



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:35 PM UTC

PDB ID : 9PDA / pdb\_00009pda  
Title : Structure of Porcine Trypsin Crystals Grown From PEG and Complexed With Crystallization Additives IV  
Authors : McPherson, A.  
Deposited on : 2025-06-30  
Resolution : 1.18 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

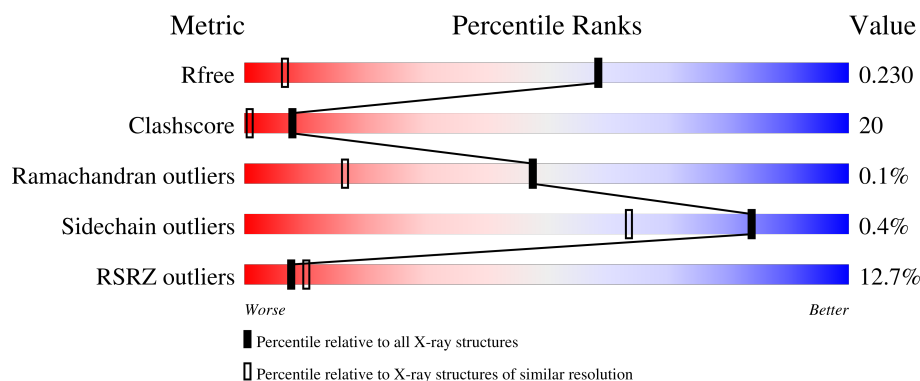
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.18 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1789 (1.20-1.16)                                      |
| Clashscore            | 190562                      | 1845 (1.20-1.16)                                      |
| Ramachandran outliers | 187476                      | 1789 (1.20-1.16)                                      |
| Sidechain outliers    | 187428                      | 1789 (1.20-1.16)                                      |
| RSRZ outliers         | 180081                      | 1787 (1.20-1.16)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 231    |                  |
| 1   | B     | 231    |                  |
| 1   | C     | 231    |                  |
| 1   | D     | 231    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | BEN  | C     | 301 | -         | -        | X       | -                |
| 5   | PEG  | B     | 325 | -         | -        | X       | -                |
| 5   | PEG  | C     | 308 | -         | -        | X       | -                |
| 5   | PEG  | C     | 309 | -         | -        | X       | -                |
| 5   | PEG  | C     | 312 | -         | -        | X       | -                |
| 5   | PEG  | C     | 316 | -         | -        | X       | -                |
| 5   | PEG  | D     | 319 | -         | -        | X       | -                |
| 5   | PEG  | D     | 320 | -         | -        | X       | -                |
| 5   | PEG  | D     | 321 | -         | -        | X       | -                |
| 8   | PG4  | D     | 333 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

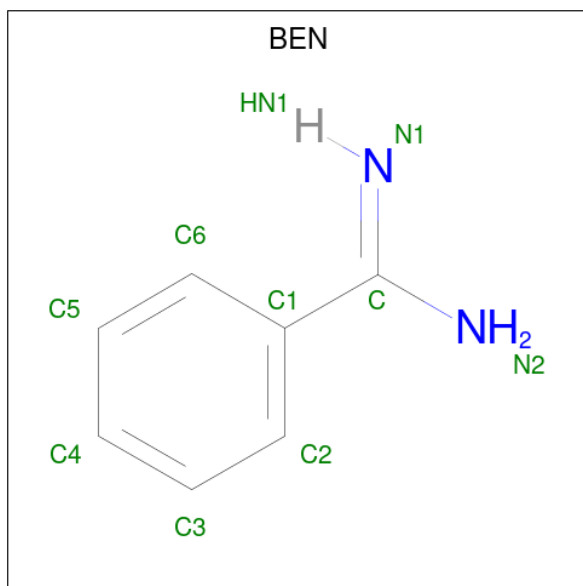
There are 12 unique types of molecules in this entry. The entry contains 16671 atoms, of which 7751 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Trypsin.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 223      | Total | C    | H    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 3258  | 1027 | 1604 | 288 | 325 | 14 |         |         |       |
| 1   | B     | 223      | Total | C    | H    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 3238  | 1020 | 1596 | 287 | 321 | 14 |         |         |       |
| 1   | C     | 223      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3237  | 1020 | 1595 | 287 | 321 | 14 |         |         |       |
| 1   | D     | 223      | Total | C    | H    | N   | O   | S  | 0       | 5       | 0     |
|     |       |          | 3293  | 1038 | 1624 | 291 | 326 | 14 |         |         |       |

- Molecule 2 is BENZAMIDINE (CCD ID: BEN) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



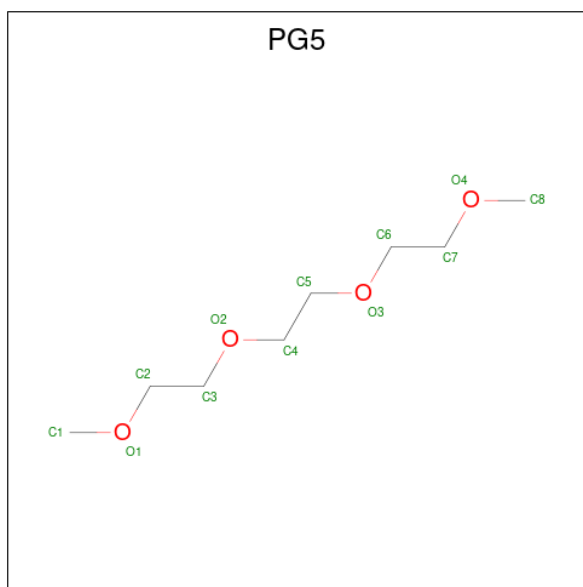
| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C | H | N | 0       | 0       |
|     |       |          | 17    | 7 | 8 | 2 |         |         |
| 2   | B     | 1        | Total | C | H | N | 0       | 0       |
|     |       |          | 17    | 7 | 8 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 2   | B     | 1        | Total | C  | H  | N | 0       | 0       |
|     |       |          | 17    | 7  | 8  | 2 |         |         |
| 2   | B     | 1        | Total | C  | H  | N | 0       | 0       |
|     |       |          | 17    | 7  | 8  | 2 |         |         |
| 2   | C     | 1        | Total | C  | H  | N | 0       | 0       |
|     |       |          | 17    | 7  | 8  | 2 |         |         |
| 2   | C     | 1        | Total | C  | H  | N | 0       | 0       |
|     |       |          | 17    | 7  | 8  | 2 |         |         |
| 2   | C     | 1        | Total | C  | H  | N | 0       | 0       |
|     |       |          | 17    | 7  | 8  | 2 |         |         |
| 2   | D     | 1        | Total | C  | H  | N | 0       | 0       |
|     |       |          | 17    | 7  | 8  | 2 |         |         |
| 2   | D     | 1        | Total | C  | H  | N | 0       | 1       |
|     |       |          | 34    | 14 | 16 | 4 |         |         |
| 2   | D     | 1        | Total | C  | H  | N | 0       | 0       |
|     |       |          | 17    | 7  | 8  | 2 |         |         |

- Molecule 3 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (CCD ID: PG5) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>4</sub>).



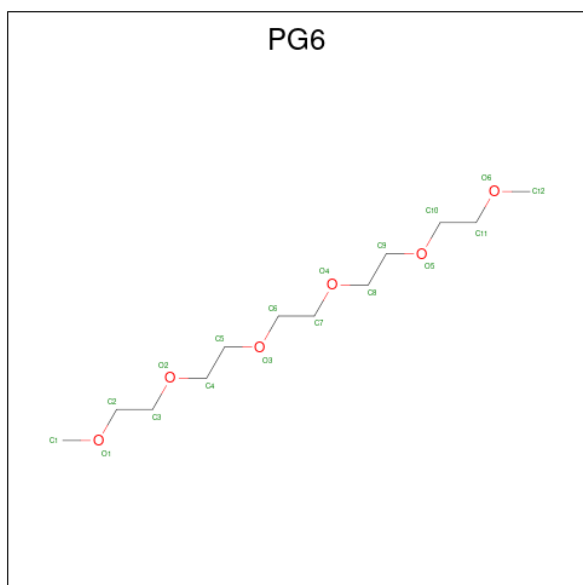
| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 30    | 8 | 18 | 4 |         |         |
| 3   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 30    | 8 | 18 | 4 |         |         |
| 3   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 30    | 8 | 18 | 4 |         |         |

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| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 3   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 30    | 8 | 18 | 4 |         |         |
| 3   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 30    | 8 | 18 | 4 |         |         |
| 3   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 30    | 8 | 18 | 4 |         |         |
| 3   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 30    | 8 | 18 | 4 |         |         |
| 3   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 30    | 8 | 18 | 4 |         |         |
| 3   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 30    | 8 | 18 | 4 |         |         |
| 3   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 29    | 8 | 17 | 4 |         |         |
| 3   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 30    | 8 | 18 | 4 |         |         |
| 3   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 30    | 8 | 18 | 4 |         |         |

- Molecule 4 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANE (CCD ID: PG6) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 4   | A     | 1        | Total | C  | H  | O | 0       | 0       |
|     |       |          | 44    | 12 | 26 | 6 |         |         |

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 5   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 1       |
|     |       |          | 34    | 8 | 20 | 6 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 16    | 4 | 9  | 3 |         |         |
| 5   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 5   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | C     | 1        | Total | C | H  | O | 0       | 1       |
|     |       |          | 34    | 8 | 20 | 6 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 1       |
|     |       |          | 34    | 8 | 20 | 6 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 16    | 4 | 9  | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 15    | 4 | 8  | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |

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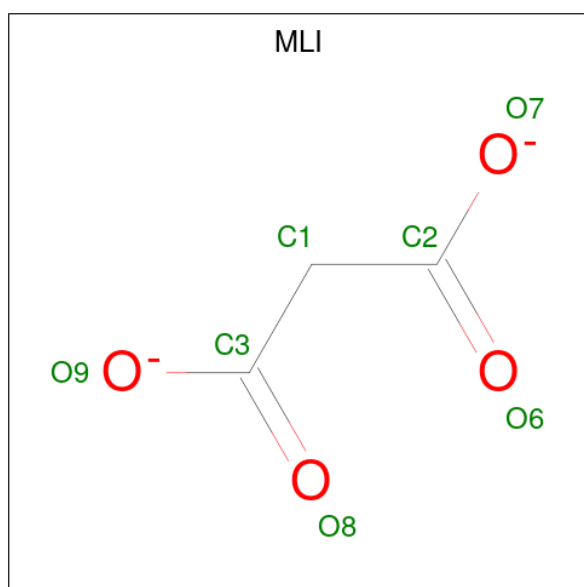
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| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 5   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

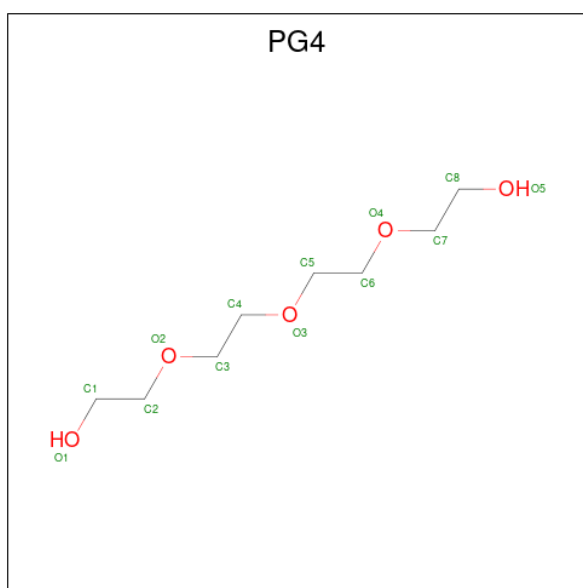
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | B     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | C     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | D     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 7 is MALONATE ION (CCD ID: MLI) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 7   | A     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 9     | 3 | 2 | 4 |         |         |
| 7   | B     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 9     | 3 | 2 | 4 |         |         |
| 7   | C     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 9     | 3 | 2 | 4 |         |         |
| 7   | D     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 9     | 3 | 2 | 4 |         |         |

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



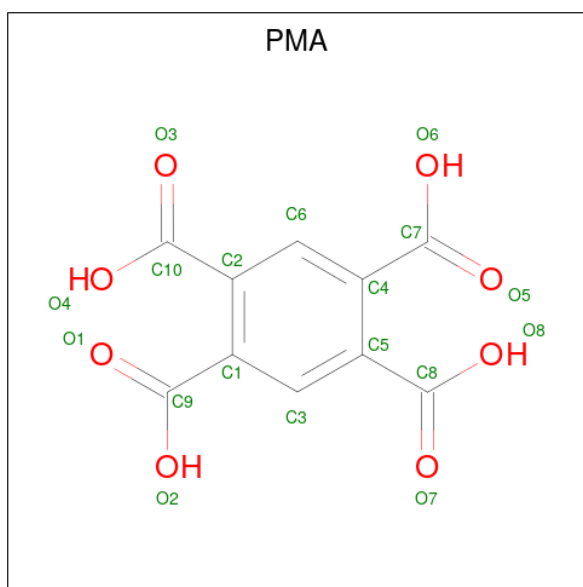
| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 8   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 29    | 8 | 17 | 4 |         |         |
| 8   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 30    | 8 | 17 | 5 |         |         |
| 8   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |
| 8   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |
| 8   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |
| 8   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |
| 8   | B     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |
| 8   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 8   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |
| 8   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |
| 8   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |
| 8   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |
| 8   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |
| 8   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |
| 8   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |
| 8   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |
| 8   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 31    | 8 | 18 | 5 |         |         |

- Molecule 9 is PYROMELLITIC ACID (CCD ID: PMA) (formula:  $C_{10}H_6O_8$ ) (labeled as "Ligand of Interest" by depositor).



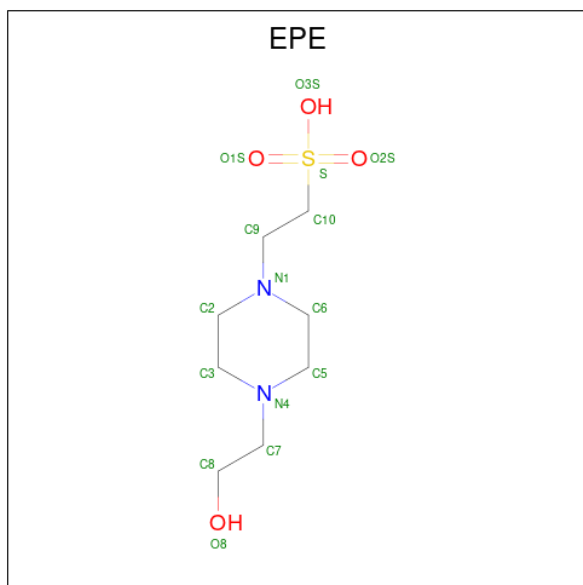
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 9   | B     | 1        | Total | C  | H | O | 0       | 0       |
|     |       |          | 20    | 10 | 2 | 8 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 9   | D     | 1        | Total | C  | H | O | 0       | 0       |
|     |       |          | 20    | 10 | 2 | 8 |         |         |

- Molecule 10 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---|---|---------|---------|
| 10  | C     | 1        | Total | C | H  | N | O | S | 0       | 0       |
|     |       |          | 31    | 8 | 16 | 2 | 4 | 1 |         |         |
| 10  | D     | 1        | Total | C | H  | N | O | S | 0       | 0       |
|     |       |          | 32    | 8 | 17 | 2 | 4 | 1 |         |         |

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 11  | D     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 12 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 12  | A     | 292      | Total | O   | 0       | 7       |
|     |       |          | 294   | 294 |         |         |
| 12  | B     | 263      | Total | O   | 0       | 14      |
|     |       |          | 269   | 269 |         |         |

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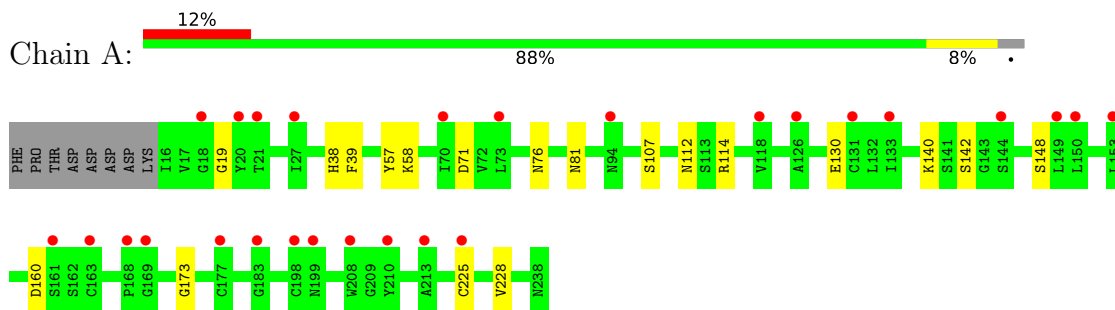
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 12  | C     | 358      | Total<br>361 | O<br>361 | 0       | 8       |
| 12  | D     | 344      | Total<br>347 | O<br>347 | 0       | 6       |

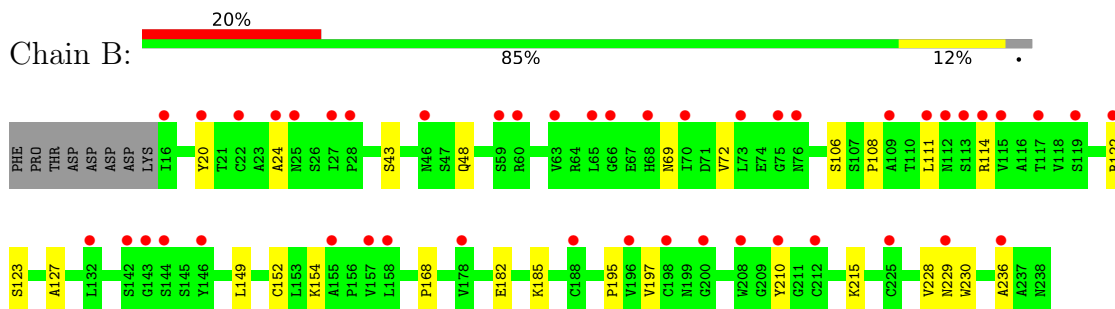
### 3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

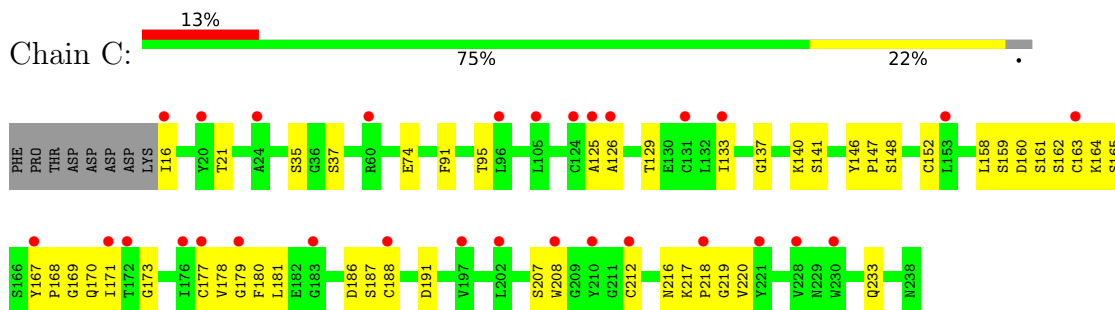
- Molecule 1: Trypsin



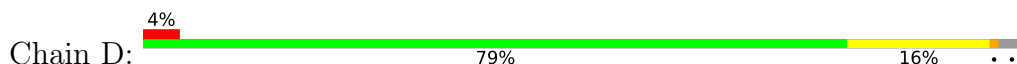
- Molecule 1: Trypsin

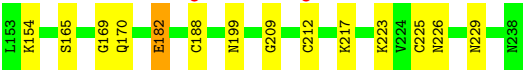
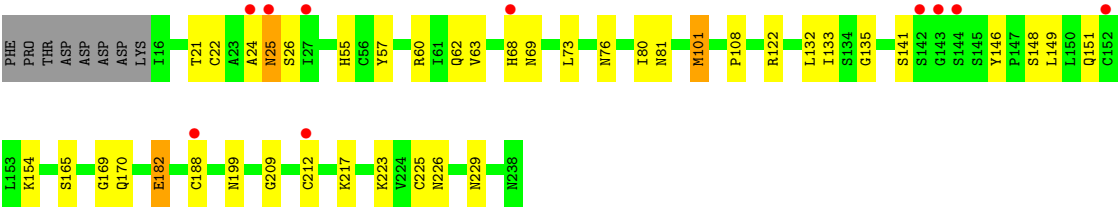


- Molecule 1: Trypsin



- Molecule 1: Trypsin





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 70.66Å 50.72Å 125.69Å<br>90.00° 99.52° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 39.25 – 1.18<br>39.25 – 1.18                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.1 (39.25-1.18)<br>91.1 (39.25-1.18)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.06                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.60 (at 1.18Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.21.1_5286                                          | Depositor        |
| R, $R_{free}$                                                           | 0.195 , 0.230<br>0.195 , 0.230                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 13014 reflections (4.52%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 15.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.214                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 45.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.97                                                        | EDS              |
| Total number of atoms                                                   | 16671                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 28.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0847e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PMA, BEN, CA, PG4, MLI, PG5, PEG, EPE, PG6, CL

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

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$   |
| 1   | A     | 0.55         | 0/1689      | 0.71        | 0/2293        |
| 1   | B     | 0.47         | 0/1674      | 0.63        | 0/2273        |
| 1   | C     | 0.61         | 0/1674      | 0.74        | 0/2273        |
| 1   | D     | 0.62         | 0/1713      | 0.74        | 1/2326 (0.0%) |
| All | All   | 0.56         | 0/6750      | 0.71        | 1/9165 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1   | D     | 101 | MET  | CA-CB-CG | 5.32 | 124.73      | 114.10   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1654  | 1604     | 1605     | 18      | 3            |
| 1   | B     | 1642  | 1596     | 1595     | 31      | 1            |
| 1   | C     | 1642  | 1595     | 1595     | 105     | 0            |
| 1   | D     | 1669  | 1624     | 1630     | 69      | 2            |
| 2   | A     | 9     | 8        | 7        | 0       | 0            |
| 2   | B     | 27    | 24       | 21       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | C     | 27    | 24       | 21       | 4       | 0            |
| 2   | D     | 36    | 32       | 28       | 1       | 0            |
| 3   | A     | 36    | 54       | 54       | 6       | 0            |
| 3   | B     | 48    | 72       | 72       | 8       | 0            |
| 3   | C     | 24    | 36       | 36       | 4       | 0            |
| 3   | D     | 36    | 53       | 54       | 8       | 0            |
| 4   | A     | 18    | 26       | 26       | 2       | 0            |
| 5   | A     | 56    | 80       | 80       | 3       | 0            |
| 5   | B     | 133   | 189      | 190      | 24      | 0            |
| 5   | C     | 112   | 160      | 160      | 26      | 0            |
| 5   | D     | 147   | 207      | 210      | 27      | 1            |
| 6   | A     | 1     | 0        | 0        | 0       | 0            |
| 6   | B     | 1     | 0        | 0        | 0       | 0            |
| 6   | C     | 1     | 0        | 0        | 0       | 0            |
| 6   | D     | 2     | 0        | 0        | 0       | 0            |
| 7   | A     | 7     | 2        | 2        | 1       | 0            |
| 7   | B     | 7     | 2        | 2        | 1       | 0            |
| 7   | C     | 7     | 2        | 2        | 0       | 0            |
| 7   | D     | 7     | 2        | 2        | 0       | 0            |
| 8   | A     | 51    | 70       | 69       | 3       | 2            |
| 8   | B     | 39    | 54       | 54       | 7       | 0            |
| 8   | C     | 65    | 90       | 90       | 11      | 0            |
| 8   | D     | 78    | 108      | 108      | 14      | 4            |
| 9   | B     | 18    | 2        | 2        | 3       | 0            |
| 9   | D     | 18    | 2        | 2        | 4       | 0            |
| 10  | C     | 15    | 16       | 18       | 3       | 0            |
| 10  | D     | 15    | 17       | 17       | 3       | 0            |
| 11  | D     | 1     | 0        | 0        | 0       | 1            |
| 12  | A     | 294   | 0        | 0        | 13      | 10           |
| 12  | B     | 269   | 0        | 0        | 23      | 10           |
| 12  | C     | 361   | 0        | 0        | 97      | 14           |
| 12  | D     | 347   | 0        | 0        | 61      | 5            |
| All | All   | 8920  | 7751     | 7752     | 303     | 28           |

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 20.

All (303) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:D:225:CYS:SG | 12:D:419:HOH:O | 1.92                     | 1.26              |

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| Atom-1             | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------|--------------------------|-------------------|
| 1:C:177:CYS:SG     | 12:C:679:HOH:O | 1.91                     | 1.25              |
| 1:D:101:MET:SD     | 12:D:682:HOH:O | 1.96                     | 1.22              |
| 1:C:188:CYS:SG     | 12:C:580:HOH:O | 2.02                     | 1.18              |
| 1:C:163:CYS:SG     | 12:C:679:HOH:O | 2.02                     | 1.15              |
| 1:A:142:SER:O      | 12:A:401:HOH:O | 1.68                     | 1.11              |
| 1:C:161:SER:O      | 12:C:403:HOH:O | 1.67                     | 1.09              |
| 1:C:126:ALA:O      | 12:C:404:HOH:O | 1.69                     | 1.09              |
| 1:D:229[A]:ASN:OD1 | 8:D:333:PG4:O5 | 1.71                     | 1.07              |
| 1:C:164:LYS:N      | 12:C:403:HOH:O | 1.90                     | 1.03              |
| 1:C:178:VAL:O      | 12:C:407:HOH:O | 1.77                     | 1.03              |
| 1:C:163:CYS:O      | 12:C:405:HOH:O | 1.74                     | 1.02              |
| 3:D:312:PG5:O1     | 12:D:401:HOH:O | 1.78                     | 1.00              |
| 1:C:161:SER:O      | 12:C:406:HOH:O | 1.77                     | 1.00              |
| 1:C:167:TYR:OH     | 12:C:408:HOH:O | 1.79                     | 0.99              |
| 5:D:335:PEG:O4     | 12:D:403:HOH:O | 1.82                     | 0.98              |
| 1:D:135:GLY:O      | 12:D:402:HOH:O | 1.81                     | 0.98              |
| 1:B:229:ASN:OD1    | 12:B:402:HOH:O | 1.81                     | 0.97              |
| 1:C:233:GLN:OE1    | 12:C:409:HOH:O | 1.81                     | 0.97              |
| 9:B:302:PMA:O3     | 12:B:403:HOH:O | 1.81                     | 0.96              |
| 1:C:212:CYS:SG     | 12:C:470:HOH:O | 2.22                     | 0.96              |
| 1:D:25[A]:ASN:ND2  | 12:D:410:HOH:O | 2.00                     | 0.95              |
| 1:C:187:SER:O      | 12:C:410:HOH:O | 1.83                     | 0.95              |
| 1:D:151:GLN:O      | 12:D:402:HOH:O | 1.84                     | 0.94              |
| 1:D:199:ASN:OD1    | 12:D:404:HOH:O | 1.86                     | 0.94              |
| 1:B:106:SER:O      | 12:B:405:HOH:O | 1.87                     | 0.93              |
| 1:C:219:GLY:O      | 12:C:407:HOH:O | 1.84                     | 0.93              |
| 1:C:158:LEU:HD11   | 12:C:476:HOH:O | 1.70                     | 0.91              |
| 1:D:63:VAL:O       | 12:D:405:HOH:O | 1.89                     | 0.91              |
| 1:D:169:GLY:O      | 12:D:401:HOH:O | 1.88                     | 0.90              |
| 1:C:140:LYS:NZ     | 12:C:420:HOH:O | 2.04                     | 0.90              |
| 1:C:233:GLN:OE1    | 12:C:411:HOH:O | 1.88                     | 0.90              |
| 1:C:212:CYS:SG     | 12:C:410:HOH:O | 2.30                     | 0.89              |
| 1:C:133:ILE:O      | 12:C:413:HOH:O | 1.90                     | 0.88              |
| 1:C:91:PHE:O       | 12:C:412:HOH:O | 1.90                     | 0.88              |
| 5:C:316:PEG:O4     | 12:C:415:HOH:O | 1.93                     | 0.86              |
| 1:D:212:CYS:O      | 12:D:407:HOH:O | 1.92                     | 0.86              |
| 1:C:191:ASP:OD2    | 12:C:414:HOH:O | 1.92                     | 0.85              |
| 1:C:186:ASP:CG     | 12:C:401:HOH:O | 2.19                     | 0.85              |
| 1:C:141:SER:O      | 12:C:416:HOH:O | 1.93                     | 0.85              |
| 5:B:316:PEG:O4     | 12:B:404:HOH:O | 1.85                     | 0.84              |
| 5:C:312:PEG:O4     | 12:C:417:HOH:O | 1.94                     | 0.84              |

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| Atom-1             | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-----------------|--------------------------|-------------------|
| 5:D:335:PEG:O1     | 12:D:408:HOH:O  | 1.95                     | 0.84              |
| 1:C:216:ASN:HA     | 12:C:430:HOH:O  | 1.76                     | 0.83              |
| 5:B:317[A]:PEG:O4  | 12:B:407:HOH:O  | 1.97                     | 0.83              |
| 5:B:317[B]:PEG:O4  | 12:B:408:HOH:O  | 1.97                     | 0.82              |
| 1:C:186:ASP:OD2    | 12:C:418:HOH:O  | 1.96                     | 0.82              |
| 1:C:16:ILE:N       | 12:C:423:HOH:O  | 2.13                     | 0.81              |
| 1:C:188:CYS:HA     | 12:C:410:HOH:O  | 1.78                     | 0.81              |
| 1:D:209:GLY:O      | 12:D:409:HOH:O  | 1.99                     | 0.81              |
| 5:B:316:PEG:O4     | 12:B:409:HOH:O  | 1.99                     | 0.80              |
| 1:C:188:CYS:O      | 12:C:414:HOH:O  | 2.00                     | 0.80              |
| 1:D:22:CYS:O       | 12:D:411:HOH:O  | 2.00                     | 0.79              |
| 1:C:191:ASP:CG     | 12:C:414:HOH:O  | 2.26                     | 0.78              |
| 1:D:151:GLN:N      | 12:D:402:HOH:O  | 2.14                     | 0.78              |
| 1:A:130[B]:GLU:OE1 | 12:A:405:HOH:O  | 1.95                     | 0.78              |
| 5:B:306:PEG:O4     | 12:B:410:HOH:O  | 2.02                     | 0.77              |
| 9:B:302:PMA:O2     | 12:B:403:HOH:O  | 2.00                     | 0.77              |
| 1:C:165:SER:N      | 12:C:403:HOH:O  | 1.96                     | 0.77              |
| 1:C:167:TYR:CE2    | 12:C:402:HOH:O  | 2.38                     | 0.76              |
| 8:B:330:PG4:O5     | 12:B:411:HOH:O  | 2.03                     | 0.76              |
| 1:B:24:ALA:O       | 12:B:412:HOH:O  | 2.04                     | 0.75              |
| 1:C:21:THR:N       | 12:C:422:HOH:O  | 2.18                     | 0.75              |
| 1:B:152:CYS:SG     | 12:B:539:HOH:O  | 2.45                     | 0.74              |
| 1:A:225:CYS:O      | 12:A:406:HOH:O  | 2.04                     | 0.74              |
| 1:C:218:PRO:N      | 12:C:402:HOH:O  | 2.22                     | 0.73              |
| 1:C:217:LYS:C      | 12:C:402:HOH:O  | 2.31                     | 0.72              |
| 1:C:164:LYS:HA     | 5:C:308:PEG:H41 | 1.71                     | 0.71              |
| 1:C:181:LEU:HD22   | 12:C:430:HOH:O  | 1.89                     | 0.71              |
| 1:D:229[B]:ASN:OD1 | 12:D:413:HOH:O  | 2.09                     | 0.71              |
| 3:D:312:PG5:H41    | 12:D:487:HOH:O  | 1.91                     | 0.70              |
| 1:D:57:TYR:HA      | 12:D:682:HOH:O  | 1.91                     | 0.70              |
| 1:D:108:PRO:HG3    | 5:D:317:PEG:H11 | 1.72                     | 0.70              |
| 1:C:164:LYS:CA     | 5:C:308:PEG:H41 | 2.22                     | 0.70              |
| 1:C:181:LEU:HB3    | 12:C:430:HOH:O  | 1.92                     | 0.69              |
| 5:D:319:PEG:C1     | 5:D:320:PEG:H32 | 2.23                     | 0.69              |
| 2:C:301:BEN:N2     | 12:C:401:HOH:O  | 2.25                     | 0.69              |
| 1:B:114:ARG:NH1    | 12:B:415:HOH:O  | 2.22                     | 0.68              |
| 1:C:164:LYS:HB2    | 12:C:406:HOH:O  | 1.92                     | 0.68              |
| 1:B:210:TYR:CG     | 2:B:304:BEN:H3  | 2.29                     | 0.68              |
| 1:D:25[B]:ASN:ND2  | 12:D:412:HOH:O  | 2.01                     | 0.67              |
| 1:A:140:LYS:HD3    | 12:A:401:HOH:O  | 1.94                     | 0.67              |
| 1:C:16:ILE:CA      | 12:C:423:HOH:O  | 2.43                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:21:THR:OG1   | 12:C:422:HOH:O    | 2.11                     | 0.66              |
| 1:D:62:GLN:HG2   | 12:D:405:HOH:O    | 1.95                     | 0.66              |
| 1:B:123:SER:OG   | 8:B:329:PG4:H51   | 1.96                     | 0.66              |
| 1:C:181:LEU:CB   | 12:C:430:HOH:O    | 2.44                     | 0.66              |
| 1:C:218:PRO:HB3  | 12:C:476:HOH:O    | 1.96                     | 0.65              |
| 1:D:76:ASN:ND2   | 12:D:417:HOH:O    | 2.19                     | 0.65              |
| 1:C:129:THR:HB   | 12:C:404:HOH:O    | 1.97                     | 0.65              |
| 1:A:173:GLY:O    | 12:A:407:HOH:O    | 2.15                     | 0.64              |
| 1:C:74:GLU:OE2   | 12:C:493[B]:HOH:O | 2.15                     | 0.64              |
| 1:D:182:GLU:OE2  | 12:D:415:HOH:O    | 2.15                     | 0.63              |
| 1:C:129:THR:CB   | 12:C:404:HOH:O    | 2.45                     | 0.63              |
| 1:B:228:VAL:HG11 | 3:B:307:PG5:H41   | 1.80                     | 0.62              |
| 1:C:207:SER:HB3  | 12:C:428:HOH:O    | 1.98                     | 0.62              |
| 1:B:210:TYR:HB3  | 2:B:304:BEN:H2    | 1.82                     | 0.62              |
| 1:C:168:PRO:HA   | 5:C:308:PEG:H42   | 1.81                     | 0.61              |
| 1:C:179:GLY:C    | 12:C:476:HOH:O    | 2.43                     | 0.61              |
| 1:C:208:TRP:CD1  | 12:C:428:HOH:O    | 2.53                     | 0.61              |
| 1:C:217:LYS:NZ   | 5:C:320:PEG:O1    | 2.33                     | 0.61              |
| 1:D:68:HIS:CE1   | 12:D:411:HOH:O    | 2.53                     | 0.61              |
| 1:D:60:ARG:NH1   | 12:D:423:HOH:O    | 2.33                     | 0.61              |
| 1:D:21:THR:HG21  | 8:D:331:PG4:H51   | 1.82                     | 0.61              |
| 1:D:81:ASN:HB3   | 8:D:329:PG4:H12   | 1.83                     | 0.61              |
| 5:B:324:PEG:O4   | 12:B:406:HOH:O    | 1.92                     | 0.60              |
| 1:C:220:VAL:C    | 12:C:428:HOH:O    | 2.44                     | 0.60              |
| 5:D:319:PEG:C2   | 5:D:320:PEG:H32   | 2.30                     | 0.60              |
| 3:A:304:PG5:O4   | 12:A:409:HOH:O    | 2.16                     | 0.60              |
| 2:C:301:BEN:C    | 12:C:401:HOH:O    | 2.48                     | 0.60              |
| 1:C:125:ALA:HB1  | 12:C:404:HOH:O    | 2.02                     | 0.60              |
| 7:A:311:MLI:O9   | 12:A:408:HOH:O    | 2.16                     | 0.59              |
| 5:D:308:PEG:H12  | 12:D:593:HOH:O    | 2.03                     | 0.59              |
| 5:A:306:PEG:O4   | 12:A:403:HOH:O    | 1.84                     | 0.59              |
| 3:D:303:PG5:H13  | 3:D:304:PG5:H42   | 1.83                     | 0.59              |
| 1:B:108:PRO:HB2  | 3:B:305:PG5:H42   | 1.85                     | 0.58              |
| 9:D:302:PMA:H6   | 8:D:333:PG4:H51   | 1.85                     | 0.58              |
| 2:C:301:BEN:C    | 12:C:410:HOH:O    | 2.51                     | 0.58              |
| 1:A:148:SER:H    | 8:A:317:PG4:H42   | 1.68                     | 0.58              |
| 1:D:62:GLN:CG    | 12:D:405:HOH:O    | 2.49                     | 0.58              |
| 1:A:107:SER:OG   | 12:A:410:HOH:O    | 2.17                     | 0.58              |
| 1:D:217:LYS:O    | 12:D:416:HOH:O    | 2.17                     | 0.57              |
| 1:C:167:TYR:O    | 5:C:308:PEG:H42   | 2.04                     | 0.57              |
| 9:D:302:PMA:C6   | 8:D:333:PG4:H51   | 2.35                     | 0.56              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 8:D:329:PG4:C6   | 12:D:459:HOH:O     | 2.54                     | 0.56              |
| 1:C:161:SER:OG   | 5:C:316:PEG:H22    | 2.06                     | 0.56              |
| 1:D:148:SER:OG   | 5:D:320:PEG:H42    | 2.05                     | 0.55              |
| 1:B:123:SER:OG   | 8:B:329:PG4:C5     | 2.53                     | 0.55              |
| 1:D:80:ILE:N     | 12:D:405:HOH:O     | 2.29                     | 0.55              |
| 1:D:24:ALA:CB    | 12:D:690:HOH:O     | 2.55                     | 0.55              |
| 3:D:312:PG5:C3   | 12:D:433:HOH:O     | 2.55                     | 0.55              |
| 1:B:149:LEU:HD12 | 1:B:149:LEU:N      | 2.22                     | 0.54              |
| 1:D:182:GLU:H    | 1:D:182:GLU:CD     | 2.14                     | 0.54              |
| 8:D:330:PG4:H22  | 12:D:621:HOH:O     | 2.07                     | 0.54              |
| 1:C:147:PRO:HA   | 8:C:324:PG4:H61    | 1.89                     | 0.54              |
| 1:D:108:PRO:CG   | 5:D:317:PEG:H11    | 2.38                     | 0.54              |
| 1:B:154:LYS:NZ   | 12:B:424:HOH:O     | 2.41                     | 0.53              |
| 1:C:152:CYS:HA   | 12:C:447:HOH:O     | 2.07                     | 0.53              |
| 1:C:173:GLY:O    | 12:C:426:HOH:O     | 2.18                     | 0.53              |
| 2:D:309:BEN:H4   | 12:D:477:HOH:O     | 2.08                     | 0.53              |
| 1:C:217:LYS:HB3  | 12:C:408:HOH:O     | 2.08                     | 0.53              |
| 1:C:164:LYS:HB3  | 5:C:308:PEG:H31    | 1.90                     | 0.53              |
| 5:D:319:PEG:O2   | 5:D:320:PEG:H21    | 2.09                     | 0.53              |
| 1:B:168:PRO:HG3  | 5:B:319:PEG:H42    | 1.91                     | 0.53              |
| 1:C:140:LYS:HD3  | 12:C:472:HOH:O     | 2.07                     | 0.53              |
| 1:C:162:SER:C    | 12:C:403:HOH:O     | 2.52                     | 0.53              |
| 1:D:141:SER:HA   | 8:D:330:PG4:H11    | 1.90                     | 0.53              |
| 1:C:146:TYR:O    | 8:C:325:PG4:H72    | 2.09                     | 0.53              |
| 5:D:337:PEG:H31  | 12:D:670:HOH:O     | 2.08                     | 0.52              |
| 1:C:171:ILE:C    | 12:C:434:HOH:O     | 2.52                     | 0.52              |
| 3:B:311:PG5:H81  | 7:B:321:MLI:H12    | 1.92                     | 0.52              |
| 1:C:180:PHE:O    | 12:C:424:HOH:O     | 2.18                     | 0.52              |
| 1:C:159:SER:HB2  | 5:C:309:PEG:H32    | 1.92                     | 0.51              |
| 1:A:71:ASP:OD2   | 3:A:302:PG5:H52    | 2.10                     | 0.51              |
| 1:C:158:LEU:CB   | 12:C:429:HOH:O     | 2.58                     | 0.51              |
| 3:B:311:PG5:H83  | 5:B:317[A]:PEG:H21 | 1.91                     | 0.51              |
| 1:D:25[A]:ASN:HA | 12:D:432:HOH:O     | 2.11                     | 0.51              |
| 1:C:165:SER:N    | 12:C:406:HOH:O     | 2.44                     | 0.51              |
| 1:C:167:TYR:HB2  | 12:C:405:HOH:O     | 2.11                     | 0.51              |
| 1:C:35:SER:OG    | 12:C:425:HOH:O     | 2.18                     | 0.50              |
| 1:C:146:TYR:HB3  | 8:C:325:PG4:H61    | 1.92                     | 0.50              |
| 1:C:158:LEU:HB2  | 12:C:429:HOH:O     | 2.09                     | 0.50              |
| 1:D:226:ASN:N    | 12:D:419:HOH:O     | 2.44                     | 0.50              |
| 1:B:230:TRP:HB2  | 5:B:325:PEG:H21    | 1.94                     | 0.50              |
| 1:C:161:SER:OG   | 5:C:309:PEG:O2     | 2.29                     | 0.50              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:B:311:PG5:H83     | 5:B:317[B]:PEG:H21 | 1.92                     | 0.50              |
| 1:C:129:THR:OG1     | 12:C:404:HOH:O     | 2.17                     | 0.50              |
| 1:C:164:LYS:HA      | 12:C:405:HOH:O     | 2.11                     | 0.50              |
| 10:D:305:EPE:H71    | 12:D:548:HOH:O     | 2.11                     | 0.50              |
| 1:D:146:TYR:O       | 5:D:320:PEG:H41    | 2.11                     | 0.49              |
| 1:C:164:LYS:CA      | 12:C:403:HOH:O     | 2.48                     | 0.49              |
| 1:D:68:HIS:CE1      | 1:D:149:LEU:HB3    | 2.47                     | 0.49              |
| 1:A:57:TYR:O        | 8:A:318:PG4:H61    | 2.12                     | 0.49              |
| 1:B:111:LEU:H       | 3:B:305:PG5:H71    | 1.77                     | 0.49              |
| 1:C:181:LEU:CD2     | 12:C:430:HOH:O     | 2.53                     | 0.49              |
| 1:D:25[B]:ASN:ND2   | 12:D:420:HOH:O     | 2.30                     | 0.49              |
| 5:D:321:PEG:H32     | 5:D:322:PEG:C2     | 2.43                     | 0.49              |
| 1:C:180:PHE:C       | 12:C:424:HOH:O     | 2.54                     | 0.49              |
| 1:B:20:TYR:HB2      | 5:B:317[A]:PEG:H31 | 1.95                     | 0.49              |
| 5:D:321:PEG:H32     | 5:D:322:PEG:H22    | 1.96                     | 0.48              |
| 1:C:148:SER:H       | 8:C:324:PG4:C6     | 2.26                     | 0.48              |
| 8:C:325:PG4:H82     | 12:C:417:HOH:O     | 2.13                     | 0.48              |
| 1:B:236:ALA:O       | 5:B:312:PEG:H31    | 2.14                     | 0.48              |
| 5:D:319:PEG:O2      | 5:D:320:PEG:C2     | 2.62                     | 0.48              |
| 1:A:160:ASP:H       | 4:A:303:PG6:H11    | 1.79                     | 0.48              |
| 8:C:324:PG4:H42     | 12:C:449:HOH:O     | 2.14                     | 0.47              |
| 1:D:25[B]:ASN:HA    | 12:D:432:HOH:O     | 2.14                     | 0.47              |
| 5:D:319:PEG:H22     | 5:D:320:PEG:H32    | 1.96                     | 0.47              |
| 1:D:63:VAL:N        | 12:D:405:HOH:O     | 2.45                     | 0.47              |
| 1:D:229[A]:ASN:HB3  | 8:D:333:PG4:H52    | 1.97                     | 0.47              |
| 9:B:302:PMA:O3      | 9:B:302:PMA:O2     | 2.32                     | 0.47              |
| 1:B:69:ASN:CG       | 1:B:72:VAL:HG22    | 2.39                     | 0.47              |
| 1:C:181:LEU:HA      | 12:C:424:HOH:O     | 2.14                     | 0.47              |
| 1:C:161:SER:OG      | 5:C:316:PEG:C2     | 2.63                     | 0.47              |
| 1:C:164:LYS:HE2     | 5:C:308:PEG:H12    | 1.97                     | 0.47              |
| 10:C:303:EPE:H72    | 12:C:474:HOH:O     | 2.13                     | 0.47              |
| 3:C:306:PG5:H82     | 8:C:322:PG4:H71    | 1.96                     | 0.47              |
| 8:A:316:PG4:O4      | 8:A:316:PG4:H42    | 2.15                     | 0.47              |
| 1:D:151:GLN:CA      | 12:D:402:HOH:O     | 2.60                     | 0.47              |
| 1:D:132[B]:LEU:HD23 | 1:D:133:ILE:N      | 2.30                     | 0.47              |
| 1:C:133:ILE:HG13    | 12:C:431:HOH:O     | 2.14                     | 0.46              |
| 8:C:326:PG4:C1      | 12:C:538:HOH:O     | 2.63                     | 0.46              |
| 1:C:167:TYR:N       | 12:C:405:HOH:O     | 2.30                     | 0.46              |
| 1:D:26:SER:N        | 12:D:432:HOH:O     | 2.49                     | 0.46              |
| 5:A:307:PEG:O1      | 12:A:402:HOH:O     | 1.76                     | 0.46              |
| 1:B:197:VAL:HG11    | 5:B:309:PEG:H42    | 1.98                     | 0.46              |

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| Atom-1          | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|--------------------|--------------------------|-------------------|
| 1:D:122:ARG:HG2 | 3:D:303:PG5:H71    | 1.98                     | 0.46              |
| 1:D:223:LYS:HG2 | 12:D:419:HOH:O     | 2.16                     | 0.46              |
| 5:C:312:PEG:H21 | 8:C:325:PG4:O3     | 2.16                     | 0.46              |
| 1:C:126:ALA:N   | 12:C:404:HOH:O     | 2.48                     | 0.46              |
| 1:C:168:PRO:HA  | 5:C:308:PEG:H32    | 1.97                     | 0.46              |
| 1:D:108:PRO:HB3 | 5:D:317:PEG:H42    | 1.98                     | 0.46              |
| 1:C:168:PRO:CA  | 5:C:308:PEG:H42    | 2.45                     | 0.46              |
| 5:D:316:PEG:H32 | 5:D:327:PEG:H21    | 1.97                     | 0.46              |
| 1:B:20:TYR:HA   | 12:B:407:HOH:O     | 2.16                     | 0.45              |
| 1:A:58:LYS:HA   | 3:A:305:PG5:H21    | 1.98                     | 0.45              |
| 1:C:164:LYS:HE2 | 10:C:303:EPE:H31   | 1.98                     | 0.45              |
| 1:C:188:CYS:C   | 12:C:414:HOH:O     | 2.52                     | 0.45              |
| 5:C:316:PEG:H21 | 12:C:440:HOH:O     | 2.17                     | 0.45              |
| 3:D:312:PG5:H31 | 12:D:433:HOH:O     | 2.16                     | 0.45              |
| 1:A:58:LYS:CB   | 3:A:305:PG5:H21    | 2.47                     | 0.45              |
| 1:B:114:ARG:NH2 | 12:B:436:HOH:O     | 2.49                     | 0.45              |
| 1:C:218:PRO:HB3 | 12:C:424:HOH:O     | 2.17                     | 0.45              |
| 1:A:81:ASN:HB3  | 12:A:633:HOH:O     | 2.16                     | 0.45              |
| 1:D:199:ASN:HB3 | 12:D:620:HOH:O     | 2.17                     | 0.45              |
| 1:C:167:TYR:HE2 | 12:C:402:HOH:O     | 1.88                     | 0.45              |
| 9:D:302:PMA:C1  | 8:D:333:PG4:H82    | 2.47                     | 0.45              |
| 5:B:309:PEG:O1  | 12:B:401:HOH:O     | 1.67                     | 0.44              |
| 5:C:309:PEG:H31 | 12:C:440:HOH:O     | 2.16                     | 0.44              |
| 1:D:170:GLN:HA  | 12:D:401:HOH:O     | 2.16                     | 0.44              |
| 5:B:325:PEG:O2  | 8:B:330:PG4:H71    | 2.17                     | 0.44              |
| 1:C:179:GLY:CA  | 12:C:476:HOH:O     | 2.64                     | 0.44              |
| 1:D:69:ASN:HD22 | 5:D:318[A]:PEG:C2  | 2.30                     | 0.44              |
| 1:B:48:GLN:NE2  | 12:B:413:HOH:O     | 2.19                     | 0.44              |
| 5:B:316:PEG:H22 | 12:B:407:HOH:O     | 2.18                     | 0.44              |
| 1:C:152:CYS:CA  | 12:C:447:HOH:O     | 2.66                     | 0.44              |
| 1:B:20:TYR:HB2  | 5:B:317[B]:PEG:H31 | 1.98                     | 0.44              |
| 1:B:229:ASN:HB3 | 5:B:325:PEG:O4     | 2.16                     | 0.44              |
| 8:C:326:PG4:H81 | 12:C:707:HOH:O     | 2.18                     | 0.44              |
| 1:C:164:LYS:CB  | 5:C:308:PEG:H41    | 2.48                     | 0.44              |
| 3:B:305:PG5:H51 | 12:B:524:HOH:O     | 2.18                     | 0.43              |
| 5:C:309:PEG:C4  | 12:C:440:HOH:O     | 2.66                     | 0.43              |
| 1:D:225:CYS:C   | 12:D:419:HOH:O     | 2.61                     | 0.43              |
| 5:D:321:PEG:H22 | 5:D:322:PEG:H22    | 1.99                     | 0.43              |
| 1:D:60:ARG:HG2  | 8:D:329:PG4:H61    | 1.99                     | 0.43              |
| 1:C:137:GLY:HA3 | 12:C:414:HOH:O     | 2.19                     | 0.43              |
| 4:A:303:PG6:H62 | 12:A:569:HOH:O     | 2.18                     | 0.43              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:B:230:TRP:HA      | 5:B:325:PEG:H32    | 2.01                     | 0.43              |
| 1:D:149:LEU:HD11    | 5:D:318[B]:PEG:H32 | 2.01                     | 0.43              |
| 3:D:303:PG5:H32     | 12:D:645:HOH:O     | 2.18                     | 0.43              |
| 1:B:197:VAL:HG11    | 5:B:309:PEG:C4     | 2.49                     | 0.42              |
| 2:B:303:BEN:H3      | 12:B:495:HOH:O     | 2.18                     | 0.42              |
| 5:C:312:PEG:H31     | 8:C:325:PG4:O4     | 2.18                     | 0.42              |
| 1:A:19:GLY:O        | 5:A:307:PEG:H31    | 2.18                     | 0.42              |
| 1:D:55:HIS:O        | 5:D:324:PEG:C1     | 2.67                     | 0.42              |
| 1:C:164:LYS:NZ      | 10:C:303:EPE:H71   | 2.35                     | 0.42              |
| 1:D:182:GLU:N       | 1:D:182:GLU:OE1    | 2.53                     | 0.42              |
| 5:D:336:PEG:H12     | 12:D:667:HOH:O     | 2.18                     | 0.42              |
| 1:D:25[A]:ASN:HA    | 12:D:633:HOH:O     | 2.20                     | 0.42              |
| 1:D:165:SER:HA      | 5:D:310:PEG:H41    | 2.00                     | 0.42              |
| 5:B:319:PEG:H31     | 12:B:533:HOH:O     | 2.18                     | 0.42              |
| 9:D:302:PMA:C4      | 8:D:333:PG4:H72    | 2.49                     | 0.42              |
| 1:B:149:LEU:HD22    | 3:B:311:PG5:H12    | 2.01                     | 0.42              |
| 1:C:160:ASP:H       | 3:C:306:PG5:C6     | 2.33                     | 0.42              |
| 1:C:167:TYR:OH      | 12:C:402:HOH:O     | 1.79                     | 0.42              |
| 3:C:306:PG5:H51     | 5:C:309:PEG:H32    | 2.02                     | 0.42              |
| 1:D:24:ALA:HA       | 12:D:690:HOH:O     | 2.19                     | 0.42              |
| 3:D:303:PG5:C3      | 12:D:645:HOH:O     | 2.68                     | 0.42              |
| 1:A:38:HIS:H        | 3:A:302:PG5:H81    | 1.85                     | 0.41              |
| 1:D:217:LYS:NZ      | 12:D:414:HOH:O     | 2.14                     | 0.41              |
| 5:D:320:PEG:H12     | 12:D:541:HOH:O     | 2.20                     | 0.41              |
| 2:C:301:BEN:N1      | 12:C:410:HOH:O     | 2.37                     | 0.41              |
| 5:B:308:PEG:H41     | 8:B:330:PG4:C4     | 2.51                     | 0.41              |
| 1:D:81:ASN:CB       | 8:D:329:PG4:H12    | 2.50                     | 0.41              |
| 1:A:39:PHE:HB3      | 3:A:304:PG5:H72    | 2.02                     | 0.41              |
| 1:A:228:VAL:HB      | 12:A:406:HOH:O     | 2.19                     | 0.41              |
| 1:D:132[A]:LEU:HD13 | 1:D:154:LYS:HE3    | 2.01                     | 0.41              |
| 1:B:43:SER:OG       | 1:B:195:PRO:HB3    | 2.21                     | 0.41              |
| 1:B:122:ARG:NH2     | 8:B:329:PG4:H21    | 2.35                     | 0.41              |
| 1:D:199:ASN:ND2     | 12:D:434:HOH:O     | 2.50                     | 0.41              |
| 1:C:95:THR:HG22     | 5:C:328[A]:PEG:H42 | 2.02                     | 0.41              |
| 10:D:305:EPE:H31    | 12:D:494:HOH:O     | 2.20                     | 0.41              |
| 1:A:76:ASN:CG       | 1:A:114:ARG:HD2    | 2.45                     | 0.41              |
| 1:C:37:SER:HA       | 5:C:312:PEG:O1     | 2.21                     | 0.41              |
| 1:C:220:VAL:HG12    | 12:C:428:HOH:O     | 2.20                     | 0.41              |
| 1:D:25[B]:ASN:HA    | 12:D:633:HOH:O     | 2.20                     | 0.41              |
| 1:D:68:HIS:CG       | 12:D:690:HOH:O     | 2.73                     | 0.41              |
| 1:D:73:LEU:HD21     | 5:D:311:PEG:H31    | 2.02                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:D:305:EPE:C7   | 12:D:548:HOH:O     | 2.68                     | 0.41              |
| 5:B:308:PEG:H32   | 8:B:330:PG4:O3     | 2.21                     | 0.41              |
| 1:C:220:VAL:HB    | 12:C:428:HOH:O     | 2.20                     | 0.41              |
| 1:D:229[A]:ASN:CB | 8:D:333:PG4:H52    | 2.51                     | 0.41              |
| 1:D:69:ASN:HD22   | 5:D:318[A]:PEG:H21 | 1.87                     | 0.40              |
| 1:C:170:GLN:HA    | 12:C:444:HOH:O     | 2.21                     | 0.40              |
| 5:D:319:PEG:O1    | 5:D:320:PEG:H32    | 2.21                     | 0.40              |
| 1:C:169:GLY:H     | 5:C:308:PEG:C4     | 2.34                     | 0.40              |
| 1:C:178:VAL:N     | 12:C:407:HOH:O     | 2.06                     | 0.40              |
| 3:C:305:PG5:H42   | 12:C:701:HOH:O     | 2.20                     | 0.40              |
| 5:C:313:PEG:H12   | 12:C:595:HOH:O     | 2.22                     | 0.40              |
| 1:D:57:TYR:HD1    | 12:D:682:HOH:O     | 1.99                     | 0.40              |
| 1:B:215:LYS:H     | 5:B:322:PEG:H12    | 1.86                     | 0.40              |
| 1:D:68:HIS:CD2    | 12:D:690:HOH:O     | 2.73                     | 0.40              |

All (28) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1           | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------------|--------------------------|-------------------|
| 12:B:602:HOH:O   | 12:C:683:HOH:O[1_545] | 1.38                     | 0.82              |
| 11:D:338:CL:CL   | 12:A:609:HOH:O[1_554] | 1.58                     | 0.62              |
| 8:D:333:PG4:O1   | 12:C:725:HOH:O[2_745] | 1.68                     | 0.52              |
| 12:A:404:HOH:O   | 12:C:651:HOH:O[2_746] | 1.75                     | 0.45              |
| 12:C:641:HOH:O   | 12:D:426:HOH:O[2_755] | 1.75                     | 0.45              |
| 12:A:616:HOH:O   | 12:C:706:HOH:O[2_746] | 1.77                     | 0.43              |
| 12:A:633:HOH:O   | 12:B:503:HOH:O[1_565] | 1.79                     | 0.41              |
| 12:D:605:HOH:O   | 12:D:680:HOH:O[2_745] | 1.80                     | 0.40              |
| 8:A:316:PG4:O5   | 12:C:448:HOH:O[2_746] | 1.82                     | 0.38              |
| 12:A:495:HOH:O   | 12:C:491:HOH:O[2_846] | 1.85                     | 0.35              |
| 1:A:112:ASN:ND2  | 12:B:405:HOH:O[1_565] | 1.88                     | 0.32              |
| 1:A:112:ASN:HD21 | 12:B:405:HOH:O[1_565] | 1.29                     | 0.31              |
| 12:C:453:HOH:O   | 12:D:458:HOH:O[1_565] | 1.89                     | 0.31              |
| 12:A:627:HOH:O   | 12:B:503:HOH:O[1_565] | 1.92                     | 0.28              |
| 12:A:690:HOH:O   | 12:C:706:HOH:O[2_746] | 1.99                     | 0.21              |
| 8:D:333:PG4:HO1  | 12:C:725:HOH:O[2_745] | 1.40                     | 0.20              |
| 8:D:332:PG4:O2   | 12:A:611:HOH:O[1_554] | 2.07                     | 0.13              |
| 12:A:417:HOH:O   | 12:C:452:HOH:O[2_746] | 2.12                     | 0.08              |
| 12:A:462:HOH:O   | 12:C:471:HOH:O[2_746] | 2.12                     | 0.08              |
| 12:B:427:HOH:O   | 12:C:657:HOH:O[1_545] | 2.12                     | 0.08              |
| 1:A:114:ARG:NE   | 12:B:411:HOH:O[2_756] | 2.15                     | 0.05              |

*Continued on next page...*

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| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 12:B:608:HOH:O | 12:C:541:HOH:O[1_545] | 2.15                     | 0.05              |
| 1:D:188:CYS:SG | 8:D:328:PG4:O5[2_855] | 2.15                     | 0.05              |
| 12:D:621:HOH:O | 12:D:636:HOH:O[2_855] | 2.15                     | 0.05              |
| 12:D:662:HOH:O | 12:D:738:HOH:O[1_545] | 2.17                     | 0.03              |
| 1:B:127:ALA:O  | 12:B:406:HOH:O[2_756] | 2.18                     | 0.02              |
| 8:A:315:PG4:O3 | 12:B:474:HOH:O[2_756] | 2.19                     | 0.01              |
| 1:D:21:THR:H   | 5:D:321:PEG:O2[2_855] | 1.59                     | 0.01              |

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 223/231 (96%) | 217 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | B     | 221/231 (96%) | 217 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | C     | 221/231 (96%) | 217 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | D     | 226/231 (98%) | 218 (96%) | 6 (3%)  | 2 (1%)   | 14          | 1   |
| All | All   | 891/924 (96%) | 869 (98%) | 20 (2%) | 2 (0%)   | 48          | 16  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | D     | 25[A] | ASN  |
| 1   | D     | 25[B] | ASN  |

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A     | 185/191 (97%) | 185 (100%) | 0        | 100         | 100 |
| 1   | B     | 183/191 (96%) | 181 (99%)  | 2 (1%)   | 65          | 31  |
| 1   | C     | 183/191 (96%) | 183 (100%) | 0        | 100         | 100 |
| 1   | D     | 188/191 (98%) | 187 (100%) | 1 (0%)   | 81          | 59  |
| All | All   | 739/764 (97%) | 736 (100%) | 3 (0%)   | 84          | 63  |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 182 | GLU  |
| 1   | B     | 185 | LYS  |
| 1   | D     | 182 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 151 | GLN  |
| 1   | C     | 233 | GLN  |
| 1   | D     | 203 | GLN  |

### 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 120 ligands modelled in this entry, 6 are monoatomic - leaving 114 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 |
| 5   | PEG  | D     | 316    | -    | 6,6,6        | 0.24 | 0        | 5,5,5       | 0.40 | 0        |
| 5   | PEG  | B     | 326    | -    | 6,6,6        | 0.29 | 0        | 5,5,5       | 0.69 | 0        |
| 2   | BEN  | D     | 306[A] | -    | 9,9,9        | 0.68 | 0        | 7,11,11     | 0.78 | 0        |
| 5   | PEG  | C     | 304    | -    | 6,6,6        | 0.25 | 0        | 5,5,5       | 0.19 | 0        |
| 8   | PG4  | D     | 329    | -    | 12,12,12     | 0.37 | 0        | 11,11,11    | 0.39 | 0        |
| 5   | PEG  | D     | 307    | -    | 6,6,6        | 0.24 | 0        | 5,5,5       | 0.25 | 0        |
| 3   | PG5  | D     | 312    | -    | 11,11,11     | 0.35 | 0        | 10,10,10    | 0.87 | 0        |
| 5   | PEG  | B     | 315    | -    | 6,6,6        | 0.25 | 0        | 5,5,5       | 0.25 | 0        |
| 5   | PEG  | D     | 321    | -    | 6,6,6        | 0.30 | 0        | 5,5,5       | 0.40 | 0        |
| 5   | PEG  | B     | 319    | -    | 6,6,6        | 0.22 | 0        | 5,5,5       | 0.25 | 0        |
| 9   | PMA  | B     | 302    | -    | 18,18,18     | 1.36 | 2 (11%)  | 26,26,26    | 1.55 | 5 (19%)  |
| 7   | MLI  | D     | 315    | -    | 6,6,6        | 1.54 | 1 (16%)  | 7,7,7       | 1.18 | 0        |
| 5   | PEG  | A     | 319    | -    | 6,6,6        | 0.28 | 0        | 5,5,5       | 0.67 | 0        |
| 5   | PEG  | A     | 313    | -    | 6,6,6        | 0.29 | 0        | 5,5,5       | 0.42 | 0        |
| 8   | PG4  | A     | 315    | -    | 11,11,12     | 0.28 | 0        | 10,10,11    | 0.81 | 1 (10%)  |
| 5   | PEG  | D     | 318[B] | -    | 6,6,6        | 0.25 | 0        | 5,5,5       | 0.23 | 0        |
| 5   | PEG  | D     | 336    | -    | 6,6,6        | 0.25 | 0        | 5,5,5       | 0.17 | 0        |
| 5   | PEG  | A     | 307    | -    | 6,6,6        | 0.27 | 0        | 5,5,5       | 0.28 | 0        |
| 8   | PG4  | D     | 331    | -    | 12,12,12     | 0.29 | 0        | 11,11,11    | 0.23 | 0        |
| 5   | PEG  | B     | 322    | -    | 6,6,6        | 0.25 | 0        | 5,5,5       | 0.24 | 0        |
| 5   | PEG  | D     | 319    | -    | 6,6,6        | 0.23 | 0        | 5,5,5       | 0.44 | 0        |
| 5   | PEG  | D     | 325    | -    | 6,6,6        | 0.33 | 0        | 5,5,5       | 0.23 | 0        |
| 8   | PG4  | A     | 318    | -    | 12,12,12     | 0.28 | 0        | 11,11,11    | 0.38 | 0        |
| 5   | PEG  | B     | 306    | -    | 6,6,6        | 0.22 | 0        | 5,5,5       | 0.34 | 0        |
| 2   | BEN  | C     | 302    | -    | 9,9,9        | 0.72 | 0        | 7,11,11     | 2.00 | 2 (28%)  |
| 3   | PG5  | C     | 306    | -    | 11,11,11     | 0.32 | 0        | 10,10,10    | 0.30 | 0        |
| 5   | PEG  | C     | 318    | -    | 6,6,6        | 0.23 | 0        | 5,5,5       | 0.26 | 0        |
| 5   | PEG  | B     | 316    | -    | 6,6,6        | 0.25 | 0        | 5,5,5       | 0.30 | 0        |
| 8   | PG4  | C     | 325    | -    | 12,12,12     | 0.29 | 0        | 11,11,11    | 0.34 | 0        |
| 8   | PG4  | D     | 330    | -    | 12,12,12     | 0.30 | 0        | 11,11,11    | 0.25 | 0        |
| 5   | PEG  | A     | 314    | -    | 6,6,6        | 0.24 | 0        | 5,5,5       | 0.32 | 0        |
| 3   | PG5  | B     | 327    | -    | 11,11,11     | 0.30 | 0        | 10,10,10    | 0.16 | 0        |
| 5   | PEG  | C     | 328[A] | -    | 6,6,6        | 0.25 | 0        | 5,5,5       | 0.26 | 0        |
| 5   | PEG  | D     | 324    | -    | 6,6,6        | 0.27 | 0        | 5,5,5       | 0.33 | 0        |
| 5   | PEG  | D     | 310    | -    | 6,6,6        | 0.24 | 0        | 5,5,5       | 0.25 | 0        |
| 3   | PG5  | B     | 305    | -    | 11,11,11     | 0.42 | 0        | 10,10,10    | 0.70 | 0        |
| 5   | PEG  | C     | 327    | -    | 6,6,6        | 0.24 | 0        | 5,5,5       | 0.22 | 0        |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | PEG  | D     | 308    | -    | 6,6,6        | 0.21 | 0        | 5,5,5       | 0.43 | 0        |
| 5   | PEG  | B     | 312    | -    | 6,6,6        | 0.29 | 0        | 5,5,5       | 0.19 | 0        |
| 3   | PG5  | A     | 305    | -    | 11,11,11     | 0.33 | 0        | 10,10,10    | 0.20 | 0        |
| 8   | PG4  | A     | 317    | -    | 12,12,12     | 0.34 | 0        | 11,11,11    | 0.26 | 0        |
| 5   | PEG  | B     | 309    | -    | 6,6,6        | 0.29 | 0        | 5,5,5       | 0.17 | 0        |
| 8   | PG4  | B     | 329    | -    | 12,12,12     | 0.43 | 0        | 11,11,11    | 0.93 | 0        |
| 5   | PEG  | B     | 317[A] | -    | 6,6,6        | 0.25 | 0        | 5,5,5       | 0.29 | 0        |
| 5   | PEG  | D     | 334    | -    | 6,6,6        | 0.24 | 0        | 5,5,5       | 0.23 | 0        |
| 3   | PG5  | B     | 311    | -    | 11,11,11     | 0.31 | 0        | 10,10,10    | 0.25 | 0        |
| 5   | PEG  | D     | 320    | -    | 6,6,6        | 0.28 | 0        | 5,5,5       | 0.49 | 0        |
| 8   | PG4  | C     | 324    | -    | 12,12,12     | 0.35 | 0        | 11,11,11    | 0.48 | 0        |
| 8   | PG4  | C     | 322    | -    | 12,12,12     | 0.27 | 0        | 11,11,11    | 0.24 | 0        |
| 5   | PEG  | A     | 309    | -    | 6,6,6        | 0.25 | 0        | 5,5,5       | 0.26 | 0        |
| 2   | BEN  | D     | 306[B] | 5    | 9,9,9        | 1.40 | 1 (11%)  | 7,11,11     | 1.88 | 2 (28%)  |
| 2   | BEN  | C     | 307    | -    | 9,9,9        | 0.64 | 0        | 7,11,11     | 0.99 | 1 (14%)  |
| 8   | PG4  | B     | 328    | -    | 12,12,12     | 0.28 | 0        | 11,11,11    | 0.25 | 0        |
| 8   | PG4  | D     | 328    | -    | 12,12,12     | 0.30 | 0        | 11,11,11    | 0.26 | 0        |
| 5   | PEG  | B     | 324    | -    | 6,6,6        | 0.28 | 0        | 5,5,5       | 0.15 | 0        |
| 5   | PEG  | D     | 335    | -    | 6,6,6        | 0.30 | 0        | 5,5,5       | 0.39 | 0        |
| 5   | PEG  | D     | 327    | -    | 6,6,6        | 0.27 | 0        | 5,5,5       | 0.25 | 0        |
| 5   | PEG  | B     | 310    | -    | 6,6,6        | 0.24 | 0        | 5,5,5       | 0.19 | 0        |
| 8   | PG4  | C     | 323    | -    | 12,12,12     | 0.29 | 0        | 11,11,11    | 0.23 | 0        |
| 2   | BEN  | B     | 304    | -    | 9,9,9        | 0.66 | 0        | 7,11,11     | 1.15 | 1 (14%)  |
| 5   | PEG  | D     | 326    | -    | 6,6,6        | 0.22 | 0        | 5,5,5       | 0.16 | 0        |
| 3   | PG5  | C     | 305    | -    | 11,11,11     | 0.31 | 0        | 10,10,10    | 0.20 | 0        |
| 3   | PG5  | A     | 304    | -    | 11,11,11     | 0.28 | 0        | 10,10,10    | 0.27 | 0        |
| 10  | EPE  | D     | 305    | -    | 15,15,15     | 0.87 | 1 (6%)   | 19,20,20    | 1.17 | 2 (10%)  |
| 5   | PEG  | B     | 331    | -    | 6,6,6        | 0.24 | 0        | 5,5,5       | 0.23 | 0        |
| 2   | BEN  | B     | 301    | -    | 9,9,9        | 0.55 | 0        | 7,11,11     | 1.97 | 3 (42%)  |
| 5   | PEG  | B     | 308    | -    | 6,6,6        | 0.26 | 0        | 5,5,5       | 0.30 | 0        |
| 2   | BEN  | B     | 303    | -    | 9,9,9        | 0.60 | 0        | 7,11,11     | 1.57 | 2 (28%)  |
| 5   | PEG  | B     | 325    | -    | 6,6,6        | 0.29 | 0        | 5,5,5       | 0.31 | 0        |
| 8   | PG4  | D     | 333    | -    | 12,12,12     | 0.42 | 0        | 11,11,11    | 0.68 | 0        |
| 5   | PEG  | B     | 323    | -    | 6,6,6        | 0.28 | 0        | 5,5,5       | 0.53 | 0        |
| 8   | PG4  | B     | 330    | -    | 12,12,12     | 0.34 | 0        | 11,11,11    | 0.49 | 0        |
| 5   | PEG  | B     | 314    | -    | 6,6,6        | 0.24 | 0        | 5,5,5       | 0.32 | 0        |
| 5   | PEG  | D     | 311    | -    | 6,6,6        | 0.29 | 0        | 5,5,5       | 0.25 | 0        |
| 8   | PG4  | A     | 316    | -    | 12,12,12     | 0.32 | 0        | 11,11,11    | 0.45 | 0        |
| 5   | PEG  | C     | 311    | -    | 6,6,6        | 0.27 | 0        | 5,5,5       | 0.20 | 0        |
| 5   | PEG  | D     | 318[A] | -    | 6,6,6        | 0.25 | 0        | 5,5,5       | 0.44 | 0        |
| 9   | PMA  | D     | 302    | -    | 18,18,18     | 1.25 | 3 (16%)  | 26,26,26    | 1.52 | 4 (15%)  |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | PEG  | C     | 328[B] | -    | 6,6,6        | 0.27 | 0        | 5,5,5       | 0.26 | 0        |
| 5   | PEG  | D     | 323    | -    | 6,6,6        | 0.27 | 0        | 5,5,5       | 0.36 | 0        |
| 7   | MLI  | B     | 321    | -    | 6,6,6        | 1.73 | 1 (16%)  | 7,7,7       | 1.14 | 0        |
| 5   | PEG  | C     | 316    | -    | 6,6,6        | 0.26 | 0        | 5,5,5       | 0.46 | 0        |
| 10  | EPE  | C     | 303    | -    | 15,15,15     | 0.87 | 1 (6%)   | 19,20,20    | 0.87 | 0        |
| 5   | PEG  | C     | 321    | -    | 6,6,6        | 0.23 | 0        | 5,5,5       | 0.22 | 0        |
| 5   | PEG  | A     | 312    | -    | 6,6,6        | 0.24 | 0        | 5,5,5       | 0.24 | 0        |
| 3   | PG5  | B     | 307    | -    | 11,11,11     | 0.31 | 0        | 10,10,10    | 0.20 | 0        |
| 5   | PEG  | A     | 308    | -    | 6,6,6        | 0.24 | 0        | 5,5,5       | 0.19 | 0        |
| 5   | PEG  | B     | 313    | -    | 6,6,6        | 0.25 | 0        | 5,5,5       | 0.24 | 0        |
| 5   | PEG  | C     | 309    | -    | 6,6,6        | 0.28 | 0        | 5,5,5       | 0.48 | 0        |
| 3   | PG5  | A     | 302    | -    | 11,11,11     | 0.30 | 0        | 10,10,10    | 0.28 | 0        |
| 5   | PEG  | B     | 318    | -    | 6,6,6        | 0.27 | 0        | 5,5,5       | 0.19 | 0        |
| 5   | PEG  | C     | 317    | -    | 6,6,6        | 0.26 | 0        | 5,5,5       | 0.24 | 0        |
| 5   | PEG  | B     | 317[B] | -    | 6,6,6        | 0.26 | 0        | 5,5,5       | 0.24 | 0        |
| 5   | PEG  | D     | 317    | -    | 6,6,6        | 0.32 | 0        | 5,5,5       | 0.47 | 0        |
| 7   | MLI  | A     | 311    | -    | 6,6,6        | 1.78 | 1 (16%)  | 7,7,7       | 0.99 | 0        |
| 5   | PEG  | C     | 313    | -    | 6,6,6        | 0.26 | 0        | 5,5,5       | 0.28 | 0        |
| 8   | PG4  | D     | 332    | -    | 12,12,12     | 0.29 | 0        | 11,11,11    | 0.24 | 0        |
| 4   | PG6  | A     | 303    | -    | 17,17,17     | 0.33 | 0        | 16,16,16    | 0.37 | 0        |
| 5   | PEG  | A     | 306    | -    | 6,6,6        | 0.25 | 0        | 5,5,5       | 0.22 | 0        |
| 5   | PEG  | C     | 312    | -    | 6,6,6        | 0.26 | 0        | 5,5,5       | 0.73 | 0        |
| 3   | PG5  | D     | 304    | -    | 11,11,11     | 0.30 | 0        | 10,10,10    | 0.17 | 0        |
| 5   | PEG  | C     | 308    | -    | 6,6,6        | 0.52 | 0        | 5,5,5       | 1.10 | 1 (20%)  |
| 2   | BEN  | D     | 309    | -    | 9,9,9        | 0.86 | 0        | 7,11,11     | 1.26 | 1 (14%)  |
| 2   | BEN  | D     | 301    | -    | 9,9,9        | 1.02 | 1 (11%)  | 7,11,11     | 1.92 | 3 (42%)  |
| 3   | PG5  | D     | 303    | -    | 11,11,11     | 0.29 | 0        | 10,10,10    | 0.18 | 0        |
| 2   | BEN  | A     | 301    | -    | 9,9,9        | 0.51 | 0        | 7,11,11     | 0.35 | 0        |
| 5   | PEG  | D     | 322    | 2    | 6,6,6        | 0.36 | 0        | 5,5,5       | 0.50 | 0        |
| 5   | PEG  | C     | 310    | -    | 6,6,6        | 0.26 | 0        | 5,5,5       | 0.22 | 0        |
| 5   | PEG  | C     | 320    | -    | 6,6,6        | 0.27 | 0        | 5,5,5       | 0.46 | 0        |
| 5   | PEG  | D     | 337    | -    | 6,6,6        | 0.23 | 0        | 5,5,5       | 0.27 | 0        |
| 5   | PEG  | C     | 319    | -    | 6,6,6        | 0.23 | 0        | 5,5,5       | 0.26 | 0        |
| 8   | PG4  | C     | 326    | -    | 12,12,12     | 0.26 | 0        | 11,11,11    | 0.24 | 0        |
| 7   | MLI  | C     | 315    | -    | 6,6,6        | 1.69 | 1 (16%)  | 7,7,7       | 1.18 | 0        |
| 2   | BEN  | C     | 301    | -    | 9,9,9        | 0.71 | 0        | 7,11,11     | 1.29 | 1 (14%)  |

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

| Mol | Type | Chain | Res    | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|--------|------|---------|------------|---------|
| 5   | PEG  | D     | 316    | -    | -       | 2/4/4/4    | -       |
| 5   | PEG  | B     | 326    | -    | -       | 3/4/4/4    | -       |
| 2   | BEN  | D     | 306[A] | -    | -       | 0/4/4/4    | 0/1/1/1 |
| 5   | PEG  | C     | 304    | -    | -       | 1/4/4/4    | -       |
| 8   | PG4  | D     | 329    | -    | -       | 3/10/10/10 | -       |
| 5   | PEG  | D     | 307    | -    | -       | 1/4/4/4    | -       |
| 3   | PG5  | D     | 312    | -    | -       | 7/9/9/9    | -       |
| 5   | PEG  | B     | 315    | -    | -       | 2/4/4/4    | -       |
| 5   | PEG  | D     | 321    | -    | -       | 2/4/4/4    | -       |
| 5   | PEG  | B     | 319    | -    | -       | 2/4/4/4    | -       |
| 9   | PMA  | B     | 302    | -    | -       | 6/16/16/16 | 0/1/1/1 |
| 7   | MLI  | D     | 315    | -    | -       | 0/4/4/4    | -       |
| 5   | PEG  | A     | 319    | -    | -       | 1/4/4/4    | -       |
| 5   | PEG  | A     | 313    | -    | -       | 3/4/4/4    | -       |
| 8   | PG4  | A     | 315    | -    | -       | 2/9/9/10   | -       |
| 5   | PEG  | D     | 318[B] | -    | -       | 2/4/4/4    | -       |
| 5   | PEG  | D     | 336    | -    | -       | 4/4/4/4    | -       |
| 5   | PEG  | A     | 307    | -    | -       | 1/4/4/4    | -       |
| 8   | PG4  | D     | 331    | -    | -       | 4/10/10/10 | -       |
| 5   | PEG  | B     | 322    | -    | -       | 3/4/4/4    | -       |
| 5   | PEG  | D     | 319    | -    | -       | 3/4/4/4    | -       |
| 5   | PEG  | D     | 325    | -    | -       | 1/4/4/4    | -       |
| 8   | PG4  | A     | 318    | -    | -       | 5/10/10/10 | -       |
| 5   | PEG  | B     | 306    | -    | -       | 2/4/4/4    | -       |
| 2   | BEN  | C     | 302    | -    | -       | 0/4/4/4    | 0/1/1/1 |
| 3   | PG5  | C     | 306    | -    | -       | 5/9/9/9    | -       |
| 5   | PEG  | C     | 318    | -    | -       | 0/4/4/4    | -       |
| 5   | PEG  | B     | 316    | -    | -       | 3/4/4/4    | -       |
| 8   | PG4  | C     | 325    | -    | -       | 6/10/10/10 | -       |
| 8   | PG4  | D     | 330    | -    | -       | 7/10/10/10 | -       |
| 5   | PEG  | A     | 314    | -    | -       | 1/4/4/4    | -       |
| 3   | PG5  | B     | 327    | -    | -       | 5/9/9/9    | -       |
| 5   | PEG  | C     | 328[A] | -    | -       | 1/4/4/4    | -       |
| 5   | PEG  | D     | 324    | -    | -       | 3/4/4/4    | -       |
| 5   | PEG  | D     | 310    | -    | -       | 0/4/4/4    | -       |
| 3   | PG5  | B     | 305    | -    | -       | 5/9/9/9    | -       |
| 5   | PEG  | C     | 327    | -    | -       | 2/4/4/4    | -       |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|--------|------|---------|------------|---------|
| 5   | PEG  | D     | 308    | -    | -       | 2/4/4/4    | -       |
| 5   | PEG  | B     | 312    | -    | -       | 3/4/4/4    | -       |
| 3   | PG5  | A     | 305    | -    | -       | 6/9/9/9    | -       |
| 8   | PG4  | A     | 317    | -    | -       | 7/10/10/10 | -       |
| 5   | PEG  | B     | 309    | -    | -       | 2/4/4/4    | -       |
| 8   | PG4  | B     | 329    | -    | -       | 5/10/10/10 | -       |
| 5   | PEG  | B     | 317[A] | -    | -       | 1/4/4/4    | -       |
| 5   | PEG  | D     | 334    | -    | -       | 3/4/4/4    | -       |
| 3   | PG5  | B     | 311    | -    | -       | 6/9/9/9    | -       |
| 5   | PEG  | D     | 320    | -    | -       | 2/4/4/4    | -       |
| 8   | PG4  | C     | 324    | -    | -       | 5/10/10/10 | -       |
| 8   | PG4  | C     | 322    | -    | -       | 5/10/10/10 | -       |
| 5   | PEG  | A     | 309    | -    | -       | 2/4/4/4    | -       |
| 2   | BEN  | D     | 306[B] | 5    | -       | 0/4/4/4    | 0/1/1/1 |
| 2   | BEN  | C     | 307    | -    | -       | 3/4/4/4    | 0/1/1/1 |
| 8   | PG4  | B     | 328    | -    | -       | 7/10/10/10 | -       |
| 8   | PG4  | D     | 328    | -    | -       | 4/10/10/10 | -       |
| 5   | PEG  | B     | 324    | -    | -       | 2/4/4/4    | -       |
| 5   | PEG  | D     | 335    | -    | -       | 3/4/4/4    | -       |
| 5   | PEG  | D     | 327    | -    | -       | 3/4/4/4    | -       |
| 5   | PEG  | B     | 310    | -    | -       | 1/4/4/4    | -       |
| 8   | PG4  | C     | 323    | -    | -       | 5/10/10/10 | -       |
| 2   | BEN  | B     | 304    | -    | -       | 4/4/4/4    | 0/1/1/1 |
| 5   | PEG  | D     | 326    | -    | -       | 3/4/4/4    | -       |
| 3   | PG5  | C     | 305    | -    | -       | 6/9/9/9    | -       |
| 3   | PG5  | A     | 304    | -    | -       | 4/9/9/9    | -       |
| 10  | EPE  | D     | 305    | -    | -       | 4/9/19/19  | 0/1/1/1 |
| 5   | PEG  | B     | 331    | -    | -       | 1/4/4/4    | -       |
| 2   | BEN  | B     | 301    | -    | -       | 2/4/4/4    | 0/1/1/1 |
| 5   | PEG  | B     | 308    | -    | -       | 1/4/4/4    | -       |
| 2   | BEN  | B     | 303    | -    | -       | 0/4/4/4    | 0/1/1/1 |
| 5   | PEG  | B     | 325    | -    | -       | 2/4/4/4    | -       |
| 8   | PG4  | D     | 333    | -    | -       | 5/10/10/10 | -       |
| 5   | PEG  | B     | 323    | -    | -       | 1/4/4/4    | -       |
| 8   | PG4  | B     | 330    | -    | -       | 6/10/10/10 | -       |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|--------|------|---------|------------|---------|
| 5   | PEG  | B     | 314    | -    | -       | 3/4/4/4    | -       |
| 5   | PEG  | D     | 311    | -    | -       | 3/4/4/4    | -       |
| 8   | PG4  | A     | 316    | -    | -       | 7/10/10/10 | -       |
| 5   | PEG  | C     | 311    | -    | -       | 2/4/4/4    | -       |
| 5   | PEG  | D     | 318[A] | -    | -       | 2/4/4/4    | -       |
| 9   | PMA  | D     | 302    | -    | -       | 2/16/16/16 | 0/1/1/1 |
| 5   | PEG  | C     | 328[B] | -    | -       | 1/4/4/4    | -       |
| 5   | PEG  | D     | 323    | -    | -       | 2/4/4/4    | -       |
| 7   | MLI  | B     | 321    | -    | -       | 3/4/4/4    | -       |
| 5   | PEG  | C     | 316    | -    | -       | 2/4/4/4    | -       |
| 10  | EPE  | C     | 303    | -    | -       | 3/9/19/19  | 0/1/1/1 |
| 5   | PEG  | C     | 321    | -    | -       | 3/4/4/4    | -       |
| 5   | PEG  | A     | 312    | -    | -       | 3/4/4/4    | -       |
| 3   | PG5  | B     | 307    | -    | -       | 3/9/9/9    | -       |
| 5   | PEG  | A     | 308    | -    | -       | 2/4/4/4    | -       |
| 5   | PEG  | B     | 313    | -    | -       | 2/4/4/4    | -       |
| 5   | PEG  | C     | 309    | -    | -       | 2/4/4/4    | -       |
| 3   | PG5  | A     | 302    | -    | -       | 5/9/9/9    | -       |
| 5   | PEG  | B     | 318    | -    | -       | 2/4/4/4    | -       |
| 5   | PEG  | C     | 317    | -    | -       | 2/4/4/4    | -       |
| 5   | PEG  | B     | 317[B] | -    | -       | 1/4/4/4    | -       |
| 5   | PEG  | D     | 317    | -    | -       | 2/4/4/4    | -       |
| 7   | MLI  | A     | 311    | -    | -       | 4/4/4/4    | -       |
| 5   | PEG  | C     | 313    | -    | -       | 3/4/4/4    | -       |
| 8   | PG4  | D     | 332    | -    | -       | 6/10/10/10 | -       |
| 4   | PG6  | A     | 303    | -    | -       | 7/15/15/15 | -       |
| 5   | PEG  | A     | 306    | -    | -       | 3/4/4/4    | -       |
| 5   | PEG  | C     | 312    | -    | -       | 3/4/4/4    | -       |
| 3   | PG5  | D     | 304    | -    | -       | 5/9/9/9    | -       |
| 5   | PEG  | C     | 308    | -    | -       | 4/4/4/4    | -       |
| 2   | BEN  | D     | 309    | -    | -       | 2/4/4/4    | 0/1/1/1 |
| 2   | BEN  | D     | 301    | -    | -       | 0/4/4/4    | 0/1/1/1 |
| 3   | PG5  | D     | 303    | -    | -       | 4/9/9/9    | -       |
| 2   | BEN  | A     | 301    | -    | -       | 0/4/4/4    | 0/1/1/1 |
| 5   | PEG  | D     | 322    | 2    | -       | 2/4/4/4    | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | PEG  | C     | 310 | -    | -       | 1/4/4/4    | -       |
| 5   | PEG  | C     | 320 | -    | -       | 2/4/4/4    | -       |
| 5   | PEG  | D     | 337 | -    | -       | 1/4/4/4    | -       |
| 5   | PEG  | C     | 319 | -    | -       | 4/4/4/4    | -       |
| 8   | PG4  | C     | 326 | -    | -       | 3/10/10/10 | -       |
| 7   | MLI  | C     | 315 | -    | -       | 2/4/4/4    | -       |
| 2   | BEN  | C     | 301 | -    | -       | 0/4/4/4    | 0/1/1/1 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|-------|-------------|----------|
| 2   | D     | 306[B] | BEN  | C6-C1  | 3.27  | 1.44        | 1.39     |
| 7   | B     | 321    | MLI  | C1-C3  | 2.83  | 1.55        | 1.51     |
| 7   | A     | 311    | MLI  | C1-C3  | 2.81  | 1.55        | 1.51     |
| 7   | C     | 315    | MLI  | C1-C3  | 2.71  | 1.55        | 1.51     |
| 9   | B     | 302    | PMA  | C2-C10 | 2.51  | 1.55        | 1.49     |
| 9   | D     | 302    | PMA  | O6-C7  | -2.45 | 1.23        | 1.30     |
| 10  | D     | 305    | EPE  | C10-S  | 2.36  | 1.80        | 1.77     |
| 7   | D     | 315    | MLI  | C1-C3  | 2.30  | 1.54        | 1.51     |
| 10  | C     | 303    | EPE  | C10-S  | 2.21  | 1.80        | 1.77     |
| 9   | B     | 302    | PMA  | C1-C9  | 2.20  | 1.54        | 1.49     |
| 9   | D     | 302    | PMA  | C5-C8  | 2.11  | 1.54        | 1.49     |
| 2   | D     | 301    | BEN  | C2-C1  | -2.09 | 1.36        | 1.39     |
| 9   | D     | 302    | PMA  | C2-C10 | 2.06  | 1.54        | 1.49     |

All (29) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|----------|-------|-------------|----------|
| 9   | D     | 302    | PMA  | O5-C7-C4 | -4.64 | 110.90      | 121.97   |
| 9   | B     | 302    | PMA  | O7-C8-C5 | -3.73 | 113.07      | 121.97   |
| 2   | D     | 306[B] | BEN  | C1-C-N2  | -3.36 | 112.92      | 118.01   |
| 2   | B     | 301    | BEN  | C5-C6-C1 | 3.32  | 123.63      | 120.36   |
| 2   | D     | 309    | BEN  | C1-C-N2  | -3.28 | 113.03      | 118.01   |
| 9   | B     | 302    | PMA  | O8-C8-O7 | 3.19  | 130.22      | 123.35   |
| 2   | D     | 306[B] | BEN  | C5-C6-C1 | -3.16 | 117.26      | 120.36   |
| 2   | C     | 302    | BEN  | C5-C6-C1 | -3.12 | 117.30      | 120.36   |
| 9   | D     | 302    | PMA  | O6-C7-C4 | 2.95  | 123.67      | 115.28   |
| 2   | B     | 303    | BEN  | C5-C6-C1 | -2.89 | 117.53      | 120.36   |
| 9   | D     | 302    | PMA  | O8-C8-O7 | 2.78  | 129.33      | 123.35   |
| 2   | D     | 301    | BEN  | C3-C2-C1 | 2.75  | 123.07      | 120.36   |
| 2   | C     | 302    | BEN  | C4-C3-C2 | -2.74 | 116.86      | 120.24   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | D     | 301 | BEN  | C6-C1-C2  | -2.62 | 115.23      | 118.57   |
| 10  | D     | 305 | EPE  | C6-C5-N4  | 2.55  | 115.80      | 110.65   |
| 2   | C     | 307 | BEN  | C1-C-N2   | -2.51 | 114.20      | 118.01   |
| 2   | B     | 301 | BEN  | C4-C3-C2  | 2.51  | 123.34      | 120.24   |
| 2   | B     | 303 | BEN  | C6-C1-C2  | 2.49  | 121.73      | 118.57   |
| 2   | D     | 301 | BEN  | C5-C6-C1  | 2.37  | 122.69      | 120.36   |
| 9   | B     | 302 | PMA  | C6-C4-C7  | 2.33  | 124.44      | 117.89   |
| 2   | C     | 301 | BEN  | C1-C-N2   | -2.31 | 114.51      | 118.01   |
| 5   | C     | 308 | PEG  | O4-C4-C3  | 2.29  | 125.30      | 111.82   |
| 9   | D     | 302 | PMA  | O7-C8-C5  | -2.24 | 116.62      | 121.97   |
| 8   | A     | 315 | PG4  | C7-O4-C6  | -2.22 | 105.28      | 113.06   |
| 9   | B     | 302 | PMA  | O1-C9-C1  | -2.20 | 116.72      | 121.97   |
| 2   | B     | 304 | BEN  | C1-C-N2   | -2.14 | 114.77      | 118.01   |
| 9   | B     | 302 | PMA  | O3-C10-C2 | -2.13 | 116.88      | 121.97   |
| 10  | D     | 305 | EPE  | C7-N4-C3  | 2.05  | 116.71      | 111.24   |
| 2   | B     | 301 | BEN  | C4-C5-C6  | -2.04 | 117.72      | 120.24   |

There are no chirality outliers.

All (327) torsion outliers are listed below:

| Mol | Chain | Res    | Type | Atoms       |
|-----|-------|--------|------|-------------|
| 2   | D     | 309    | BEN  | N2-C-C1-C2  |
| 2   | D     | 309    | BEN  | N2-C-C1-C6  |
| 10  | C     | 303    | EPE  | C8-C7-N4-C5 |
| 10  | D     | 305    | EPE  | N4-C7-C8-O8 |
| 3   | B     | 327    | PG5  | O3-C6-C7-O4 |
| 3   | C     | 305    | PG5  | O1-C2-C3-O2 |
| 3   | C     | 305    | PG5  | O3-C6-C7-O4 |
| 8   | A     | 316    | PG4  | O2-C3-C4-O3 |
| 8   | B     | 329    | PG4  | O3-C5-C6-O4 |
| 8   | C     | 323    | PG4  | O2-C3-C4-O3 |
| 8   | C     | 325    | PG4  | O3-C5-C6-O4 |
| 3   | B     | 311    | PG5  | O3-C6-C7-O4 |
| 3   | C     | 306    | PG5  | O3-C6-C7-O4 |
| 3   | D     | 312    | PG5  | O3-C6-C7-O4 |
| 3   | B     | 327    | PG5  | O2-C4-C5-O3 |
| 8   | D     | 330    | PG4  | O2-C3-C4-O3 |
| 8   | D     | 332    | PG4  | O2-C3-C4-O3 |
| 3   | B     | 305    | PG5  | O3-C6-C7-O4 |
| 8   | C     | 324    | PG4  | O3-C5-C6-O4 |
| 5   | B     | 309    | PEG  | O1-C1-C2-O2 |
| 5   | C     | 328[A] | PEG  | O2-C3-C4-O4 |

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| Mol | Chain | Res    | Type | Atoms       |
|-----|-------|--------|------|-------------|
| 3   | C     | 305    | PG5  | O2-C4-C5-O3 |
| 8   | A     | 317    | PG4  | O2-C3-C4-O3 |
| 8   | C     | 323    | PG4  | O3-C5-C6-O4 |
| 8   | A     | 318    | PG4  | O2-C3-C4-O3 |
| 8   | D     | 331    | PG4  | O2-C3-C4-O3 |
| 8   | B     | 329    | PG4  | O2-C3-C4-O3 |
| 8   | A     | 315    | PG4  | O3-C5-C6-O4 |
| 3   | A     | 304    | PG5  | O2-C4-C5-O3 |
| 4   | A     | 303    | PG6  | O3-C6-C7-O4 |
| 3   | D     | 304    | PG5  | O1-C2-C3-O2 |
| 4   | A     | 303    | PG6  | O1-C2-C3-O2 |
| 4   | A     | 303    | PG6  | O2-C4-C5-O3 |
| 3   | A     | 305    | PG5  | O2-C4-C5-O3 |
| 5   | B     | 315    | PEG  | O1-C1-C2-O2 |
| 5   | B     | 317[B] | PEG  | O2-C3-C4-O4 |
| 5   | C     | 308    | PEG  | O2-C3-C4-O4 |
| 5   | D     | 318[A] | PEG  | O2-C3-C4-O4 |
| 5   | D     | 321    | PEG  | O1-C1-C2-O2 |
| 5   | D     | 337    | PEG  | O2-C3-C4-O4 |
| 8   | D     | 330    | PG4  | O1-C1-C2-O2 |
| 8   | D     | 330    | PG4  | O4-C7-C8-O5 |
| 8   | D     | 332    | PG4  | O4-C7-C8-O5 |
| 8   | D     | 333    | PG4  | O1-C1-C2-O2 |
| 3   | A     | 302    | PG5  | O1-C2-C3-O2 |
| 3   | D     | 312    | PG5  | O1-C2-C3-O2 |
| 8   | D     | 330    | PG4  | O3-C5-C6-O4 |
| 8   | A     | 317    | PG4  | O3-C5-C6-O4 |
| 5   | A     | 308    | PEG  | O2-C3-C4-O4 |
| 5   | A     | 312    | PEG  | O1-C1-C2-O2 |
| 5   | B     | 326    | PEG  | O2-C3-C4-O4 |
| 5   | C     | 313    | PEG  | O1-C1-C2-O2 |
| 5   | C     | 319    | PEG  | O2-C3-C4-O4 |
| 5   | C     | 327    | PEG  | O1-C1-C2-O2 |
| 5   | C     | 328[B] | PEG  | O2-C3-C4-O4 |
| 5   | D     | 322    | PEG  | O2-C3-C4-O4 |
| 5   | D     | 336    | PEG  | O1-C1-C2-O2 |
| 8   | A     | 316    | PG4  | O1-C1-C2-O2 |
| 8   | B     | 328    | PG4  | O1-C1-C2-O2 |
| 8   | D     | 331    | PG4  | O4-C7-C8-O5 |
| 8   | D     | 333    | PG4  | O4-C7-C8-O5 |
| 3   | B     | 305    | PG5  | O2-C4-C5-O3 |
| 5   | B     | 326    | PEG  | C4-C3-O2-C2 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | B     | 330 | PG4  | O3-C5-C6-O4 |
| 5   | A     | 306 | PEG  | O1-C1-C2-O2 |
| 5   | A     | 309 | PEG  | O2-C3-C4-O4 |
| 5   | A     | 314 | PEG  | O2-C3-C4-O4 |
| 5   | C     | 317 | PEG  | O2-C3-C4-O4 |
| 5   | D     | 307 | PEG  | O2-C3-C4-O4 |
| 5   | D     | 321 | PEG  | O2-C3-C4-O4 |
| 5   | D     | 334 | PEG  | O1-C1-C2-O2 |
| 8   | D     | 332 | PG4  | O1-C1-C2-O2 |
| 3   | D     | 303 | PG5  | O2-C4-C5-O3 |
| 3   | D     | 303 | PG5  | O3-C6-C7-O4 |
| 3   | C     | 306 | PG5  | O2-C4-C5-O3 |
| 3   | A     | 302 | PG5  | O3-C6-C7-O4 |
| 3   | D     | 303 | PG5  | O1-C2-C3-O2 |
| 5   | B     | 316 | PEG  | O1-C1-C2-O2 |
| 5   | B     | 322 | PEG  | O1-C1-C2-O2 |
| 5   | B     | 324 | PEG  | O1-C1-C2-O2 |
| 5   | D     | 311 | PEG  | O1-C1-C2-O2 |
| 5   | D     | 316 | PEG  | O1-C1-C2-O2 |
| 5   | D     | 324 | PEG  | O1-C1-C2-O2 |
| 8   | A     | 317 | PG4  | O1-C1-C2-O2 |
| 8   | A     | 317 | PG4  | O4-C7-C8-O5 |
| 8   | D     | 328 | PG4  | O1-C1-C2-O2 |
| 3   | B     | 307 | PG5  | O3-C6-C7-O4 |
| 3   | A     | 305 | PG5  | O1-C2-C3-O2 |
| 5   | B     | 314 | PEG  | O2-C3-C4-O4 |
| 5   | D     | 320 | PEG  | O2-C3-C4-O4 |
| 5   | D     | 324 | PEG  | O2-C3-C4-O4 |
| 5   | D     | 334 | PEG  | O2-C3-C4-O4 |
| 8   | C     | 323 | PG4  | O4-C7-C8-O5 |
| 8   | C     | 326 | PG4  | O1-C1-C2-O2 |
| 5   | B     | 326 | PEG  | C1-C2-O2-C3 |
| 5   | A     | 307 | PEG  | O2-C3-C4-O4 |
| 5   | A     | 309 | PEG  | O1-C1-C2-O2 |
| 5   | B     | 319 | PEG  | O2-C3-C4-O4 |
| 5   | B     | 322 | PEG  | O2-C3-C4-O4 |
| 5   | C     | 308 | PEG  | O1-C1-C2-O2 |
| 5   | C     | 312 | PEG  | O1-C1-C2-O2 |
| 5   | C     | 320 | PEG  | O1-C1-C2-O2 |
| 5   | D     | 317 | PEG  | O1-C1-C2-O2 |
| 5   | D     | 319 | PEG  | O1-C1-C2-O2 |
| 5   | D     | 325 | PEG  | O1-C1-C2-O2 |

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| Mol | Chain | Res    | Type | Atoms        |
|-----|-------|--------|------|--------------|
| 5   | D     | 326    | PEG  | O1-C1-C2-O2  |
| 5   | D     | 336    | PEG  | O2-C3-C4-O4  |
| 8   | B     | 328    | PG4  | O4-C7-C8-O5  |
| 8   | C     | 322    | PG4  | O4-C7-C8-O5  |
| 8   | C     | 325    | PG4  | O4-C7-C8-O5  |
| 8   | D     | 328    | PG4  | O4-C7-C8-O5  |
| 8   | A     | 316    | PG4  | C8-C7-O4-C6  |
| 3   | B     | 311    | PG5  | O2-C4-C5-O3  |
| 8   | D     | 328    | PG4  | O3-C5-C6-O4  |
| 5   | D     | 326    | PEG  | O2-C3-C4-O4  |
| 3   | D     | 304    | PG5  | O2-C4-C5-O3  |
| 3   | B     | 307    | PG5  | O1-C2-C3-O2  |
| 4   | A     | 303    | PG6  | O4-C8-C9-O5  |
| 3   | B     | 305    | PG5  | O1-C2-C3-O2  |
| 10  | C     | 303    | EPE  | C10-C9-N1-C2 |
| 10  | C     | 303    | EPE  | C10-C9-N1-C6 |
| 10  | D     | 305    | EPE  | C10-C9-N1-C2 |
| 10  | D     | 305    | EPE  | C10-C9-N1-C6 |
| 5   | B     | 325    | PEG  | O2-C3-C4-O4  |
| 5   | C     | 321    | PEG  | O1-C1-C2-O2  |
| 5   | D     | 318[B] | PEG  | O1-C1-C2-O2  |
| 8   | B     | 328    | PG4  | O2-C3-C4-O3  |
| 8   | B     | 330    | PG4  | C6-C5-O3-C4  |
| 5   | B     | 310    | PEG  | O1-C1-C2-O2  |
| 8   | A     | 316    | PG4  | C4-C3-O2-C2  |
| 7   | A     | 311    | MLI  | C2-C1-C3-O8  |
| 5   | C     | 313    | PEG  | O2-C3-C4-O4  |
| 8   | C     | 322    | PG4  | O1-C1-C2-O2  |
| 5   | A     | 313    | PEG  | O1-C1-C2-O2  |
| 5   | B     | 316    | PEG  | O2-C3-C4-O4  |
| 5   | D     | 308    | PEG  | O1-C1-C2-O2  |
| 3   | B     | 327    | PG5  | C6-C7-O4-C8  |
| 3   | D     | 312    | PG5  | C2-C3-O2-C4  |
| 3   | D     | 312    | PG5  | C3-C2-O1-C1  |
| 7   | A     | 311    | MLI  | C2-C1-C3-O9  |
| 8   | C     | 325    | PG4  | C6-C5-O3-C4  |
| 3   | B     | 307    | PG5  | C7-C6-O3-C5  |
| 5   | D     | 318[B] | PEG  | O2-C3-C4-O4  |
| 8   | C     | 324    | PG4  | O1-C1-C2-O2  |
| 5   | C     | 311    | PEG  | C1-C2-O2-C3  |
| 8   | B     | 330    | PG4  | C5-C6-O4-C7  |
| 8   | D     | 333    | PG4  | C6-C5-O3-C4  |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | B     | 313 | PEG  | C1-C2-O2-C3 |
| 5   | D     | 335 | PEG  | C1-C2-O2-C3 |
| 5   | A     | 319 | PEG  | C1-C2-O2-C3 |
| 5   | D     | 322 | PEG  | C1-C2-O2-C3 |
| 8   | D     | 328 | PG4  | C6-C5-O3-C4 |
| 3   | B     | 311 | PG5  | C4-C5-O3-C6 |
| 5   | D     | 336 | PEG  | C1-C2-O2-C3 |
| 4   | A     | 303 | PG6  | C5-C4-O2-C3 |
| 5   | A     | 313 | PEG  | C1-C2-O2-C3 |
| 5   | D     | 308 | PEG  | C1-C2-O2-C3 |
| 8   | C     | 322 | PG4  | C1-C2-O2-C3 |
| 8   | D     | 330 | PG4  | C6-C5-O3-C4 |
| 3   | D     | 304 | PG5  | C6-C7-O4-C8 |
| 5   | D     | 311 | PEG  | C1-C2-O2-C3 |
| 5   | D     | 320 | PEG  | C4-C3-O2-C2 |
| 8   | B     | 329 | PG4  | C5-C6-O4-C7 |
| 8   | C     | 325 | PG4  | C1-C2-O2-C3 |
| 3   | C     | 306 | PG5  | C2-C3-O2-C4 |
| 5   | C     | 309 | PEG  | O2-C3-C4-O4 |
| 5   | C     | 317 | PEG  | O1-C1-C2-O2 |
| 5   | D     | 327 | PEG  | O2-C3-C4-O4 |
| 8   | C     | 325 | PG4  | O1-C1-C2-O2 |
| 8   | D     | 331 | PG4  | O1-C1-C2-O2 |
| 5   | D     | 319 | PEG  | C1-C2-O2-C3 |
| 3   | D     | 312 | PG5  | C5-C4-O2-C3 |
| 9   | B     | 302 | PMA  | C6-C4-C7-O5 |
| 9   | B     | 302 | PMA  | C6-C4-C7-O6 |
| 3   | C     | 305 | PG5  | C2-C3-O2-C4 |
| 8   | D     | 333 | PG4  | C5-C6-O4-C7 |
| 5   | B     | 312 | PEG  | C4-C3-O2-C2 |
| 8   | A     | 316 | PG4  | C5-C6-O4-C7 |
| 5   | A     | 312 | PEG  | C1-C2-O2-C3 |
| 8   | A     | 318 | PG4  | C6-C5-O3-C4 |
| 8   | C     | 322 | PG4  | C3-C4-O3-C5 |
| 3   | D     | 312 | PG5  | C7-C6-O3-C5 |
| 8   | C     | 325 | PG4  | O2-C3-C4-O3 |
| 2   | C     | 307 | BEN  | N1-C-C1-C2  |
| 2   | C     | 307 | BEN  | N2-C-C1-C6  |
| 3   | A     | 305 | PG5  | C4-C5-O3-C6 |
| 8   | B     | 330 | PG4  | O2-C3-C4-O3 |
| 5   | C     | 319 | PEG  | C4-C3-O2-C2 |
| 3   | C     | 306 | PG5  | O1-C2-C3-O2 |

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| Mol | Chain | Res    | Type | Atoms       |
|-----|-------|--------|------|-------------|
| 3   | B     | 327    | PG5  | C3-C2-O1-C1 |
| 5   | D     | 323    | PEG  | C4-C3-O2-C2 |
| 8   | A     | 318    | PG4  | C5-C6-O4-C7 |
| 8   | B     | 328    | PG4  | C6-C5-O3-C4 |
| 5   | B     | 306    | PEG  | O2-C3-C4-O4 |
| 5   | B     | 308    | PEG  | O1-C1-C2-O2 |
| 5   | B     | 306    | PEG  | C4-C3-O2-C2 |
| 3   | B     | 305    | PG5  | C5-C4-O2-C3 |
| 8   | D     | 330    | PG4  | C1-C2-O2-C3 |
| 5   | C     | 308    | PEG  | C4-C3-O2-C2 |
| 8   | D     | 330    | PG4  | C4-C3-O2-C2 |
| 5   | D     | 318[A] | PEG  | C4-C3-O2-C2 |
| 8   | D     | 329    | PG4  | C3-C4-O3-C5 |
| 8   | D     | 329    | PG4  | C1-C2-O2-C3 |
| 8   | C     | 322    | PG4  | C5-C6-O4-C7 |
| 3   | B     | 327    | PG5  | C5-C4-O2-C3 |
| 5   | A     | 306    | PEG  | C4-C3-O2-C2 |
| 5   | A     | 313    | PEG  | O2-C3-C4-O4 |
| 5   | B     | 318    | PEG  | O1-C1-C2-O2 |
| 5   | C     | 316    | PEG  | O1-C1-C2-O2 |
| 5   | D     | 311    | PEG  | O2-C3-C4-O4 |
| 5   | B     | 322    | PEG  | C4-C3-O2-C2 |
| 8   | C     | 324    | PG4  | C5-C6-O4-C7 |
| 3   | A     | 302    | PG5  | C6-C7-O4-C8 |
| 3   | A     | 305    | PG5  | C6-C7-O4-C8 |
| 5   | B     | 313    | PEG  | O1-C1-C2-O2 |
| 5   | B     | 331    | PEG  | O2-C3-C4-O4 |
| 5   | D     | 327    | PEG  | O1-C1-C2-O2 |
| 8   | B     | 329    | PG4  | O1-C1-C2-O2 |
| 5   | D     | 335    | PEG  | C4-C3-O2-C2 |
| 9   | B     | 302    | PMA  | C5-C4-C7-O5 |
| 3   | A     | 305    | PG5  | O3-C6-C7-O4 |
| 3   | C     | 305    | PG5  | C5-C4-O2-C3 |
| 5   | D     | 336    | PEG  | C4-C3-O2-C2 |
| 3   | B     | 311    | PG5  | O1-C2-C3-O2 |
| 9   | B     | 302    | PMA  | C5-C4-C7-O6 |
| 5   | C     | 310    | PEG  | O2-C3-C4-O4 |
| 5   | D     | 335    | PEG  | O2-C3-C4-O4 |
| 8   | A     | 316    | PG4  | C1-C2-O2-C3 |
| 8   | C     | 326    | PG4  | C8-C7-O4-C6 |
| 8   | C     | 324    | PG4  | C6-C5-O3-C4 |
| 3   | D     | 304    | PG5  | C3-C2-O1-C1 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | C     | 308 | PEG  | C1-C2-O2-C3 |
| 8   | D     | 332 | PG4  | C5-C6-O4-C7 |
| 8   | B     | 328 | PG4  | C5-C6-O4-C7 |
| 8   | D     | 332 | PG4  | C3-C4-O3-C5 |
| 5   | D     | 317 | PEG  | C4-C3-O2-C2 |
| 5   | C     | 309 | PEG  | C4-C3-O2-C2 |
| 7   | C     | 315 | MLI  | C2-C1-C3-O8 |
| 5   | A     | 306 | PEG  | O2-C3-C4-O4 |
| 5   | C     | 311 | PEG  | O1-C1-C2-O2 |
| 8   | B     | 330 | PG4  | O4-C7-C8-O5 |
| 5   | D     | 316 | PEG  | C1-C2-O2-C3 |
| 5   | B     | 314 | PEG  | C4-C3-O2-C2 |
| 3   | A     | 302 | PG5  | C2-C3-O2-C4 |
| 5   | B     | 309 | PEG  | C1-C2-O2-C3 |
| 3   | D     | 304 | PG5  | O3-C6-C7-O4 |
| 3   | A     | 304 | PG5  | O3-C6-C7-O4 |
| 5   | B     | 314 | PEG  | C1-C2-O2-C3 |
| 7   | C     | 315 | MLI  | C2-C1-C3-O9 |
| 5   | B     | 312 | PEG  | O2-C3-C4-O4 |
| 5   | B     | 319 | PEG  | C4-C3-O2-C2 |
| 2   | B     | 304 | BEN  | N2-C-C1-C2  |
| 2   | B     | 304 | BEN  | N2-C-C1-C6  |
| 2   | C     | 307 | BEN  | N2-C-C1-C2  |
| 8   | C     | 323 | PG4  | C4-C3-O2-C2 |
| 5   | C     | 316 | PEG  | C4-C3-O2-C2 |
| 3   | B     | 311 | PG5  | C3-C2-O1-C1 |
| 8   | B     | 329 | PG4  | C1-C2-O2-C3 |
| 3   | A     | 305 | PG5  | C5-C4-O2-C3 |
| 8   | A     | 317 | PG4  | C8-C7-O4-C6 |
| 7   | B     | 321 | MLI  | C3-C1-C2-O7 |
| 8   | A     | 316 | PG4  | O3-C5-C6-O4 |
| 8   | A     | 318 | PG4  | O1-C1-C2-O2 |
| 5   | A     | 312 | PEG  | C4-C3-O2-C2 |
| 3   | D     | 312 | PG5  | O2-C4-C5-O3 |
| 4   | A     | 303 | PG6  | C9-C8-O4-C7 |
| 5   | B     | 318 | PEG  | C4-C3-O2-C2 |
| 5   | B     | 324 | PEG  | C1-C2-O2-C3 |
| 7   | B     | 321 | MLI  | C2-C1-C3-O8 |
| 5   | B     | 325 | PEG  | O1-C1-C2-O2 |
| 8   | A     | 317 | PG4  | C6-C5-O3-C4 |
| 8   | C     | 324 | PG4  | O2-C3-C4-O3 |
| 5   | C     | 327 | PEG  | C4-C3-O2-C2 |

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| Mol | Chain | Res    | Type | Atoms       |
|-----|-------|--------|------|-------------|
| 5   | C     | 313    | PEG  | C1-C2-O2-C3 |
| 5   | C     | 319    | PEG  | C1-C2-O2-C3 |
| 3   | A     | 304    | PG5  | C6-C7-O4-C8 |
| 5   | D     | 323    | PEG  | O2-C3-C4-O4 |
| 5   | D     | 334    | PEG  | C4-C3-O2-C2 |
| 3   | C     | 306    | PG5  | C3-C2-O1-C1 |
| 9   | D     | 302    | PMA  | C3-C5-C8-O8 |
| 7   | B     | 321    | MLI  | C3-C1-C2-O6 |
| 8   | A     | 317    | PG4  | C3-C4-O3-C5 |
| 9   | B     | 302    | PMA  | C3-C5-C8-O8 |
| 5   | D     | 319    | PEG  | C4-C3-O2-C2 |
| 5   | C     | 321    | PEG  | C1-C2-O2-C3 |
| 5   | C     | 319    | PEG  | O1-C1-C2-O2 |
| 8   | D     | 332    | PG4  | O3-C5-C6-O4 |
| 9   | B     | 302    | PMA  | C3-C5-C8-O7 |
| 8   | B     | 328    | PG4  | O3-C5-C6-O4 |
| 9   | D     | 302    | PMA  | C3-C5-C8-O7 |
| 8   | C     | 326    | PG4  | O3-C5-C6-O4 |
| 8   | B     | 328    | PG4  | C4-C3-O2-C2 |
| 5   | B     | 323    | PEG  | C4-C3-O2-C2 |
| 5   | C     | 312    | PEG  | C4-C3-O2-C2 |
| 10  | D     | 305    | EPE  | C8-C7-N4-C3 |
| 5   | B     | 316    | PEG  | C1-C2-O2-C3 |
| 8   | A     | 318    | PG4  | O3-C5-C6-O4 |
| 2   | B     | 301    | BEN  | N1-C-C1-C2  |
| 2   | B     | 301    | BEN  | N2-C-C1-C2  |
| 2   | B     | 304    | BEN  | N1-C-C1-C2  |
| 2   | B     | 304    | BEN  | N1-C-C1-C6  |
| 3   | C     | 305    | PG5  | C6-C7-O4-C8 |
| 3   | D     | 303    | PG5  | C5-C4-O2-C3 |
| 8   | D     | 333    | PG4  | O3-C5-C6-O4 |
| 5   | B     | 315    | PEG  | C4-C3-O2-C2 |
| 8   | A     | 315    | PG4  | O1-C1-C2-O2 |
| 8   | D     | 329    | PG4  | C4-C3-O2-C2 |
| 5   | C     | 304    | PEG  | C1-C2-O2-C3 |
| 8   | B     | 330    | PG4  | C8-C7-O4-C6 |
| 7   | A     | 311    | MLI  | C3-C1-C2-O7 |
| 5   | B     | 317[A] | PEG  | O2-C3-C4-O4 |
| 5   | C     | 321    | PEG  | C4-C3-O2-C2 |
| 3   | B     | 305    | PG5  | C7-C6-O3-C5 |
| 8   | D     | 331    | PG4  | O3-C5-C6-O4 |
| 3   | A     | 304    | PG5  | O1-C2-C3-O2 |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 5   | D     | 326 | PEG  | C1-C2-O2-C3   |
| 7   | A     | 311 | MLI  | C3-C1-C2-O6   |
| 5   | A     | 308 | PEG  | O1-C1-C2-O2   |
| 5   | B     | 312 | PEG  | O1-C1-C2-O2   |
| 5   | C     | 320 | PEG  | O2-C3-C4-O4   |
| 5   | D     | 324 | PEG  | C1-C2-O2-C3   |
| 8   | C     | 323 | PG4  | C6-C5-O3-C4   |
| 5   | C     | 312 | PEG  | C1-C2-O2-C3   |
| 5   | D     | 327 | PEG  | C1-C2-O2-C3   |
| 3   | B     | 311 | PG5  | C6-C7-O4-C8   |
| 4   | A     | 303 | PG6  | O5-C10-C11-O6 |
| 3   | A     | 302 | PG5  | C3-C2-O1-C1   |

There are no ring outliers.

74 monomers are involved in 159 short contacts:

| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 5   | D     | 316    | PEG  | 1       | 0            |
| 8   | D     | 329    | PG4  | 4       | 0            |
| 3   | D     | 312    | PG5  | 4       | 0            |
| 5   | D     | 321    | PEG  | 3       | 1            |
| 5   | B     | 319    | PEG  | 2       | 0            |
| 9   | B     | 302    | PMA  | 3       | 0            |
| 8   | A     | 315    | PG4  | 0       | 1            |
| 5   | D     | 318[B] | PEG  | 1       | 0            |
| 5   | D     | 336    | PEG  | 1       | 0            |
| 5   | A     | 307    | PEG  | 2       | 0            |
| 8   | D     | 331    | PG4  | 1       | 0            |
| 5   | B     | 322    | PEG  | 1       | 0            |
| 5   | D     | 319    | PEG  | 6       | 0            |
| 8   | A     | 318    | PG4  | 1       | 0            |
| 5   | B     | 306    | PEG  | 1       | 0            |
| 3   | C     | 306    | PG5  | 3       | 0            |
| 5   | B     | 316    | PEG  | 3       | 0            |
| 8   | C     | 325    | PG4  | 5       | 0            |
| 8   | D     | 330    | PG4  | 2       | 0            |
| 5   | C     | 328[A] | PEG  | 1       | 0            |
| 5   | D     | 324    | PEG  | 1       | 0            |
| 5   | D     | 310    | PEG  | 1       | 0            |
| 3   | B     | 305    | PG5  | 3       | 0            |
| 5   | D     | 308    | PEG  | 1       | 0            |
| 5   | B     | 312    | PEG  | 1       | 0            |

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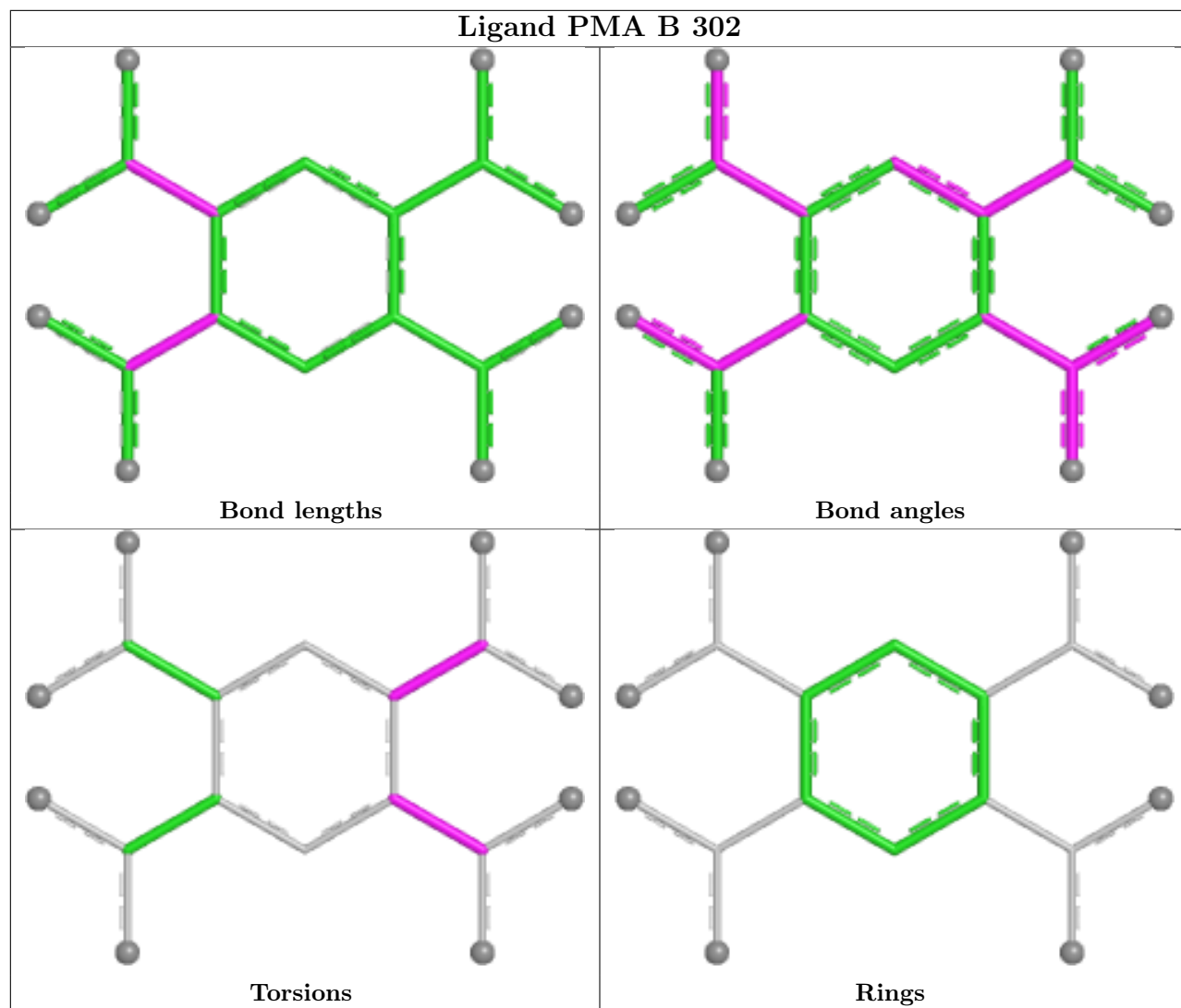
| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 3   | A     | 305    | PG5  | 2       | 0            |
| 8   | A     | 317    | PG4  | 1       | 0            |
| 5   | B     | 309    | PEG  | 3       | 0            |
| 8   | B     | 329    | PG4  | 3       | 0            |
| 5   | B     | 317[A] | PEG  | 3       | 0            |
| 3   | B     | 311    | PG5  | 4       | 0            |
| 5   | D     | 320    | PEG  | 9       | 0            |
| 8   | C     | 324    | PG4  | 3       | 0            |
| 8   | C     | 322    | PG4  | 1       | 0            |
| 8   | D     | 328    | PG4  | 0       | 1            |
| 5   | B     | 324    | PEG  | 1       | 0            |
| 5   | D     | 335    | PEG  | 2       | 0            |
| 5   | D     | 327    | PEG  | 1       | 0            |
| 2   | B     | 304    | BEN  | 2       | 0            |
| 3   | C     | 305    | PG5  | 1       | 0            |
| 3   | A     | 304    | PG5  | 2       | 0            |
| 10  | D     | 305    | EPE  | 3       | 0            |
| 5   | B     | 308    | PEG  | 2       | 0            |
| 2   | B     | 303    | BEN  | 1       | 0            |
| 5   | B     | 325    | PEG  | 4       | 0            |
| 8   | D     | 333    | PG4  | 7       | 2            |
| 8   | B     | 330    | PG4  | 4       | 0            |
| 5   | D     | 311    | PEG  | 1       | 0            |
| 8   | A     | 316    | PG4  | 1       | 1            |
| 5   | D     | 318[A] | PEG  | 2       | 0            |
| 9   | D     | 302    | PMA  | 4       | 0            |
| 7   | B     | 321    | MLI  | 1       | 0            |
| 5   | C     | 316    | PEG  | 4       | 0            |
| 10  | C     | 303    | EPE  | 3       | 0            |
| 3   | B     | 307    | PG5  | 1       | 0            |
| 5   | C     | 309    | PEG  | 5       | 0            |
| 3   | A     | 302    | PG5  | 2       | 0            |
| 5   | B     | 317[B] | PEG  | 3       | 0            |
| 5   | D     | 317    | PEG  | 3       | 0            |
| 7   | A     | 311    | MLI  | 1       | 0            |
| 5   | C     | 313    | PEG  | 1       | 0            |
| 8   | D     | 332    | PG4  | 0       | 1            |
| 4   | A     | 303    | PG6  | 2       | 0            |
| 5   | A     | 306    | PEG  | 1       | 0            |
| 5   | C     | 312    | PEG  | 4       | 0            |
| 3   | D     | 304    | PG5  | 1       | 0            |
| 5   | C     | 308    | PEG  | 10      | 0            |

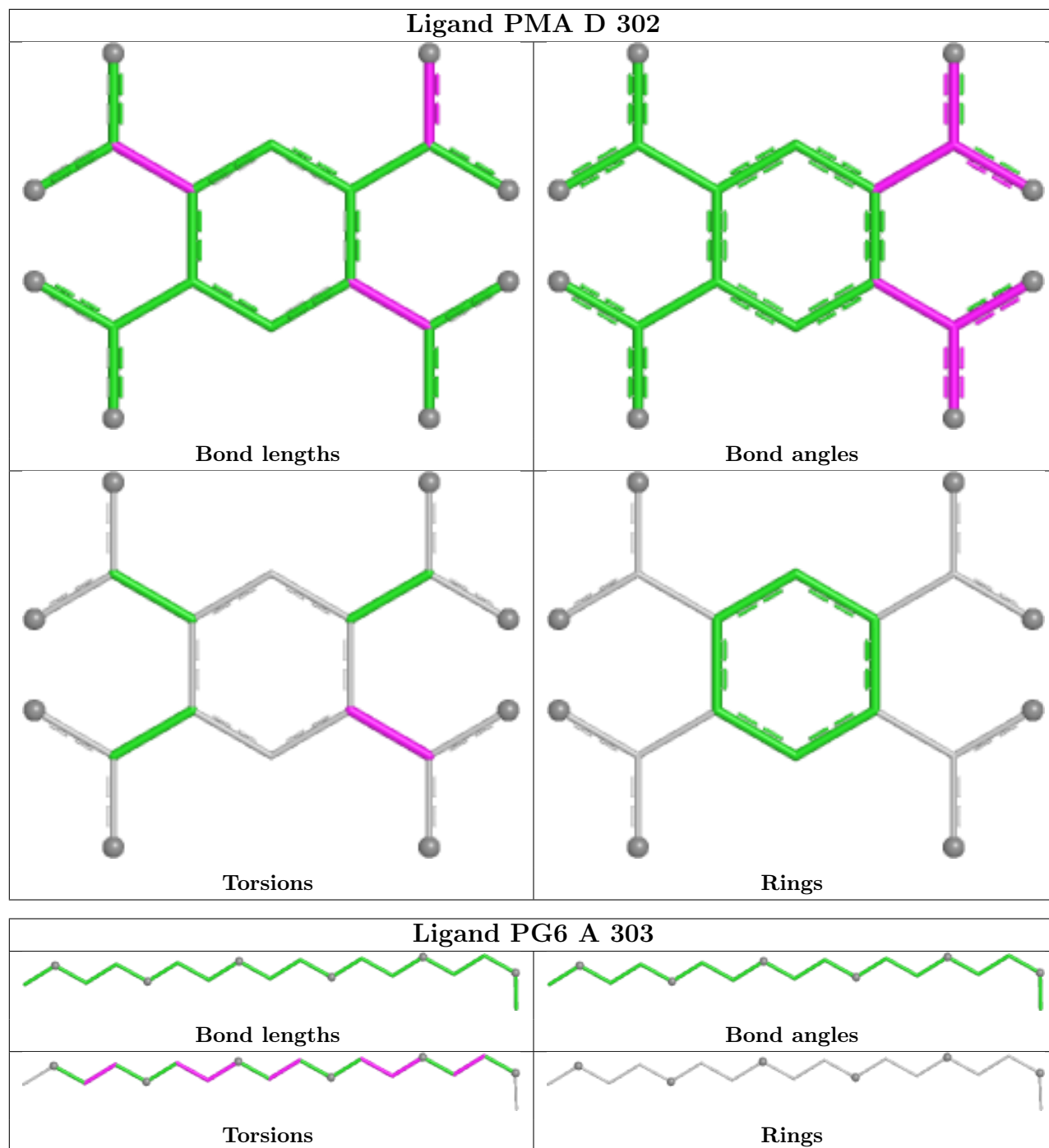
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | D     | 309 | BEN  | 1       | 0            |
| 3   | D     | 303 | PG5  | 4       | 0            |
| 5   | D     | 322 | PEG  | 3       | 0            |
| 5   | C     | 320 | PEG  | 1       | 0            |
| 5   | D     | 337 | PEG  | 1       | 0            |
| 8   | C     | 326 | PG4  | 2       | 0            |
| 2   | C     | 301 | BEN  | 4       | 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.





## 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 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|---------------|--------|----------------|-----------------------|---------|
| 1   | A     | 223/231 (96%) | 1.04   | 27 (12%) 8 11  | 15, 21, 31, 38        | 3 (1%)  |
| 1   | B     | 223/231 (96%) | 1.31   | 46 (20%) 2 4   | 18, 29, 47, 51        | 2 (0%)  |
| 1   | C     | 223/231 (96%) | 1.06   | 30 (13%) 7 9   | 14, 19, 27, 34        | 1 (0%)  |
| 1   | D     | 223/231 (96%) | 0.74   | 10 (4%) 38 41  | 10, 18, 32, 47        | 6 (2%)  |
| All | All   | 892/924 (96%) | 1.04   | 113 (12%) 8 10 | 10, 21, 38, 51        | 12 (1%) |

All (113) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 163 | CYS  | 5.7  |
| 1   | B     | 73  | LEU  | 4.8  |
| 1   | B     | 212 | CYS  | 4.6  |
| 1   | C     | 218 | PRO  | 3.9  |
| 1   | B     | 114 | ARG  | 3.9  |
| 1   | C     | 208 | TRP  | 3.8  |
| 1   | B     | 75  | GLY  | 3.7  |
| 1   | B     | 157 | VAL  | 3.6  |
| 1   | B     | 143 | GLY  | 3.4  |
| 1   | B     | 142 | SER  | 3.4  |
| 1   | D     | 212 | CYS  | 3.3  |
| 1   | A     | 169 | GLY  | 3.3  |
| 1   | B     | 188 | CYS  | 3.3  |
| 1   | B     | 144 | SER  | 3.2  |
| 1   | B     | 76  | ASN  | 3.2  |
| 1   | C     | 210 | TYR  | 3.1  |
| 1   | B     | 155 | ALA  | 3.1  |
| 1   | A     | 149 | LEU  | 3.1  |
| 1   | A     | 198 | CYS  | 3.0  |
| 1   | B     | 63  | VAL  | 3.0  |
| 1   | C     | 228 | VAL  | 3.0  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | A     | 183   | GLY  | 3.0  |
| 1   | B     | 198   | CYS  | 3.0  |
| 1   | B     | 16    | ILE  | 2.9  |
| 1   | D     | 25[A] | ASN  | 2.9  |
| 1   | C     | 20    | TYR  | 2.9  |
| 1   | A     | 133   | ILE  | 2.9  |
| 1   | C     | 131   | CYS  | 2.9  |
| 1   | D     | 27    | ILE  | 2.8  |
| 1   | C     | 183   | GLY  | 2.8  |
| 1   | B     | 60    | ARG  | 2.8  |
| 1   | B     | 27    | ILE  | 2.8  |
| 1   | B     | 22    | CYS  | 2.8  |
| 1   | A     | 199   | ASN  | 2.7  |
| 1   | A     | 73    | LEU  | 2.7  |
| 1   | C     | 221   | TYR  | 2.7  |
| 1   | A     | 225   | CYS  | 2.7  |
| 1   | C     | 126   | ALA  | 2.7  |
| 1   | A     | 210   | TYR  | 2.6  |
| 1   | A     | 153   | LEU  | 2.6  |
| 1   | B     | 196   | VAL  | 2.6  |
| 1   | A     | 94    | ASN  | 2.6  |
| 1   | C     | 179   | GLY  | 2.6  |
| 1   | C     | 96    | LEU  | 2.6  |
| 1   | A     | 161   | SER  | 2.6  |
| 1   | B     | 113   | SER  | 2.5  |
| 1   | A     | 168   | PRO  | 2.5  |
| 1   | B     | 65    | LEU  | 2.5  |
| 1   | B     | 200   | GLY  | 2.5  |
| 1   | A     | 118   | VAL  | 2.5  |
| 1   | C     | 176   | ILE  | 2.5  |
| 1   | A     | 126   | ALA  | 2.5  |
| 1   | B     | 236   | ALA  | 2.5  |
| 1   | C     | 24    | ALA  | 2.5  |
| 1   | B     | 112   | ASN  | 2.4  |
| 1   | C     | 177   | CYS  | 2.4  |
| 1   | D     | 188   | CYS  | 2.4  |
| 1   | B     | 122   | ARG  | 2.4  |
| 1   | A     | 70    | ILE  | 2.4  |
| 1   | C     | 171   | ILE  | 2.4  |
| 1   | B     | 115   | VAL  | 2.4  |
| 1   | C     | 197   | VAL  | 2.4  |
| 1   | A     | 144   | SER  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 208 | TRP  | 2.3  |
| 1   | B     | 210 | TYR  | 2.3  |
| 1   | C     | 60  | ARG  | 2.3  |
| 1   | D     | 142 | SER  | 2.3  |
| 1   | B     | 24  | ALA  | 2.3  |
| 1   | B     | 111 | LEU  | 2.3  |
| 1   | B     | 132 | LEU  | 2.3  |
| 1   | B     | 225 | CYS  | 2.3  |
| 1   | A     | 18  | GLY  | 2.3  |
| 1   | D     | 24  | ALA  | 2.3  |
| 1   | A     | 163 | CYS  | 2.2  |
| 1   | C     | 124 | CYS  | 2.2  |
| 1   | C     | 167 | TYR  | 2.2  |
| 1   | C     | 230 | TRP  | 2.2  |
| 1   | C     | 105 | LEU  | 2.2  |
| 1   | A     | 177 | CYS  | 2.2  |
| 1   | B     | 20  | TYR  | 2.2  |
| 1   | D     | 152 | CYS  | 2.2  |
| 1   | B     | 119 | SER  | 2.2  |
| 1   | B     | 28  | PRO  | 2.2  |
| 1   | C     | 172 | THR  | 2.2  |
| 1   | A     | 27  | ILE  | 2.2  |
| 1   | C     | 133 | ILE  | 2.2  |
| 1   | B     | 158 | LEU  | 2.2  |
| 1   | D     | 68  | HIS  | 2.2  |
| 1   | D     | 144 | SER  | 2.2  |
| 1   | A     | 20  | TYR  | 2.2  |
| 1   | B     | 66  | GLY  | 2.1  |
| 1   | C     | 188 | CYS  | 2.1  |
| 1   | C     | 16  | ILE  | 2.1  |
| 1   | B     | 68  | HIS  | 2.1  |
| 1   | A     | 131 | CYS  | 2.1  |
| 1   | C     | 212 | CYS  | 2.1  |
| 1   | A     | 208 | TRP  | 2.1  |
| 1   | C     | 125 | ALA  | 2.1  |
| 1   | B     | 25  | ASN  | 2.1  |
| 1   | B     | 46  | ASN  | 2.1  |
| 1   | B     | 229 | ASN  | 2.1  |
| 1   | C     | 153 | LEU  | 2.0  |
| 1   | C     | 202 | LEU  | 2.0  |
| 1   | B     | 70  | ILE  | 2.0  |
| 1   | B     | 178 | VAL  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 146 | TYR  | 2.0  |
| 1   | A     | 21  | THR  | 2.0  |
| 1   | B     | 117 | THR  | 2.0  |
| 1   | A     | 213 | ALA  | 2.0  |
| 1   | B     | 59  | SER  | 2.0  |
| 1   | B     | 109 | ALA  | 2.0  |
| 1   | D     | 143 | GLY  | 2.0  |
| 1   | A     | 150 | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|----------------------------|-------|
| 7   | MLI  | A     | 311    | 7/7   | 0.39 | 0.15 | 48,72,86,91                | 0     |
| 5   | PEG  | D     | 322    | 7/7   | 0.40 | 0.17 | 52,63,71,71                | 17    |
| 5   | PEG  | D     | 318[A] | 7/7   | 0.45 | 0.20 | 30,55,66,66                | 17    |
| 5   | PEG  | D     | 318[B] | 7/7   | 0.45 | 0.20 | 37,53,67,72                | 17    |
| 5   | PEG  | C     | 328[A] | 7/7   | 0.45 | 0.24 | 42,57,69,69                | 17    |
| 5   | PEG  | C     | 328[B] | 7/7   | 0.45 | 0.24 | 46,60,72,74                | 17    |
| 8   | PG4  | B     | 330    | 13/13 | 0.47 | 0.21 | 35,57,74,77                | 31    |
| 5   | PEG  | D     | 319    | 7/7   | 0.50 | 0.21 | 46,57,69,71                | 16    |
| 5   | PEG  | D     | 327    | 7/7   | 0.51 | 0.13 | 52,65,81,84                | 0     |
| 5   | PEG  | B     | 317[A] | 7/7   | 0.51 | 0.15 | 38,60,72,72                | 17    |
| 5   | PEG  | B     | 317[B] | 7/7   | 0.51 | 0.15 | 49,59,69,69                | 17    |
| 5   | PEG  | C     | 309    | 7/7   | 0.53 | 0.20 | 25,57,68,78                | 17    |
| 5   | PEG  | B     | 322    | 7/7   | 0.55 | 0.18 | 42,59,67,77                | 17    |
| 8   | PG4  | C     | 325    | 13/13 | 0.55 | 0.20 | 32,57,68,71                | 31    |
| 5   | PEG  | C     | 320    | 7/7   | 0.56 | 0.18 | 34,54,65,65                | 17    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 7   | MLI  | C     | 315 | 7/7   | 0.56 | 0.19 | 30,62,71,73                 | 9     |
| 8   | PG4  | A     | 317 | 13/13 | 0.56 | 0.20 | 25,59,77,78                 | 31    |
| 5   | PEG  | D     | 326 | 7/7   | 0.56 | 0.20 | 44,57,69,69                 | 17    |
| 3   | PG5  | D     | 304 | 12/12 | 0.56 | 0.16 | 38,64,73,78                 | 30    |
| 8   | PG4  | C     | 323 | 13/13 | 0.58 | 0.17 | 47,60,66,68                 | 31    |
| 3   | PG5  | B     | 327 | 12/12 | 0.58 | 0.19 | 48,60,66,66                 | 30    |
| 3   | PG5  | B     | 307 | 12/12 | 0.59 | 0.21 | 22,46,66,66                 | 30    |
| 5   | PEG  | C     | 308 | 7/7   | 0.59 | 0.19 | 31,62,79,91                 | 0     |
| 2   | BEN  | C     | 307 | 9/9   | 0.60 | 0.15 | 45,63,87,87                 | 0     |
| 5   | PEG  | D     | 308 | 7/7   | 0.60 | 0.24 | 26,54,64,67                 | 17    |
| 8   | PG4  | D     | 331 | 13/13 | 0.60 | 0.18 | 42,56,69,71                 | 31    |
| 8   | PG4  | D     | 332 | 13/13 | 0.60 | 0.17 | 44,54,64,64                 | 31    |
| 7   | MLI  | B     | 321 | 7/7   | 0.61 | 0.11 | 55,64,74,75                 | 0     |
| 5   | PEG  | B     | 324 | 7/7   | 0.61 | 0.20 | 28,53,77,77                 | 17    |
| 5   | PEG  | D     | 324 | 7/7   | 0.62 | 0.25 | 21,56,69,75                 | 17    |
| 5   | PEG  | A     | 308 | 7/7   | 0.62 | 0.16 | 53,64,71,75                 | 0     |
| 7   | MLI  | D     | 315 | 7/7   | 0.62 | 0.15 | 37,47,49,59                 | 9     |
| 3   | PG5  | C     | 306 | 12/12 | 0.63 | 0.24 | 41,52,63,63                 | 30    |
| 8   | PG4  | C     | 322 | 13/13 | 0.63 | 0.17 | 45,55,67,67                 | 31    |
| 8   | PG4  | B     | 328 | 13/13 | 0.63 | 0.18 | 43,58,66,68                 | 31    |
| 3   | PG5  | B     | 311 | 12/12 | 0.64 | 0.16 | 30,52,60,60                 | 30    |
| 5   | PEG  | D     | 321 | 7/7   | 0.64 | 0.17 | 29,49,68,68                 | 17    |
| 3   | PG5  | D     | 303 | 12/12 | 0.64 | 0.26 | 21,36,59,59                 | 29    |
| 5   | PEG  | D     | 316 | 7/7   | 0.65 | 0.16 | 48,58,70,70                 | 17    |
| 5   | PEG  | B     | 325 | 7/7   | 0.66 | 0.23 | 36,58,67,67                 | 17    |
| 8   | PG4  | D     | 330 | 13/13 | 0.66 | 0.22 | 35,59,71,74                 | 31    |
| 4   | PG6  | A     | 303 | 18/18 | 0.66 | 0.18 | 23,54,67,74                 | 44    |
| 5   | PEG  | D     | 337 | 7/7   | 0.66 | 0.21 | 45,54,61,61                 | 17    |
| 5   | PEG  | B     | 318 | 7/7   | 0.67 | 0.21 | 33,51,62,62                 | 17    |
| 5   | PEG  | B     | 308 | 7/7   | 0.67 | 0.18 | 34,56,78,78                 | 17    |
| 3   | PG5  | C     | 305 | 12/12 | 0.67 | 0.18 | 33,60,73,84                 | 30    |
| 5   | PEG  | C     | 321 | 7/7   | 0.67 | 0.12 | 47,56,67,69                 | 17    |
| 3   | PG5  | A     | 304 | 12/12 | 0.67 | 0.20 | 32,56,63,72                 | 30    |
| 5   | PEG  | C     | 317 | 7/7   | 0.68 | 0.19 | 32,50,60,60                 | 17    |
| 5   | PEG  | D     | 335 | 7/7   | 0.68 | 0.18 | 28,46,66,79                 | 17    |
| 5   | PEG  | C     | 318 | 7/7   | 0.68 | 0.15 | 47,56,68,68                 | 17    |
| 3   | PG5  | A     | 302 | 12/12 | 0.68 | 0.18 | 29,52,66,70                 | 30    |
| 10  | EPE  | C     | 303 | 15/15 | 0.68 | 0.17 | 27,49,61,64                 | 31    |
| 5   | PEG  | D     | 310 | 7/7   | 0.69 | 0.20 | 29,47,60,60                 | 17    |
| 5   | PEG  | A     | 307 | 7/7   | 0.69 | 0.24 | 38,59,71,75                 | 17    |
| 5   | PEG  | B     | 331 | 7/7   | 0.69 | 0.12 | 48,57,61,63                 | 17    |
| 5   | PEG  | C     | 327 | 7/7   | 0.69 | 0.18 | 34,53,64,64                 | 17    |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 8   | PG4  | A     | 316    | 13/13 | 0.69 | 0.16 | 37,57,68,79                 | 30    |
| 5   | PEG  | B     | 314    | 7/7   | 0.70 | 0.15 | 53,63,66,67                 | 17    |
| 5   | PEG  | B     | 316    | 7/7   | 0.70 | 0.14 | 49,63,76,79                 | 17    |
| 3   | PG5  | D     | 312    | 12/12 | 0.71 | 0.27 | 23,53,73,76                 | 30    |
| 8   | PG4  | D     | 329    | 13/13 | 0.71 | 0.20 | 20,53,65,67                 | 31    |
| 3   | PG5  | A     | 305    | 12/12 | 0.71 | 0.17 | 28,51,62,68                 | 30    |
| 8   | PG4  | C     | 326    | 13/13 | 0.72 | 0.24 | 34,53,62,63                 | 31    |
| 5   | PEG  | B     | 319    | 7/7   | 0.72 | 0.21 | 26,48,60,60                 | 17    |
| 5   | PEG  | C     | 304    | 7/7   | 0.72 | 0.22 | 27,58,70,71                 | 17    |
| 2   | BEN  | D     | 309    | 9/9   | 0.72 | 0.16 | 27,63,80,81                 | 0     |
| 5   | PEG  | A     | 306    | 7/7   | 0.72 | 0.17 | 40,55,66,66                 | 17    |
| 5   | PEG  | A     | 314    | 7/7   | 0.72 | 0.15 | 32,51,76,76                 | 0     |
| 5   | PEG  | B     | 326    | 7/7   | 0.73 | 0.17 | 40,50,65,67                 | 16    |
| 5   | PEG  | B     | 312    | 7/7   | 0.73 | 0.14 | 31,49,67,67                 | 17    |
| 5   | PEG  | D     | 323    | 7/7   | 0.73 | 0.16 | 31,58,66,67                 | 17    |
| 5   | PEG  | C     | 310    | 7/7   | 0.73 | 0.15 | 27,60,73,73                 | 17    |
| 5   | PEG  | A     | 309    | 7/7   | 0.73 | 0.16 | 38,50,62,65                 | 17    |
| 5   | PEG  | B     | 313    | 7/7   | 0.74 | 0.14 | 35,58,70,70                 | 17    |
| 5   | PEG  | D     | 311    | 7/7   | 0.75 | 0.22 | 19,48,66,66                 | 17    |
| 8   | PG4  | A     | 318    | 13/13 | 0.75 | 0.21 | 24,53,65,76                 | 31    |
| 5   | PEG  | D     | 320    | 7/7   | 0.75 | 0.16 | 47,58,65,72                 | 15    |
| 5   | PEG  | C     | 319    | 7/7   | 0.75 | 0.22 | 22,52,63,63                 | 17    |
| 8   | PG4  | D     | 328    | 13/13 | 0.75 | 0.22 | 35,55,65,74                 | 31    |
| 8   | PG4  | A     | 315    | 12/13 | 0.76 | 0.28 | 27,52,59,64                 | 29    |
| 5   | PEG  | D     | 317    | 7/7   | 0.76 | 0.13 | 29,50,70,70                 | 0     |
| 5   | PEG  | A     | 312    | 7/7   | 0.77 | 0.14 | 42,56,64,64                 | 17    |
| 8   | PG4  | B     | 329    | 13/13 | 0.78 | 0.25 | 17,48,67,68                 | 31    |
| 5   | PEG  | B     | 306    | 7/7   | 0.78 | 0.17 | 29,45,73,73                 | 17    |
| 2   | BEN  | D     | 306[A] | 9/9   | 0.78 | 0.17 | 37,52,66,73                 | 17    |
| 2   | BEN  | D     | 306[B] | 9/9   | 0.78 | 0.17 | 34,49,74,74                 | 17    |
| 5   | PEG  | D     | 307    | 7/7   | 0.78 | 0.21 | 41,57,76,76                 | 17    |
| 3   | PG5  | B     | 305    | 12/12 | 0.78 | 0.22 | 23,45,70,78                 | 30    |
| 8   | PG4  | C     | 324    | 13/13 | 0.79 | 0.15 | 27,57,73,77                 | 31    |
| 5   | PEG  | C     | 312    | 7/7   | 0.79 | 0.15 | 30,58,70,78                 | 17    |
| 5   | PEG  | B     | 310    | 7/7   | 0.79 | 0.12 | 37,57,69,78                 | 17    |
| 10  | EPE  | D     | 305    | 15/15 | 0.79 | 0.16 | 27,54,80,83                 | 32    |
| 8   | PG4  | D     | 333    | 13/13 | 0.80 | 0.26 | 24,53,64,70                 | 31    |
| 5   | PEG  | D     | 325    | 7/7   | 0.80 | 0.14 | 25,51,83,83                 | 17    |
| 5   | PEG  | B     | 323    | 7/7   | 0.80 | 0.16 | 17,55,69,70                 | 17    |
| 2   | BEN  | B     | 304    | 9/9   | 0.81 | 0.28 | 37,54,73,80                 | 17    |
| 5   | PEG  | A     | 319    | 7/7   | 0.81 | 0.17 | 31,50,77,77                 | 17    |
| 5   | PEG  | D     | 334    | 7/7   | 0.81 | 0.16 | 25,54,69,69                 | 17    |

*Continued on next page...*

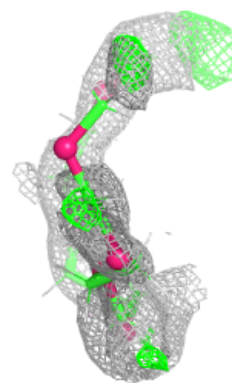
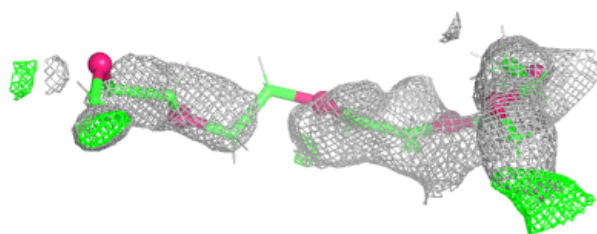
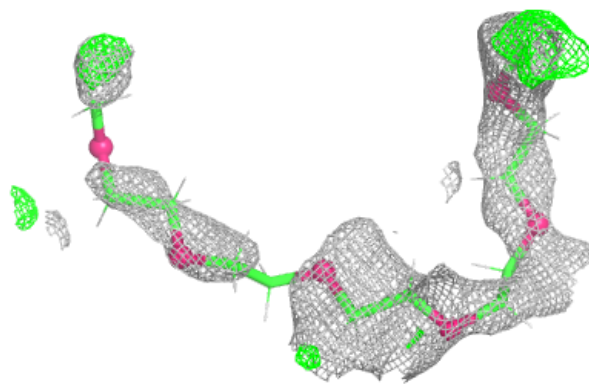
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 5   | PEG  | B     | 315 | 7/7   | 0.81 | 0.12 | 46,56,67,68                 | 17    |
| 5   | PEG  | D     | 336 | 7/7   | 0.81 | 0.17 | 23,46,64,64                 | 17    |
| 5   | PEG  | C     | 311 | 7/7   | 0.83 | 0.18 | 20,50,67,67                 | 17    |
| 5   | PEG  | A     | 313 | 7/7   | 0.84 | 0.19 | 22,39,58,58                 | 17    |
| 2   | BEN  | C     | 301 | 9/9   | 0.84 | 0.11 | 17,22,26,28                 | 0     |
| 5   | PEG  | C     | 316 | 7/7   | 0.85 | 0.16 | 32,54,64,65                 | 17    |
| 5   | PEG  | B     | 309 | 7/7   | 0.85 | 0.20 | 22,33,50,60                 | 17    |
| 5   | PEG  | C     | 313 | 7/7   | 0.85 | 0.12 | 23,52,66,66                 | 17    |
| 2   | BEN  | A     | 301 | 9/9   | 0.88 | 0.09 | 18,23,29,30                 | 0     |
| 9   | PMA  | B     | 302 | 18/18 | 0.90 | 0.09 | 23,29,50,74                 | 0     |
| 2   | BEN  | B     | 301 | 9/9   | 0.93 | 0.10 | 20,25,30,33                 | 0     |
| 2   | BEN  | B     | 303 | 9/9   | 0.93 | 0.08 | 19,24,32,32                 | 0     |
| 2   | BEN  | D     | 301 | 9/9   | 0.94 | 0.08 | 17,22,26,26                 | 0     |
| 9   | PMA  | D     | 302 | 18/18 | 0.94 | 0.07 | 15,16,23,25                 | 0     |
| 6   | CA   | B     | 320 | 1/1   | 0.94 | 0.07 | 37,37,37,37                 | 0     |
| 2   | BEN  | C     | 302 | 9/9   | 0.94 | 0.08 | 15,19,26,27                 | 0     |
| 11  | CL   | D     | 338 | 1/1   | 0.94 | 0.15 | 25,25,25,25                 | 0     |
| 6   | CA   | D     | 314 | 1/1   | 0.96 | 0.21 | 32,32,32,32                 | 0     |
| 6   | CA   | D     | 313 | 1/1   | 0.96 | 0.05 | 20,20,20,20                 | 0     |
| 6   | CA   | C     | 314 | 1/1   | 0.97 | 0.05 | 15,15,15,15                 | 0     |
| 6   | CA   | A     | 310 | 1/1   | 0.97 | 0.05 | 19,19,19,19                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

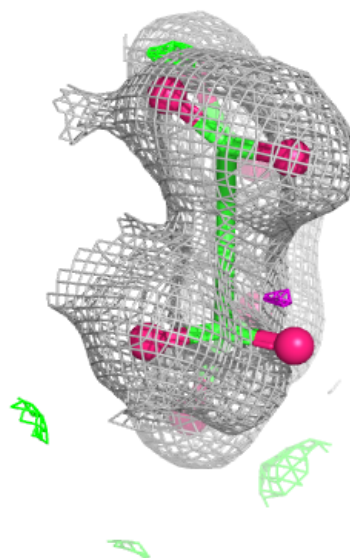
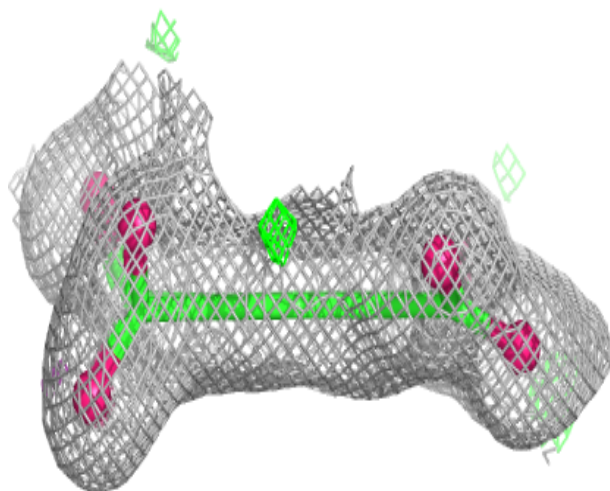
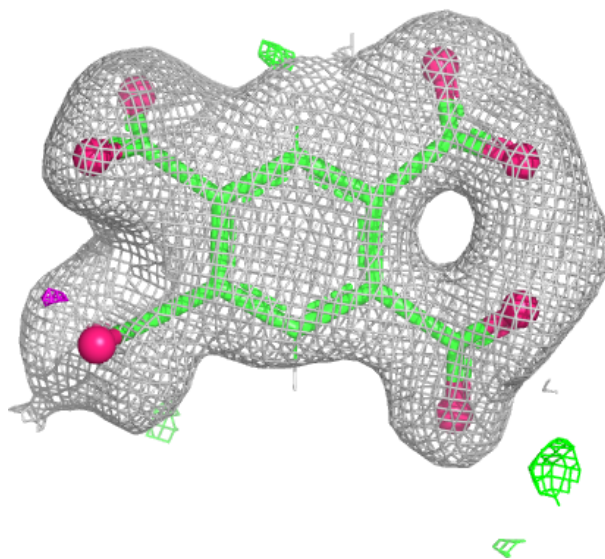
**Electron density around PG6 A 303:**

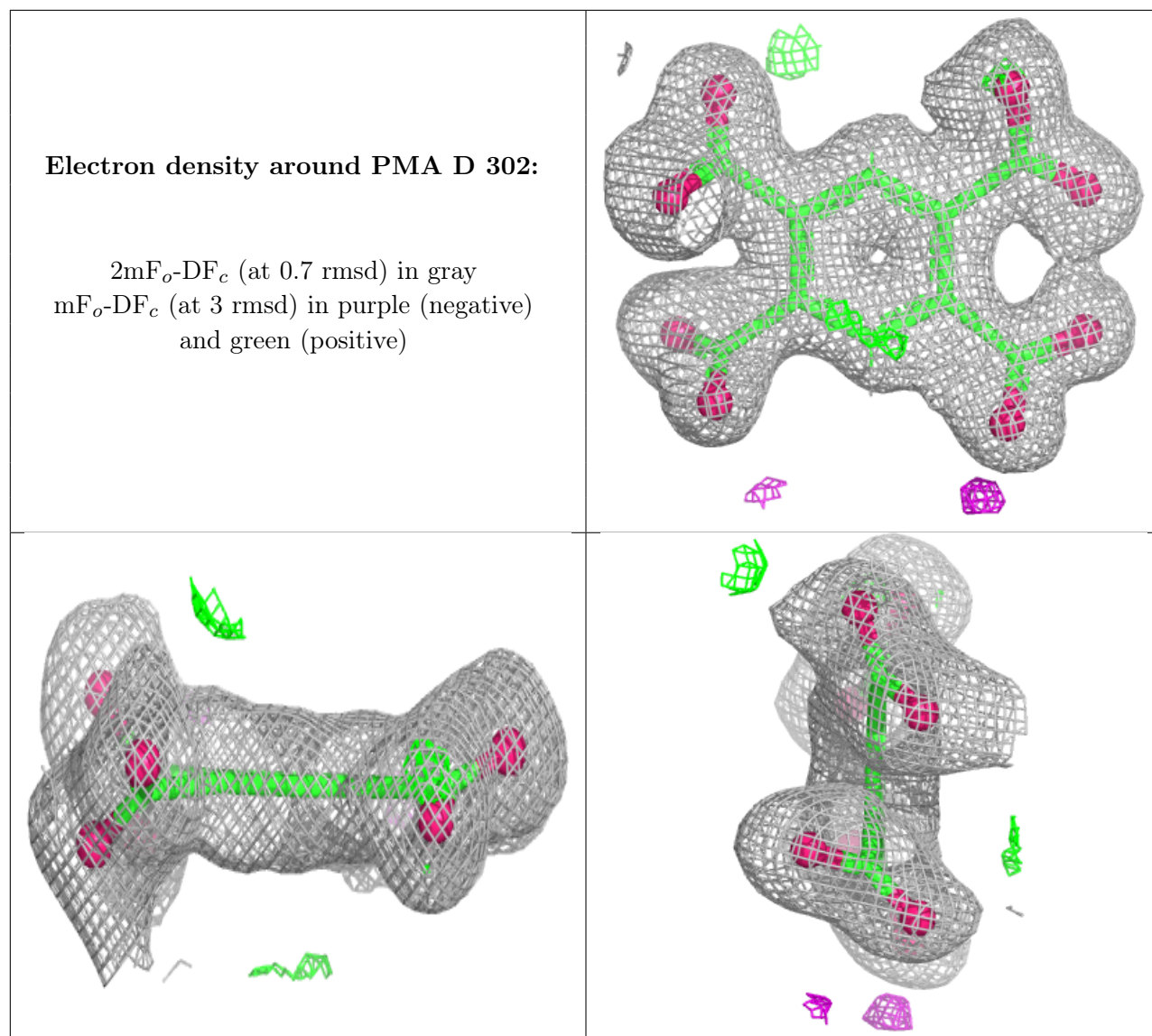
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PMA B 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.