1-O1-CM1    |
| 8   | 2     | 103 | SPO  | C3-C1-O1-CM1    |
| 8   | 8     | 101 | SPO  | C3-C1-O1-CM1    |
| 8   | D     | 101 | SPO  | C3-C1-O1-CM1    |
| 8   | D     | 103 | SPO  | C2-C1-O1-CM1    |
| 8   | I     | 102 | SPO  | C2-C1-O1-CM1    |
| 8   | I     | 102 | SPO  | C3-C1-O1-CM1    |
| 8   | S     | 103 | SPO  | C3-C1-O1-CM1    |
| 8   | U     | 102 | SPO  | C3-C1-O1-CM1    |
| 8   | Z     | 101 | SPO  | C2-C1-O1-CM1    |
| 8   | 9     | 102 | SPO  | C29-C28-C30-C31 |
| 8   | D     | 103 | SPO  | C29-C28-C30-C31 |
| 12  | L     | 306 | U10  | C30-C29-C31-C32 |
| 12  | X     | 101 | U10  | C25-C24-C26-C27 |
| 7   | E     | 101 | BCL  | C5-C6-C7-C8     |
| 7   | Q     | 101 | BCL  | C8-C10-C11-C12  |
| 7   | W     | 102 | BCL  | C13-C15-C16-C17 |
| 7   | 3     | 101 | BCL  | C11-C10-C8-C9   |
| 7   | 3     | 101 | BCL  | C14-C13-C15-C16 |
| 7   | C     | 101 | BCL  | C11-C12-C13-C14 |
| 7   | E     | 101 | BCL  | C14-C13-C15-C16 |
| 7   | F     | 102 | BCL  | C6-C7-C8-C9     |
| 7   | R     | 103 | BCL  | C14-C13-C15-C16 |
| 7   | U     | 101 | BCL  | C13-C15-C16-C17 |
| 7   | R     | 103 | BCL  | C10-C11-C12-C13 |
| 9   | M     | 402 | PC1  | C32-C31-O31-C3  |
| 7   | 3     | 102 | BCL  | C12-C13-C15-C16 |
| 7   | 9     | 101 | BCL  | C12-C13-C15-C16 |
| 7   | D     | 102 | BCL  | C6-C7-C8-C10    |
| 7   | D     | 102 | BCL  | C11-C10-C8-C7   |
| 7   | E     | 101 | BCL  | C11-C10-C8-C7   |
| 7   | F     | 102 | BCL  | C6-C7-C8-C10    |
| 7   | F     | 102 | BCL  | C11-C10-C8-C7   |
| 7   | I     | 101 | BCL  | C6-C7-C8-C10    |
| 7   | K     | 101 | BCL  | C12-C13-C15-C16 |
| 7   | P     | 102 | BCL  | C11-C10-C8-C7   |
| 7   | V     | 101 | BCL  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | L     | 303 | BPH  | C11-C10-C8-C7   |
| 7   | R     | 103 | BCL  | C16-C17-C18-C19 |
| 11  | L     | 311 | BPH  | C6-C7-C8-C10    |
| 7   | A     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 7   | D     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 7   | F     | 102 | BCL  | C4-C3-C5-C6     |
| 7   | b     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 8   | M     | 406 | SPO  | C34-C33-C35-C36 |
| 7   | F     | 102 | BCL  | C15-C16-C17-C18 |
| 7   | R     | 103 | BCL  | C8-C10-C11-C12  |
| 7   | 8     | 102 | BCL  | C16-C17-C18-C19 |
| 7   | K     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 9   | L     | 305 | PC1  | C1-C2-C3-O31    |
| 9   | W     | 103 | PC1  | C1-C2-C3-O31    |
| 10  | M     | 407 | CDL  | CA3-CA4-CA6-OA8 |
| 7   | b     | 101 | BCL  | C11-C12-C13-C14 |
| 10  | M     | 407 | CDL  | C52-C53-C54-C55 |
| 7   | 0     | 101 | BCL  | C1-C2-C3-C4     |
| 7   | J     | 102 | BCL  | C1-C2-C3-C4     |
| 7   | K     | 101 | BCL  | C1-C2-C3-C4     |
| 7   | L     | 302 | BCL  | C1-C2-C3-C4     |
| 7   | O     | 101 | BCL  | C1-C2-C3-C4     |
| 7   | Q     | 101 | BCL  | C1-C2-C3-C4     |
| 7   | U     | 101 | BCL  | C1-C2-C3-C4     |
| 7   | 9     | 101 | BCL  | C4-C3-C5-C6     |
| 7   | A     | 101 | BCL  | C4-C3-C5-C6     |
| 8   | A     | 102 | SPO  | C34-C33-C35-C36 |
| 8   | P     | 101 | SPO  | C29-C28-C30-C31 |
| 11  | L     | 311 | BPH  | C4-C3-C5-C6     |
| 7   | F     | 102 | BCL  | C2-C3-C5-C6     |
| 8   | 9     | 102 | SPO  | C27-C28-C30-C31 |
| 8   | D     | 103 | SPO  | C27-C28-C30-C31 |
| 12  | X     | 101 | U10  | C23-C24-C26-C27 |
| 12  | L     | 306 | U10  | C4-C3-O3-C3M    |
| 9   | H     | 301 | PC1  | O11-C1-C2-O21   |
| 10  | F     | 101 | CDL  | OA5-CA3-CA4-OA6 |
| 7   | 3     | 102 | BCL  | C15-C16-C17-C18 |
| 7   | 3     | 102 | BCL  | CBD-CGD-O2D-CED |
| 7   | C     | 101 | BCL  | C16-C17-C18-C19 |
| 7   | J     | 102 | BCL  | C16-C17-C18-C19 |
| 7   | V     | 101 | BCL  | C16-C17-C18-C20 |
| 7   | S     | 102 | BCL  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | 9     | 103 | PC1  | O21-C2-C3-O31   |
| 8   | M     | 406 | SPO  | C32-C33-C35-C36 |
| 8   | P     | 101 | SPO  | C27-C28-C30-C31 |
| 8   | S     | 103 | SPO  | C27-C28-C30-C31 |
| 10  | M     | 407 | CDL  | C73-C74-C75-C76 |
| 7   | 0     | 101 | BCL  | C1-C2-C3-C5     |
| 7   | L     | 302 | BCL  | C1-C2-C3-C5     |
| 7   | M     | 403 | BCL  | C1-C2-C3-C5     |
| 7   | O     | 101 | BCL  | C1-C2-C3-C5     |
| 7   | Q     | 101 | BCL  | C1-C2-C3-C5     |
| 7   | W     | 102 | BCL  | C1-C2-C3-C5     |
| 7   | S     | 102 | BCL  | C16-C17-C18-C20 |
| 7   | C     | 101 | BCL  | C4B-C3B-CAB-OB  |
| 7   | D     | 102 | BCL  | C11-C10-C8-C9   |
| 7   | I     | 101 | BCL  | C11-C12-C13-C14 |
| 7   | O     | 101 | BCL  | C6-C7-C8-C9     |
| 7   | P     | 102 | BCL  | C16-C17-C18-C20 |
| 8   | 9     | 102 | SPO  | C33-C35-C36-C37 |
| 8   | N     | 101 | SPO  | C28-C30-C31-C32 |
| 8   | U     | 102 | SPO  | C28-C30-C31-C32 |
| 10  | F     | 101 | CDL  | C76-C77-C78-C79 |
| 7   | b     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 7   | I     | 101 | BCL  | C16-C17-C18-C20 |
| 7   | I     | 101 | BCL  | C10-C11-C12-C13 |
| 8   | 8     | 101 | SPO  | C24-C23-C25-C26 |
| 7   | 1     | 102 | BCL  | C11-C10-C8-C7   |
| 7   | 9     | 101 | BCL  | C6-C7-C8-C10    |
| 7   | C     | 101 | BCL  | C11-C10-C8-C7   |
| 7   | J     | 102 | BCL  | C6-C7-C8-C10    |
| 7   | Q     | 101 | BCL  | C12-C13-C15-C16 |
| 7   | T     | 101 | BCL  | C11-C12-C13-C15 |
| 7   | V     | 101 | BCL  | C11-C10-C8-C7   |
| 8   | 2     | 103 | SPO  | C1-C4-C5-C6     |
| 8   | U     | 103 | SPO  | C1-C4-C5-C6     |
| 8   | S     | 103 | SPO  | C10-C11-C12-C14 |
| 8   | U     | 103 | SPO  | C10-C11-C12-C14 |
| 7   | K     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 12  | L     | 310 | U10  | C1-C6-C7-C8     |
| 7   | J     | 102 | BCL  | C15-C16-C17-C18 |
| 7   | A     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 7   | L     | 301 | BCL  | C16-C17-C18-C19 |
| 8   | D     | 103 | SPO  | C34-C33-C35-C36 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | R     | 101 | SPO  | C29-C28-C30-C31 |
| 12  | L     | 306 | U10  | C15-C14-C16-C17 |
| 7   | D     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 9   | M     | 402 | PC1  | O32-C31-O31-C3  |
| 9   | L     | 305 | PC1  | C33-C34-C35-C36 |
| 11  | L     | 303 | BPH  | O2A-C1-C2-C3    |
| 8   | O     | 102 | SPO  | C33-C35-C36-C37 |
| 9   | M     | 401 | PC1  | C1-C2-C3-O31    |
| 9   | M     | 410 | PC1  | C1-C2-C3-O31    |
| 7   | 8     | 102 | BCL  | C16-C17-C18-C20 |
| 7   | B     | 101 | BCL  | C4-C3-C5-C6     |
| 10  | F     | 101 | CDL  | C32-C31-CA7-OA8 |
| 7   | 9     | 101 | BCL  | C2-C3-C5-C6     |
| 10  | F     | 101 | CDL  | C71-C72-C73-C74 |
| 9   | 9     | 103 | PC1  | C12-C11-O13-P   |
| 9   | L     | 305 | PC1  | C12-C11-O13-P   |
| 9   | M     | 402 | PC1  | C12-C11-O13-P   |
| 9   | W     | 103 | PC1  | C12-C11-O13-P   |
| 12  | L     | 310 | U10  | C5-C6-C7-C8     |
| 7   | T     | 101 | BCL  | O1D-CGD-O2D-CED |
| 9   | M     | 401 | PC1  | O21-C2-C3-O31   |
| 7   | 8     | 102 | BCL  | C6-C7-C8-C9     |
| 9   | A     | 104 | PC1  | C2-C1-O11-P     |
| 9   | A     | 104 | PC1  | O13-C11-C12-N   |
| 9   | F     | 103 | PC1  | O13-C11-C12-N   |
| 9   | M     | 401 | PC1  | O13-C11-C12-N   |
| 9   | M     | 409 | PC1  | O13-C11-C12-N   |
| 9   | W     | 103 | PC1  | O13-C11-C12-N   |
| 12  | L     | 306 | U10  | C13-C14-C16-C17 |
| 12  | L     | 306 | U10  | C28-C29-C31-C32 |
| 7   | J     | 102 | BCL  | C10-C11-C12-C13 |
| 9   | H     | 301 | PC1  | C32-C33-C34-C35 |
| 7   | A     | 101 | BCL  | CBD-CGD-O2D-CED |
| 7   | B     | 101 | BCL  | C15-C16-C17-C18 |
| 9   | 9     | 103 | PC1  | C25-C26-C27-C28 |
| 9   | M     | 409 | PC1  | C2C-C2D-C2E-C2F |
| 7   | R     | 103 | BCL  | C16-C17-C18-C20 |
| 8   | D     | 101 | SPO  | C28-C30-C31-C32 |
| 7   | b     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 8   | S     | 103 | SPO  | C29-C28-C30-C31 |
| 8   | S     | 103 | SPO  | C34-C33-C35-C36 |
| 9   | W     | 103 | PC1  | O21-C21-C22-C23 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | 8     | 101 | SPO  | C22-C23-C25-C26 |
| 9   | H     | 301 | PC1  | O11-C1-C2-C3    |
| 10  | M     | 408 | CDL  | OB5-CB3-CB4-CB6 |
| 9   | 9     | 103 | PC1  | C2D-C2E-C2F-C2G |
| 7   | A     | 101 | BCL  | C6-C7-C8-C10    |
| 7   | N     | 102 | BCL  | C6-C7-C8-C10    |
| 7   | T     | 101 | BCL  | C11-C10-C8-C7   |
| 7   | V     | 101 | BCL  | C6-C7-C8-C10    |
| 7   | b     | 101 | BCL  | C11-C10-C8-C7   |
| 7   | E     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 8   | 0     | 102 | SPO  | C3-C1-C4-C5     |
| 7   | 3     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 7   | J     | 102 | BCL  | C4-C3-C5-C6     |
| 7   | U     | 101 | BCL  | C16-C17-C18-C19 |
| 7   | B     | 101 | BCL  | C2-C3-C5-C6     |
| 9   | W     | 103 | PC1  | O11-C1-C2-O21   |
| 10  | M     | 408 | CDL  | OB5-CB3-CB4-OB6 |
| 7   | E     | 101 | BCL  | C3-C5-C6-C7     |
| 7   | 0     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 7   | R     | 103 | BCL  | C2A-CAA-CBA-CGA |
| 7   | E     | 101 | BCL  | C11-C10-C8-C9   |
| 7   | N     | 102 | BCL  | C14-C13-C15-C16 |
| 10  | F     | 101 | CDL  | C74-C75-C76-C77 |
| 7   | M     | 403 | BCL  | C8-C10-C11-C12  |
| 9   | M     | 402 | PC1  | C24-C25-C26-C27 |
| 10  | M     | 407 | CDL  | OA6-CA4-CA6-OA8 |
| 10  | M     | 407 | CDL  | OB6-CB4-CB6-OB8 |
| 9   | H     | 301 | PC1  | C36-C37-C38-C39 |
| 9   | 9     | 103 | PC1  | C1-C2-C3-O31    |
| 10  | M     | 407 | CDL  | CB3-CB4-CB6-OB8 |
| 8   | R     | 101 | SPO  | C27-C28-C30-C31 |
| 7   | M     | 403 | BCL  | CAD-CBD-CGD-O2D |
| 8   | 0     | 103 | SPO  | C4-C1-O1-CM1    |
| 7   | V     | 101 | BCL  | C13-C15-C16-C17 |
| 7   | J     | 102 | BCL  | C5-C6-C7-C8     |
| 7   | b     | 101 | BCL  | C11-C12-C13-C15 |
| 7   | 3     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 12  | M     | 405 | U10  | C5-C4-O4-C4M    |
| 7   | J     | 102 | BCL  | CHA-CBD-CGD-O1D |
| 7   | L     | 302 | BCL  | CHA-CBD-CGD-O1D |
| 7   | L     | 302 | BCL  | CHA-CBD-CGD-O2D |
| 7   | M     | 403 | BCL  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | 9     | 103 | PC1  | C11-O13-P-O12   |
| 9   | A     | 103 | PC1  | C1-O11-P-O12    |
| 9   | A     | 104 | PC1  | C11-O13-P-O11   |
| 9   | F     | 103 | PC1  | C1-O11-P-O12    |
| 9   | H     | 301 | PC1  | C1-O11-P-O14    |
| 9   | M     | 402 | PC1  | C11-O13-P-O14   |
| 10  | F     | 101 | CDL  | CA3-OA5-PA1-OA2 |
| 10  | F     | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 10  | F     | 101 | CDL  | CB2-OB2-PB2-OB3 |
| 10  | M     | 407 | CDL  | CB2-OB2-PB2-OB3 |
| 10  | M     | 407 | CDL  | CB2-OB2-PB2-OB4 |
| 10  | M     | 407 | CDL  | CB2-OB2-PB2-OB5 |
| 10  | M     | 408 | CDL  | CB3-OB5-PB2-OB3 |
| 8   | D     | 103 | SPO  | C32-C33-C35-C36 |
| 7   | K     | 101 | BCL  | C16-C17-C18-C20 |
| 7   | 8     | 102 | BCL  | C15-C16-C17-C18 |
| 7   | B     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 10  | F     | 101 | CDL  | C41-C42-C43-C44 |
| 10  | M     | 407 | CDL  | C40-C41-C42-C43 |
| 7   | b     | 101 | BCL  | C2B-C3B-CAB-CBB |
| 9   | H     | 301 | PC1  | C3-C2-O21-C21   |
| 8   | 0     | 102 | SPO  | C14-C15-C16-C17 |
| 8   | 2     | 101 | SPO  | C23-C25-C26-C27 |
| 8   | 2     | 102 | SPO  | C9-C10-C11-C12  |
| 8   | 2     | 103 | SPO  | C9-C10-C11-C12  |
| 8   | 3     | 103 | SPO  | C14-C15-C16-C17 |
| 8   | E     | 102 | SPO  | C14-C15-C16-C17 |
| 8   | K     | 102 | SPO  | C14-C15-C16-C17 |
| 8   | S     | 101 | SPO  | C14-C15-C16-C17 |
| 8   | S     | 103 | SPO  | C14-C15-C16-C17 |
| 8   | Z     | 101 | SPO  | C23-C25-C26-C27 |
| 8   | A     | 102 | SPO  | C32-C33-C35-C36 |
| 11  | L     | 311 | BPH  | C2-C3-C5-C6     |
| 9   | M     | 402 | PC1  | C11-C12-N-C14   |
| 7   | 1     | 102 | BCL  | C11-C10-C8-C9   |
| 7   | 7     | 101 | BCL  | C6-C7-C8-C9     |
| 7   | M     | 403 | BCL  | C14-C13-C15-C16 |
| 7   | S     | 102 | BCL  | C14-C13-C15-C16 |
| 7   | T     | 101 | BCL  | C11-C12-C13-C14 |
| 10  | M     | 408 | CDL  | C73-C74-C75-C76 |
| 7   | O     | 101 | BCL  | C6-C7-C8-C10    |
| 8   | 2     | 101 | SPO  | C16-C17-C19-C20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | 3     | 102 | BCL  | O1D-CGD-O2D-CED |
| 12  | L     | 307 | U10  | C35-C34-C36-C37 |
| 7   | M     | 403 | BCL  | CAA-CBA-CGA-O2A |
| 7   | a     | 101 | BCL  | C2-C3-C5-C6     |
| 12  | L     | 306 | U10  | C5-C4-O4-C4M    |
| 8   | M     | 406 | SPO  | C30-C31-C32-C33 |
| 7   | A     | 101 | BCL  | O1D-CGD-O2D-CED |
| 9   | F     | 103 | PC1  | O21-C2-C3-O31   |
| 7   | 8     | 102 | BCL  | C5-C6-C7-C8     |
| 7   | 9     | 101 | BCL  | C13-C15-C16-C17 |
| 8   | M     | 406 | SPO  | C33-C35-C36-C37 |
| 8   | R     | 102 | SPO  | C28-C30-C31-C32 |
| 8   | S     | 103 | SPO  | C28-C30-C31-C32 |
| 9   | M     | 402 | PC1  | C27-C28-C29-C2A |
| 9   | 9     | 103 | PC1  | C29-C2A-C2B-C2C |
| 8   | 0     | 102 | SPO  | C3-C1-O1-CM1    |
| 8   | 2     | 103 | SPO  | C2-C1-O1-CM1    |
| 8   | 8     | 101 | SPO  | C2-C1-O1-CM1    |
| 8   | A     | 102 | SPO  | C2-C1-O1-CM1    |
| 8   | D     | 103 | SPO  | C3-C1-O1-CM1    |
| 8   | S     | 103 | SPO  | C2-C1-O1-CM1    |
| 8   | U     | 102 | SPO  | C2-C1-O1-CM1    |
| 8   | W     | 101 | SPO  | C2-C1-O1-CM1    |
| 8   | W     | 101 | SPO  | C3-C1-O1-CM1    |
| 7   | Q     | 101 | BCL  | C2A-CAA-CBA-CGA |
| 8   | 2     | 101 | SPO  | C25-C26-C27-C28 |
| 8   | Z     | 101 | SPO  | C25-C26-C27-C28 |
| 12  | L     | 307 | U10  | C33-C34-C36-C37 |
| 9   | M     | 402 | PC1  | C11-C12-N-C15   |
| 7   | C     | 101 | BCL  | C4B-C3B-CAB-CBB |
| 7   | 9     | 101 | BCL  | C6-C7-C8-C9     |
| 7   | A     | 101 | BCL  | C6-C7-C8-C9     |
| 7   | 8     | 102 | BCL  | C10-C11-C12-C13 |
| 12  | M     | 405 | U10  | C35-C34-C36-C37 |
| 7   | J     | 102 | BCL  | C2-C3-C5-C6     |
| 7   | 8     | 102 | BCL  | C6-C7-C8-C10    |
| 7   | T     | 101 | BCL  | C12-C13-C15-C16 |
| 7   | L     | 301 | BCL  | C3-C5-C6-C7     |
| 10  | F     | 101 | CDL  | C36-C37-C38-C39 |
| 12  | L     | 307 | U10  | C20-C19-C21-C22 |
| 8   | 2     | 103 | SPO  | C8-C7-C9-C10    |
| 8   | 2     | 103 | SPO  | C13-C12-C14-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | 3     | 103 | SPO  | C8-C7-C9-C10    |
| 8   | 3     | 103 | SPO  | C13-C12-C14-C15 |
| 8   | 3     | 103 | SPO  | C18-C17-C19-C20 |
| 8   | E     | 102 | SPO  | C8-C7-C9-C10    |
| 8   | K     | 102 | SPO  | C8-C7-C9-C10    |
| 7   | R     | 103 | BCL  | C2-C1-O2A-CGA   |
| 7   | F     | 104 | BCL  | C8-C10-C11-C12  |
| 10  | M     | 407 | CDL  | C1-CA2-OA2-PA1  |
| 7   | 0     | 101 | BCL  | C4-C3-C5-C6     |
| 12  | L     | 304 | U10  | C25-C24-C26-C27 |
| 8   | S     | 103 | SPO  | C32-C33-C35-C36 |
| 7   | L     | 301 | BCL  | C16-C17-C18-C20 |
| 12  | L     | 308 | U10  | C5-C4-O4-C4M    |
| 12  | L     | 310 | U10  | C5-C4-O4-C4M    |
| 9   | F     | 103 | PC1  | C1-C2-C3-O31    |
| 9   | L     | 305 | PC1  | O32-C31-C32-C33 |
| 7   | F     | 102 | BCL  | C11-C12-C13-C14 |
| 7   | K     | 101 | BCL  | C11-C12-C13-C14 |
| 7   | L     | 309 | BCL  | C11-C10-C8-C9   |
| 7   | O     | 101 | BCL  | C14-C13-C15-C16 |
| 7   | Q     | 101 | BCL  | C6-C7-C8-C9     |
| 7   | Q     | 101 | BCL  | C11-C12-C13-C14 |
| 9   | A     | 104 | PC1  | C1-C2-O21-C21   |
| 9   | L     | 305 | PC1  | C1-C2-O21-C21   |
| 9   | W     | 103 | PC1  | C1-C2-O21-C21   |
| 7   | 3     | 102 | BCL  | C1-C2-C3-C4     |
| 7   | E     | 101 | BCL  | C1-C2-C3-C4     |
| 7   | M     | 403 | BCL  | C1-C2-C3-C4     |
| 7   | W     | 102 | BCL  | C1-C2-C3-C4     |
| 12  | L     | 304 | U10  | C23-C24-C26-C27 |
| 12  | L     | 307 | U10  | C18-C19-C21-C22 |
| 7   | 0     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 7   | 8     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 7   | A     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 7   | D     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 7   | U     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 8   | 2     | 103 | SPO  | C6-C7-C9-C10    |
| 8   | 2     | 103 | SPO  | C11-C12-C14-C15 |
| 8   | 3     | 103 | SPO  | C6-C7-C9-C10    |
| 8   | 3     | 103 | SPO  | C11-C12-C14-C15 |
| 8   | 3     | 103 | SPO  | C16-C17-C19-C20 |
| 8   | E     | 102 | SPO  | C6-C7-C9-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | K     | 102 | SPO  | C6-C7-C9-C10    |
| 9   | M     | 402 | PC1  | C11-C12-N-C13   |
| 10  | F     | 101 | CDL  | O1-C1-CA2-OA2   |
| 9   | W     | 103 | PC1  | O11-C1-C2-C3    |
| 12  | M     | 405 | U10  | C33-C34-C36-C37 |
| 12  | X     | 101 | U10  | C21-C22-C23-C24 |
| 7   | 7     | 101 | BCL  | C6-C7-C8-C10    |
| 7   | B     | 101 | BCL  | C6-C7-C8-C10    |
| 7   | L     | 309 | BCL  | C11-C12-C13-C15 |
| 7   | W     | 102 | BCL  | C6-C7-C8-C10    |
| 7   | W     | 102 | BCL  | C11-C12-C13-C15 |
| 8   | 8     | 101 | SPO  | C28-C30-C31-C32 |
| 10  | M     | 407 | CDL  | C59-C60-C61-C62 |
| 8   | 2     | 101 | SPO  | C3-C1-C4-C5     |
| 12  | L     | 304 | U10  | C5-C4-O4-C4M    |
| 10  | F     | 101 | CDL  | CA2-C1-CB2-OB2  |
| 7   | 1     | 102 | BCL  | C4-C3-C5-C6     |
| 7   | b     | 101 | BCL  | C4-C3-C5-C6     |
| 7   | 0     | 101 | BCL  | C2-C3-C5-C6     |
| 7   | 1     | 101 | BCL  | C1-C2-C3-C5     |
| 7   | C     | 101 | BCL  | C1-C2-C3-C5     |
| 7   | J     | 102 | BCL  | C1-C2-C3-C5     |
| 7   | b     | 101 | BCL  | C1-C2-C3-C5     |
| 7   | 3     | 101 | BCL  | C15-C16-C17-C18 |
| 7   | L     | 309 | BCL  | C14-C13-C15-C16 |
| 7   | O     | 101 | BCL  | C11-C12-C13-C14 |
| 7   | B     | 101 | BCL  | C13-C15-C16-C17 |
| 8   | 2     | 101 | SPO  | C35-C36-C37-C38 |
| 7   | O     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 7   | E     | 101 | BCL  | C4-C3-C5-C6     |
| 8   | D     | 101 | SPO  | C29-C28-C30-C31 |
| 7   | U     | 101 | BCL  | C16-C17-C18-C20 |
| 9   | M     | 410 | PC1  | C11-C12-N-C13   |
| 7   | O     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 7   | W     | 102 | BCL  | C15-C16-C17-C18 |
| 8   | 8     | 101 | SPO  | C4-C1-O1-CM1    |
| 8   | D     | 103 | SPO  | C4-C1-O1-CM1    |
| 8   | Z     | 101 | SPO  | C34-C33-C35-C36 |
| 7   | b     | 101 | BCL  | C2-C3-C5-C6     |
| 12  | L     | 306 | U10  | C6-C7-C8-C9     |
| 12  | L     | 307 | U10  | C2-C3-O3-C3M    |
| 7   | T     | 101 | BCL  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | H     | 301 | PC1  | C25-C26-C27-C28 |
| 11  | L     | 303 | BPH  | CHA-CBD-CGD-O1D |
| 11  | L     | 303 | BPH  | CHA-CBD-CGD-O2D |
| 10  | M     | 408 | CDL  | C1-CB2-OB2-PB2  |
| 7   | 9     | 101 | BCL  | C11-C12-C13-C15 |
| 7   | F     | 104 | BCL  | C11-C10-C8-C9   |
| 7   | I     | 101 | BCL  | C2-C1-O2A-CGA   |
| 7   | 8     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 7   | B     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 11  | L     | 311 | BPH  | C3A-C2A-CAA-CBA |
| 7   | F     | 104 | BCL  | CAA-CBA-CGA-O2A |
| 7   | E     | 101 | BCL  | C2-C3-C5-C6     |
| 9   | M     | 409 | PC1  | C25-C26-C27-C28 |
| 7   | M     | 403 | BCL  | C16-C17-C18-C19 |
| 9   | L     | 305 | PC1  | C3-C2-O21-C21   |
| 9   | M     | 409 | PC1  | C1-C2-O21-C21   |
| 9   | M     | 409 | PC1  | C3-C2-O21-C21   |
| 10  | M     | 407 | CDL  | C38-C39-C40-C41 |
| 10  | M     | 407 | CDL  | C35-C36-C37-C38 |
| 8   | 2     | 103 | SPO  | C34-C33-C35-C36 |
| 8   | Z     | 101 | SPO  | C32-C33-C35-C36 |
| 10  | M     | 408 | CDL  | CB5-C51-C52-C53 |
| 7   | 0     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 7   | P     | 102 | BCL  | O1A-CGA-O2A-C1  |
| 7   | 8     | 102 | BCL  | C14-C13-C15-C16 |
| 7   | M     | 403 | BCL  | C11-C10-C8-C9   |
| 7   | R     | 103 | BCL  | C11-C12-C13-C14 |
| 7   | T     | 101 | BCL  | C11-C10-C8-C9   |
| 7   | b     | 101 | BCL  | C11-C10-C8-C9   |
| 9   | M     | 409 | PC1  | O11-C1-C2-C3    |
| 8   | K     | 102 | SPO  | C5-C6-C7-C9     |
| 7   | L     | 301 | BCL  | C2A-CAA-CBA-CGA |
| 7   | C     | 101 | BCL  | C12-C13-C15-C16 |
| 7   | F     | 102 | BCL  | C11-C12-C13-C15 |
| 7   | K     | 101 | BCL  | C11-C12-C13-C15 |
| 7   | L     | 309 | BCL  | C12-C13-C15-C16 |
| 7   | O     | 101 | BCL  | C11-C12-C13-C15 |
| 7   | Q     | 101 | BCL  | C6-C7-C8-C10    |
| 7   | Q     | 101 | BCL  | C11-C12-C13-C15 |
| 7   | U     | 101 | BCL  | C6-C7-C8-C10    |
| 7   | W     | 102 | BCL  | C12-C13-C15-C16 |
| 7   | 3     | 101 | BCL  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | b     | 101 | BCL  | CAA-CBA-CGA-O1A |
| 7   | 7     | 101 | BCL  | C8-C10-C11-C12  |
| 12  | L     | 307 | U10  | C15-C14-C16-C17 |
| 10  | M     | 408 | CDL  | C32-C31-CA7-OA8 |
| 7   | V     | 101 | BCL  | C2-C3-C5-C6     |
| 9   | F     | 103 | PC1  | C33-C34-C35-C36 |
| 7   | C     | 101 | BCL  | C8-C10-C11-C12  |
| 7   | U     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 9   | 9     | 103 | PC1  | O21-C21-C22-C23 |
| 9   | 9     | 103 | PC1  | O31-C31-C32-C33 |
| 9   | F     | 103 | PC1  | O31-C31-C32-C33 |
| 12  | L     | 306 | U10  | C25-C24-C26-C27 |
| 9   | F     | 103 | PC1  | C32-C33-C34-C35 |
| 7   | D     | 102 | BCL  | C11-C12-C13-C14 |
| 7   | V     | 101 | BCL  | C6-C7-C8-C9     |
| 10  | M     | 407 | CDL  | C72-C71-CB7-OB8 |
| 10  | M     | 407 | CDL  | C36-C37-C38-C39 |
| 7   | 7     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 7   | B     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 9   | M     | 410 | PC1  | C11-C12-N-C14   |
| 9   | M     | 410 | PC1  | C11-C12-N-C15   |
| 7   | P     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 7   | U     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 7   | V     | 101 | BCL  | C4-C3-C5-C6     |
| 8   | 0     | 103 | SPO  | C35-C36-C37-C38 |
| 8   | U     | 103 | SPO  | C15-C16-C17-C19 |
| 9   | H     | 301 | PC1  | O22-C21-O21-C2  |
| 9   | F     | 103 | PC1  | C22-C23-C24-C25 |
| 9   | F     | 103 | PC1  | C24-C25-C26-C27 |
| 10  | F     | 101 | CDL  | C53-C54-C55-C56 |
| 10  | F     | 101 | CDL  | CB2-C1-CA2-OA2  |
| 7   | 8     | 102 | BCL  | C2-C1-O2A-CGA   |
| 7   | 3     | 101 | BCL  | C11-C12-C13-C15 |
| 7   | P     | 102 | BCL  | C11-C12-C13-C15 |
| 7   | P     | 102 | BCL  | C12-C13-C15-C16 |
| 11  | L     | 303 | BPH  | C6-C7-C8-C10    |
| 9   | A     | 104 | PC1  | C32-C33-C34-C35 |
| 7   | C     | 101 | BCL  | C2B-C3B-CAB-OB  |
| 7   | C     | 101 | BCL  | O2A-C1-C2-C3    |
| 9   | A     | 104 | PC1  | C3-C2-O21-C21   |
| 10  | M     | 407 | CDL  | CB6-CB4-OB6-CB5 |
| 8   | M     | 406 | SPO  | C2-C1-C4-C5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | U     | 103 | SPO  | C3-C1-C4-C5     |
| 9   | M     | 402 | PC1  | C25-C26-C27-C28 |
| 8   | R     | 102 | SPO  | C35-C36-C37-C38 |
| 7   | B     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 10  | M     | 408 | CDL  | C32-C31-CA7-OA9 |
| 7   | K     | 101 | BCL  | O1D-CGD-O2D-CED |
| 7   | U     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 9   | M     | 409 | PC1  | C26-C27-C28-C29 |
| 10  | F     | 101 | CDL  | C32-C31-CA7-OA9 |
| 10  | M     | 407 | CDL  | OA5-CA3-CA4-OA6 |
| 7   | R     | 103 | BCL  | CAA-CBA-CGA-O2A |
| 8   | R     | 101 | SPO  | C35-C36-C37-C38 |
| 7   | E     | 101 | BCL  | C6-C7-C8-C9     |
| 7   | F     | 104 | BCL  | C14-C13-C15-C16 |
| 7   | L     | 309 | BCL  | C11-C12-C13-C14 |
| 7   | W     | 102 | BCL  | C6-C7-C8-C9     |
| 9   | 9     | 103 | PC1  | O22-C21-C22-C23 |
| 9   | W     | 103 | PC1  | O22-C21-C22-C23 |
| 9   | F     | 103 | PC1  | C28-C29-C2A-C2B |
| 9   | 9     | 103 | PC1  | O32-C31-C32-C33 |
| 7   | 1     | 102 | BCL  | C2-C3-C5-C6     |
| 8   | 0     | 102 | SPO  | C1-C4-C5-C6     |
| 8   | 2     | 102 | SPO  | C1-C4-C5-C6     |
| 8   | A     | 102 | SPO  | C1-C4-C5-C6     |
| 8   | D     | 101 | SPO  | C1-C4-C5-C6     |
| 8   | M     | 406 | SPO  | C1-C4-C5-C6     |
| 8   | S     | 103 | SPO  | C1-C4-C5-C6     |
| 8   | Z     | 101 | SPO  | C1-C4-C5-C6     |
| 8   | J     | 101 | SPO  | C10-C11-C12-C14 |
| 10  | M     | 408 | CDL  | CA2-C1-CB2-OB2  |
| 7   | 0     | 101 | BCL  | CAA-CBA-CGA-O1A |
| 8   | E     | 102 | SPO  | C28-C30-C31-C32 |
| 12  | L     | 304 | U10  | C30-C29-C31-C32 |
| 8   | 2     | 102 | SPO  | C35-C36-C37-C38 |
| 8   | E     | 102 | SPO  | C35-C36-C37-C38 |
| 8   | U     | 103 | SPO  | C30-C31-C32-C33 |
| 7   | P     | 102 | BCL  | CAA-CBA-CGA-O2A |
| 7   | 9     | 101 | BCL  | CAD-CBD-CGD-O2D |
| 9   | M     | 401 | PC1  | O21-C21-C22-C23 |
| 9   | F     | 103 | PC1  | O32-C31-C32-C33 |
| 7   | 3     | 101 | BCL  | C1-C2-C3-C4     |
| 7   | 7     | 101 | BCL  | C1-C2-C3-C4     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | F     | 102 | BCL  | C1-C2-C3-C4     |
| 7   | N     | 102 | BCL  | C1-C2-C3-C4     |
| 7   | P     | 102 | BCL  | C1-C2-C3-C4     |
| 12  | X     | 101 | U10  | C11-C12-C13-C14 |
| 10  | M     | 407 | CDL  | C72-C71-CB7-OB9 |
| 7   | a     | 101 | BCL  | C3-C5-C6-C7     |
| 7   | 3     | 101 | BCL  | CBD-CGD-O2D-CED |

There are no ring outliers.

81 monomers are involved in 500 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | U     | 101 | BCL  | 12      | 0            |
| 8   | D     | 101 | SPO  | 2       | 0            |
| 8   | R     | 102 | SPO  | 4       | 0            |
| 7   | R     | 103 | BCL  | 7       | 0            |
| 7   | B     | 101 | BCL  | 8       | 0            |
| 8   | M     | 406 | SPO  | 8       | 0            |
| 8   | 2     | 102 | SPO  | 5       | 0            |
| 8   | Z     | 101 | SPO  | 8       | 0            |
| 8   | 2     | 101 | SPO  | 18      | 0            |
| 8   | R     | 101 | SPO  | 5       | 0            |
| 8   | 0     | 102 | SPO  | 8       | 0            |
| 7   | N     | 102 | BCL  | 22      | 0            |
| 8   | P     | 101 | SPO  | 8       | 0            |
| 8   | W     | 101 | SPO  | 3       | 0            |
| 7   | b     | 101 | BCL  | 4       | 0            |
| 7   | V     | 101 | BCL  | 7       | 0            |
| 7   | D     | 102 | BCL  | 4       | 0            |
| 8   | A     | 102 | SPO  | 8       | 0            |
| 12  | L     | 306 | U10  | 6       | 0            |
| 11  | L     | 303 | BPH  | 5       | 0            |
| 8   | J     | 101 | SPO  | 11      | 0            |
| 9   | F     | 103 | PC1  | 5       | 0            |
| 8   | S     | 103 | SPO  | 7       | 0            |
| 7   | 9     | 101 | BCL  | 12      | 0            |
| 8   | 3     | 103 | SPO  | 1       | 0            |
| 7   | a     | 101 | BCL  | 21      | 0            |
| 7   | M     | 403 | BCL  | 9       | 0            |
| 8   | 0     | 103 | SPO  | 2       | 0            |
| 10  | M     | 407 | CDL  | 3       | 0            |
| 12  | L     | 304 | U10  | 4       | 0            |

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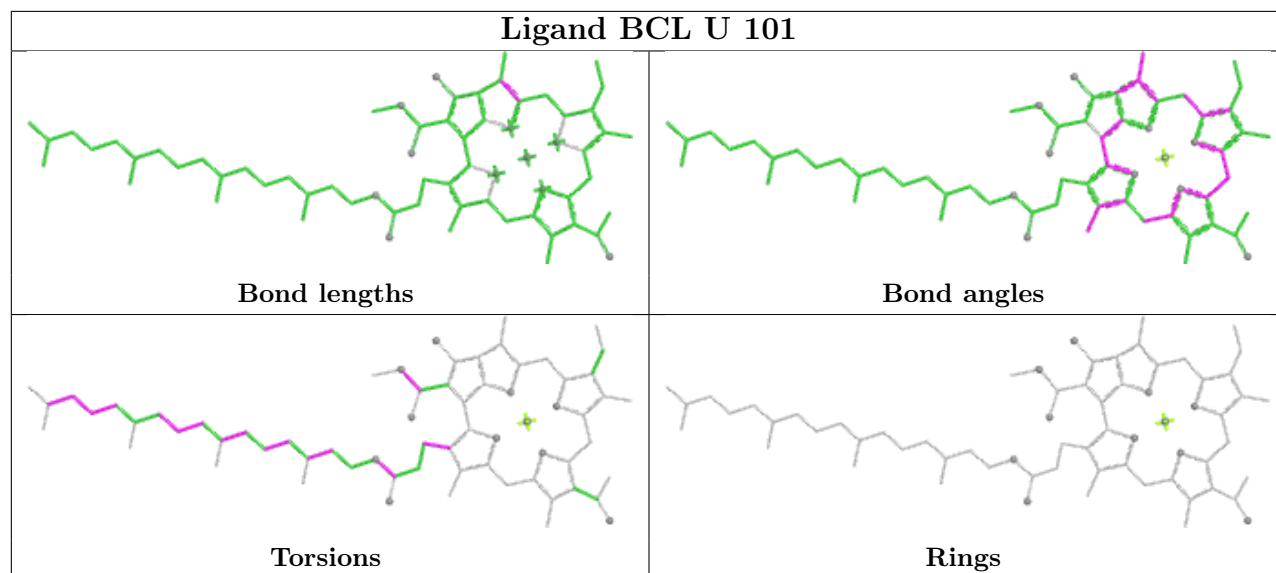
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | F     | 102 | BCL  | 18      | 0            |
| 7   | W     | 102 | BCL  | 13      | 0            |
| 10  | F     | 101 | CDL  | 1       | 0            |
| 12  | X     | 101 | U10  | 12      | 0            |
| 7   | J     | 102 | BCL  | 14      | 0            |
| 7   | 0     | 101 | BCL  | 11      | 0            |
| 9   | M     | 401 | PC1  | 2       | 0            |
| 7   | K     | 101 | BCL  | 13      | 0            |
| 9   | 9     | 103 | PC1  | 3       | 0            |
| 7   | 1     | 101 | BCL  | 14      | 0            |
| 9   | M     | 409 | PC1  | 3       | 0            |
| 7   | L     | 301 | BCL  | 7       | 0            |
| 8   | I     | 102 | SPO  | 5       | 0            |
| 12  | M     | 405 | U10  | 4       | 0            |
| 8   | S     | 101 | SPO  | 3       | 0            |
| 7   | I     | 101 | BCL  | 8       | 0            |
| 7   | 8     | 102 | BCL  | 5       | 0            |
| 9   | A     | 103 | PC1  | 3       | 0            |
| 7   | 7     | 101 | BCL  | 7       | 0            |
| 8   | O     | 102 | SPO  | 1       | 0            |
| 10  | M     | 408 | CDL  | 2       | 0            |
| 12  | L     | 307 | U10  | 3       | 0            |
| 8   | F     | 105 | SPO  | 3       | 0            |
| 7   | P     | 102 | BCL  | 8       | 0            |
| 7   | O     | 101 | BCL  | 12      | 0            |
| 8   | N     | 101 | SPO  | 9       | 0            |
| 12  | L     | 308 | U10  | 1       | 0            |
| 7   | 3     | 102 | BCL  | 13      | 0            |
| 7   | F     | 104 | BCL  | 10      | 0            |
| 8   | 9     | 102 | SPO  | 9       | 0            |
| 12  | L     | 310 | U10  | 5       | 0            |
| 7   | L     | 309 | BCL  | 12      | 0            |
| 8   | D     | 103 | SPO  | 3       | 0            |
| 11  | L     | 311 | BPH  | 6       | 0            |
| 7   | 3     | 101 | BCL  | 19      | 0            |
| 7   | 1     | 102 | BCL  | 14      | 0            |
| 7   | A     | 101 | BCL  | 11      | 0            |
| 7   | C     | 101 | BCL  | 16      | 0            |
| 7   | S     | 102 | BCL  | 8       | 0            |
| 9   | A     | 104 | PC1  | 1       | 0            |
| 8   | 2     | 103 | SPO  | 1       | 0            |
| 7   | T     | 101 | BCL  | 13      | 0            |

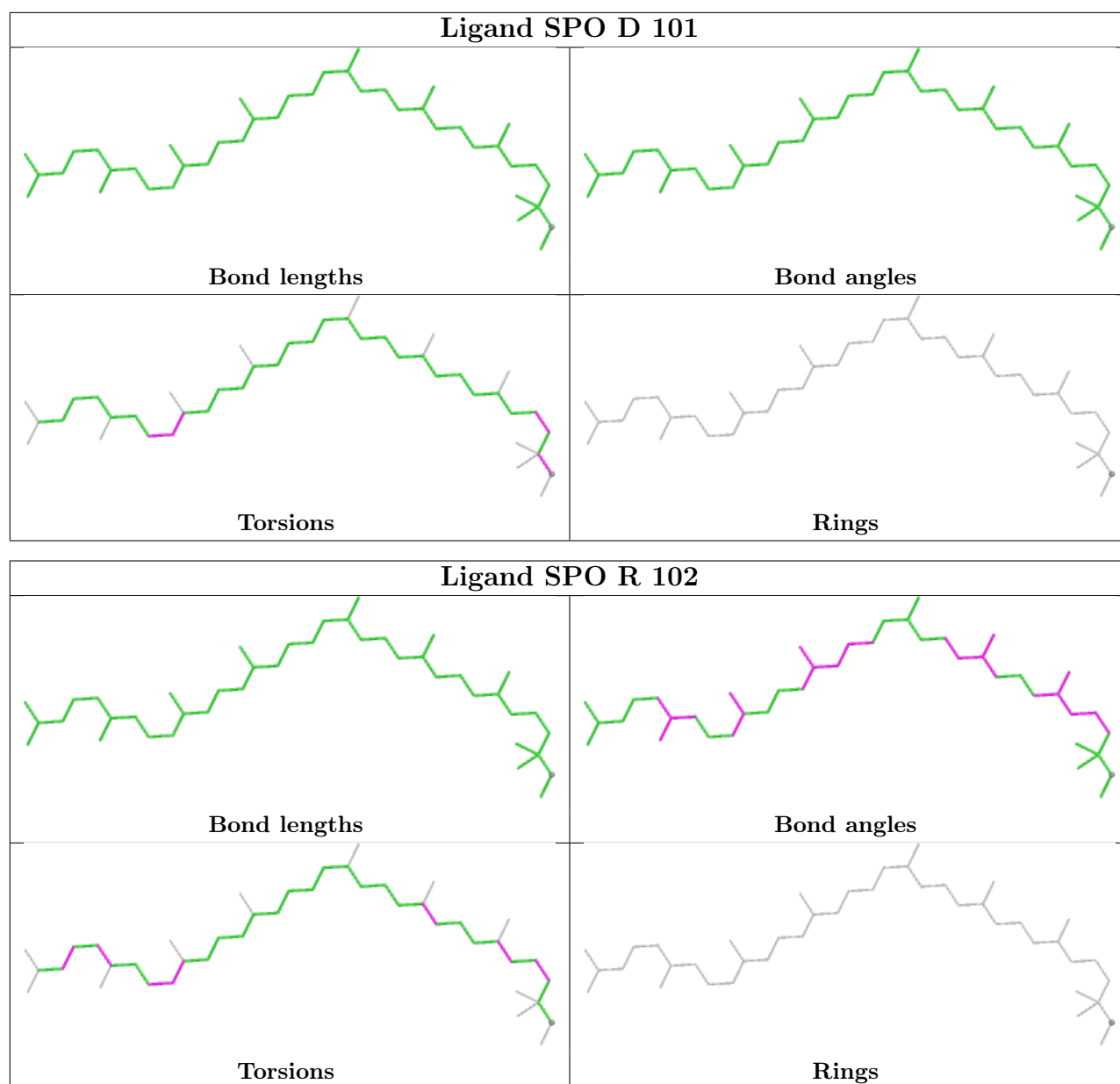
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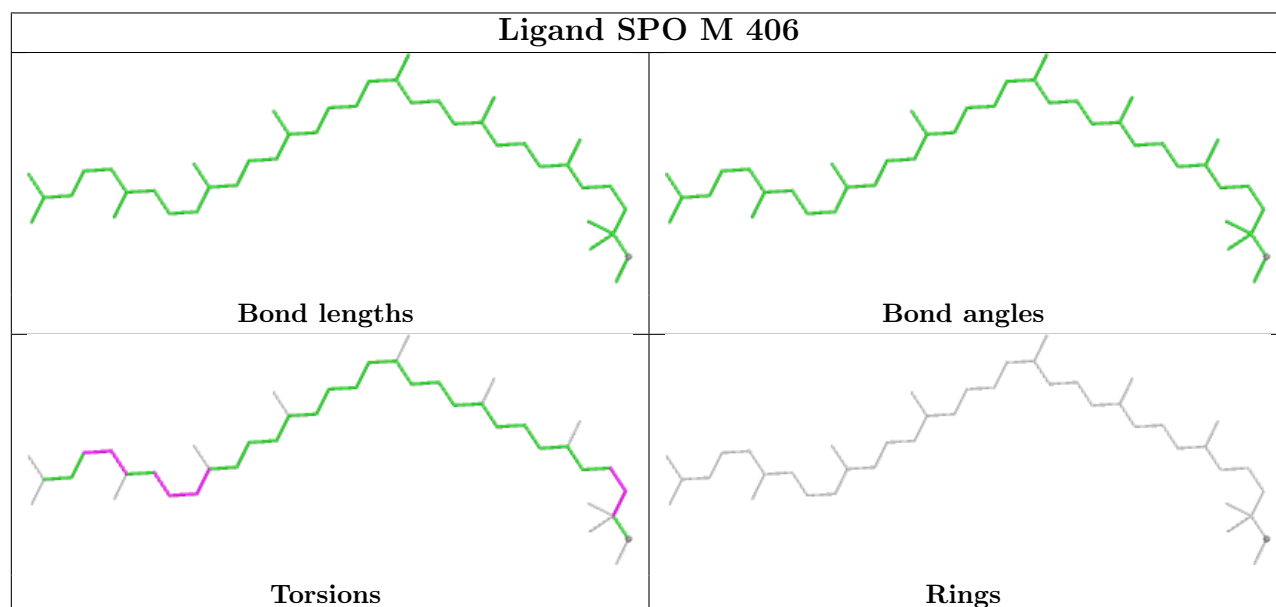
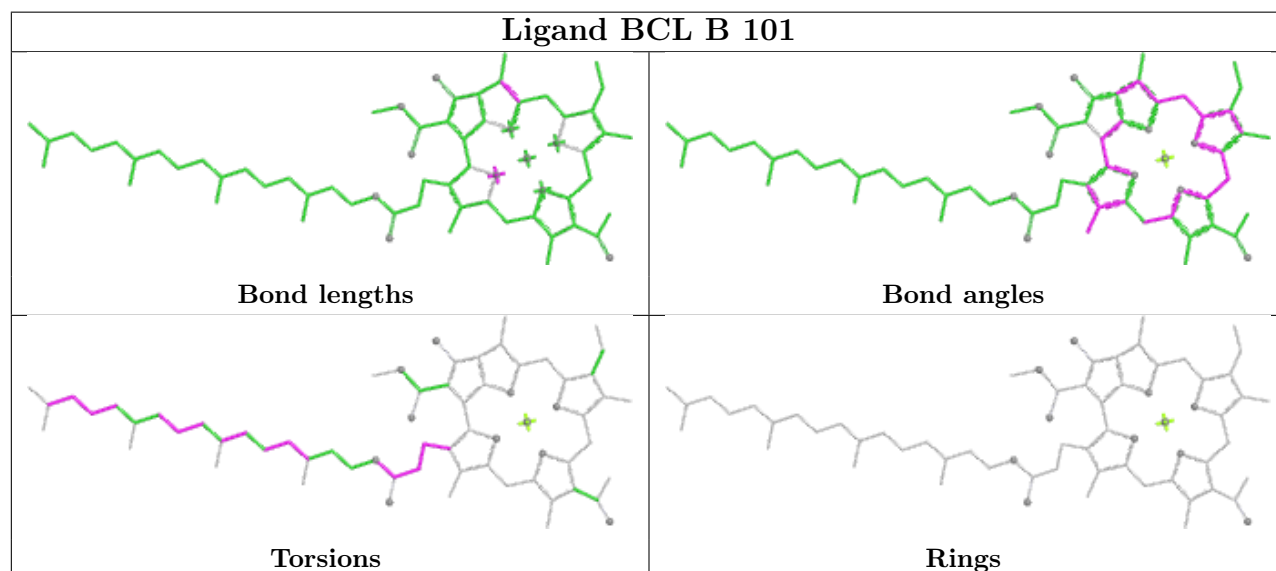
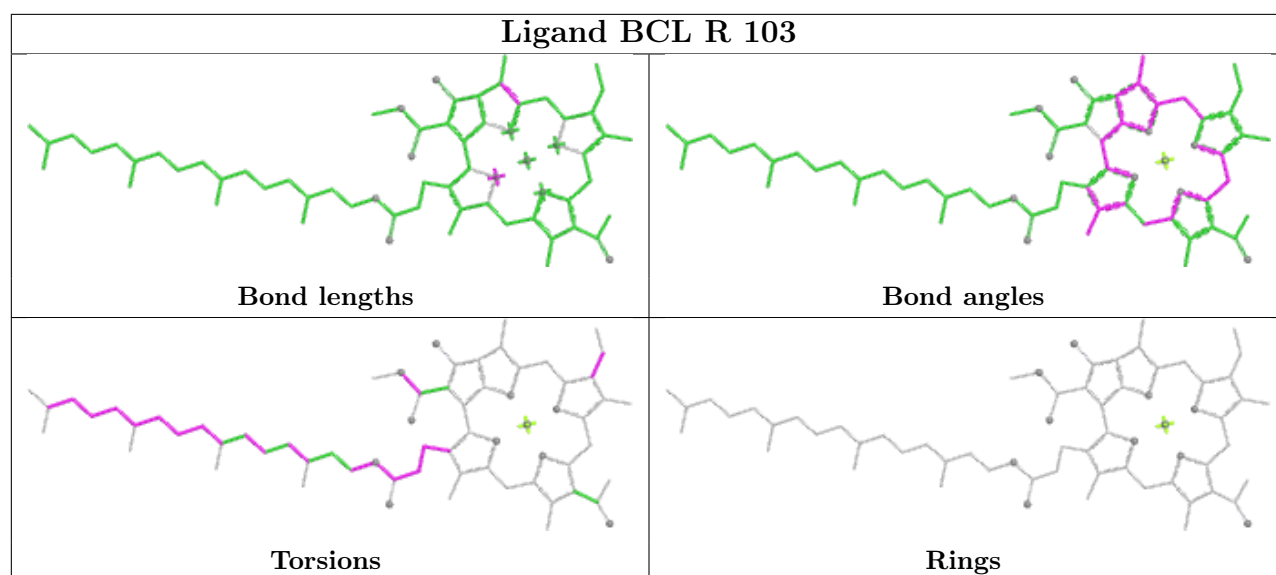
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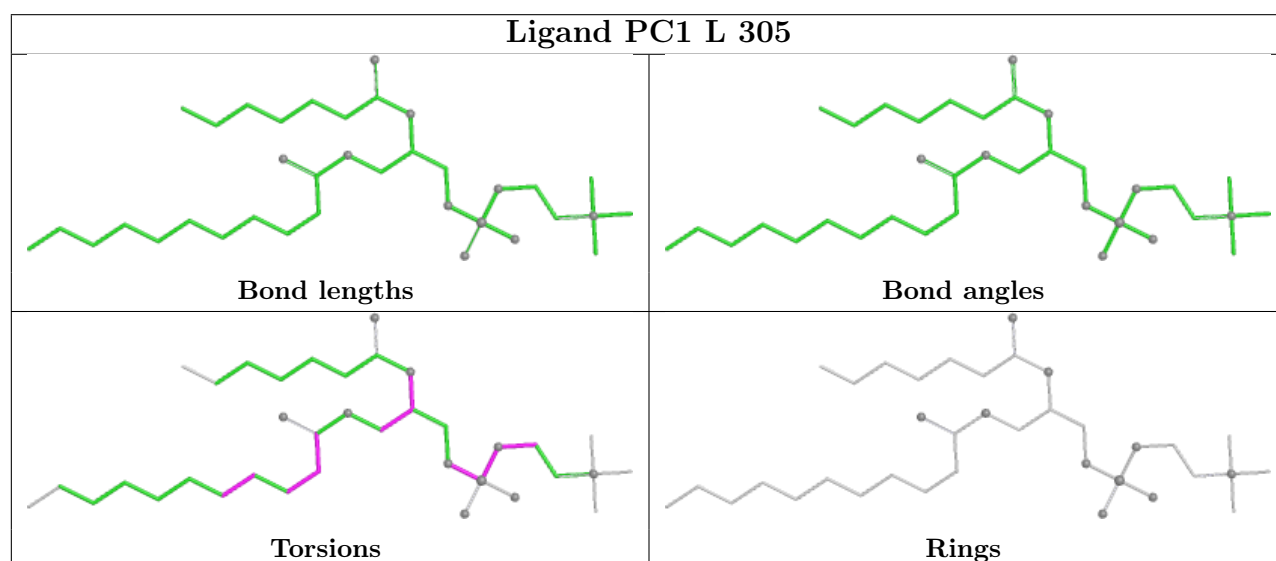
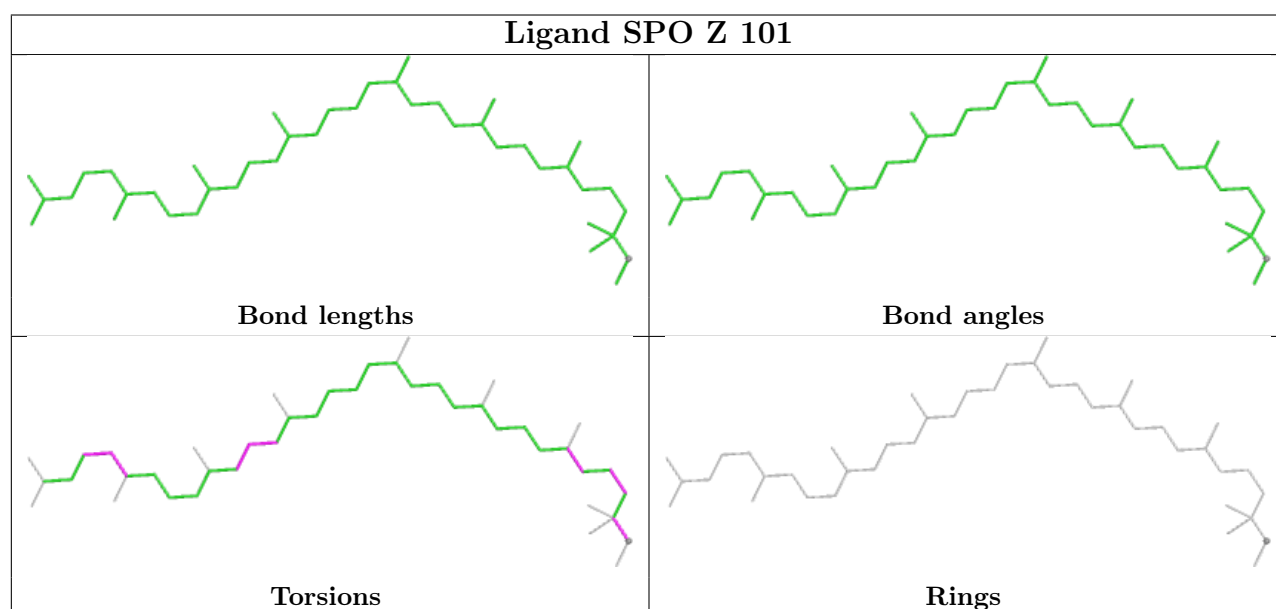
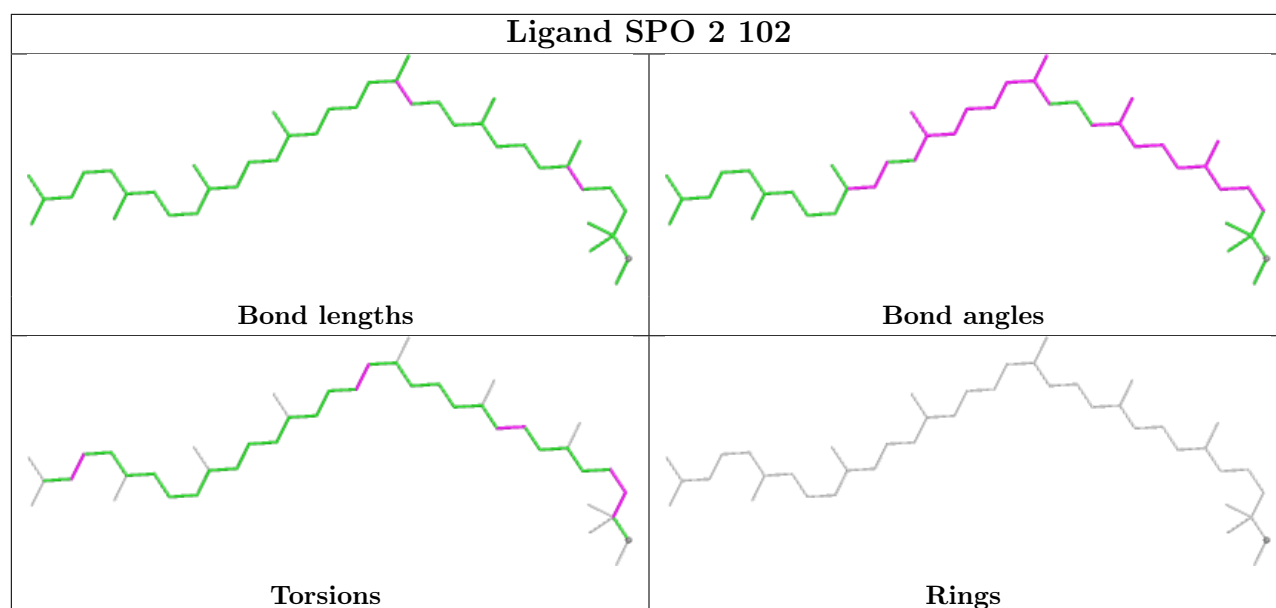
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | E     | 101 | BCL  | 14      | 0            |
| 7   | Q     | 101 | BCL  | 14      | 0            |
| 8   | E     | 102 | SPO  | 4       | 0            |
| 9   | W     | 103 | PC1  | 2       | 0            |
| 8   | T     | 102 | SPO  | 4       | 0            |
| 7   | L     | 302 | BCL  | 5       | 0            |
| 8   | K     | 102 | SPO  | 5       | 0            |
| 8   | U     | 102 | SPO  | 4       | 0            |
| 8   | U     | 103 | SPO  | 8       | 0            |

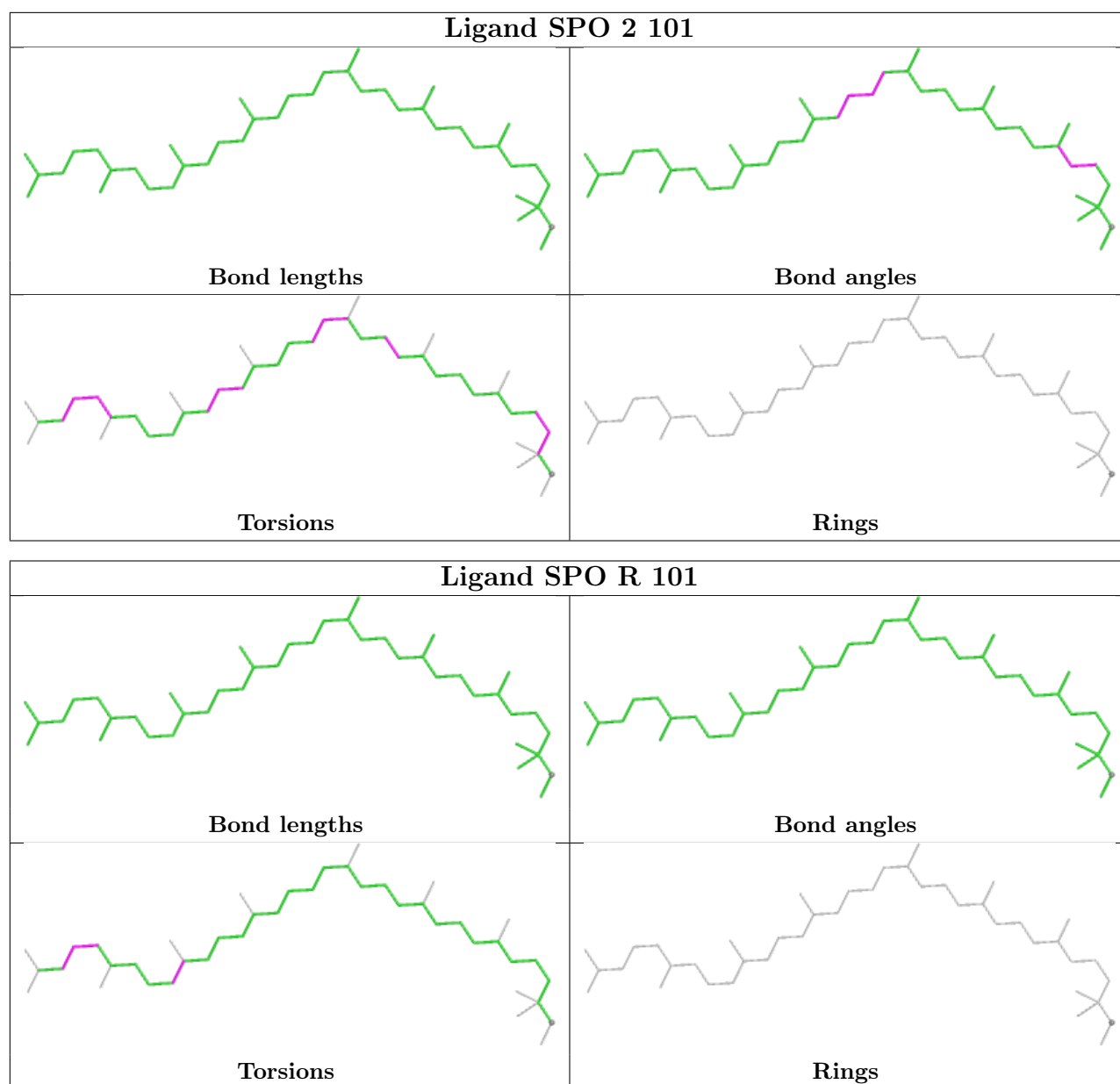
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

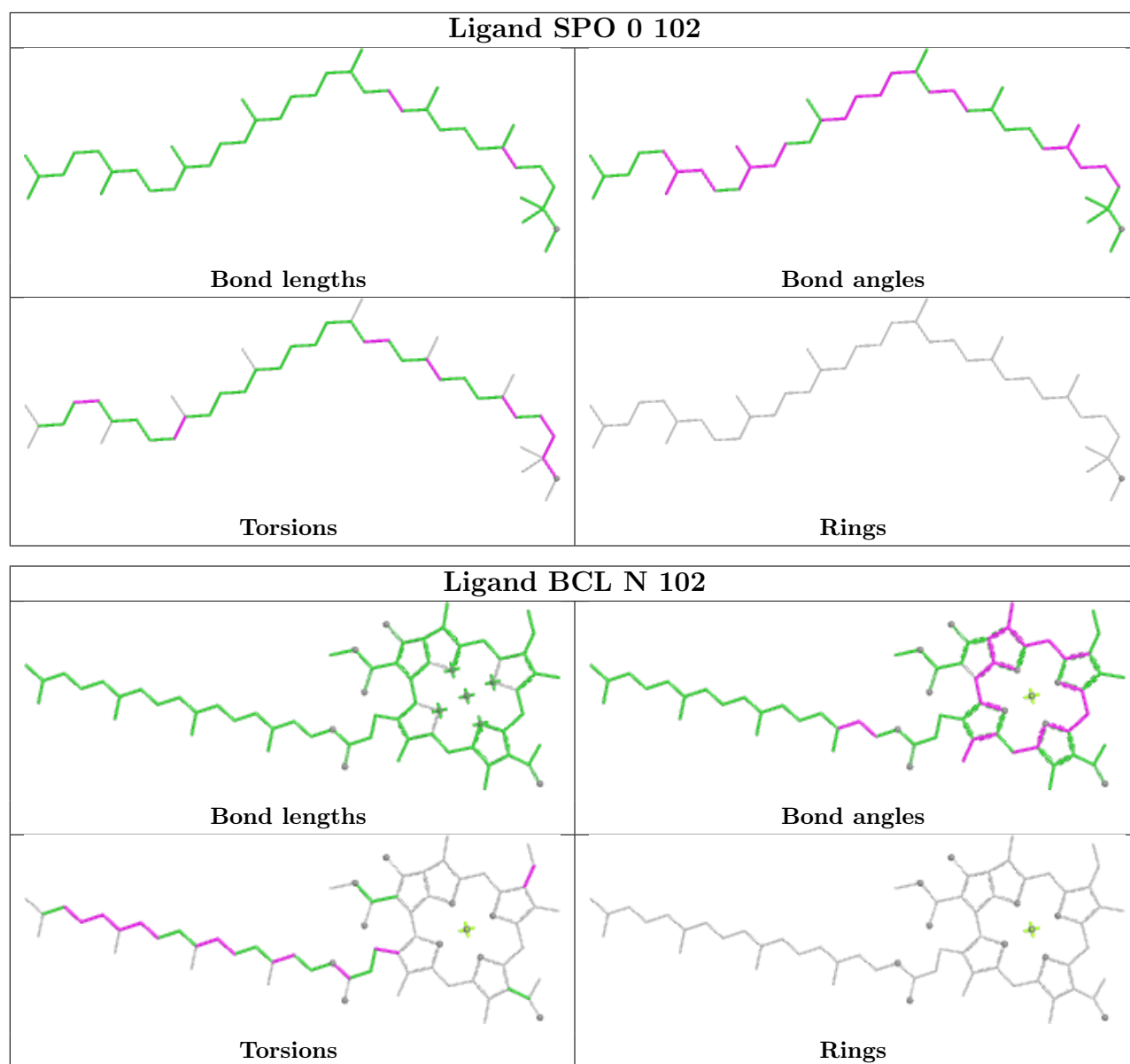


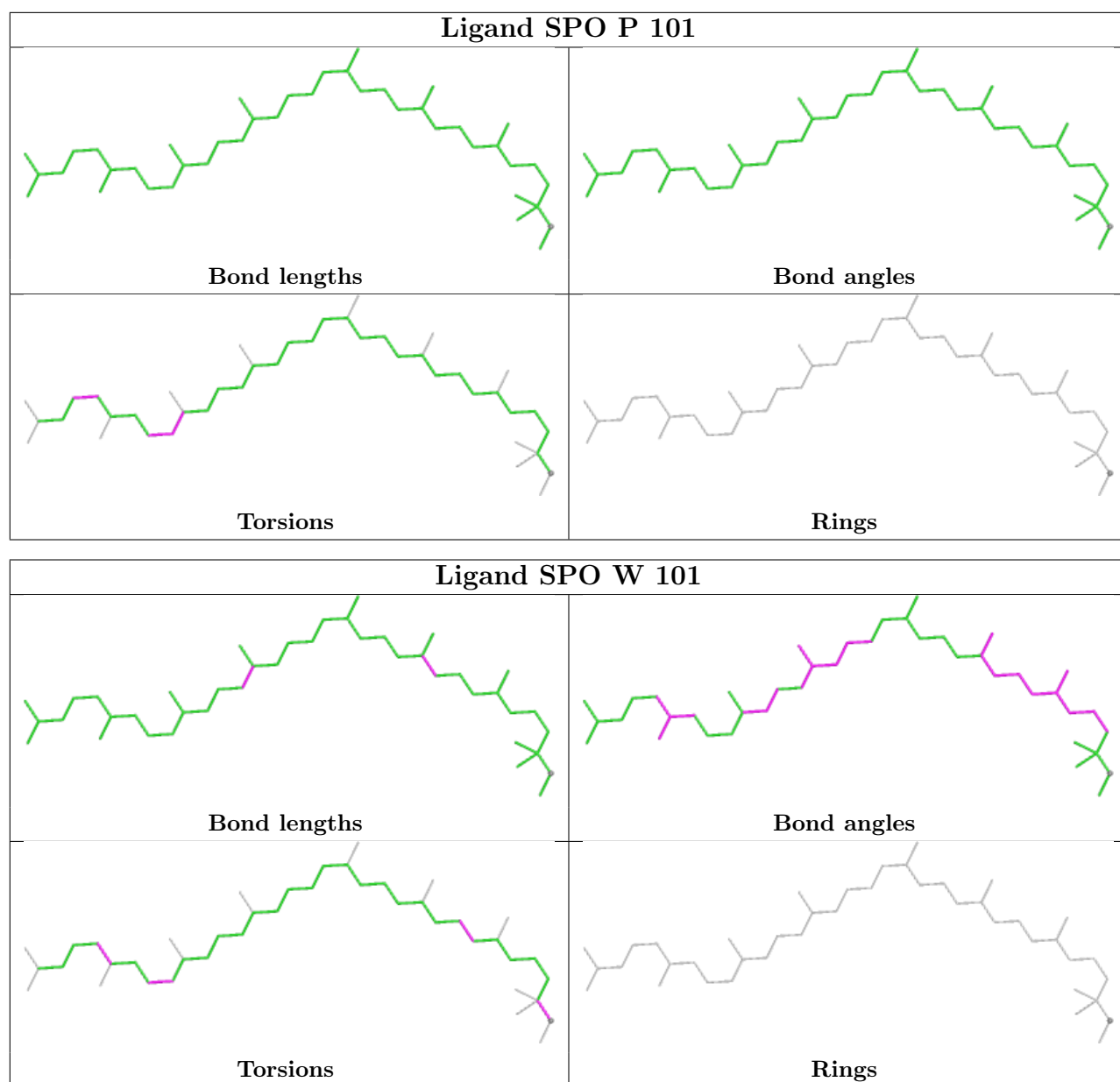


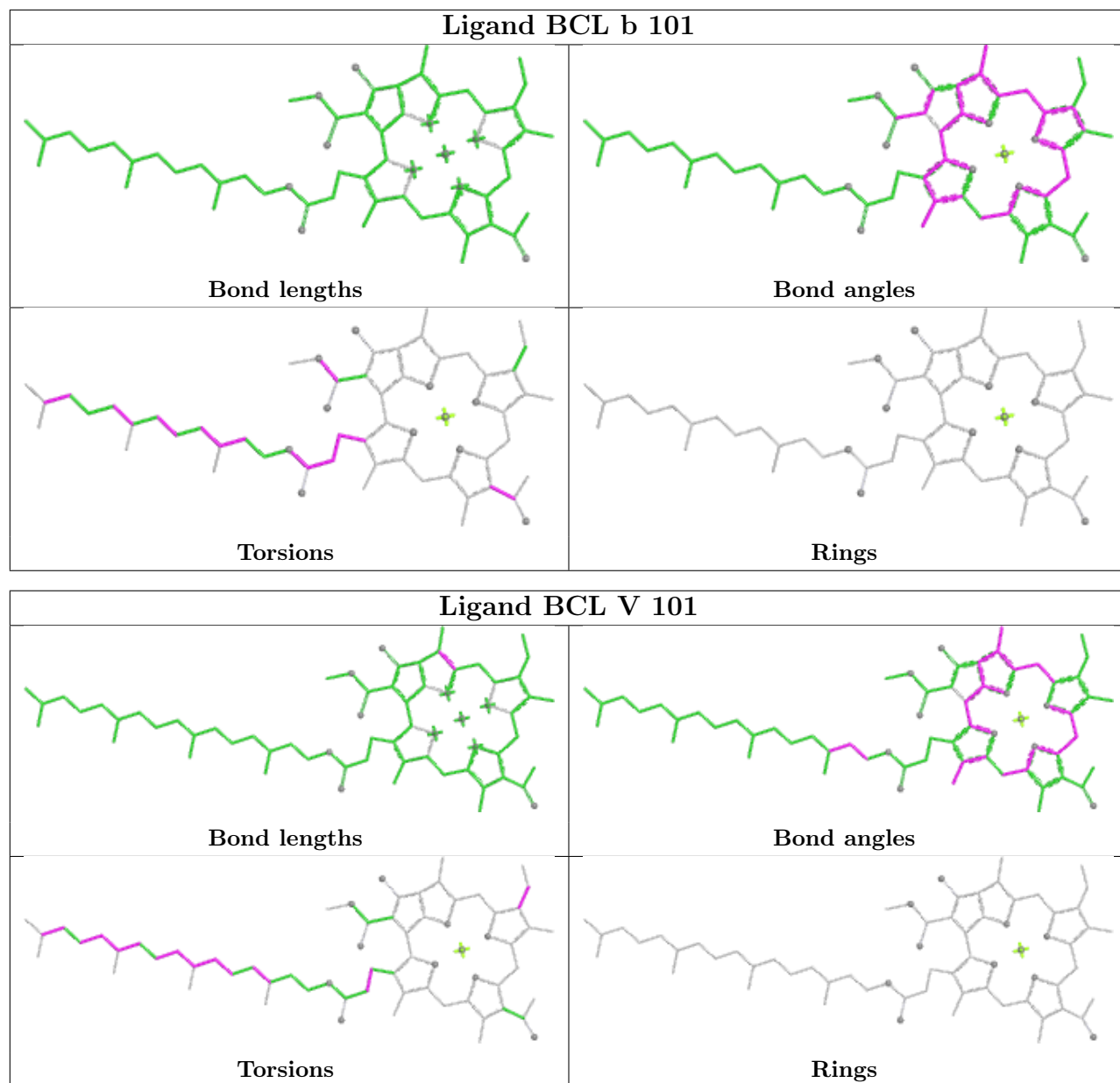


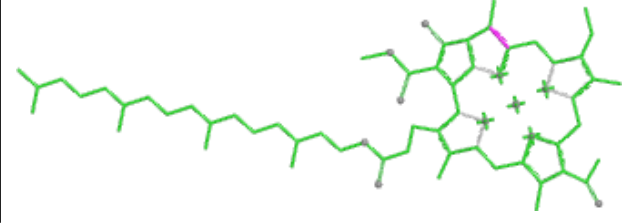
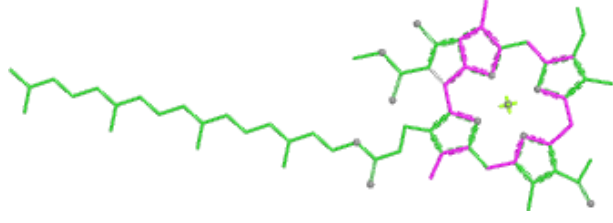
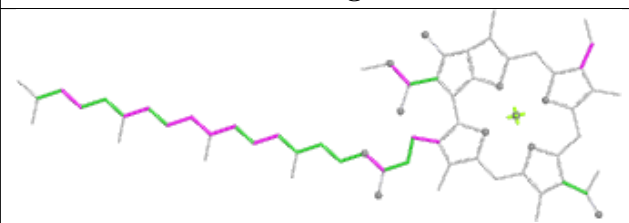
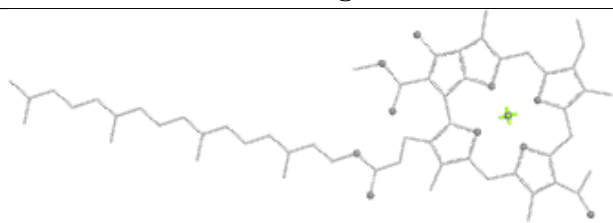
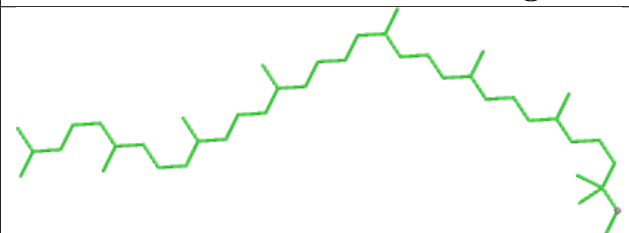
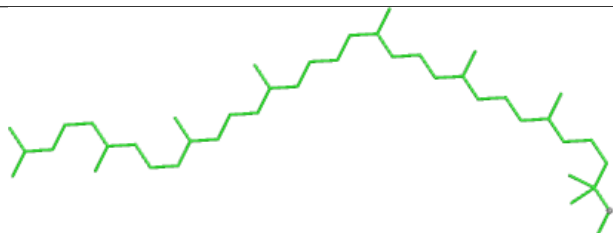
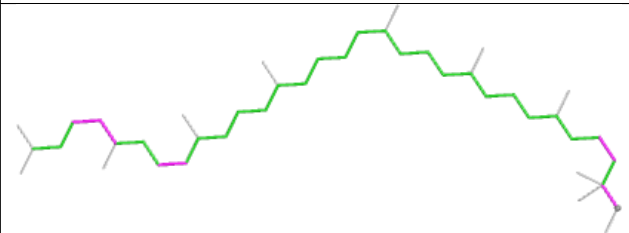
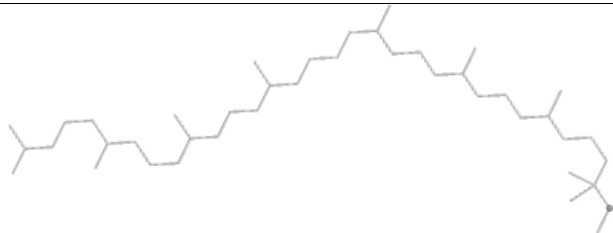
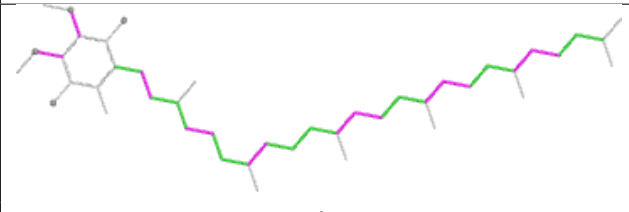
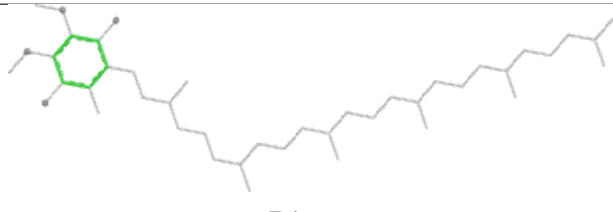


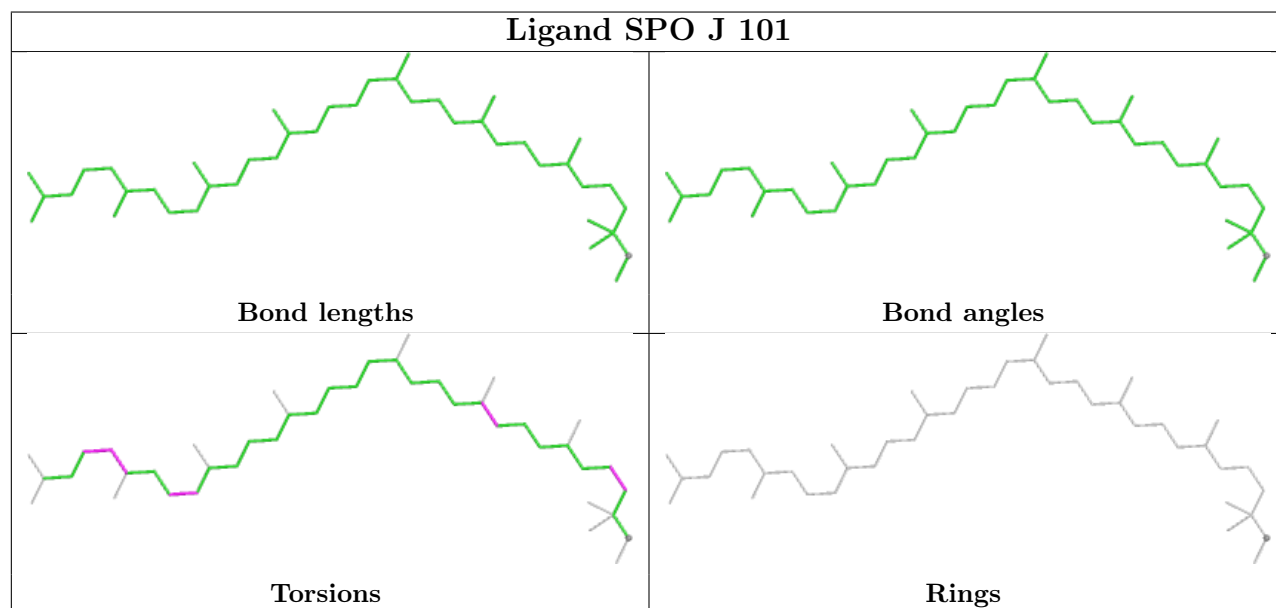
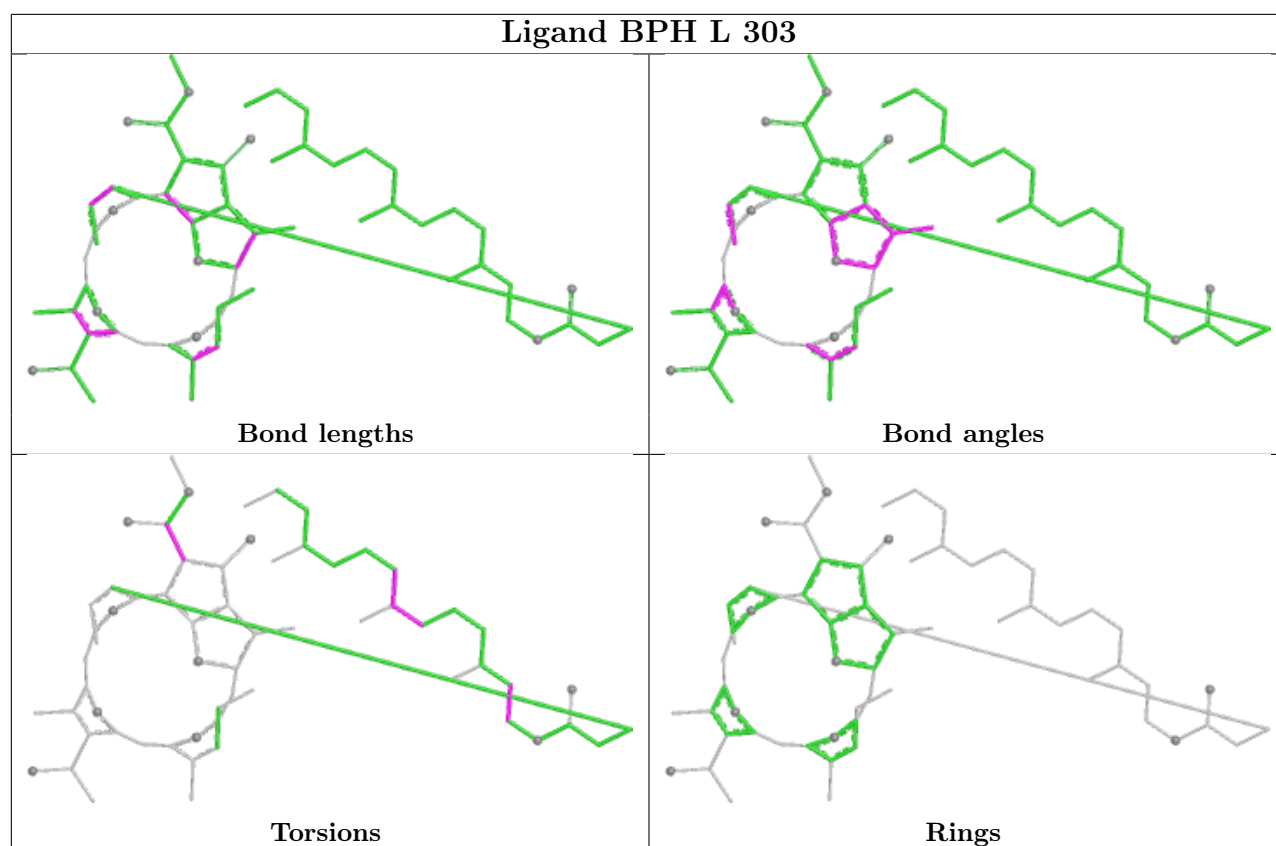


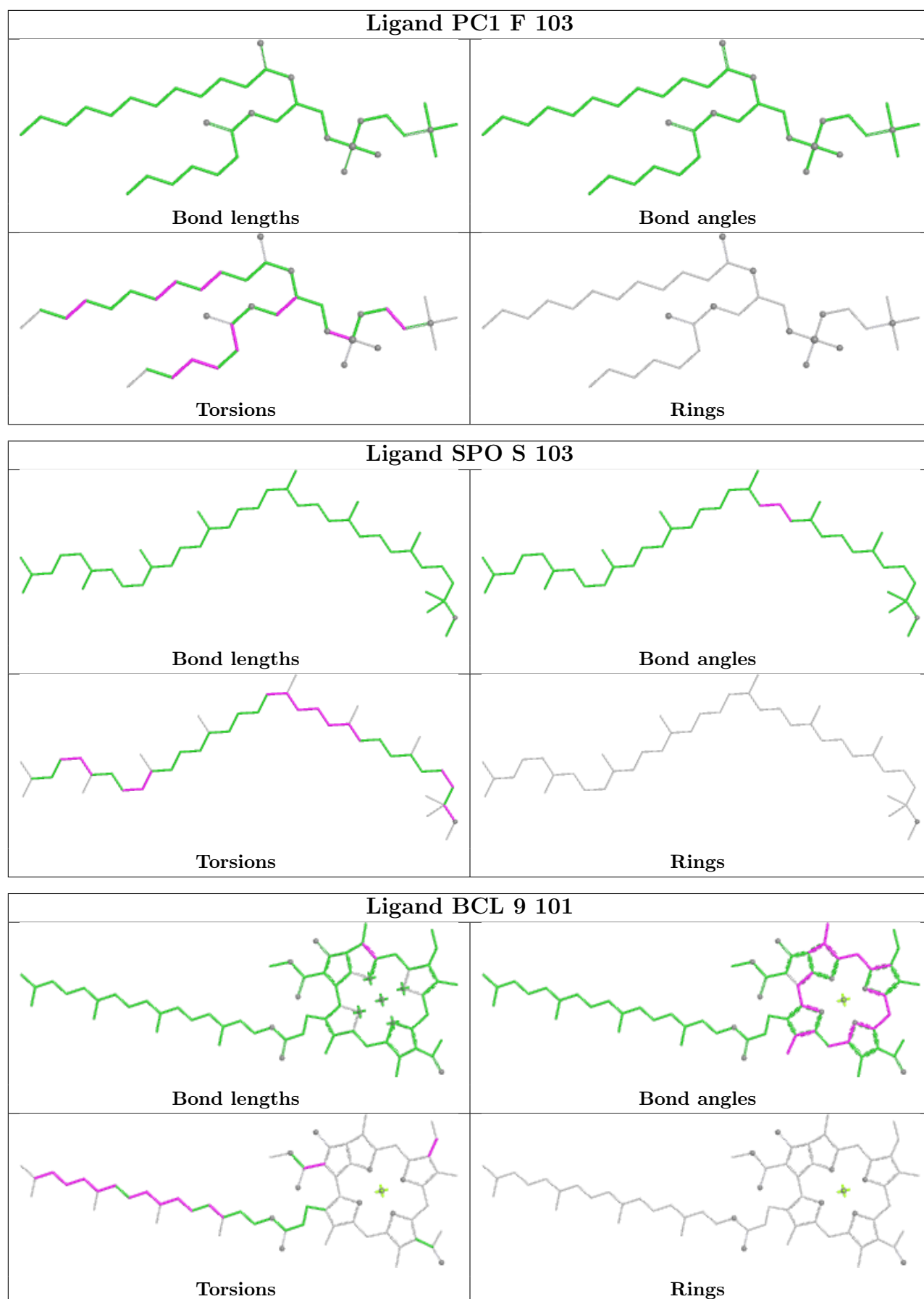


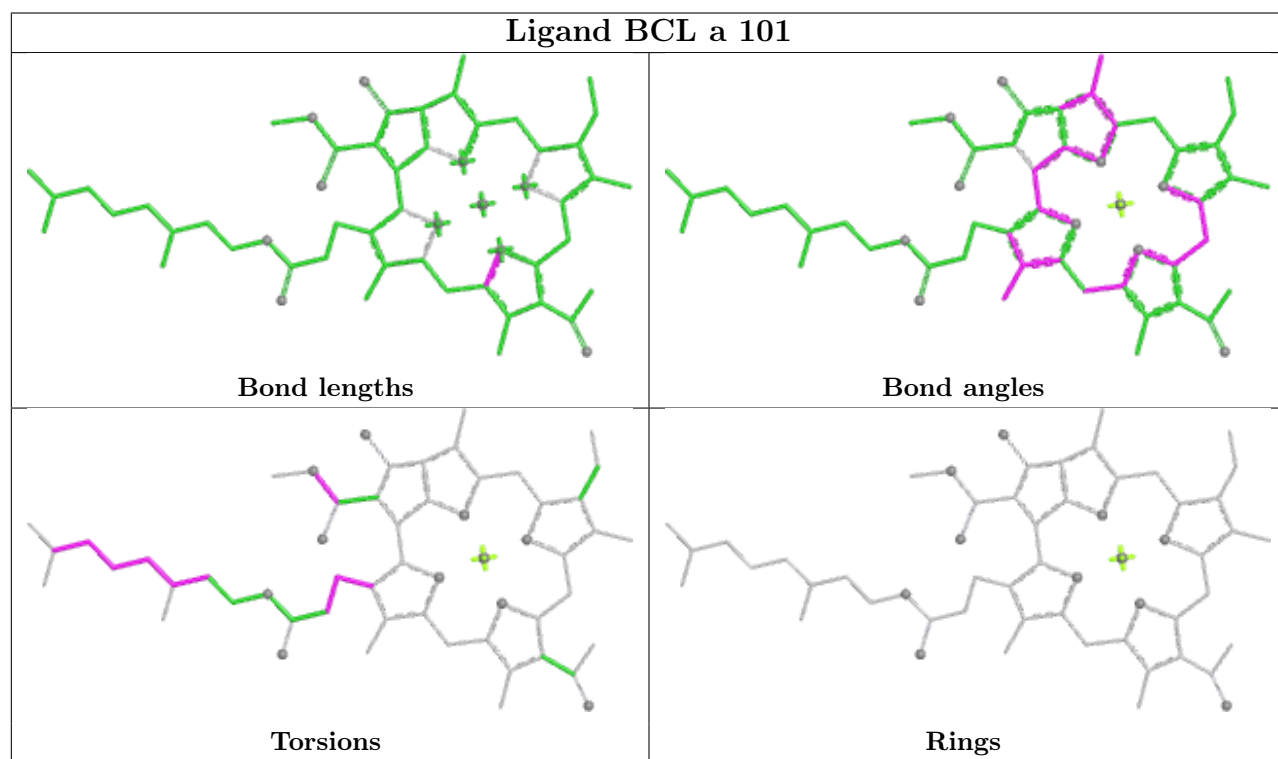
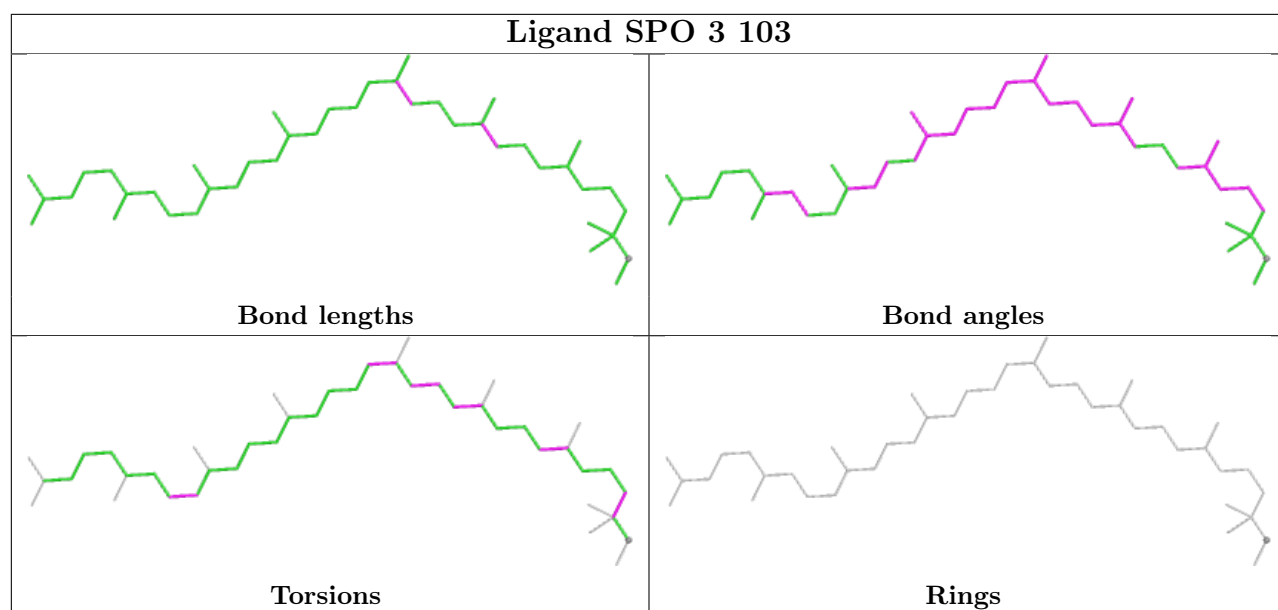


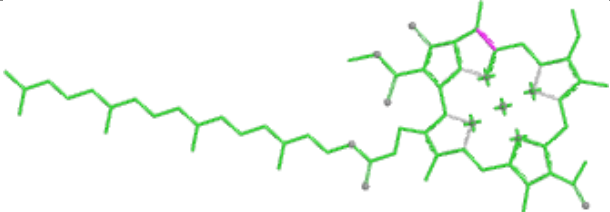
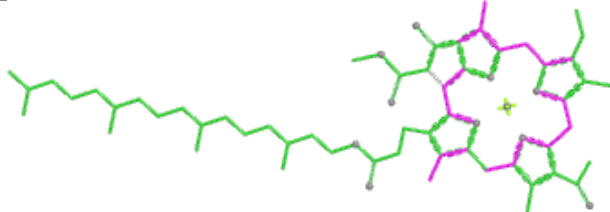
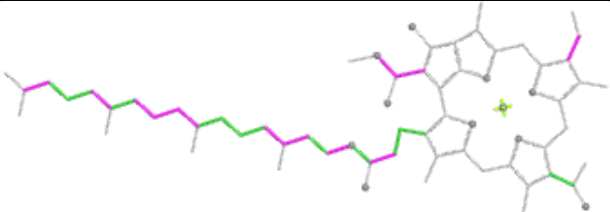
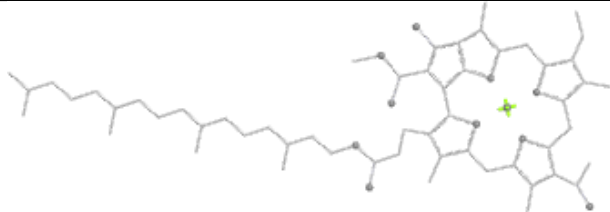
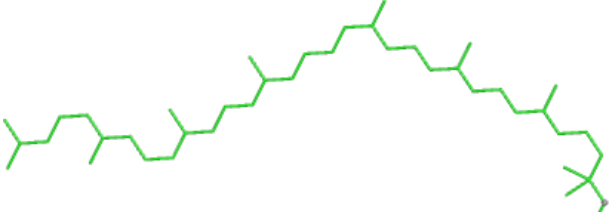
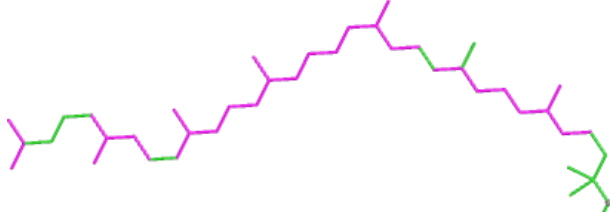
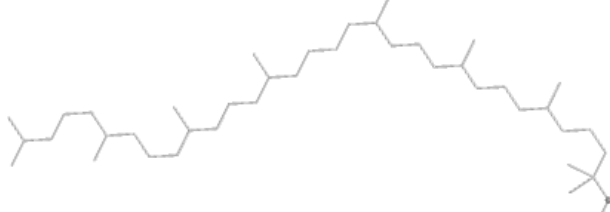


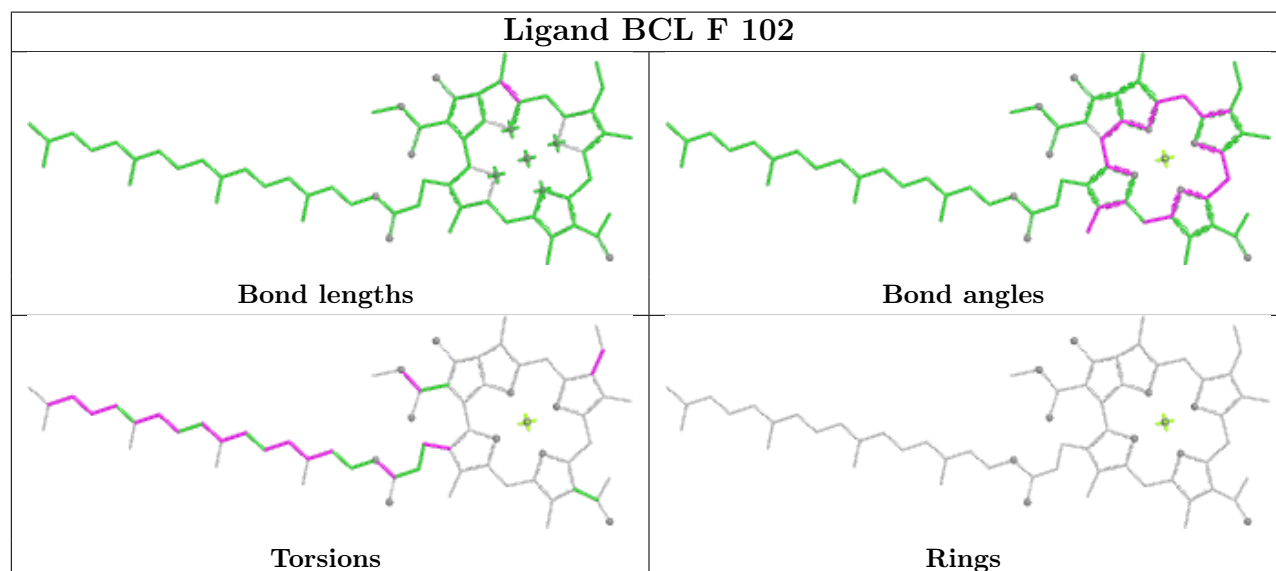
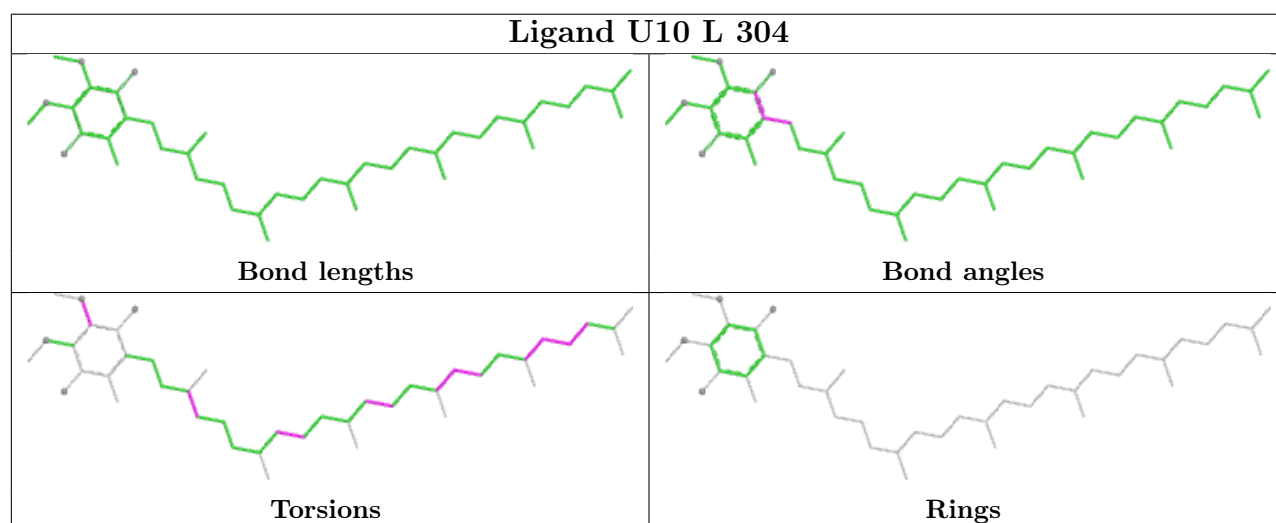
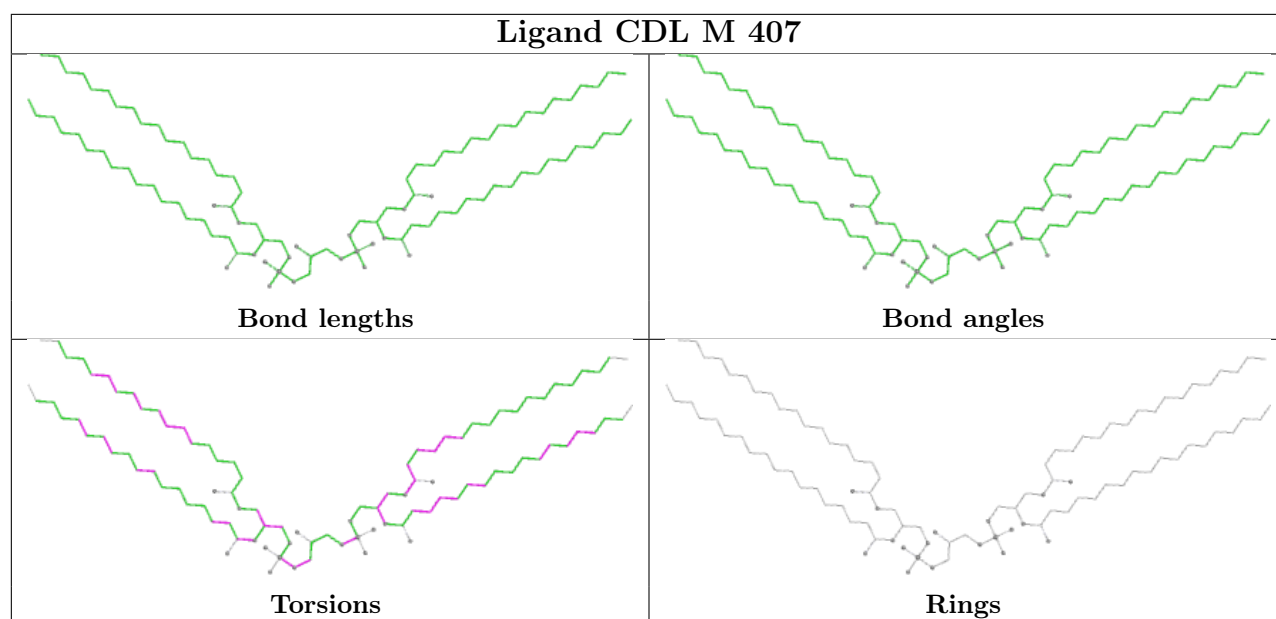
| Ligand BCL D 102                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand SPO A 102                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>  |  <p>Bond angles</p>  |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand U10 L 306                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

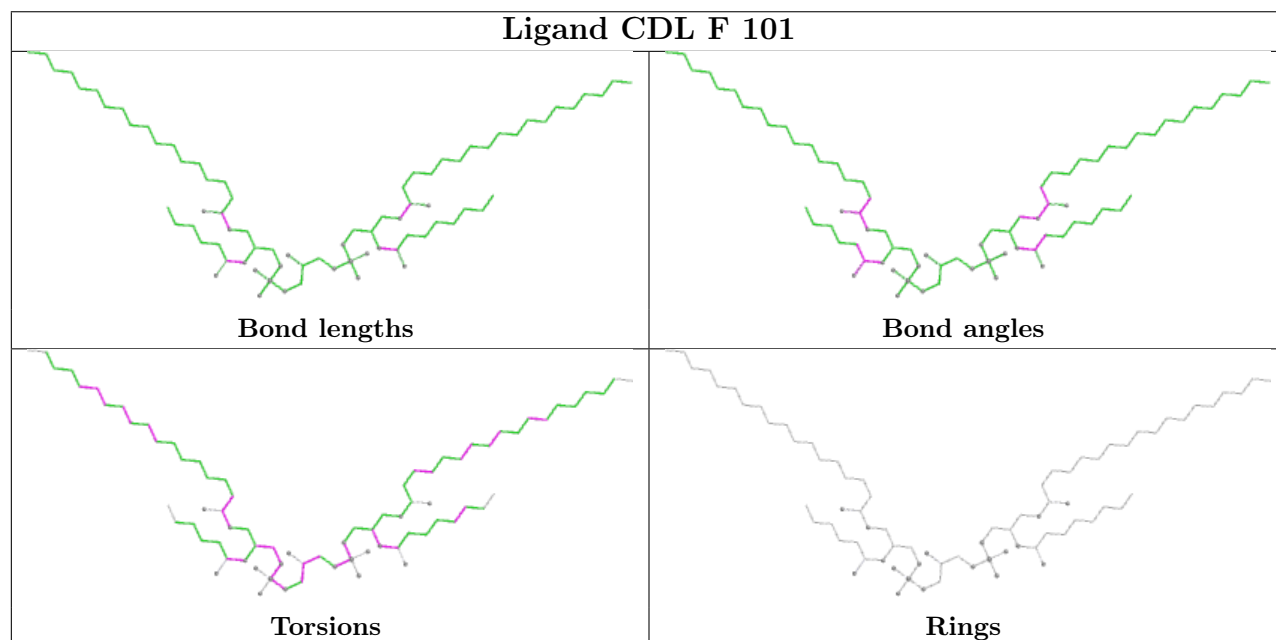
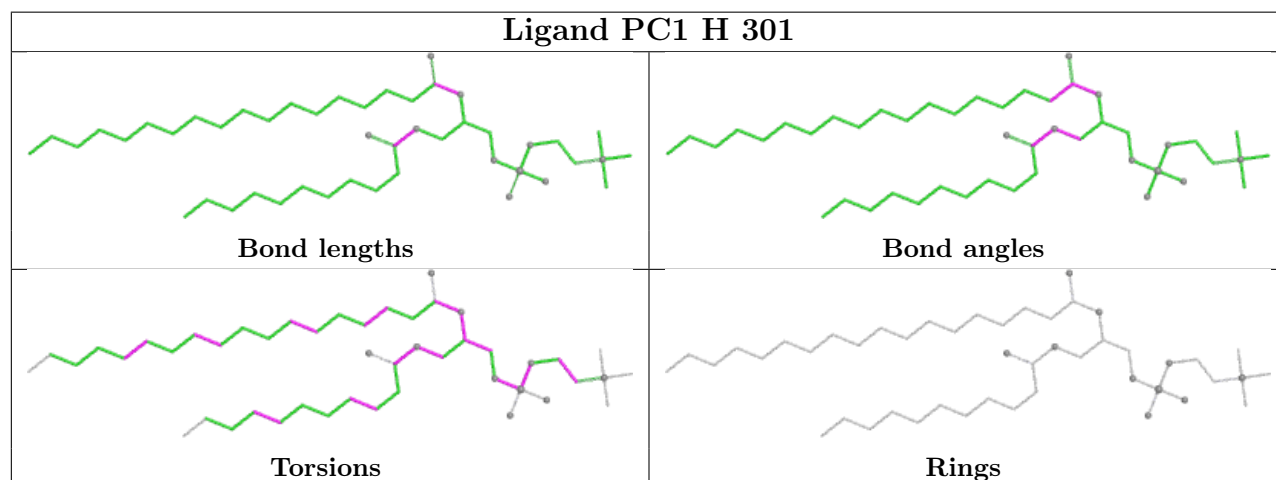
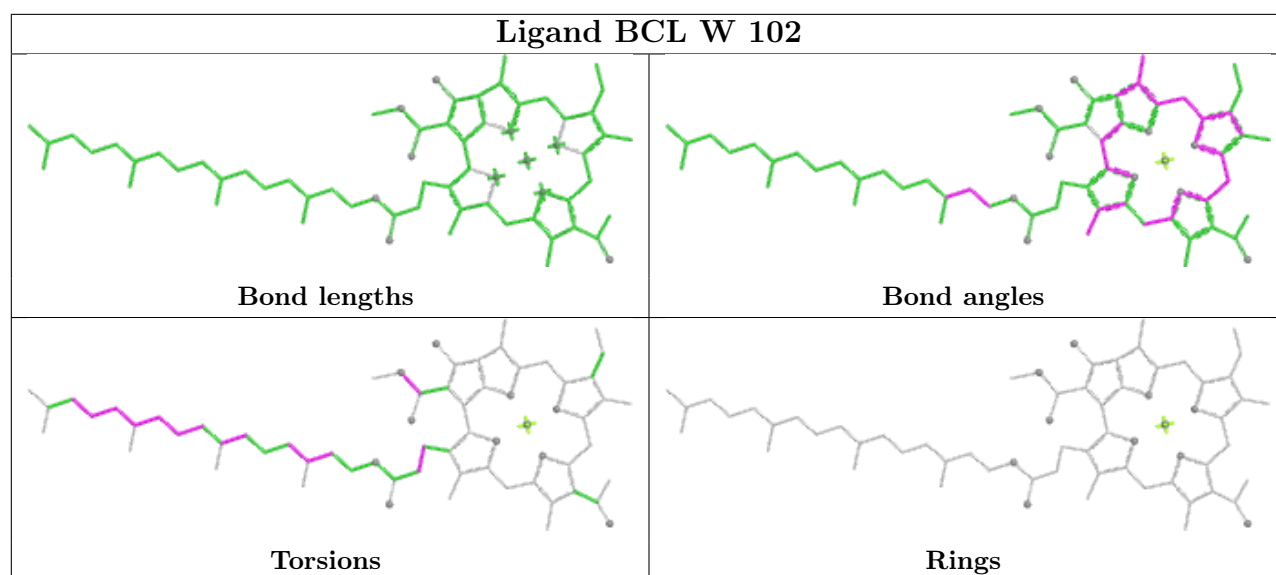


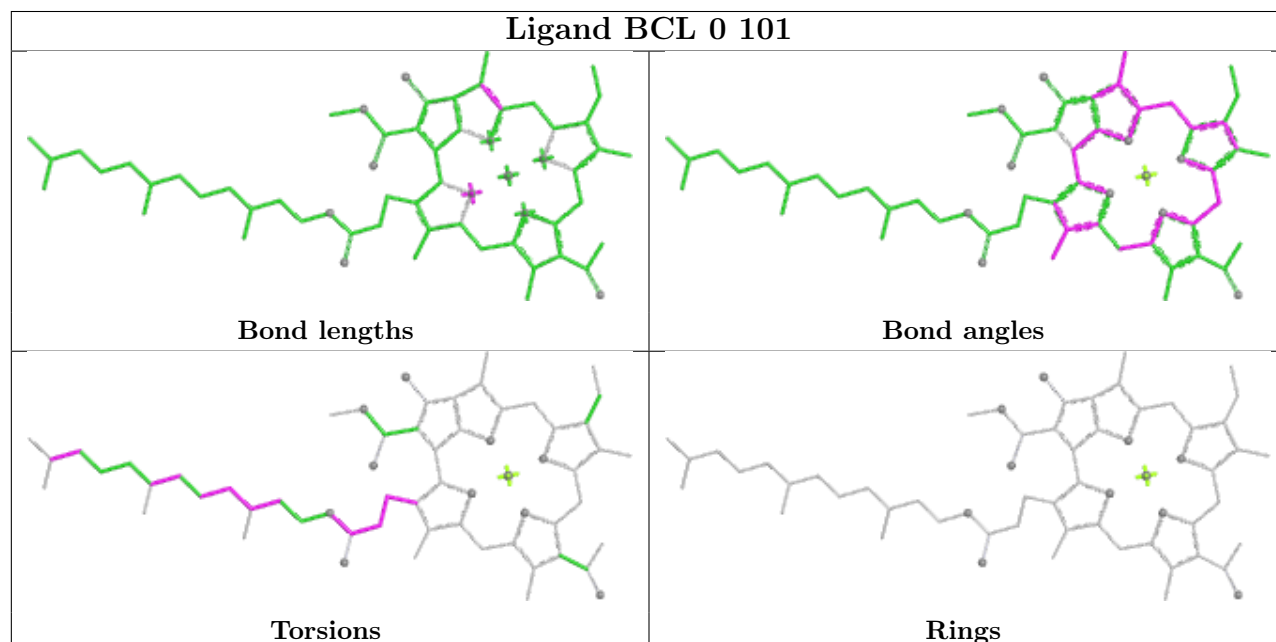
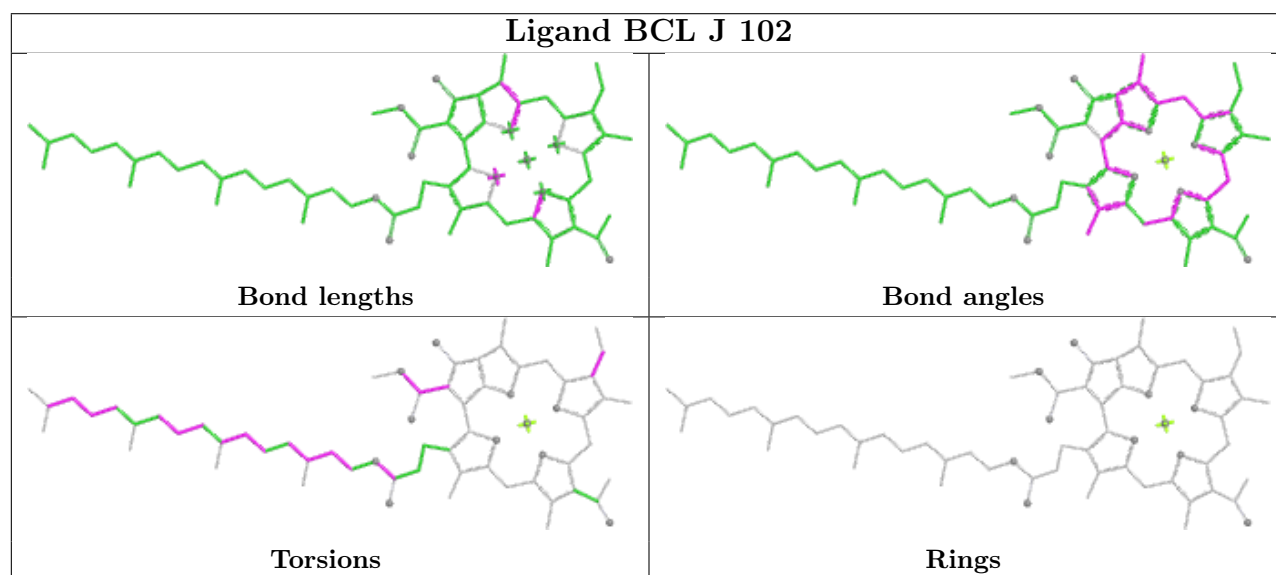
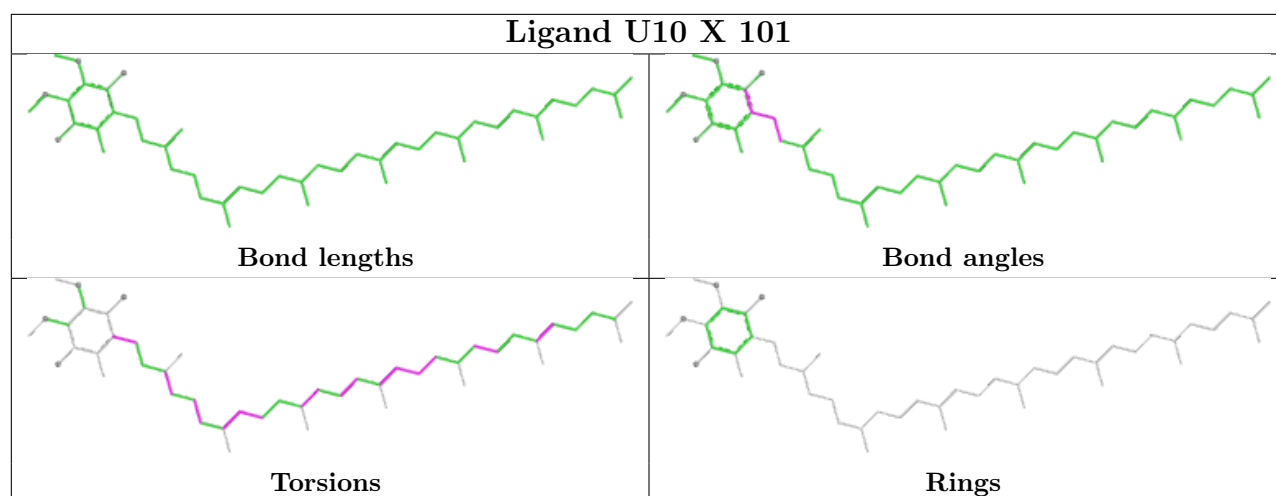


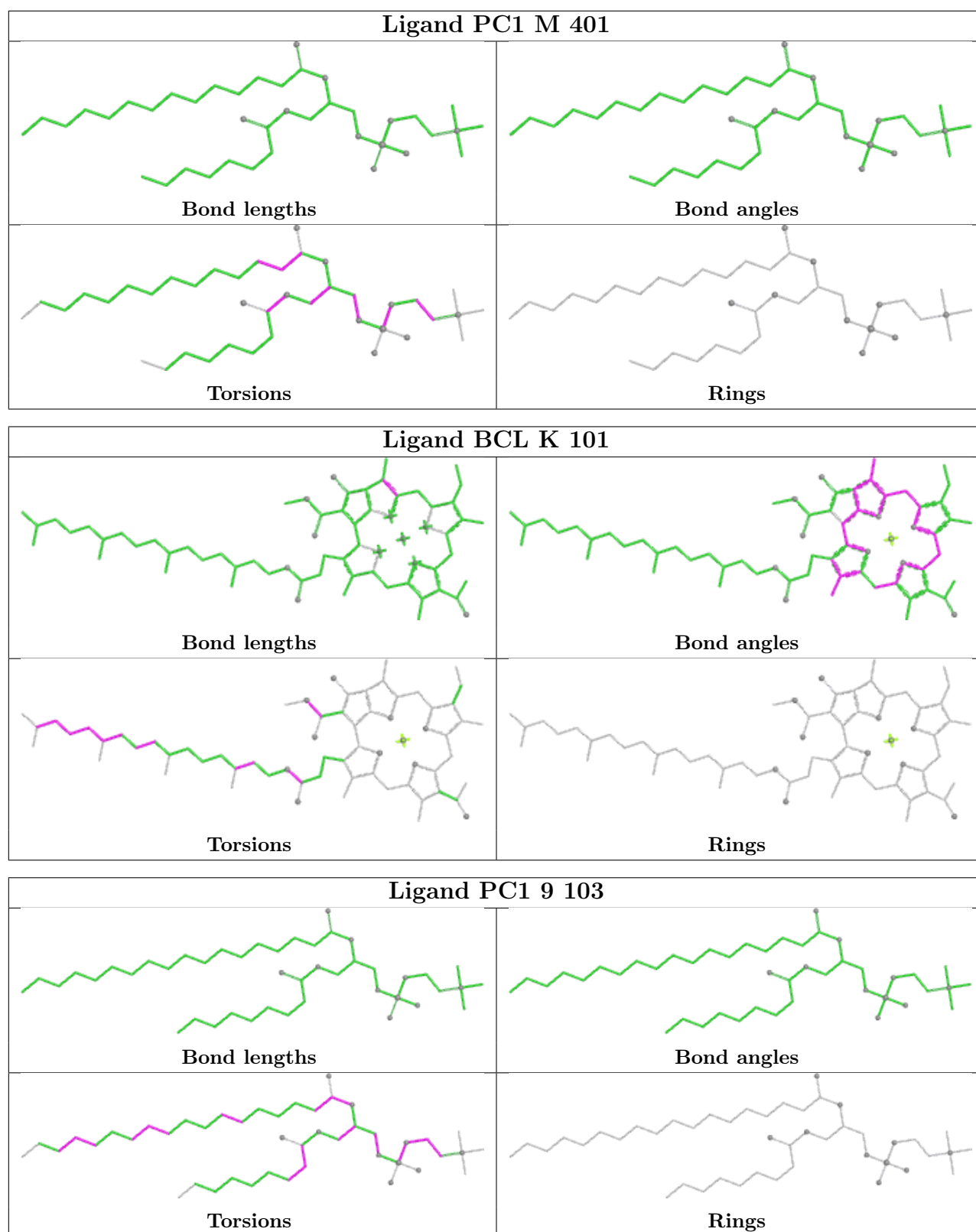


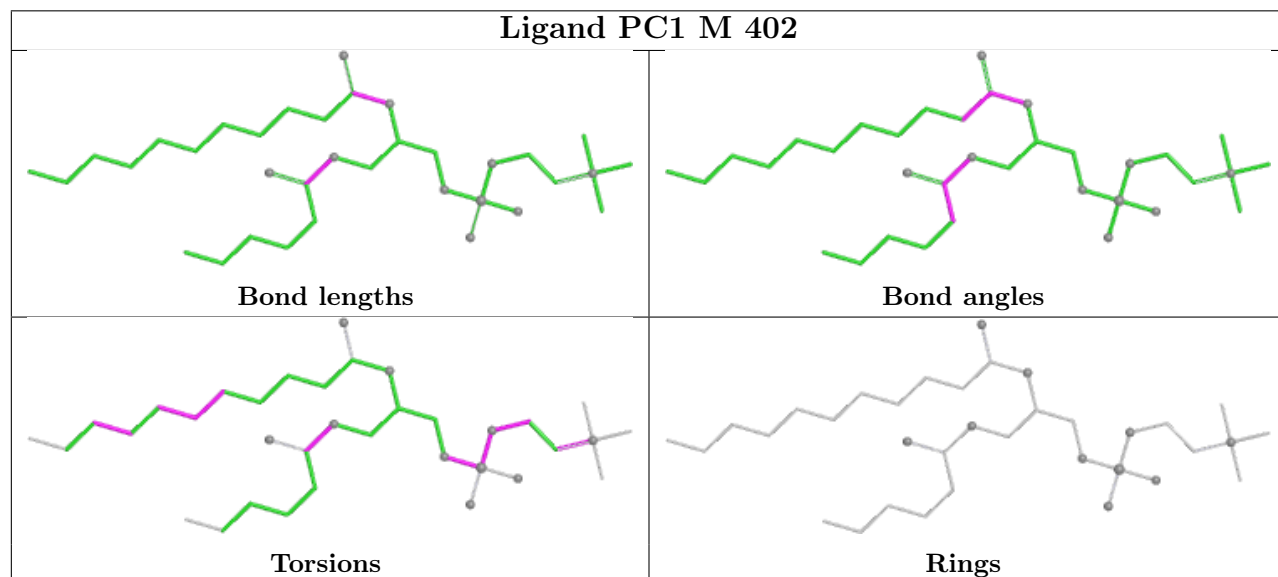
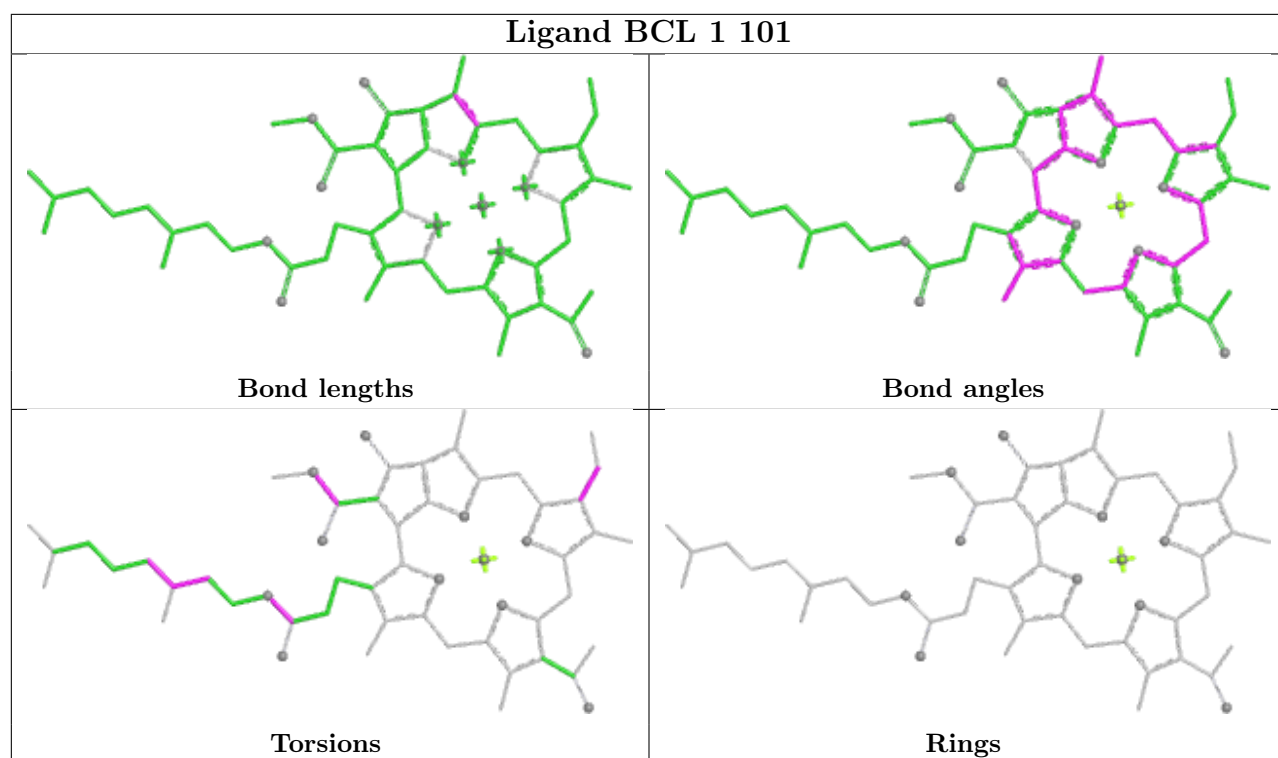
| Ligand BCL M 403                                                                                      |                                                                                                       |
|-------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand SPO 0 103                                                                                      |                                                                                                       |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>   |  <p>Rings</p>     |

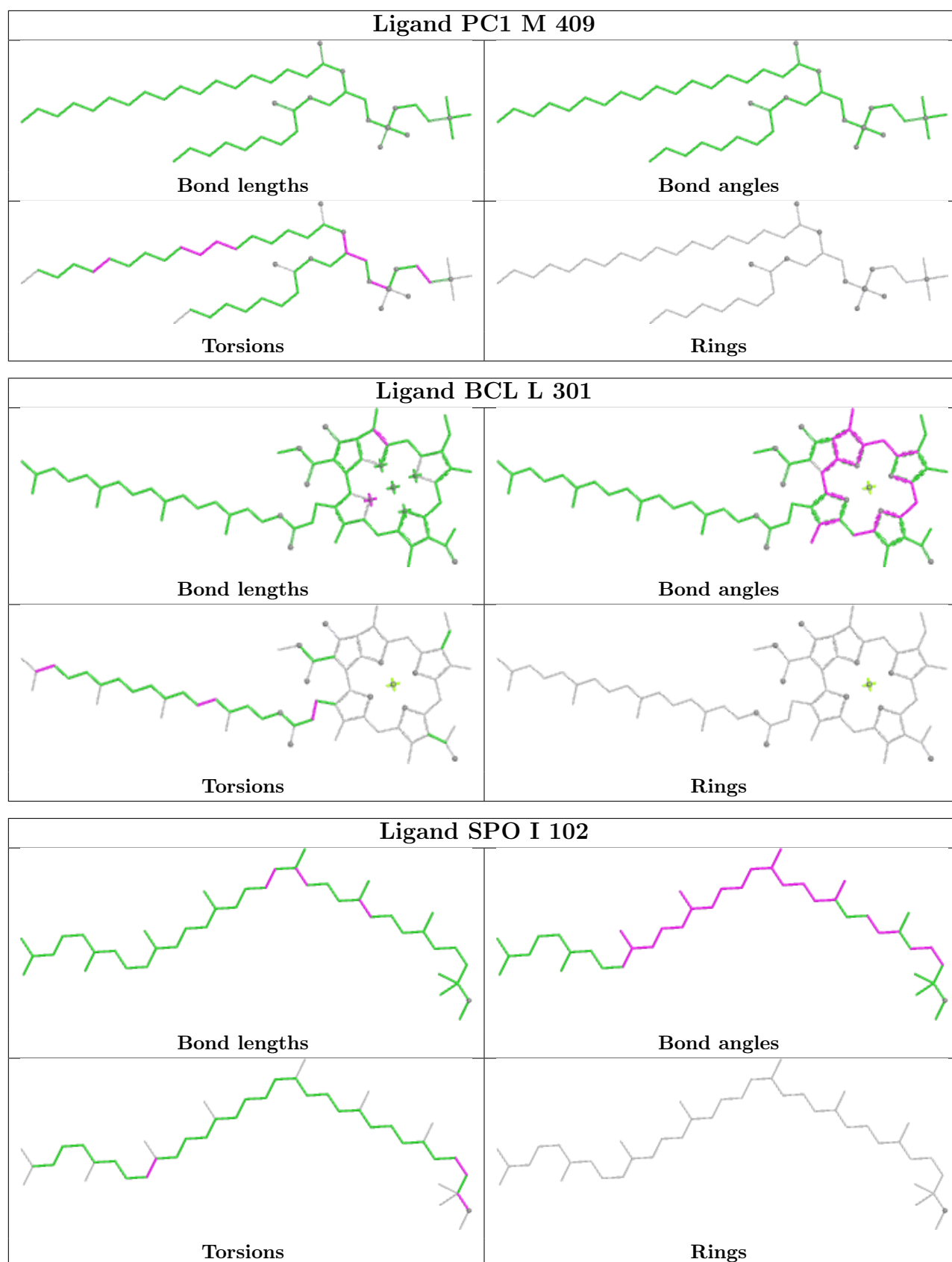


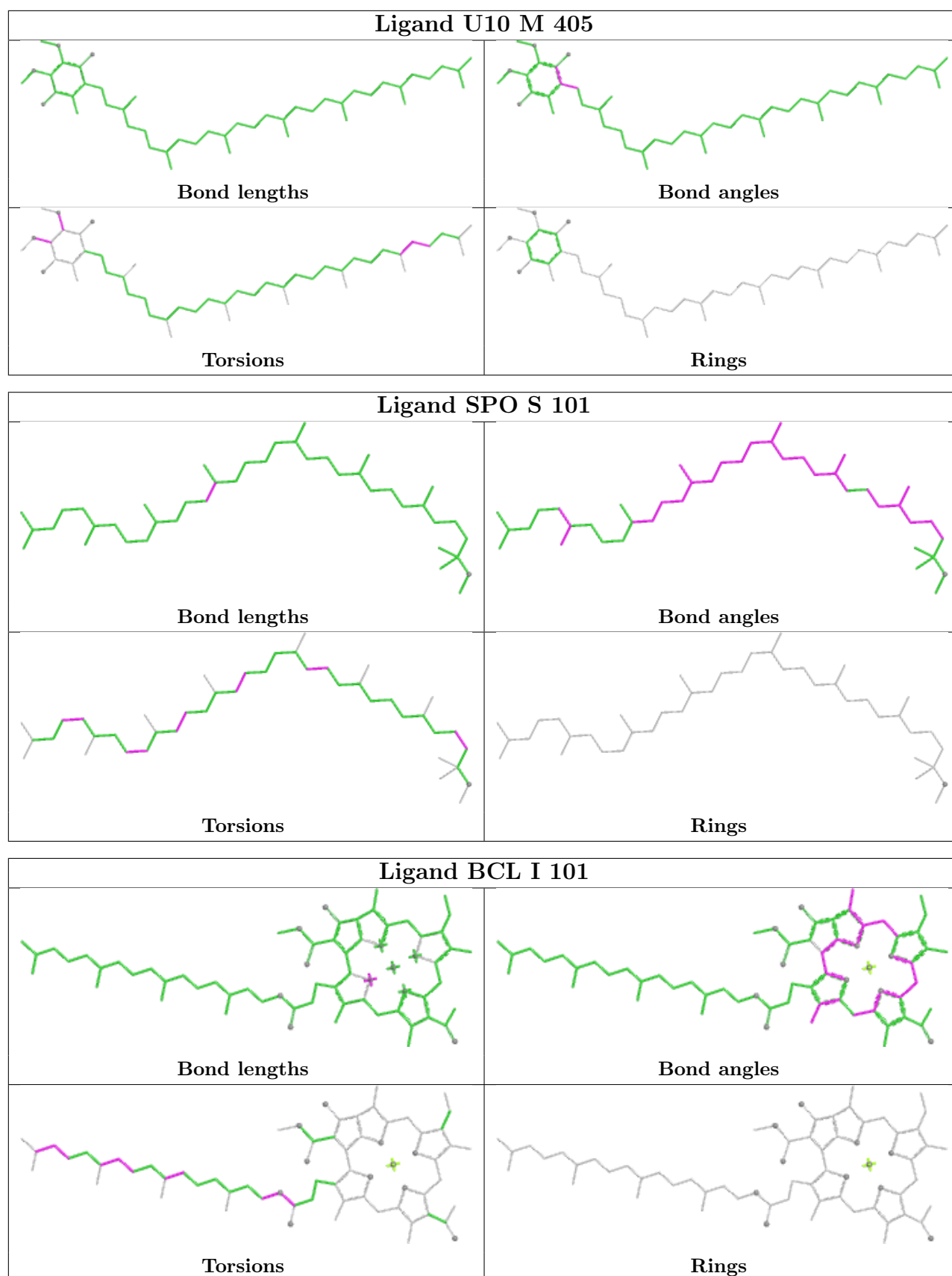


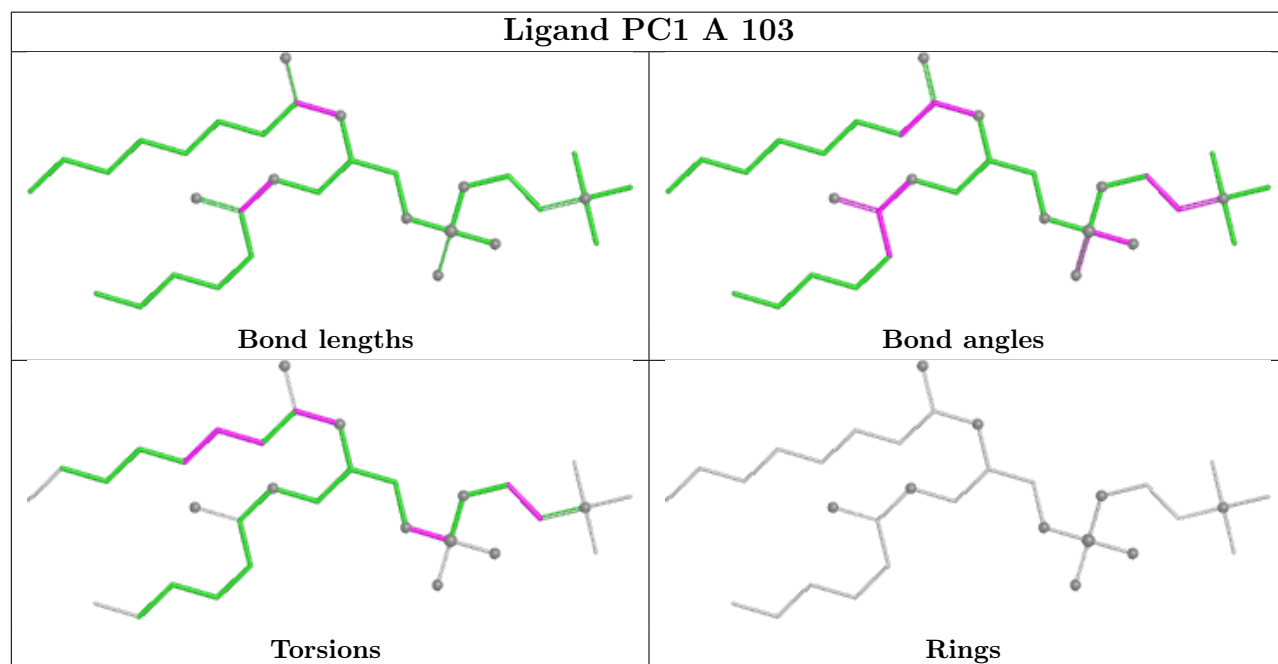
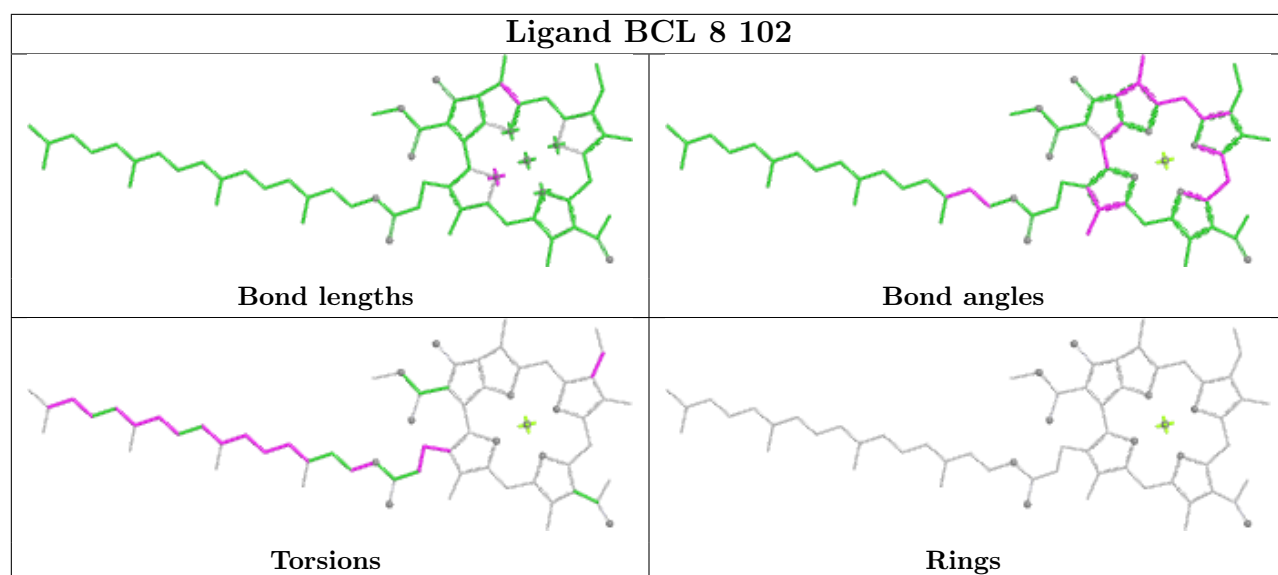


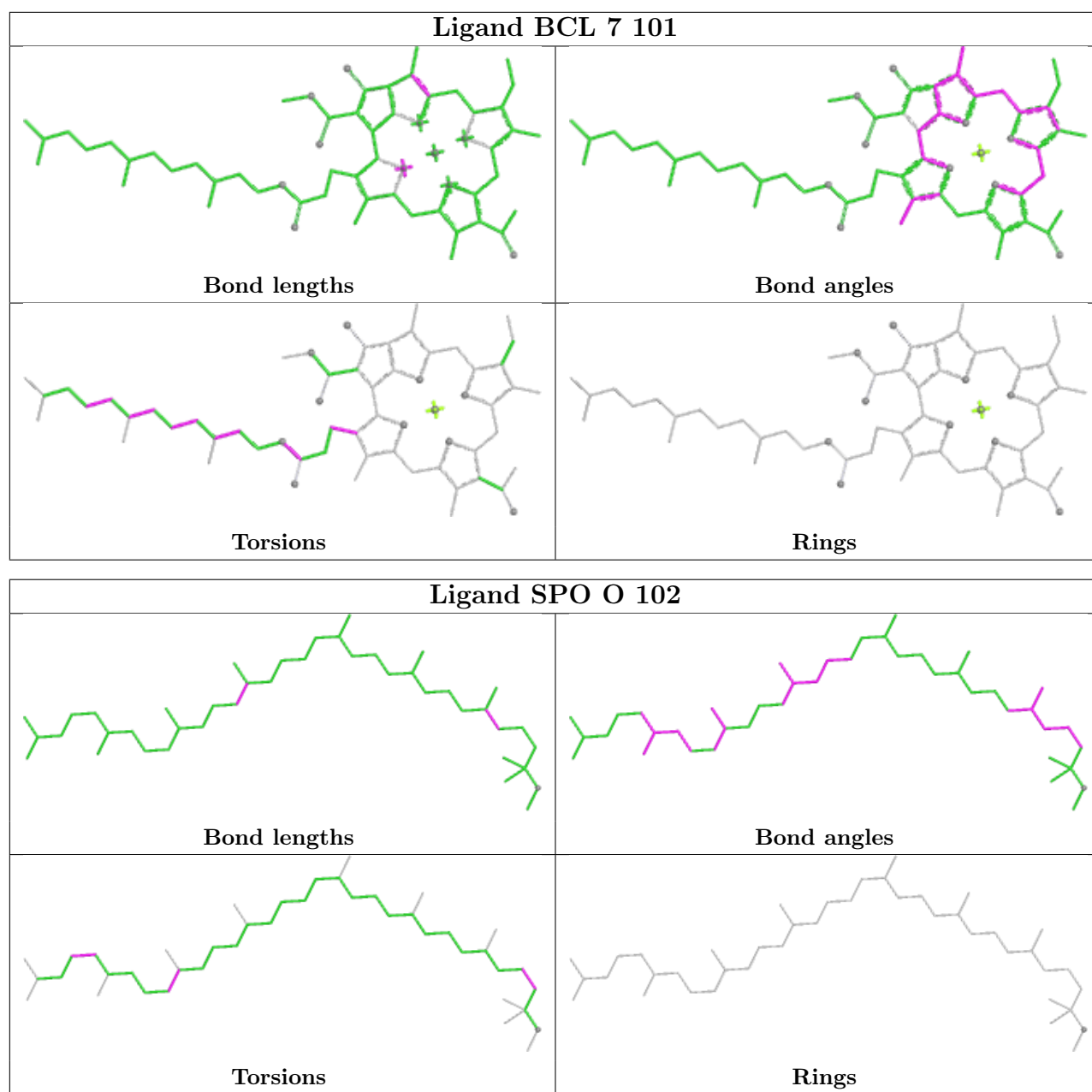


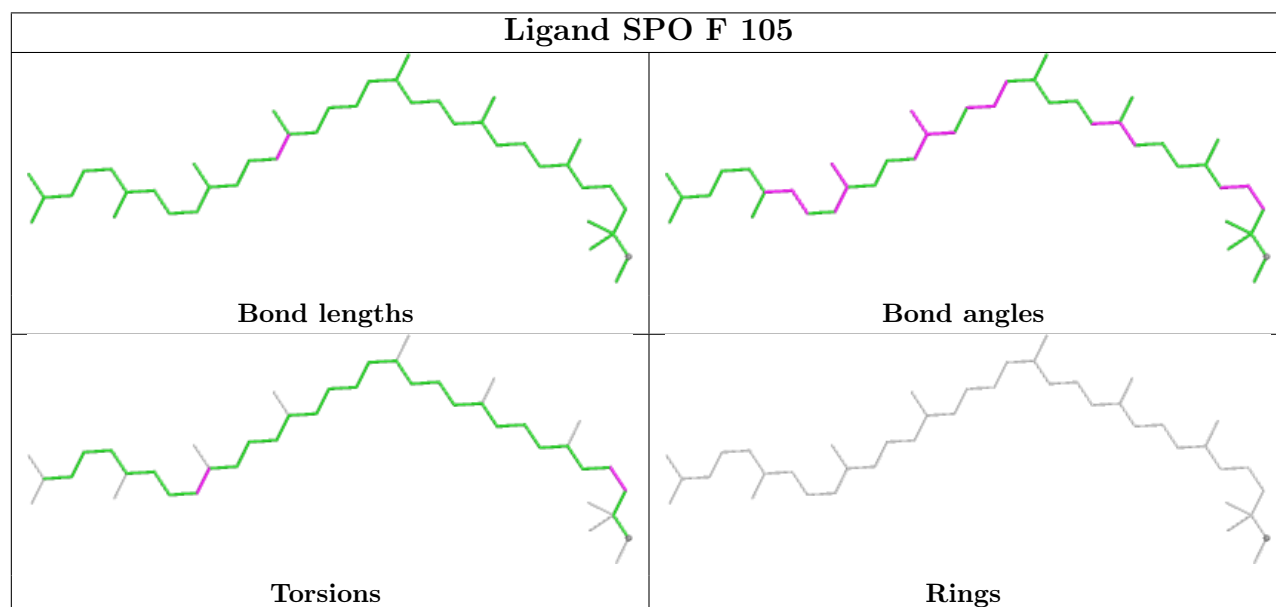
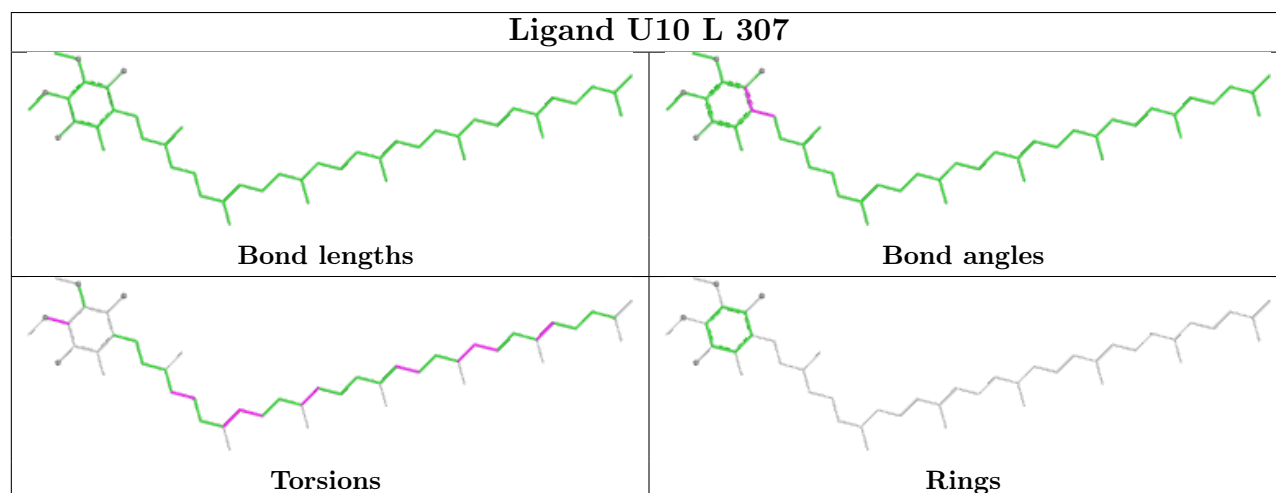
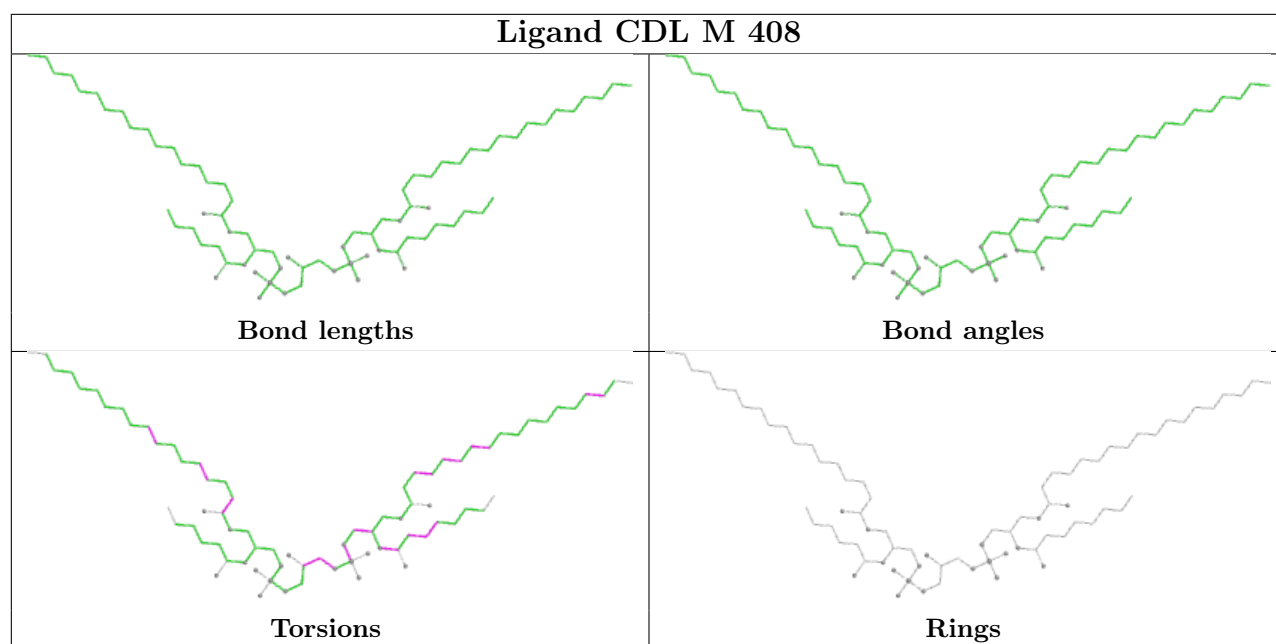


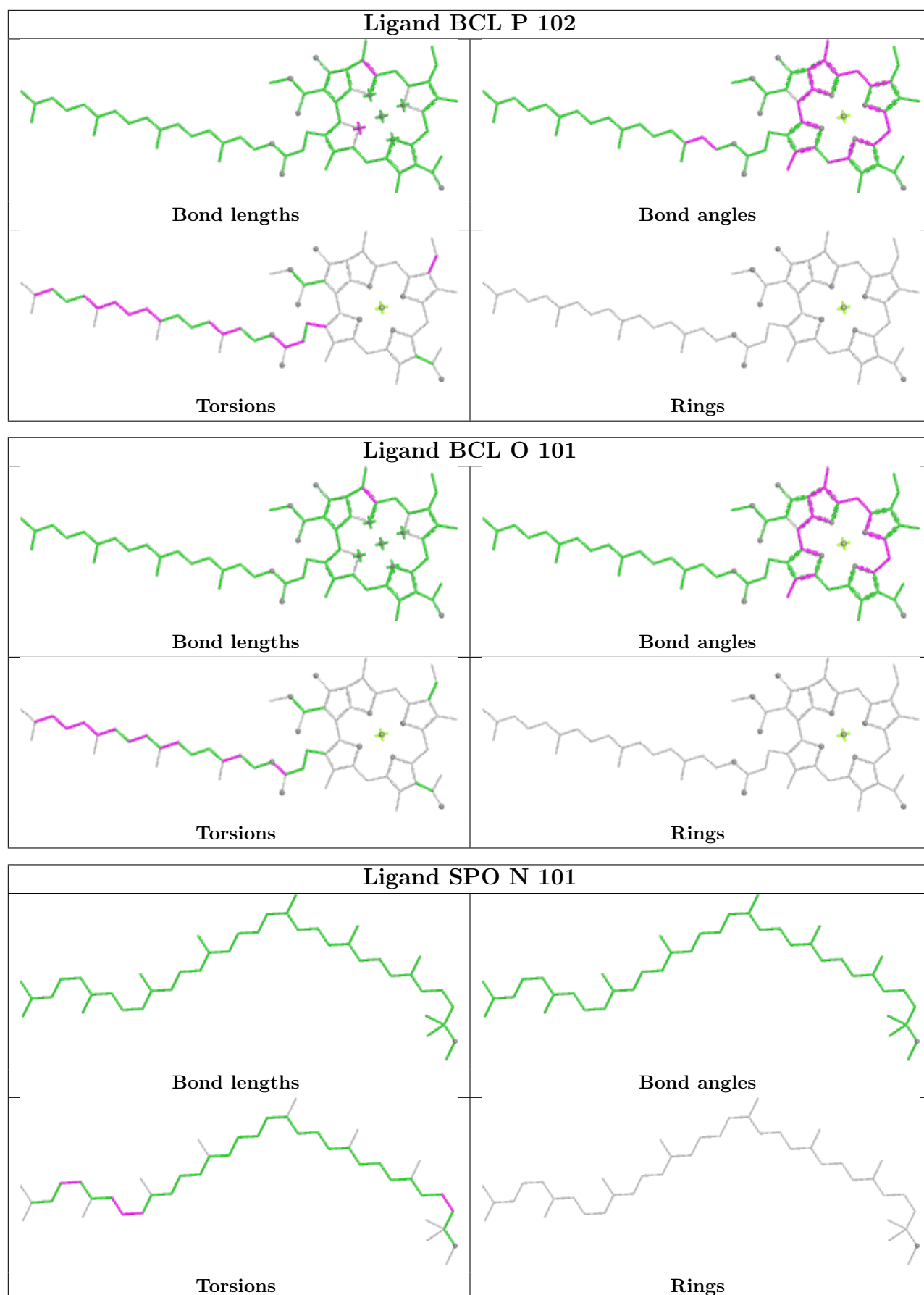


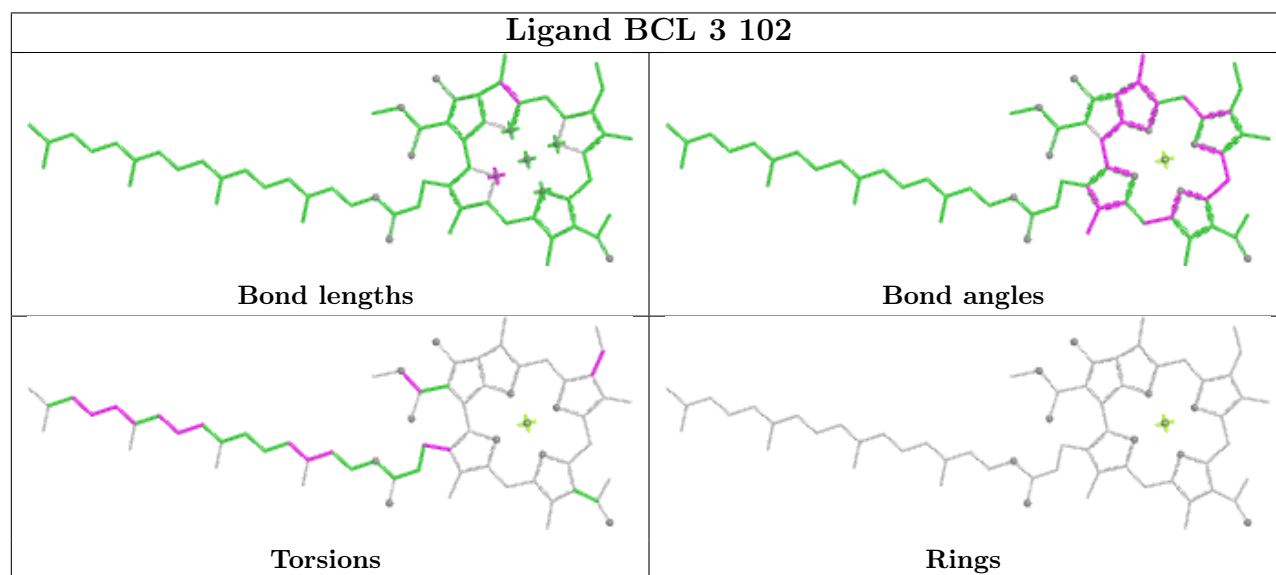
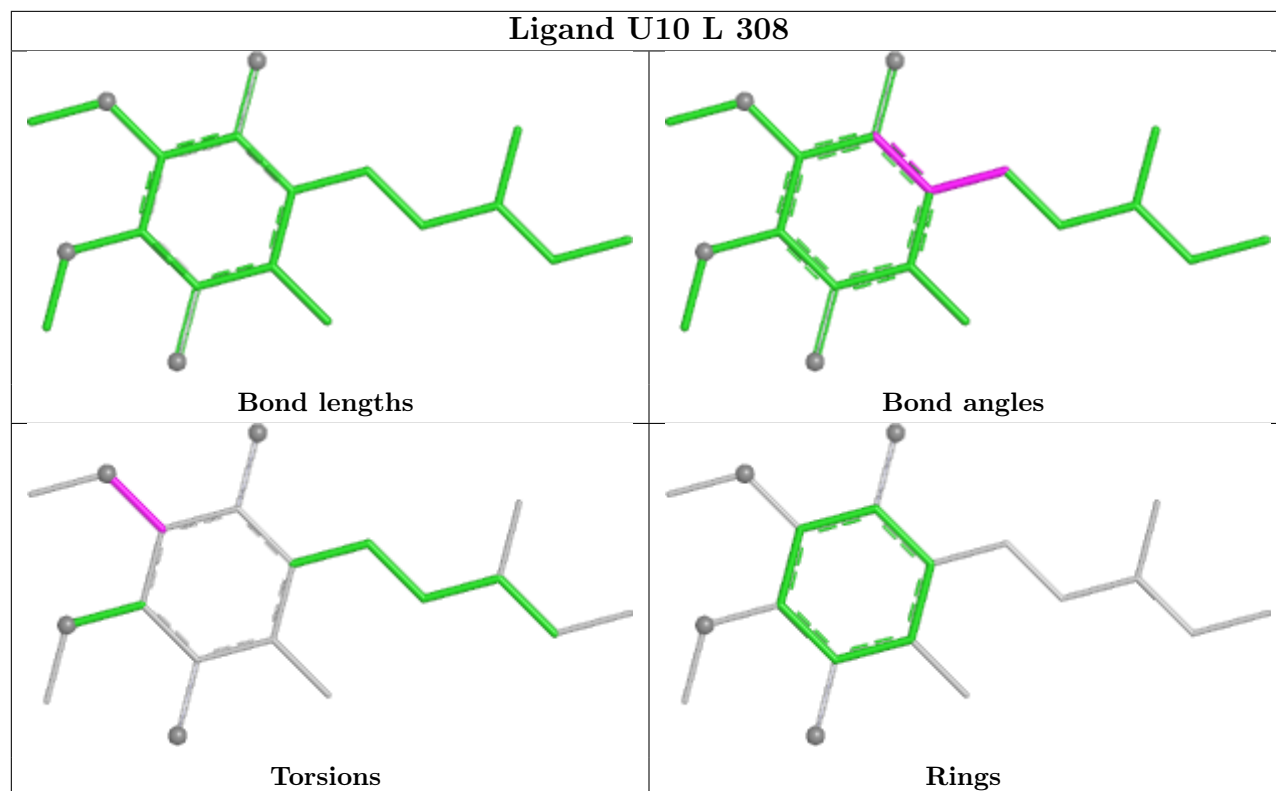


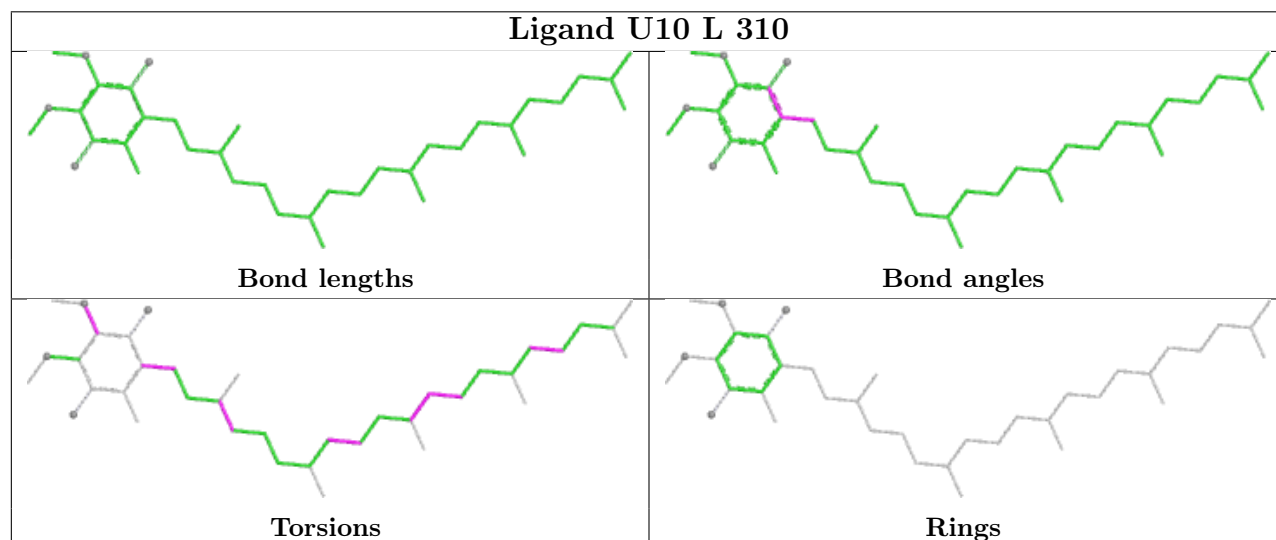
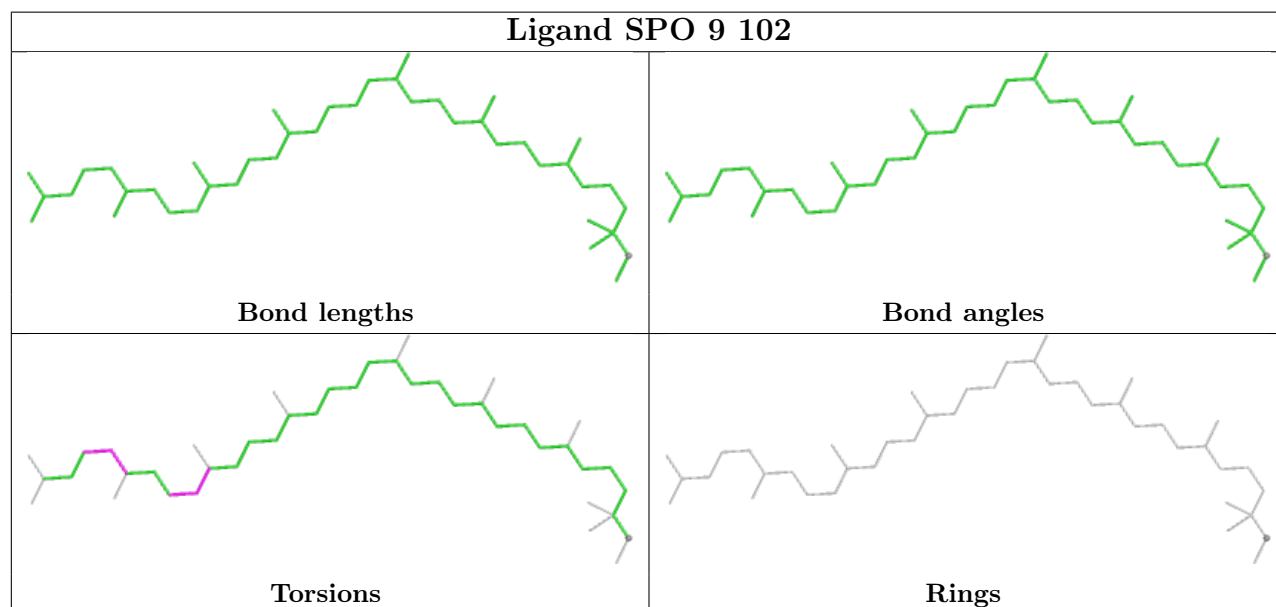
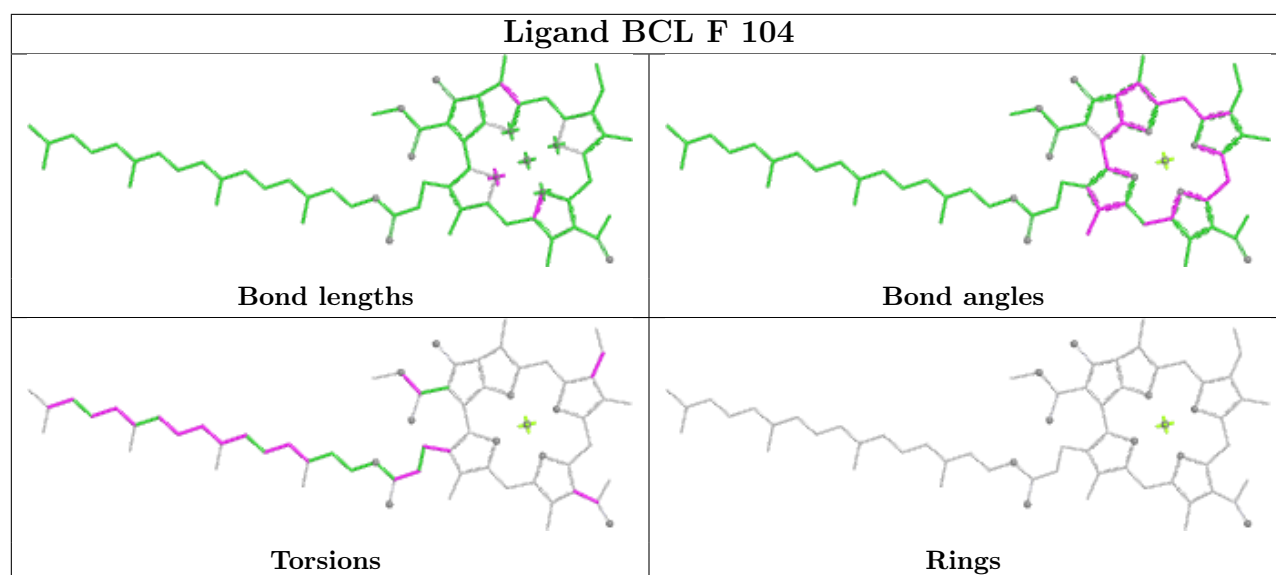


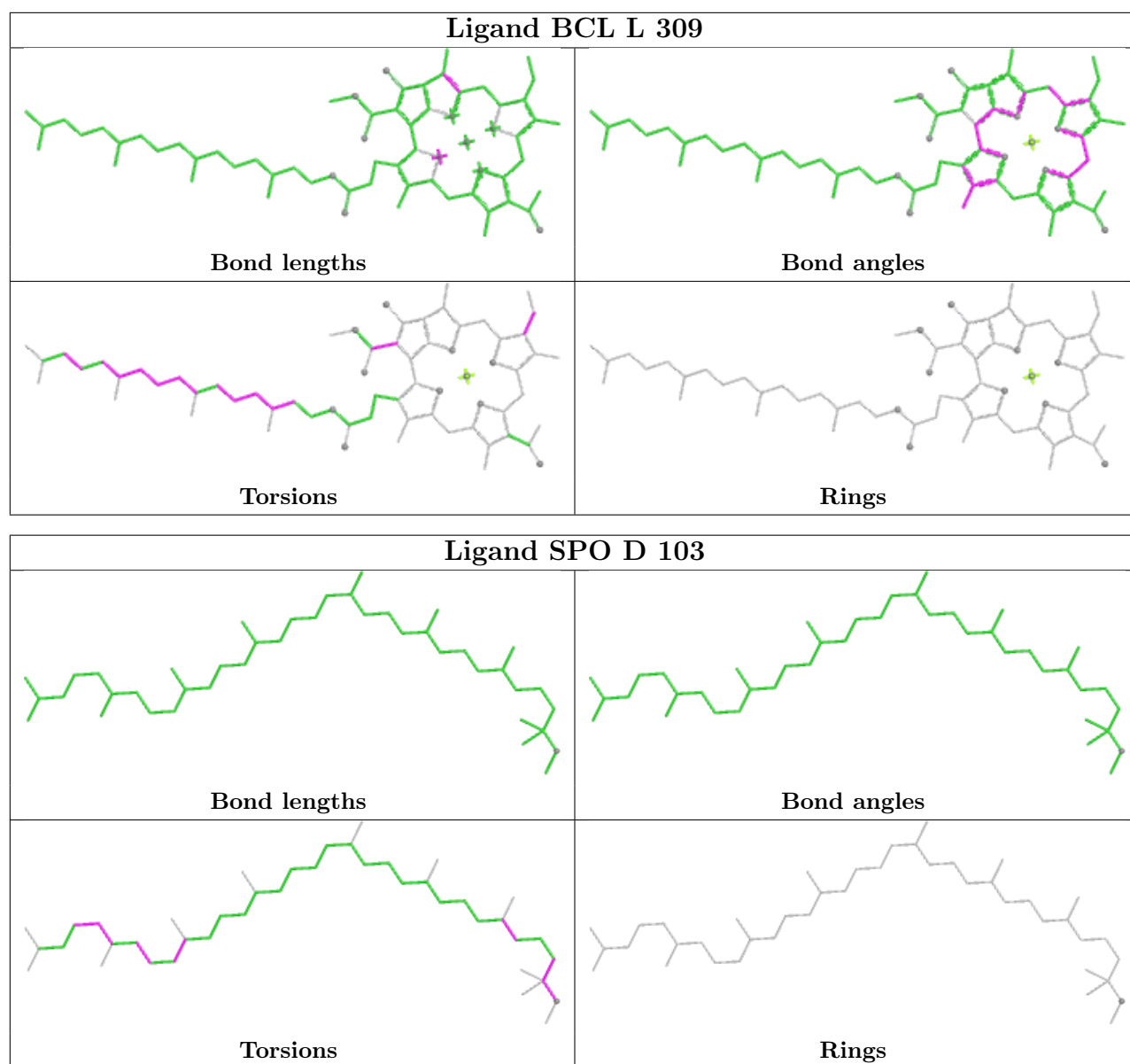




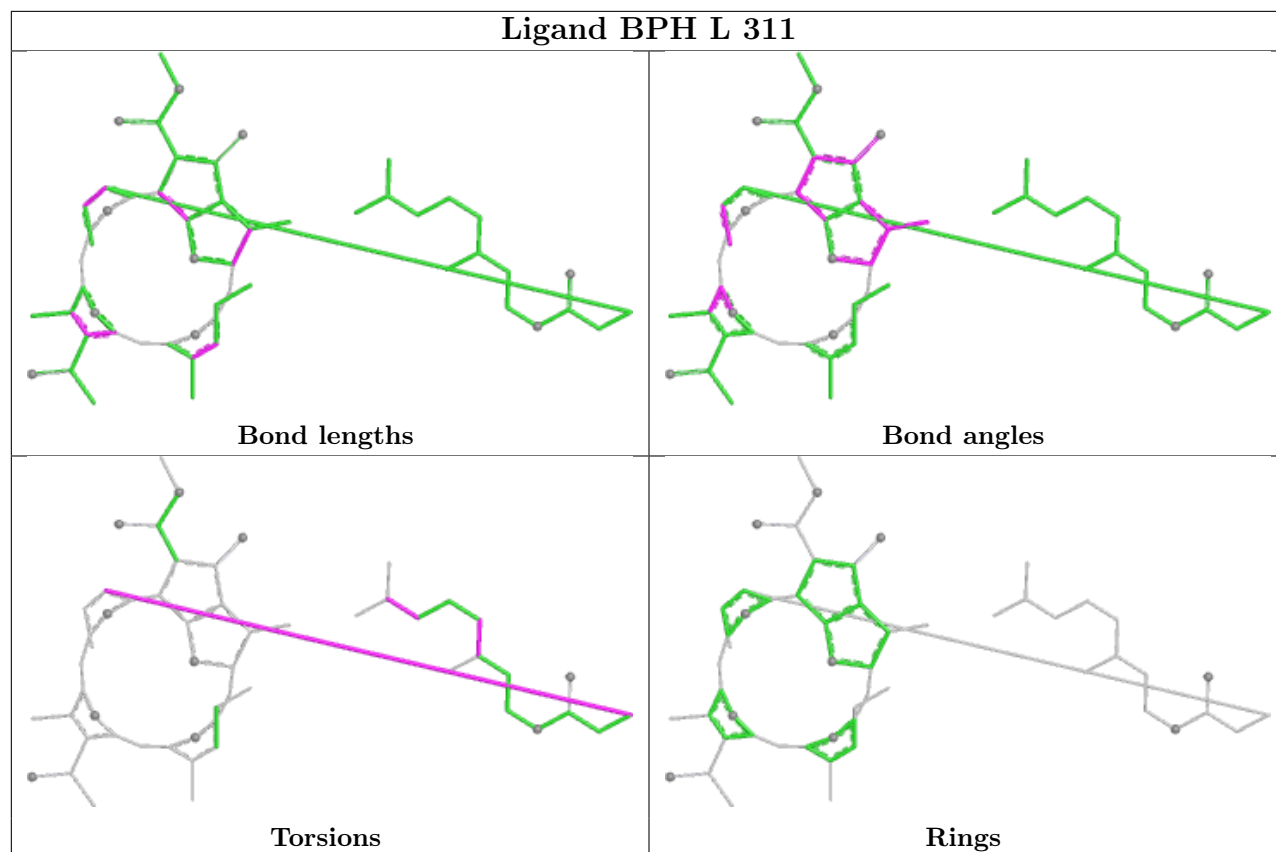




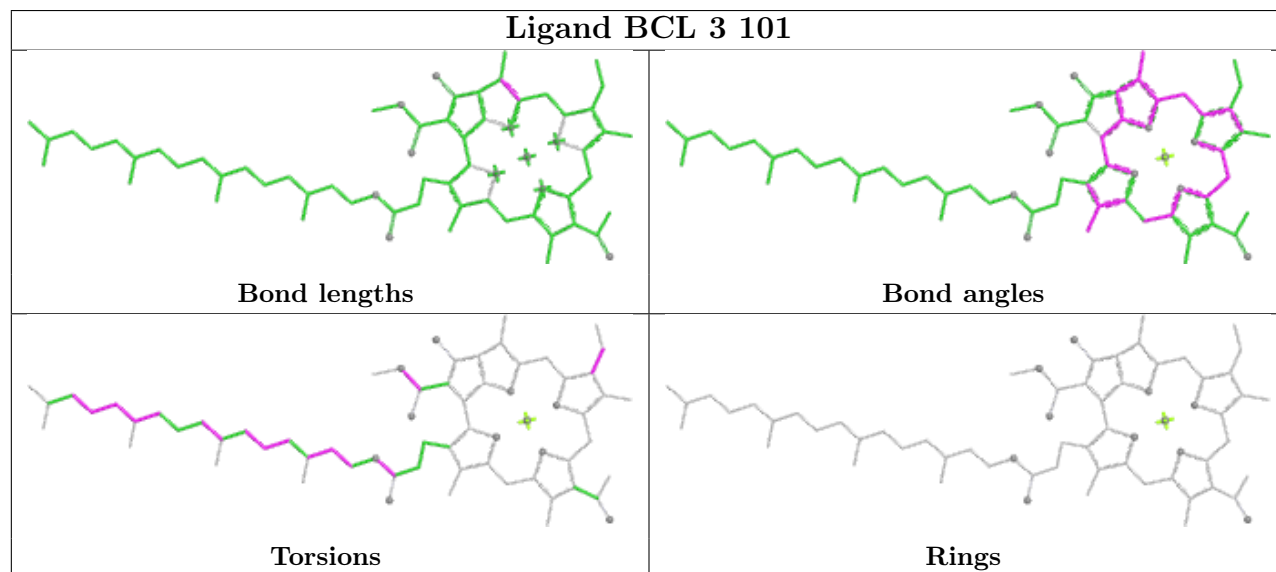


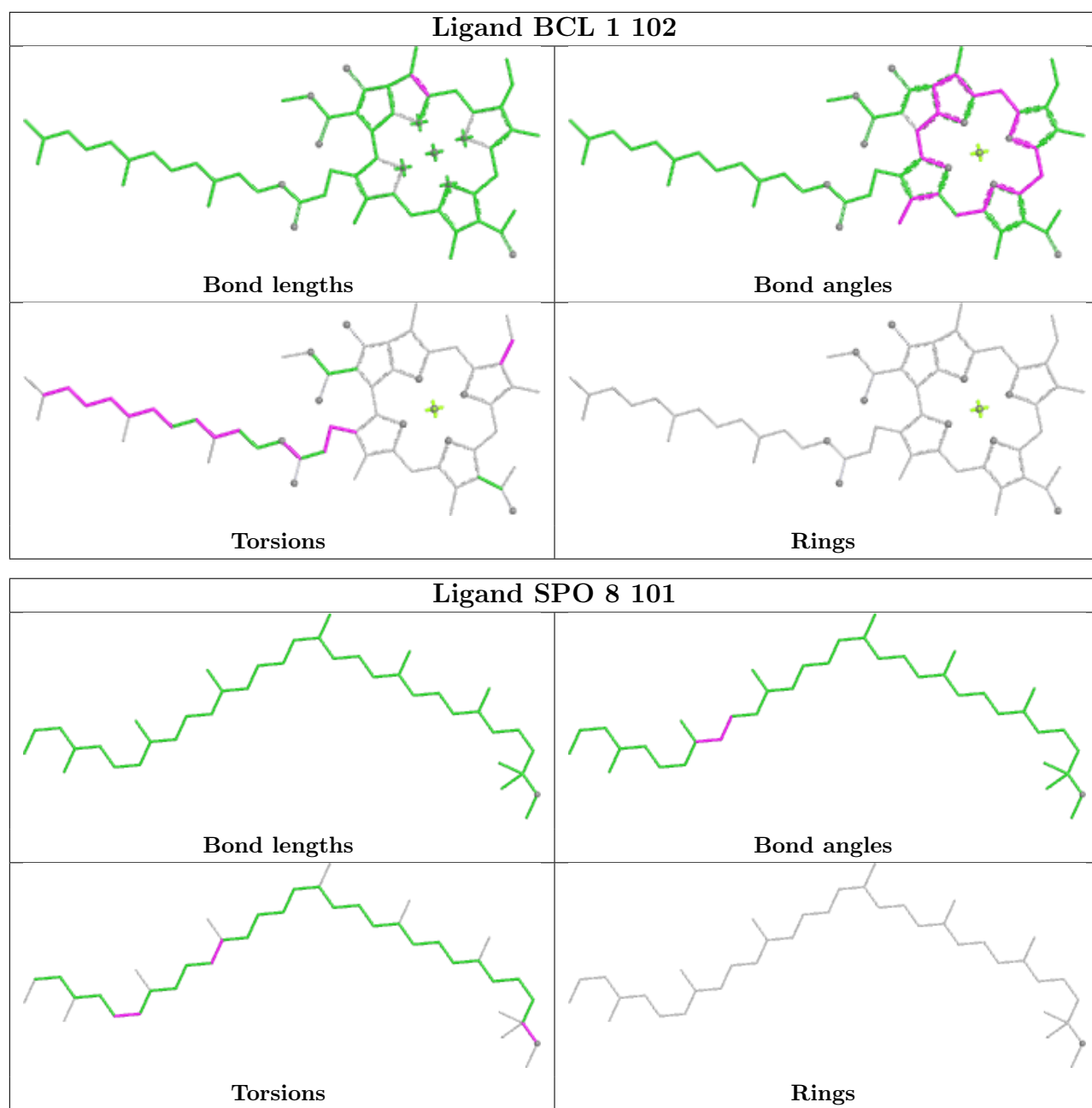


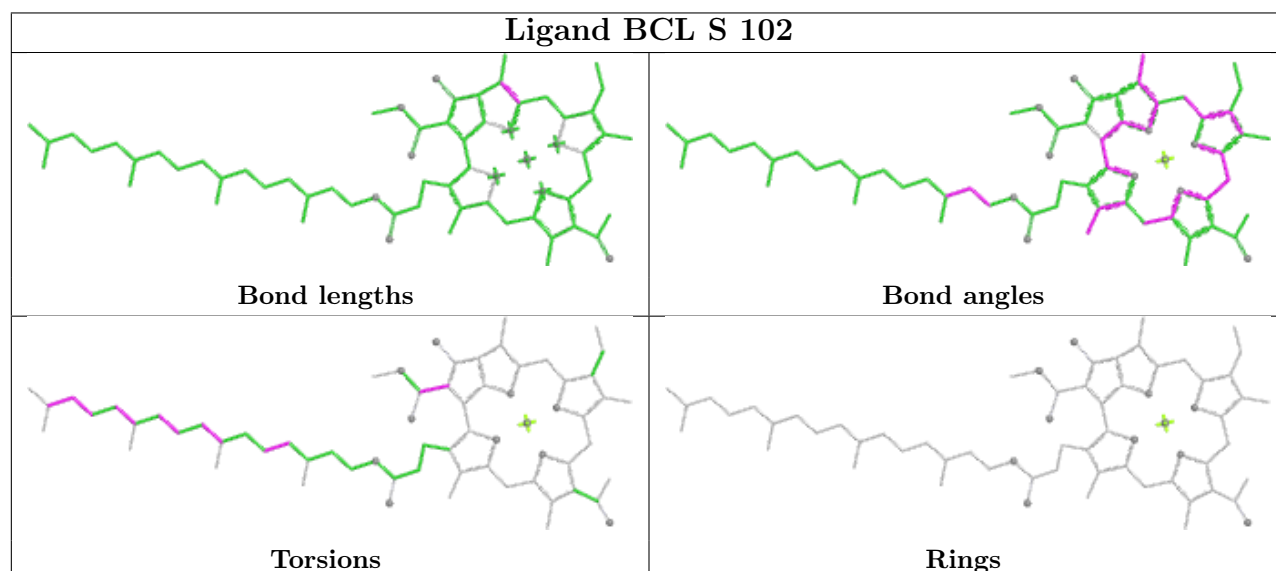
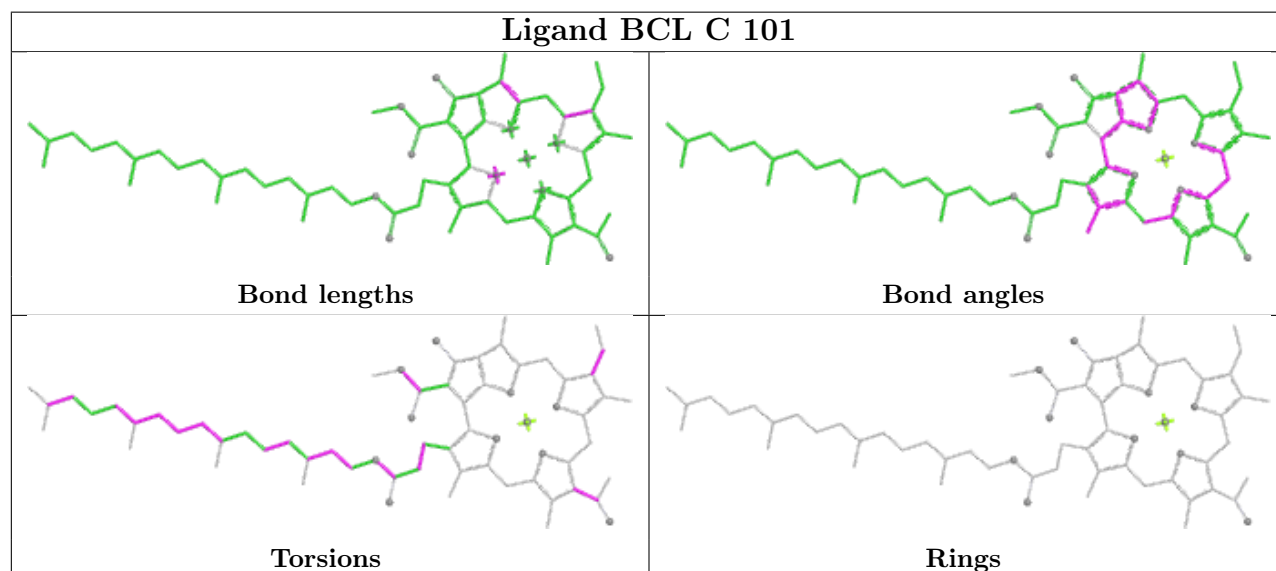
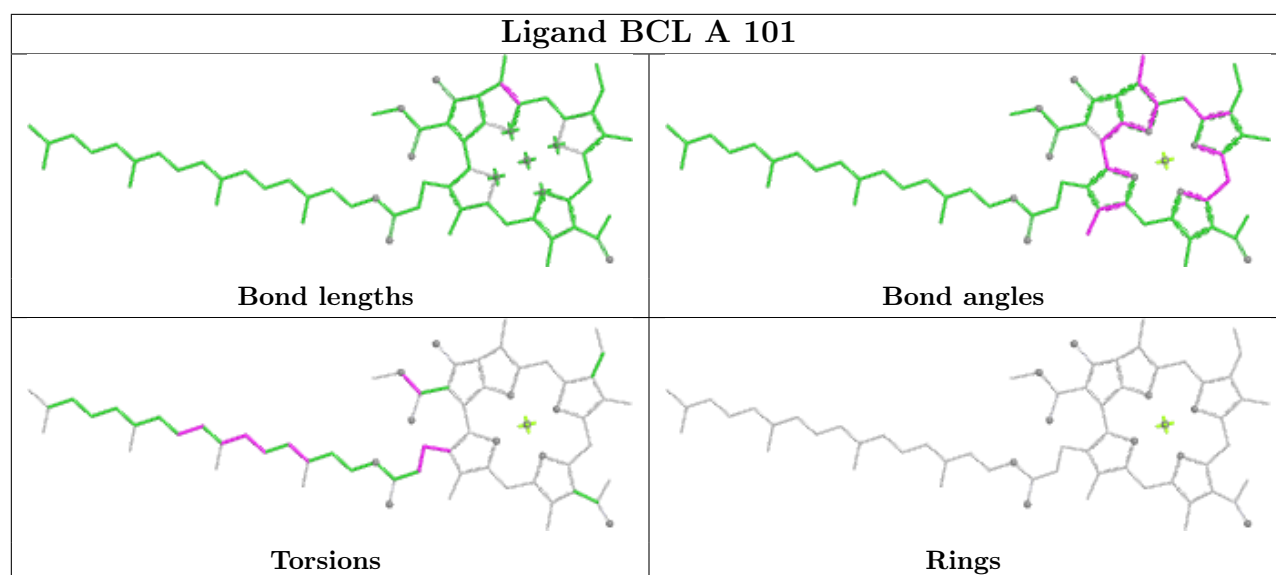
## Ligand BPH L 311

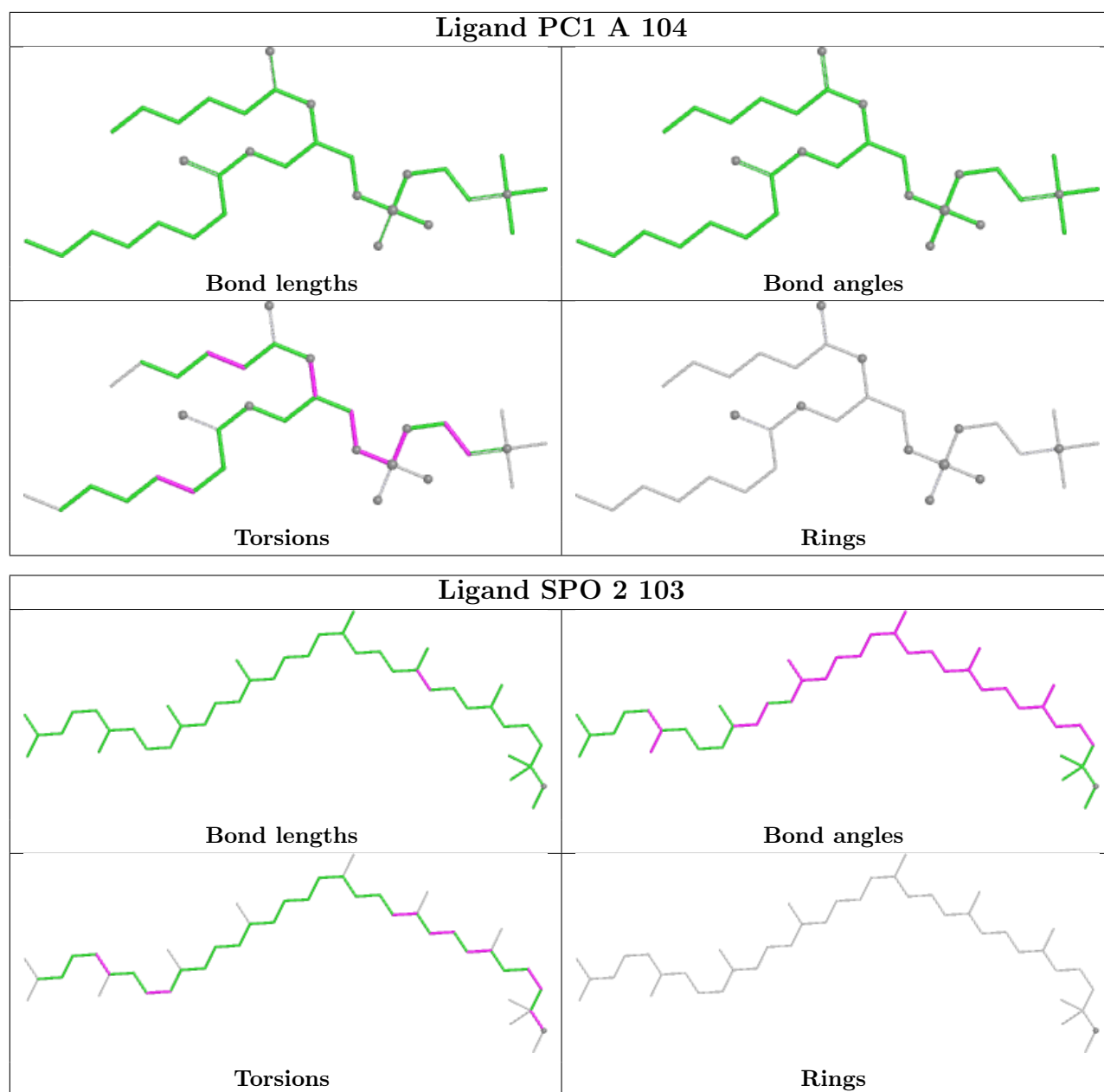


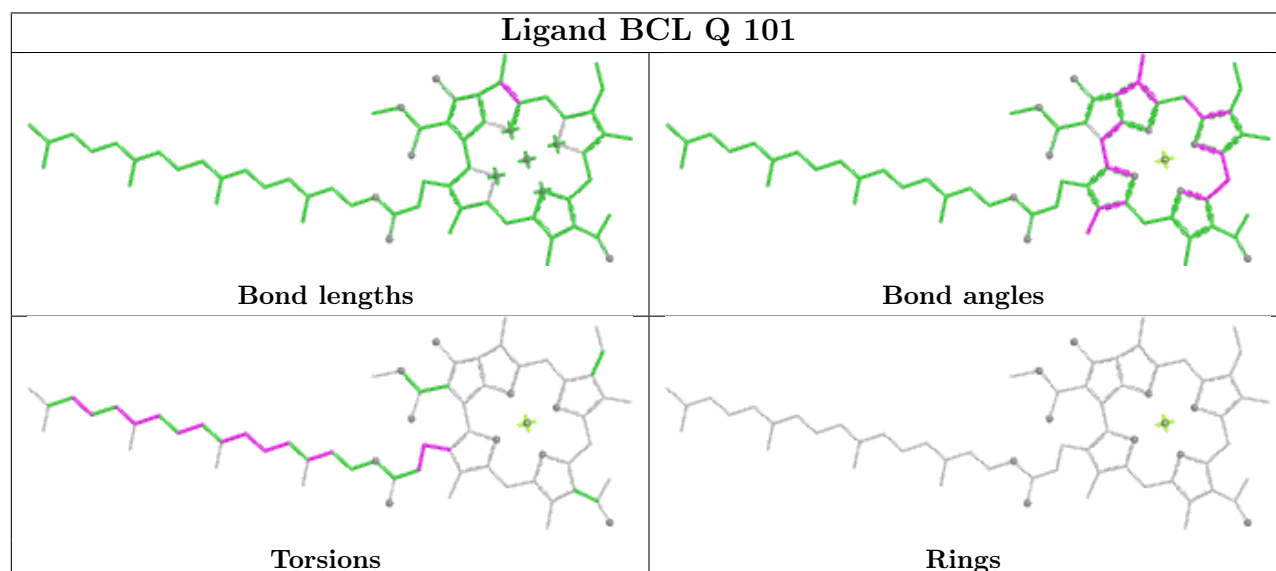
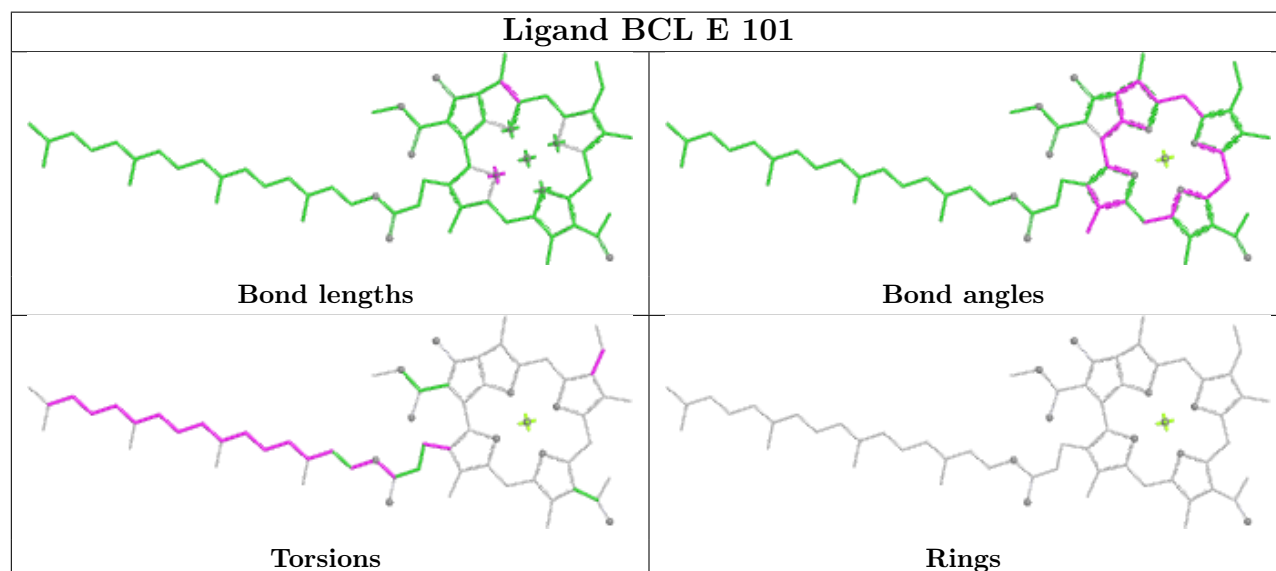
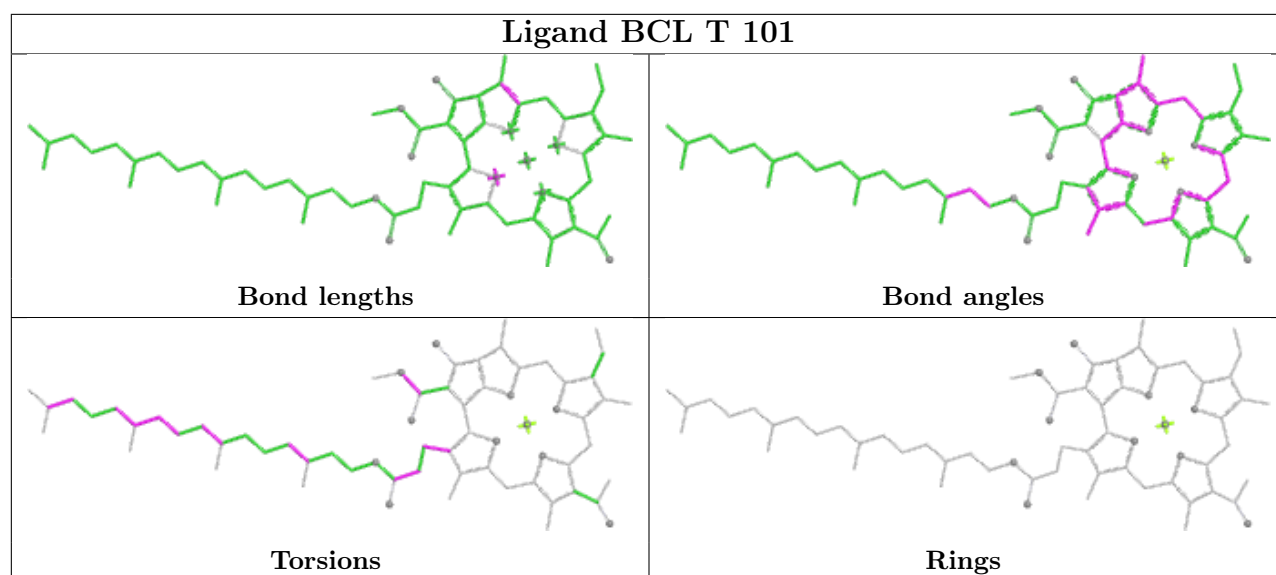
## Ligand BCL 3 101

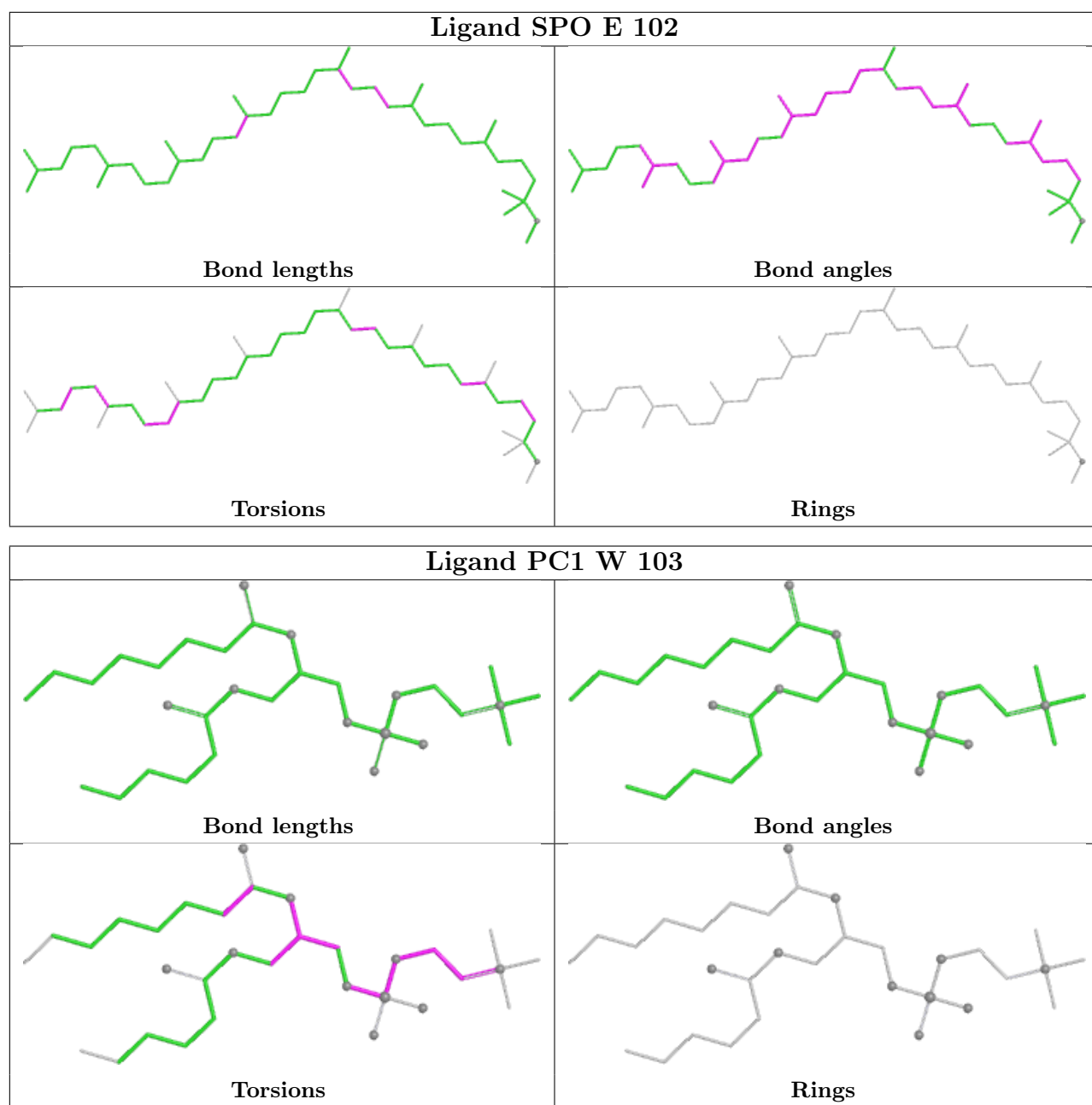


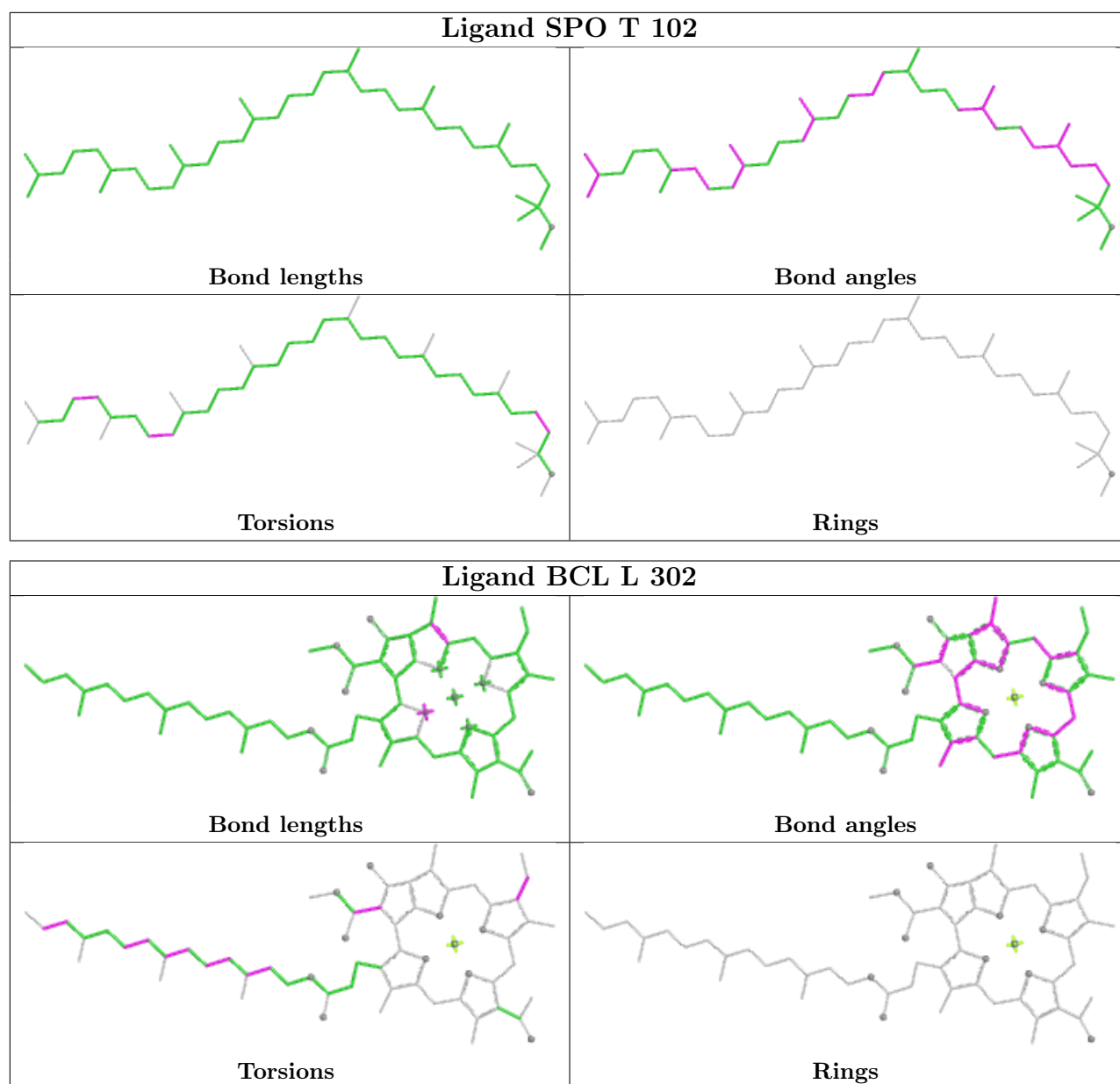


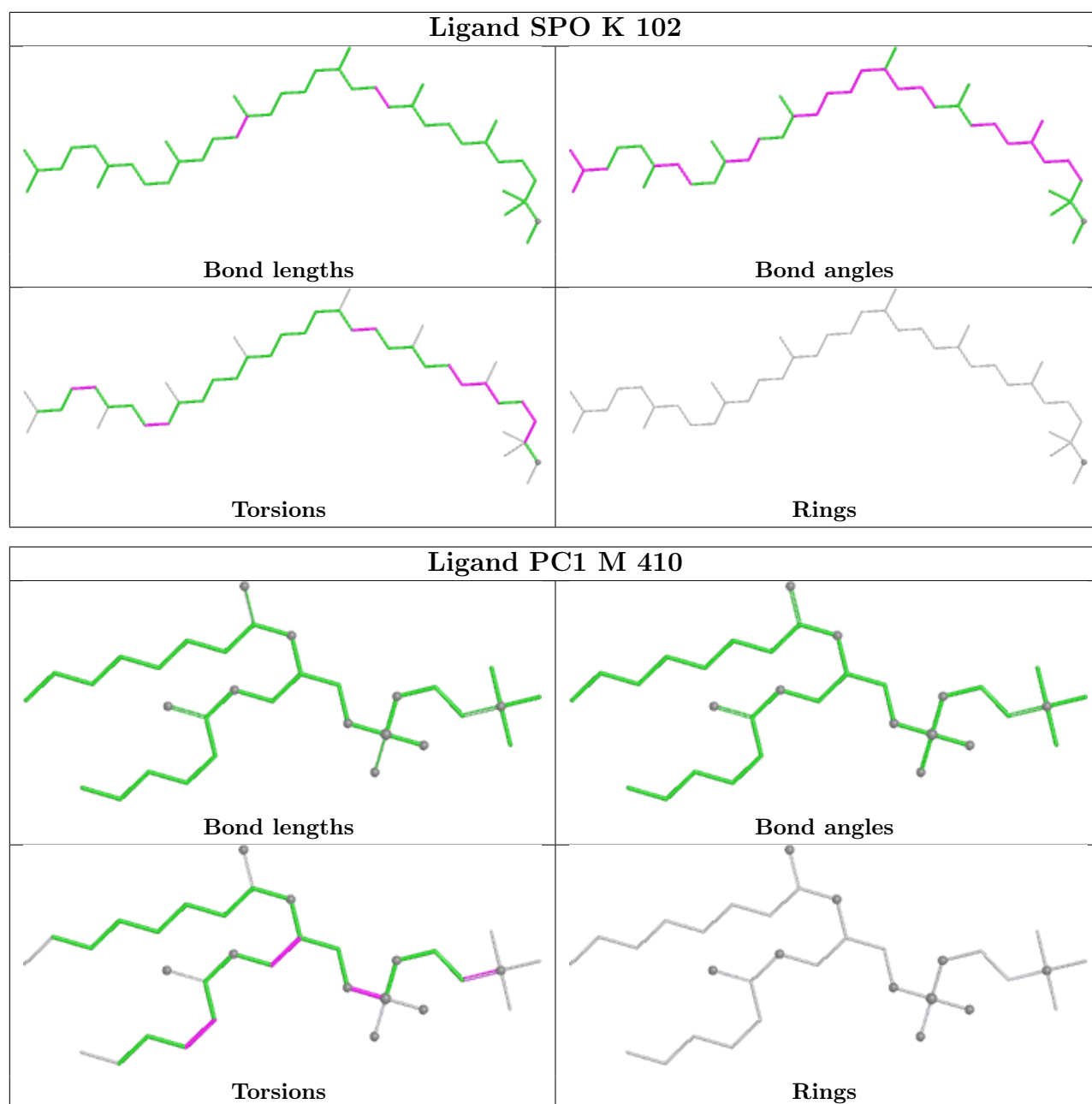


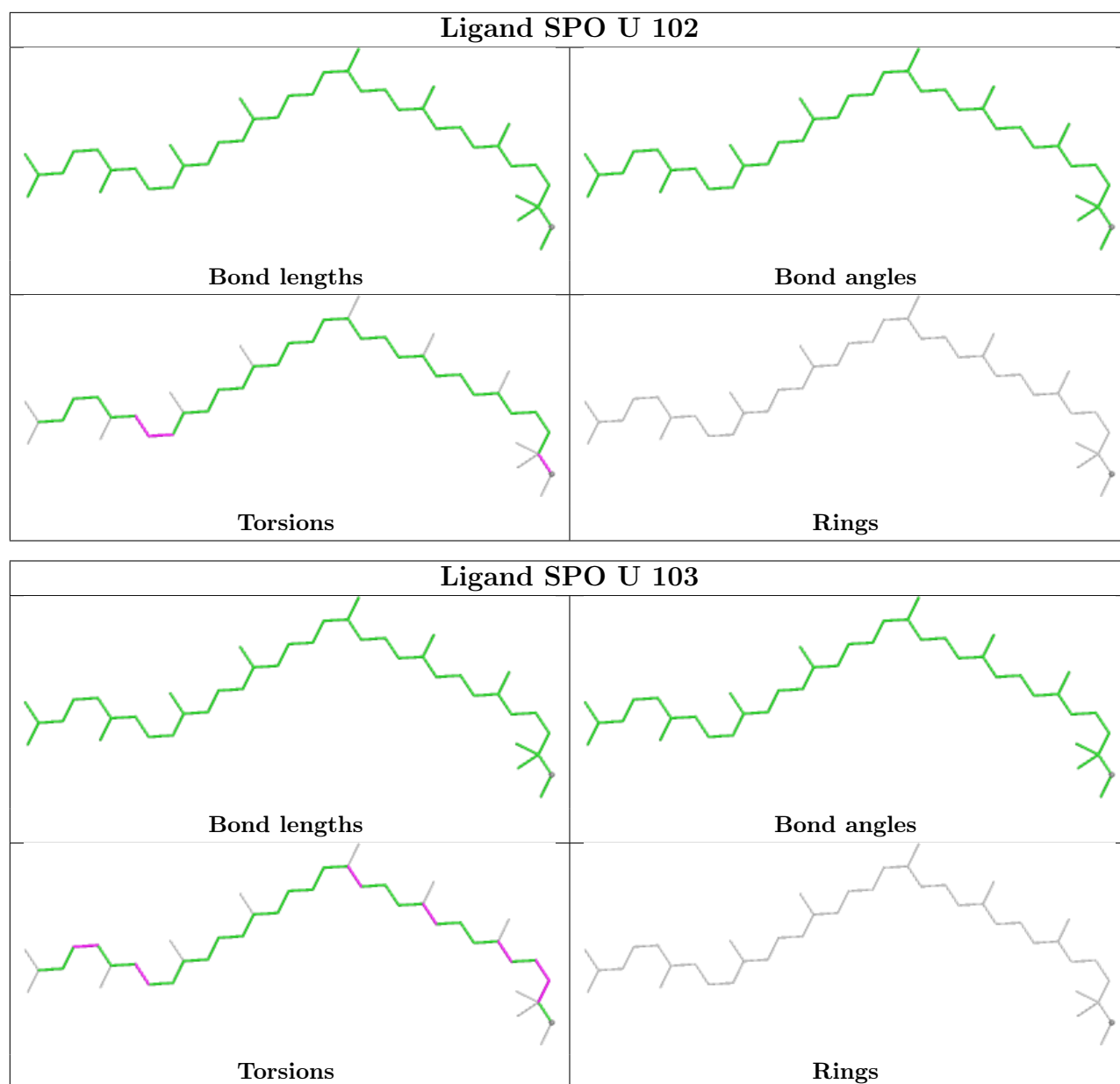












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

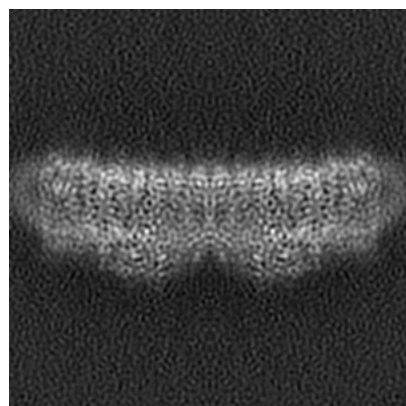
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39244. These allow visual inspection of the internal detail of the map and identification of artifacts.

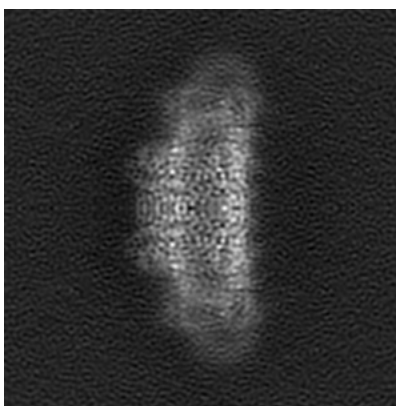
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

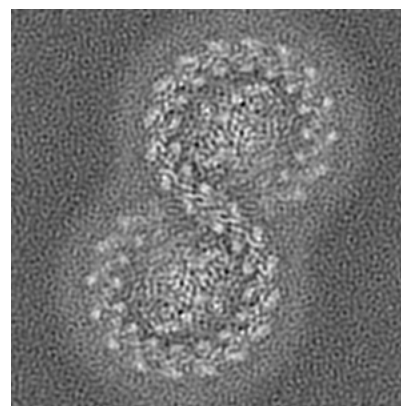
#### 6.1.1 Primary map



X

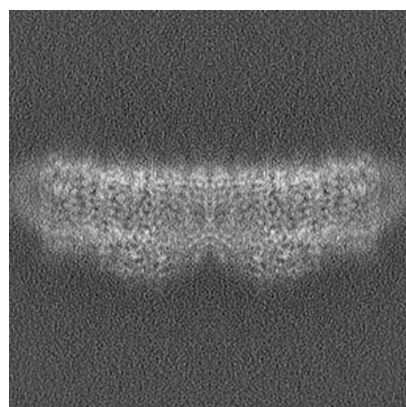


Y

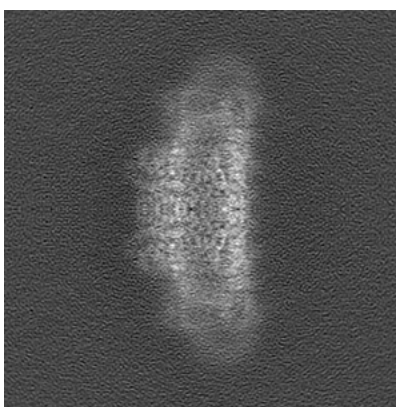


Z

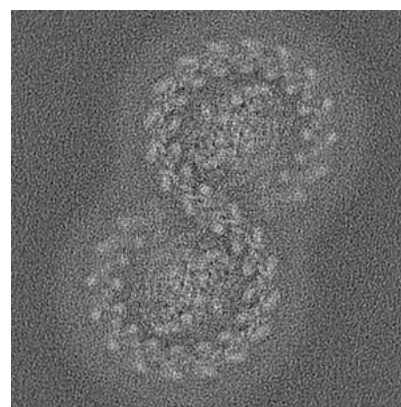
#### 6.1.2 Raw map



X



Y

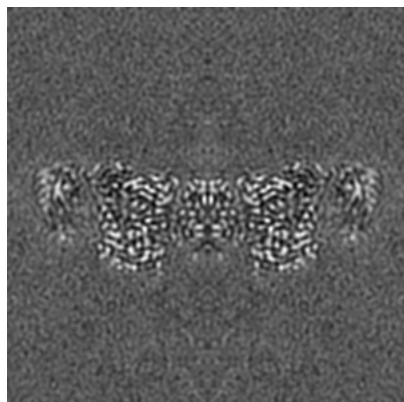


Z

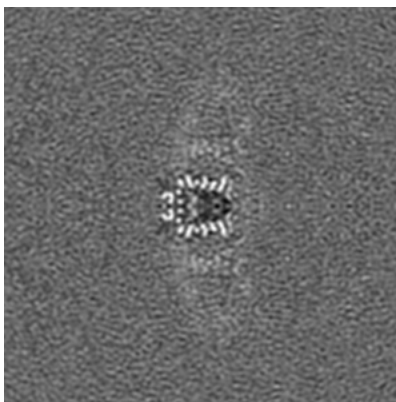
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

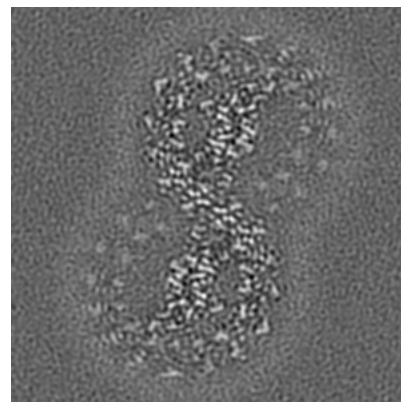
### 6.2.1 Primary map



X Index: 128

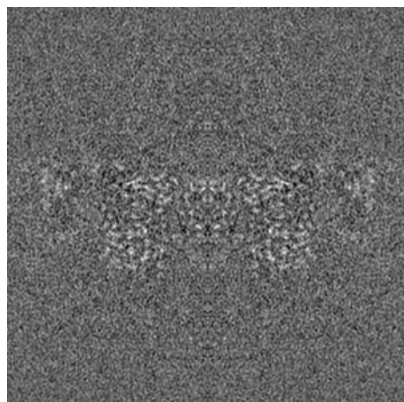


Y Index: 128

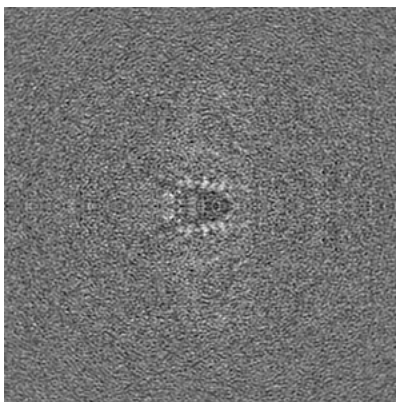


Z Index: 128

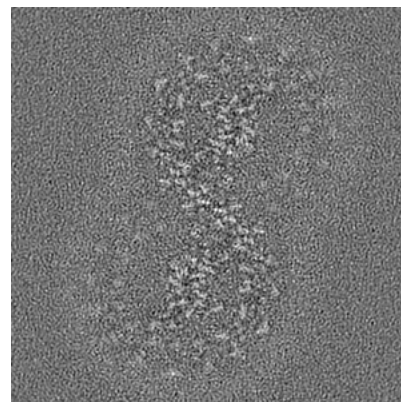
### 6.2.2 Raw map



X Index: 128



Y Index: 128

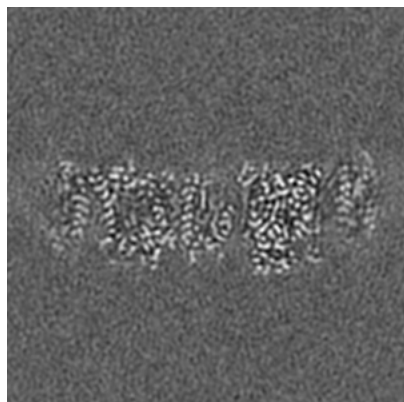


Z Index: 128

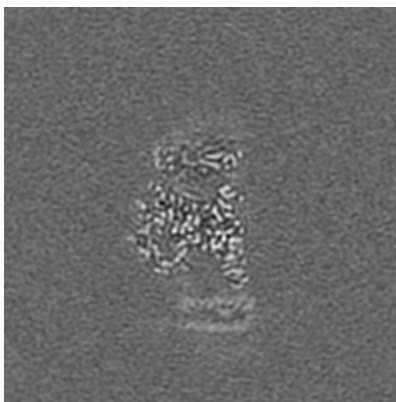
The images above show central slices of the map in three orthogonal directions.

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

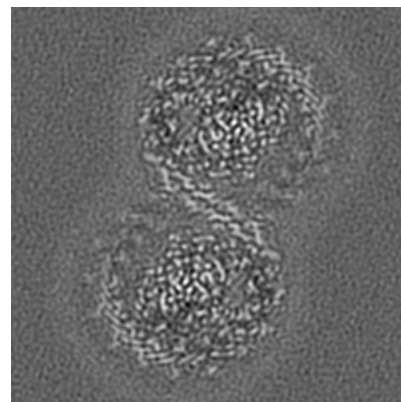
### 6.3.1 Primary map



X Index: 134

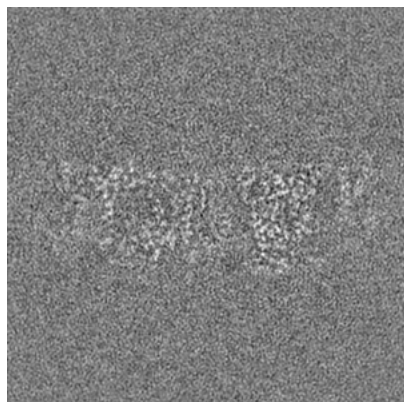


Y Index: 81

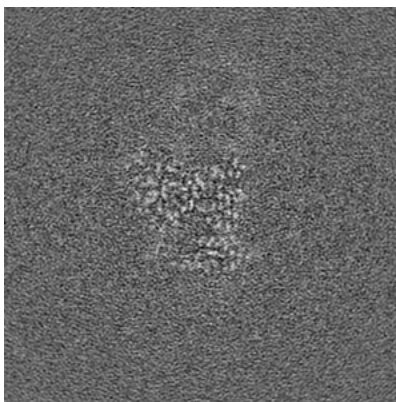


Z Index: 144

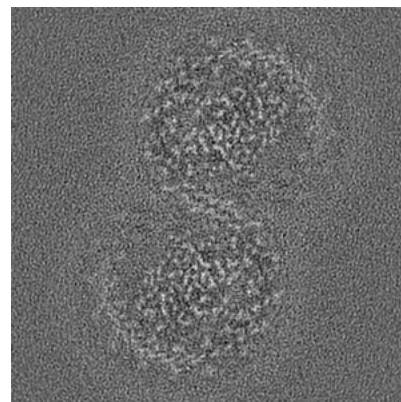
### 6.3.2 Raw map



X Index: 134



Y Index: 165

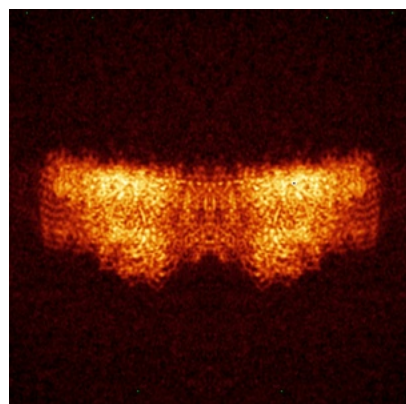


Z Index: 143

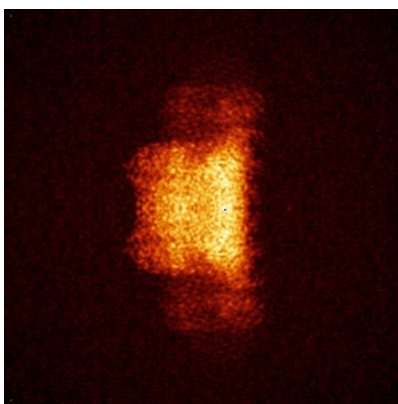
The images above show the largest variance slices of the map in three orthogonal directions.

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

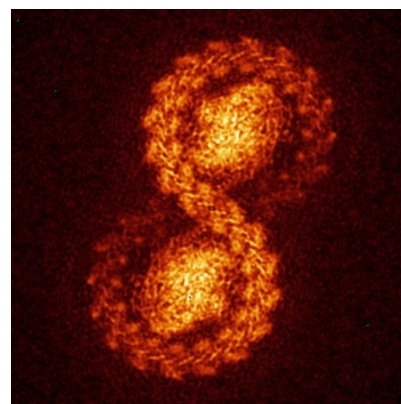
### 6.4.1 Primary map



X

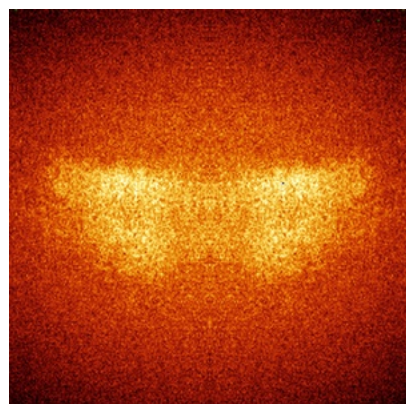


Y

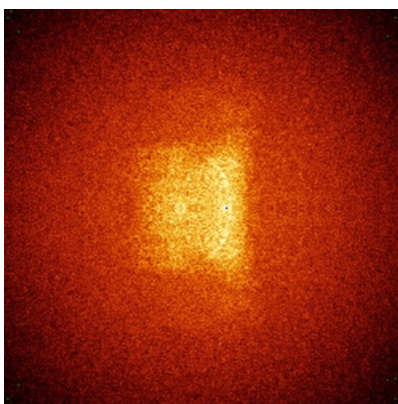


Z

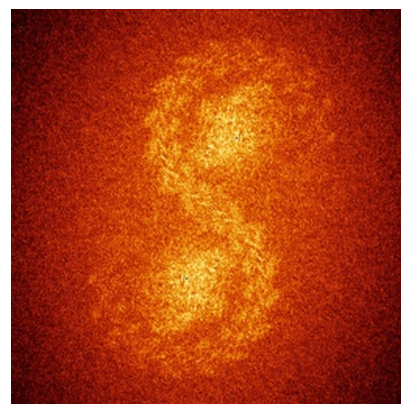
### 6.4.2 Raw map



X



Y

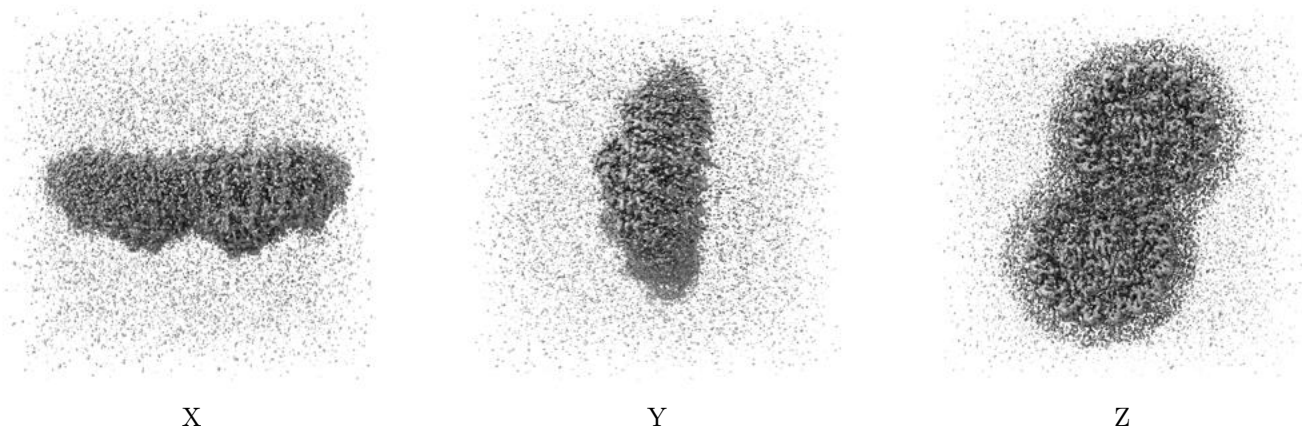


Z

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

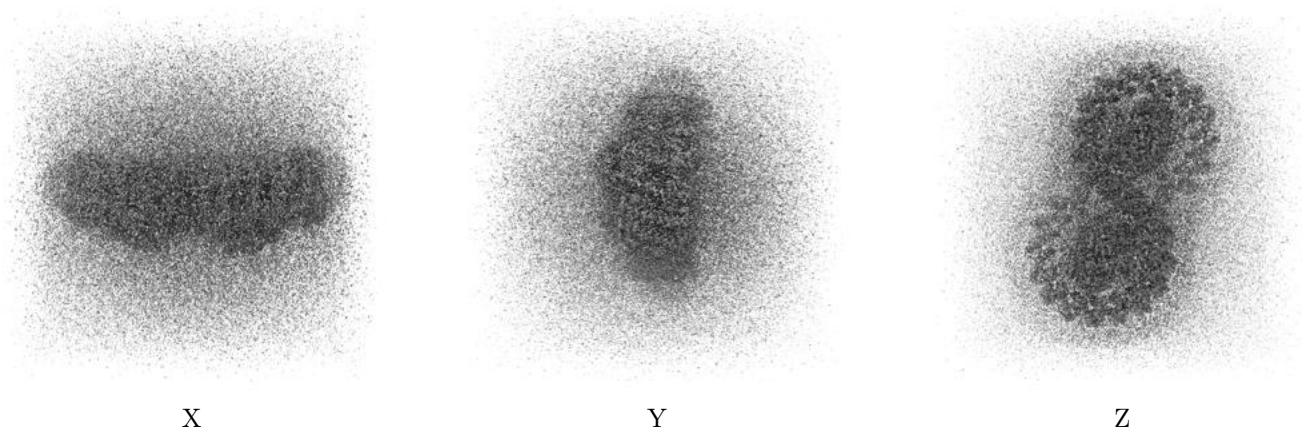
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

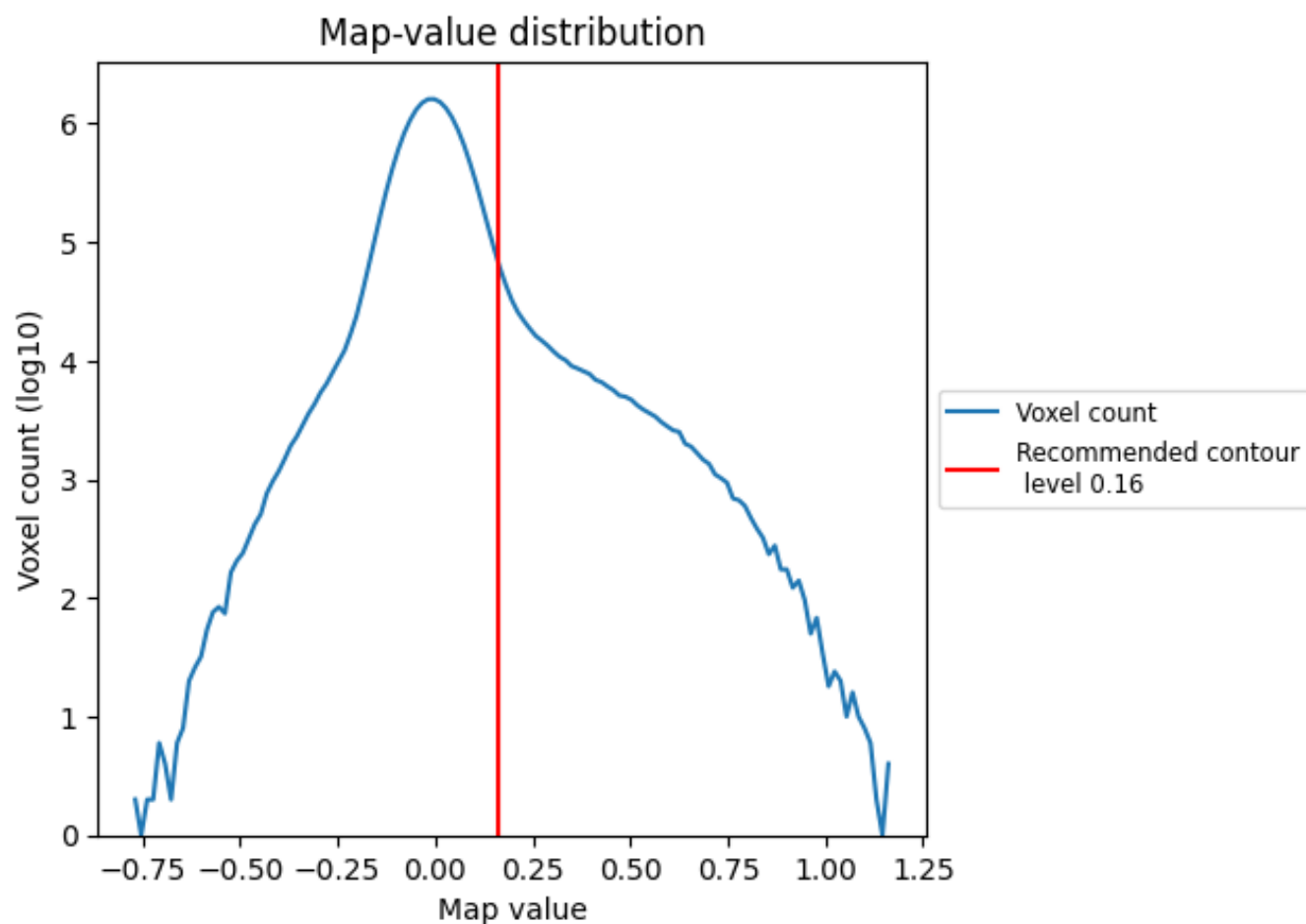
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

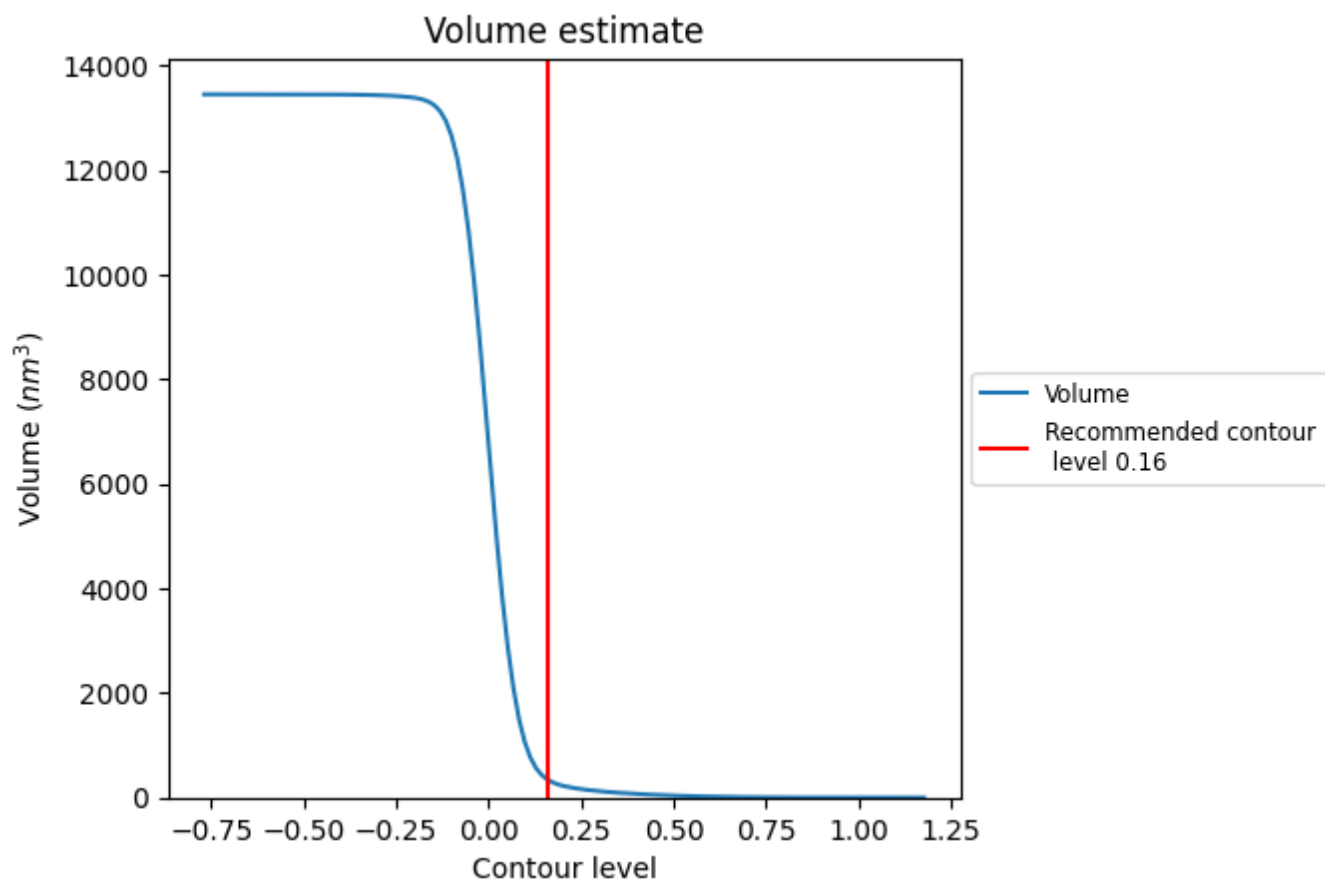
This section contains the results of statistical analysis of the map.

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



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

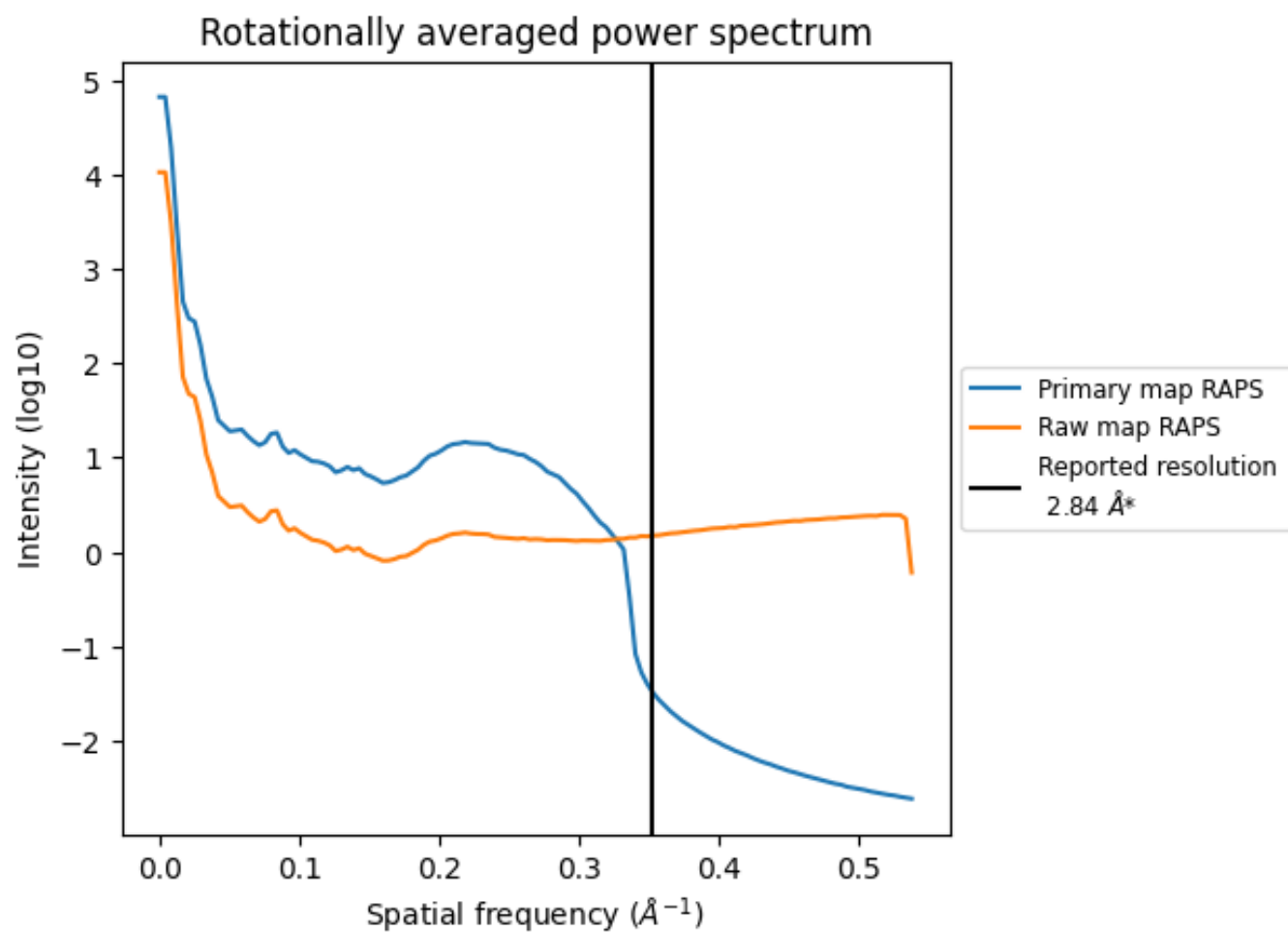
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 342 nm<sup>3</sup>; this corresponds to an approximate mass of 309 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 ⓘ

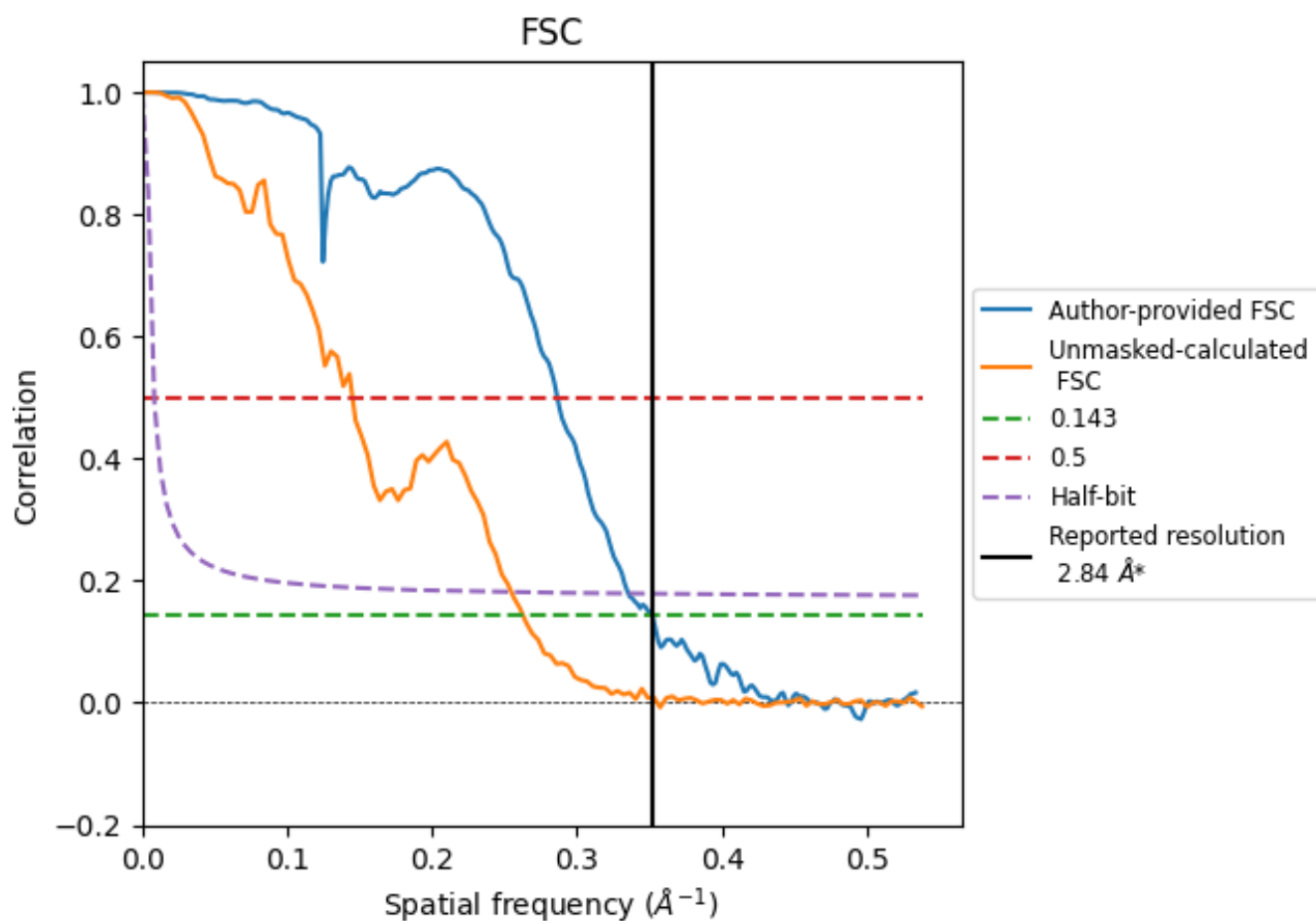


\*Reported resolution corresponds to spatial frequency of 0.352  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.84                               | -    | -        |
| Author-provided FSC curve | 2.84                               | 3.49 | 2.97     |
| Unmasked-calculated*      | 3.81                               | 6.89 | 3.93     |

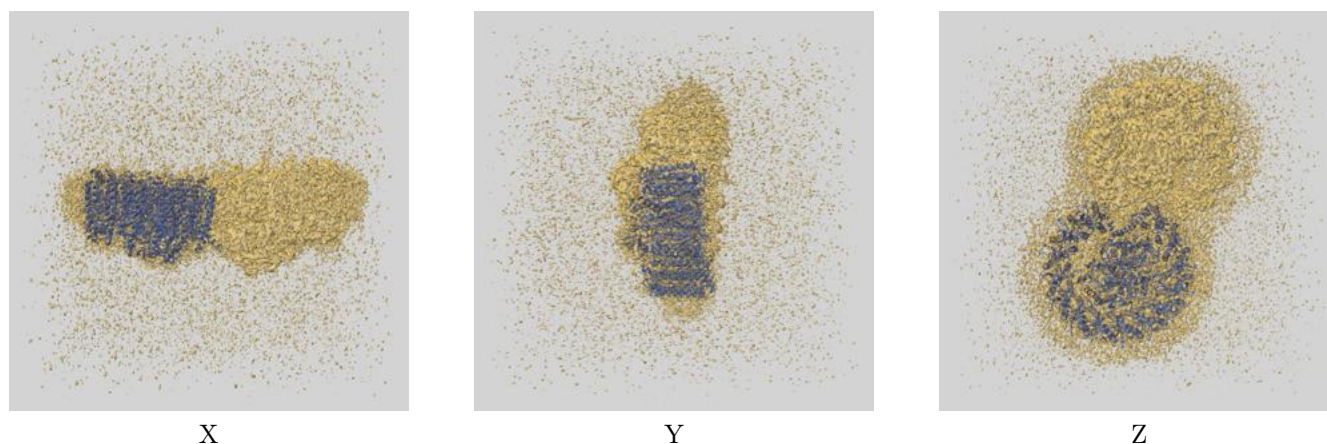
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.81 differs from the reported value 2.84 by more than 10 %

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

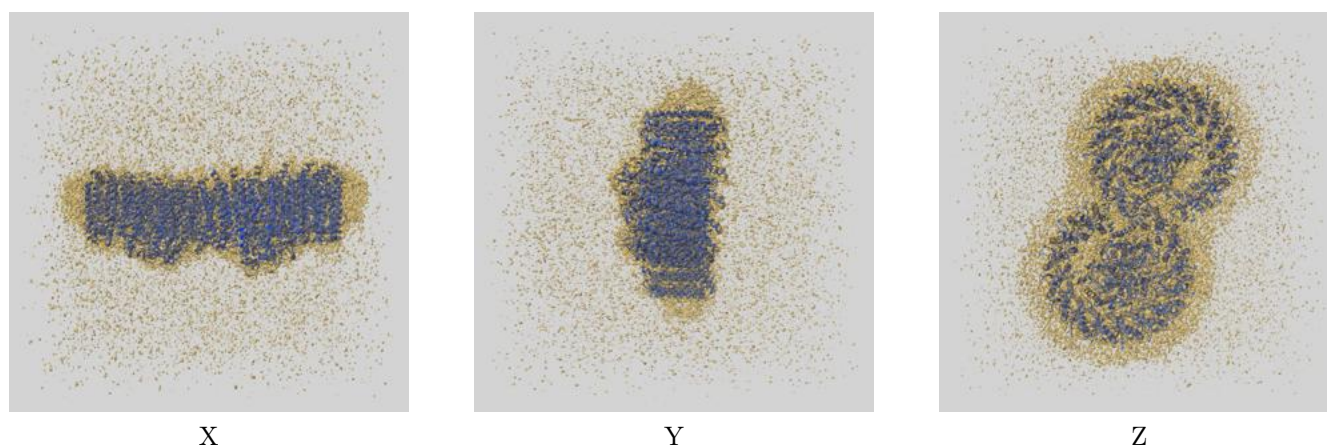
This section contains information regarding the fit between EMDB map EMD-39244 and PDB model 8YGD. Per-residue inclusion information can be found in section [3](#) on page [15](#).

### 9.1 Map-model overlays

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

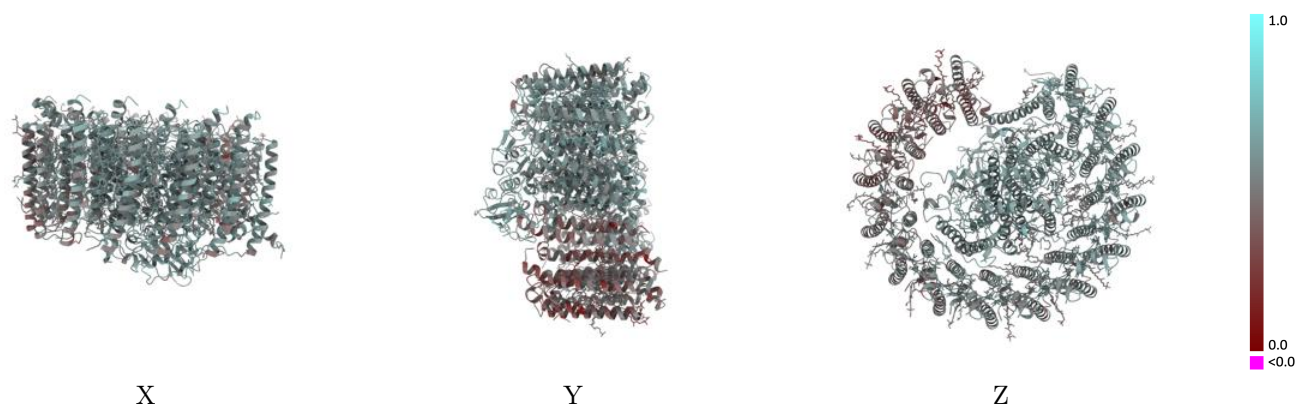


#### 9.1.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.16 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](#)

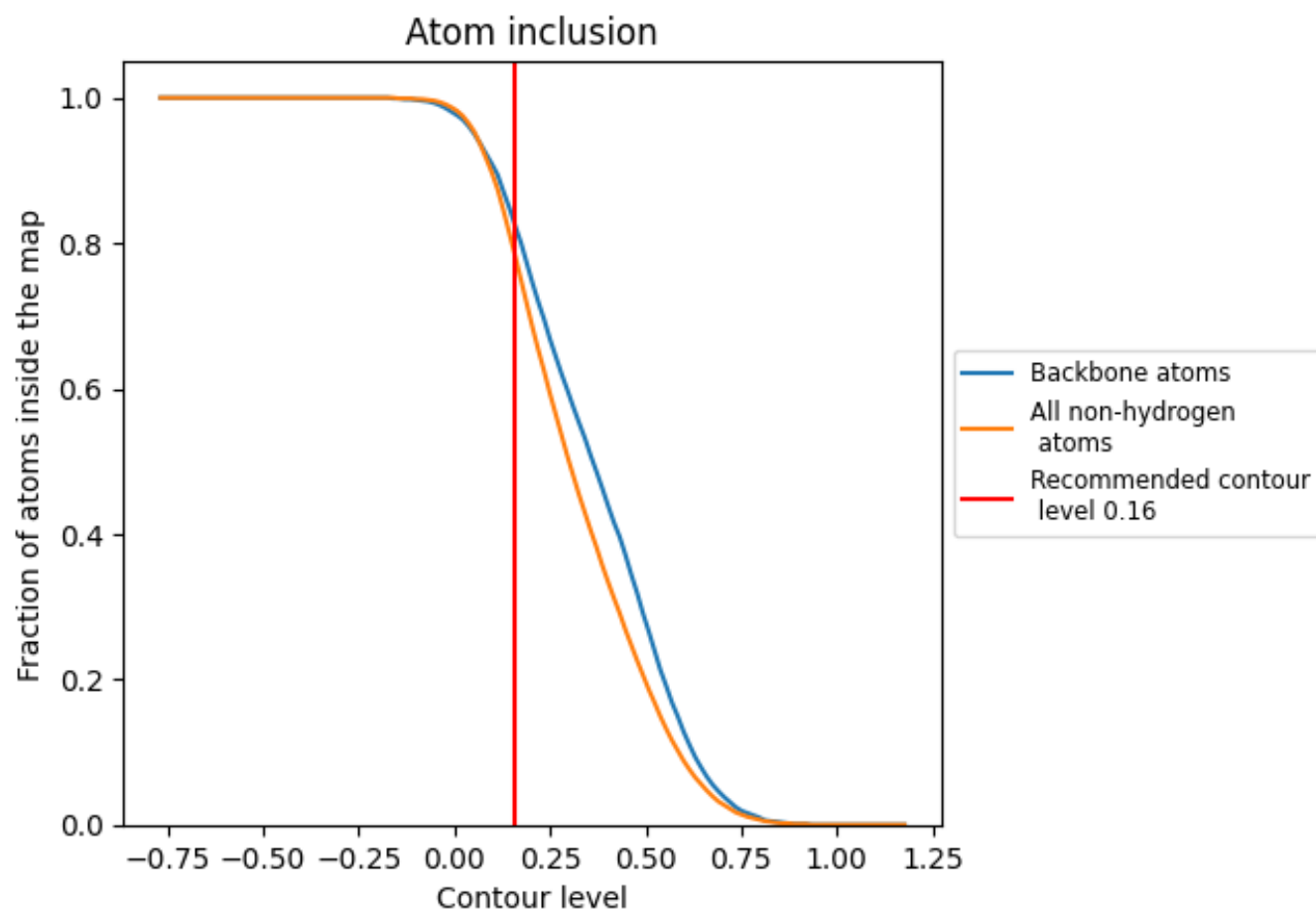


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.16) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7800   |  0.5170   |
| 0     |  0.8460   |  0.5400   |
| 1     |  0.5350   |  0.3930   |
| 2     |  0.4540   |  0.3430   |
| 3     |  0.5160   |  0.4100   |
| 7     |  0.9210   |  0.5730   |
| 8     |  0.8390   |  0.5570   |
| 9     |  0.8780   |  0.5730   |
| A     |  0.8660   |  0.5660   |
| B     |  0.8350   |  0.5370   |
| C     |  0.5550   |  0.3730   |
| D     |  0.9040   |  0.5680   |
| E     |  0.8150   |  0.5290   |
| F     |  0.8280   |  0.5400   |
| G     |  0.8440  |  0.5220  |
| H     |  0.8740 |  0.5680 |
| I     |  0.8130 |  0.5190 |
| J     |  0.8060 |  0.5160 |
| K     |  0.7980 |  0.5050 |
| L     |  0.8700 |  0.5770 |
| M     |  0.8580 |  0.5640 |
| N     |  0.7330 |  0.4690 |
| O     |  0.7700 |  0.5130 |
| P     |  0.7480 |  0.4960 |
| Q     |  0.8080 |  0.5140 |
| R     |  0.7010 |  0.4760 |
| S     |  0.7440 |  0.4890 |
| T     |  0.7060 |  0.4610 |
| U     |  0.6980 |  0.4760 |
| V     |  0.6810 |  0.4420 |
| W     |  0.6350 |  0.4590 |
| X     |  0.7870 |  0.5370 |
| Z     |  0.4910 |  0.3700 |
| a     |  0.5070 |  0.3920 |
| b     |  0.6090 |  0.4210 |

