# Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 10:32 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 1JZ3 |
| Title | : | E. COLI (lacZ) BETA-GALACTOSIDASE-TRAPPED 2-DEOXY-GALACTOSYL ENZYME INTERMEDIATE |
| Authors | : | Juers, D.H.; Matthews, B.W. |
| Deposited on | : | 2001-09-13 |
| Resolution | : | 1.75 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

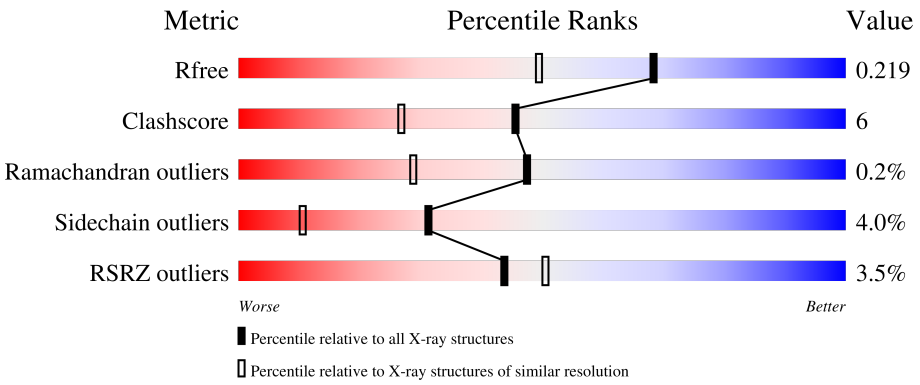
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 2340 (1.76-1.76) |
| Clashscore | 141614 | 2466 (1.76-1.76) |
| Ramachandran outliers | 138981 | 2437 (1.76-1.76) |
| Sidechain outliers | 138945 | 2437 (1.76-1.76) |
| RSRZ outliers | 127900 | 2298 (1.76-1.76) |

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 >=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 <=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 | 1023 | 3% 74% 21% • • |
| 1 | B | 1023 | 3% 75% 21% • • |
| 1 | C | 1023 | 3% 72% 22% • • |
| 1 | D | 1023 | 4% 75% 20% • • |

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 |
|---|---|---|---|---|---|---|---|
| 6 | DMS | C | 8425 | - | - | X | - |
| 6 | DMS | D | 8703 | - | - | X | - |

# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 37369 atoms, of which 0 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 Beta-Galactosidase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 1011 | 8125 | 5138 | 1440 | 1509 | 38 | 0 | 0 | 0 |
| 1 | B | 1011 | 8131 | 5144 | 1440 | 1509 | 38 | 0 | 1 | 0 |
| 1 | C | 1011 | 8125 | 5138 | 1440 | 1509 | 38 | 0 | 0 | 0 |
| 1 | D | 1011 | 8125 | 5138 | 1440 | 1509 | 38 | 0 | 0 | 0 |

There are 32 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | GLY | THR | cloning artifact | ? P00722 |
| A | 2 | SER | MET | cloning artifact | ? P00722 |
| A | 3 | HIS | ILE | cloning artifact | ? P00722 |
| A | 4 | MET | THR | cloning artifact | ? P00722 |
| A | 5 | LEU | ASP | cloning artifact | ? P00722 |
| A | 6 | GLU | SER | cloning artifact | ? P00722 |
| A | 7 | ASP | LEU | cloning artifact | ? P00722 |
| A | 8 | PRO | ALA | cloning artifact | ? P00722 |
| B | 1 | GLY | THR | cloning artifact | ? P00722 |
| B | 2 | SER | MET | cloning artifact | ? P00722 |
| B | 3 | HIS | ILE | cloning artifact | ? P00722 |
| B | 4 | MET | THR | cloning artifact | ? P00722 |
| B | 5 | LEU | ASP | cloning artifact | ? P00722 |
| B | 6 | GLU | SER | cloning artifact | ? P00722 |
| B | 7 | ASP | LEU | cloning artifact | ? P00722 |
| B | 8 | PRO | ALA | cloning artifact | ? P00722 |
| C | 1 | GLY | THR | cloning artifact | ? P00722 |
| C | 2 | SER | MET | cloning artifact | ? P00722 |
| C | 3 | HIS | ILE | cloning artifact | ? P00722 |
| C | 4 | MET | THR | cloning artifact | ? P00722 |
| C | 5 | LEU | ASP | cloning artifact | ? P00722 |

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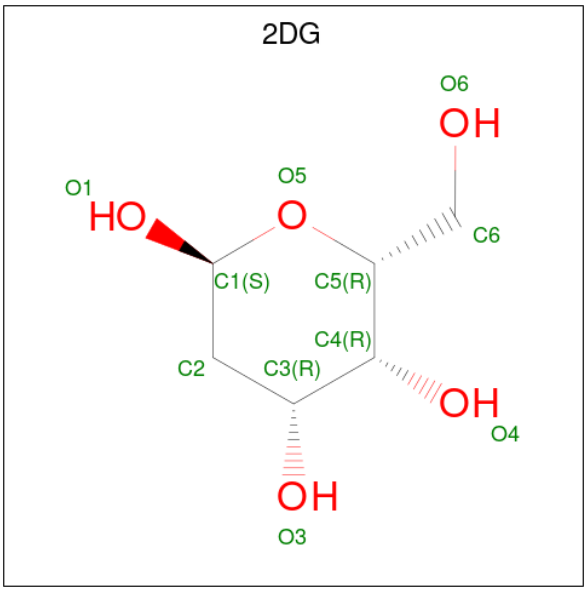
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | 6 | GLU | SER | cloning artifact | ? P00722 |
| C | 7 | ASP | LEU | cloning artifact | ? P00722 |
| C | 8 | PRO | ALA | cloning artifact | ? P00722 |
| D | 1 | GLY | THR | cloning artifact | ? P00722 |
| D | 2 | SER | MET | cloning artifact | ? P00722 |
| D | 3 | HIS | ILE | cloning artifact | ? P00722 |
| D | 4 | MET | THR | cloning artifact | ? P00722 |
| D | 5 | LEU | ASP | cloning artifact | ? P00722 |
| D | 6 | GLU | SER | cloning artifact | ? P00722 |
| D | 7 | ASP | LEU | cloning artifact | ? P00722 |
| D | 8 | PRO | ALA | cloning artifact | ? P00722 |

- Molecule 2 is 2-deoxy-alpha-D-galactopyranose (three-letter code: 2DG) (formula: $C_6H_{12}O_5$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | | |
| 2 | A | 1 | 10 | 6 | 4 | | 0 | 0 |
| | | | Total | C | O | | | |
| 2 | B | 1 | 10 | 6 | 4 | | 0 | 0 |
| | | | Total | C | O | | | |
| 2 | C | 1 | 10 | 6 | 4 | | 0 | 0 |
| | | | Total | C | O | | | |
| 2 | D | 1 | 10 | 6 | 4 | | 0 | 0 |

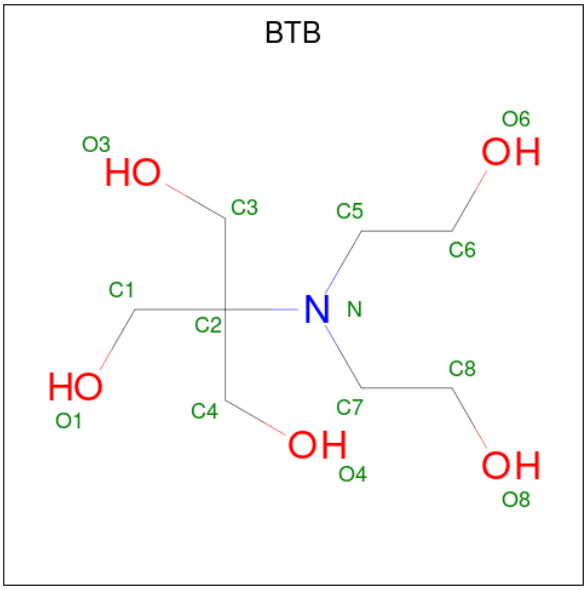
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 3 | A | 4 | 4 | 4 | 0 | 0 |
| | | | Total | Mg | | |
| 3 | B | 3 | 3 | 3 | 0 | 0 |
| | | | Total | Mg | | |
| 3 | C | 6 | 6 | 6 | 0 | 0 |
| | | | Total | Mg | | |
| 3 | D | 4 | 4 | 4 | 0 | 0 |

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Na | | |
| 4 | A | 4 | 4 | 4 | 0 | 0 |
| | | | Total | Na | | |
| 4 | B | 4 | 4 | 4 | 0 | 0 |
| | | | Total | Na | | |
| 4 | C | 4 | 4 | 4 | 0 | 0 |
| | | | Total | Na | | |
| 4 | D | 4 | 4 | 4 | 0 | 0 |

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 5 | A | 1 | 14 | 8 | 1 | 5 | 0 | 0 |

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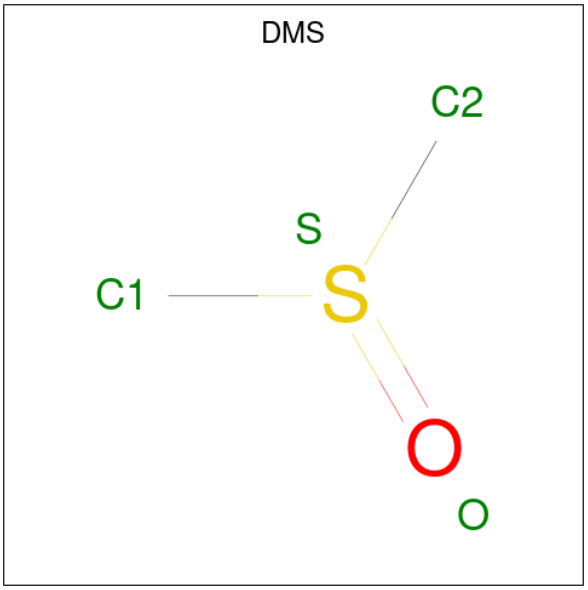
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 5 | B | 1 | 14 | 8 | 1 | 5 | 0 | 0 |
| | | | Total | C | N | O | | |
| 5 | C | 1 | 14 | 8 | 1 | 5 | 0 | 0 |
| | | | Total | C | N | O | | |
| 5 | D | 1 | 14 | 8 | 1 | 5 | 0 | 0 |

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: $C_2H_6OS$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | A | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | B | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | C | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |
| | | | Total | C | O | S | | |
| 6 | D | 1 | 4 | 2 | 1 | 1 | 0 | 0 |

- Molecule 7 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 7 | A | 1090 | 1090 | 1090 | 0 | 0 |

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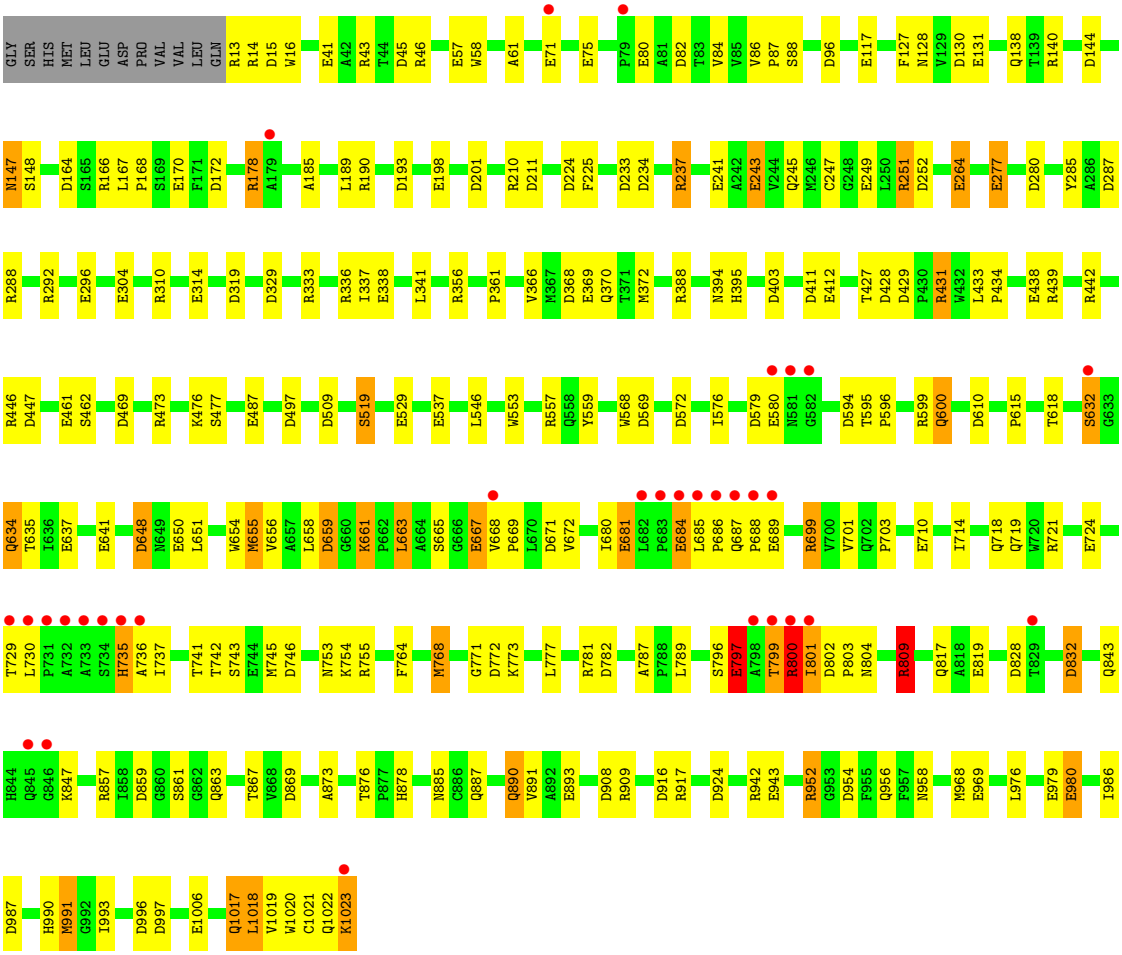
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 7 | B | 1091 | 1091 | 1091 | 0 | 0 |
| | | | Total | O | | |
| 7 | C | 1034 | 1034 | 1034 | 0 | 0 |
| | | | Total | O | | |
| 7 | D | 1079 | 1079 | 1079 | 0 | 0 |

# 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.

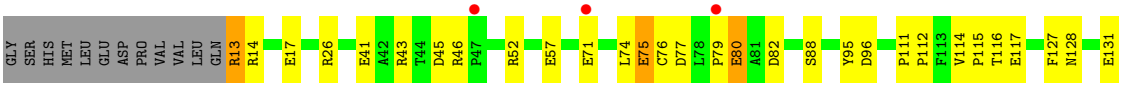
- Molecule 1: Beta-Galactosidase

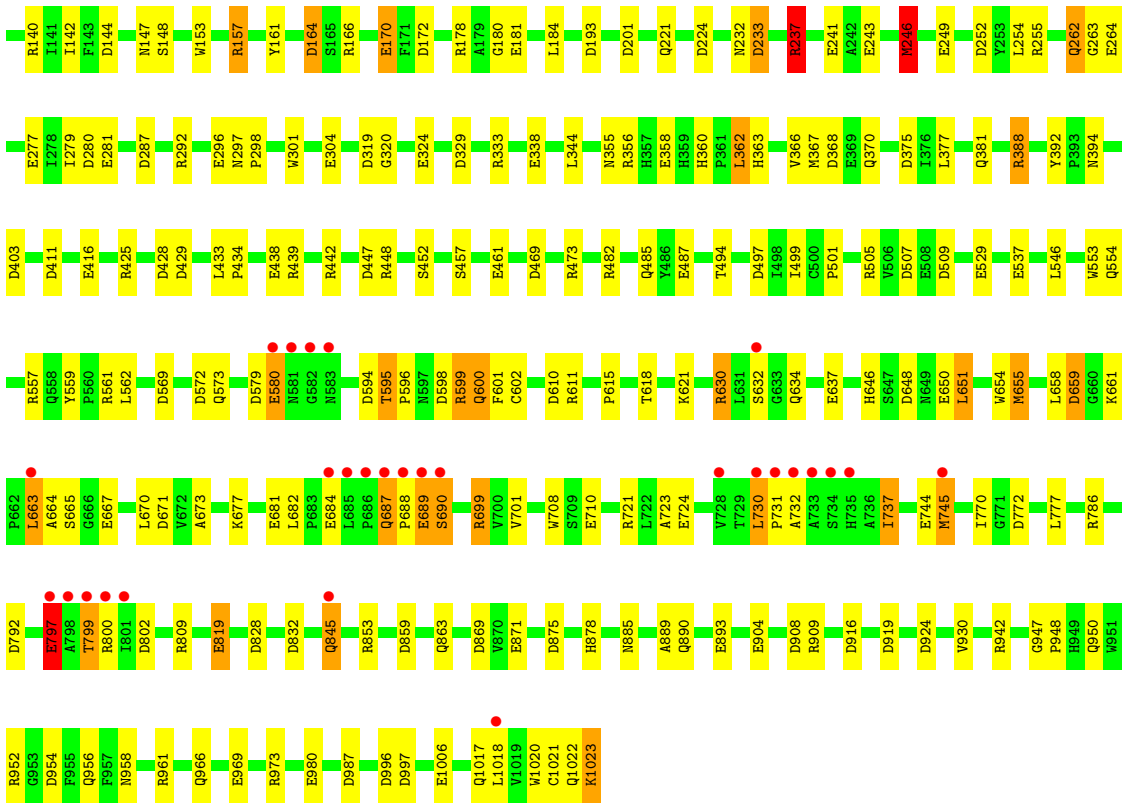
Chain A:




- Molecule 1: Beta-Galactosidase

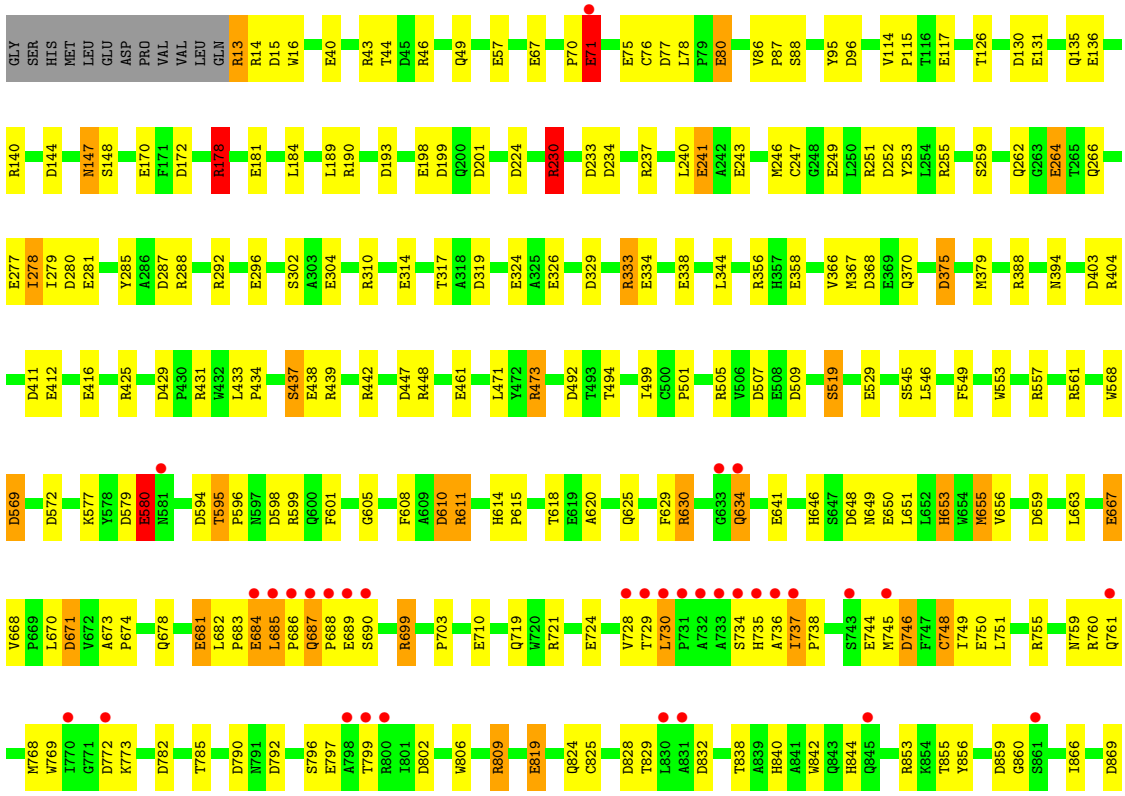
Chain B:





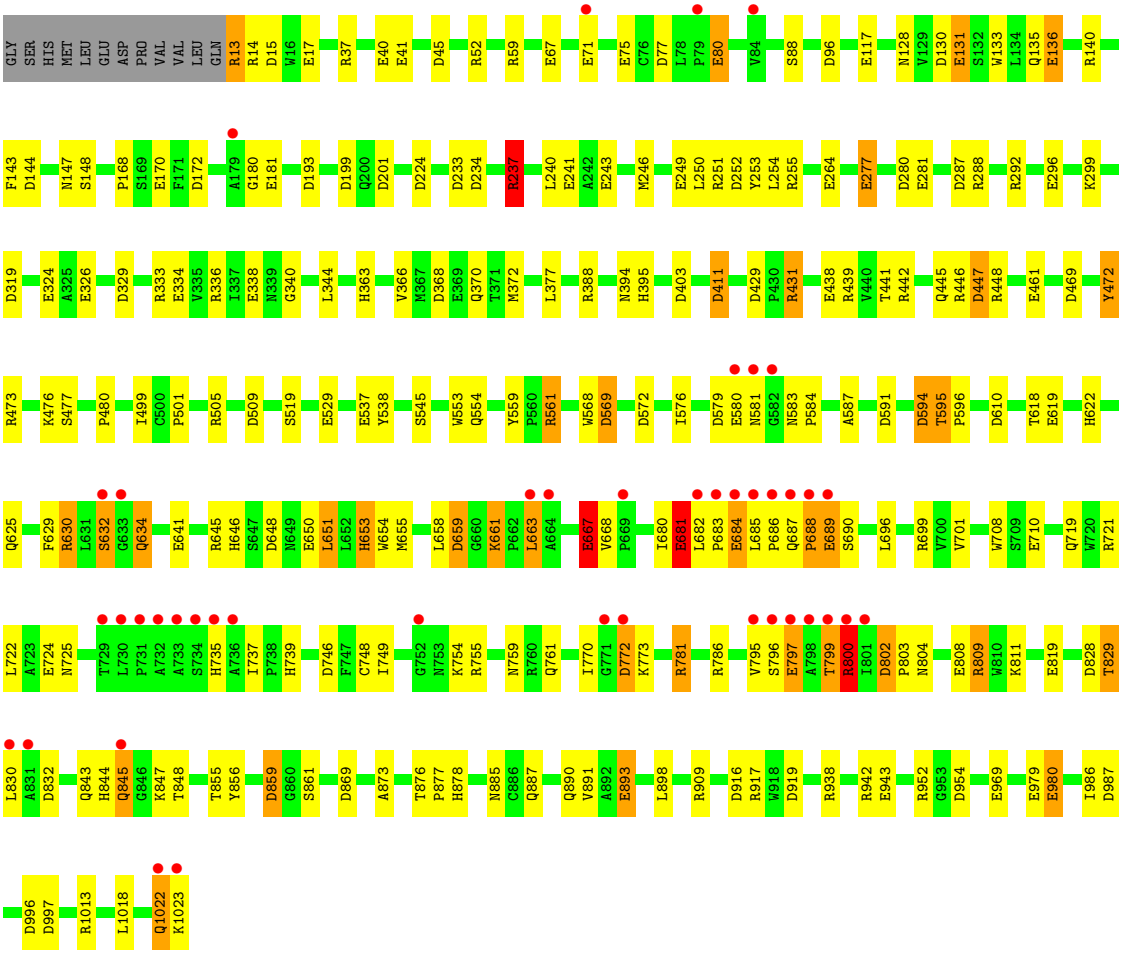

- Molecule 1: Beta-Galactosidase

Chain C: 3% 72% 22%



- Molecule 1: Beta-Galactosidase

Chain D:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 149.56Å 168.19Å 200.69Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 16.00 – 1.75<br>15.97 – 1.75 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 93.8 (16.00-1.75)<br>93.4 (15.97-1.75) | Depositor<br>EDS |
| $R_{merge}$ | 0.06 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.36 (at 1.75Å) | Xtriage |
| Refinement program | TNT | Depositor |
| R, $R_{free}$ | 0.158 , 0.222<br>0.163 , 0.219 | Depositor<br>DCC |
| $R_{free}$ test set | 6833 reflections (1.45%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 14.8 | Xtriage |
| Anisotropy | 0.425 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.35 , 97.6 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.33$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.97 | EDS |
| Total number of atoms | 37369 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 23.0 | 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 36.43 % 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 5.0078e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, BTB, MG, 2DG, DMS

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 | 1.05 | 42/8367 (0.5%) | 1.56 | 150/11415 (1.3%) |
| 1 | B | 1.06 | 43/8379 (0.5%) | 1.60 | 152/11431 (1.3%) |
| 1 | C | 1.04 | 47/8367 (0.6%) | 1.56 | 156/11415 (1.4%) |
| 1 | D | 1.07 | 43/8367 (0.5%) | 1.56 | 144/11415 (1.3%) |
| All | All | 1.06 | 175/33480 (0.5%) | 1.57 | 602/45676 (1.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 1 | 0 |

All (175) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 71 | GLU | CD-OE2 | 10.77 | 1.37 | 1.25 |
| 1 | D | 537 | GLU | CD-OE2 | 8.83 | 1.35 | 1.25 |
| 1 | B | 461 | GLU | CD-OE2 | 8.74 | 1.35 | 1.25 |
| 1 | C | 80 | GLU | CD-OE2 | 8.60 | 1.35 | 1.25 |
| 1 | D | 75 | GLU | CD-OE2 | 8.46 | 1.34 | 1.25 |
| 1 | C | 529 | GLU | CD-OE2 | 8.33 | 1.34 | 1.25 |
| 1 | B | 650 | GLU | CD-OE2 | 8.04 | 1.34 | 1.25 |
| 1 | D | 650 | GLU | CD-OE2 | 7.95 | 1.34 | 1.25 |
| 1 | A | 487 | GLU | CD-OE2 | 7.89 | 1.34 | 1.25 |
| 1 | D | 170 | GLU | CD-OE2 | 7.78 | 1.34 | 1.25 |
| 1 | A | 537 | GLU | CD-OE2 | 7.74 | 1.34 | 1.25 |
| 1 | C | 304 | GLU | CD-OE2 | 7.70 | 1.34 | 1.25 |
| 1 | D | 461 | GLU | CD-OE2 | 7.61 | 1.34 | 1.25 |
| 1 | C | 170 | GLU | CD-OE2 | 7.61 | 1.34 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 243 | GLU | CD-OE2 | 7.50 | 1.33 | 1.25 |
| 1 | A | 943 | GLU | CD-OE2 | 7.48 | 1.33 | 1.25 |
| 1 | B | 71 | GLU | CD-OE2 | 7.48 | 1.33 | 1.25 |
| 1 | D | 819 | GLU | CD-OE2 | 7.38 | 1.33 | 1.25 |
| 1 | D | 980 | GLU | CD-OE2 | 7.33 | 1.33 | 1.25 |
| 1 | A | 249 | GLU | CD-OE2 | 7.33 | 1.33 | 1.25 |
| 1 | B | 689 | GLU | CD-OE2 | 7.33 | 1.33 | 1.25 |
| 1 | B | 324 | GLU | CD-OE2 | 7.30 | 1.33 | 1.25 |
| 1 | A | 681 | GLU | CD-OE2 | 7.26 | 1.33 | 1.25 |
| 1 | C | 893 | GLU | CD-OE2 | 7.21 | 1.33 | 1.25 |
| 1 | D | 40 | GLU | CD-OE2 | 7.20 | 1.33 | 1.25 |
| 1 | B | 358 | GLU | CD-OE2 | 7.09 | 1.33 | 1.25 |
| 1 | A | 296 | GLU | CD-OE2 | 7.00 | 1.33 | 1.25 |
| 1 | B | 819 | GLU | CD-OE2 | 6.97 | 1.33 | 1.25 |
| 1 | A | 969 | GLU | CD-OE2 | 6.95 | 1.33 | 1.25 |
| 1 | D | 80 | GLU | CD-OE2 | 6.93 | 1.33 | 1.25 |
| 1 | C | 461 | GLU | CD-OE2 | 6.92 | 1.33 | 1.25 |
| 1 | A | 1006 | GLU | CD-OE2 | 6.91 | 1.33 | 1.25 |
| 1 | D | 580 | GLU | CD-OE2 | 6.90 | 1.33 | 1.25 |
| 1 | C | 416 | GLU | CD-OE2 | 6.87 | 1.33 | 1.25 |
| 1 | D | 136 | GLU | CD-OE2 | 6.83 | 1.33 | 1.25 |
| 1 | A | 689 | GLU | CD-OE2 | 6.82 | 1.33 | 1.25 |
| 1 | A | 277 | GLU | CD-OE2 | 6.81 | 1.33 | 1.25 |
| 1 | A | 580 | GLU | CD-OE2 | 6.75 | 1.33 | 1.25 |
| 1 | A | 80 | GLU | CD-OE2 | 6.74 | 1.33 | 1.25 |
| 1 | C | 744 | GLU | CD-OE2 | 6.72 | 1.33 | 1.25 |
| 1 | C | 710 | GLU | CD-OE2 | 6.68 | 1.32 | 1.25 |
| 1 | D | 681 | GLU | CD-OE2 | 6.68 | 1.32 | 1.25 |
| 1 | C | 71 | GLU | CD-OE2 | 6.67 | 1.32 | 1.25 |
| 1 | D | 667 | GLU | CD-OE2 | 6.61 | 1.32 | 1.25 |
| 1 | B | 684 | GLU | CD-OE2 | 6.60 | 1.32 | 1.25 |
| 1 | A | 71 | GLU | CD-OE2 | 6.57 | 1.32 | 1.25 |
| 1 | C | 334 | GLU | CD-OE2 | 6.56 | 1.32 | 1.25 |
| 1 | C | 934 | GLU | CD-OE2 | 6.56 | 1.32 | 1.25 |
| 1 | D | 689 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 1 | A | 170 | GLU | CD-OE2 | 6.54 | 1.32 | 1.25 |
| 1 | A | 243 | GLU | CD-OE2 | 6.53 | 1.32 | 1.25 |
| 1 | C | 684 | GLU | CD-OE2 | 6.52 | 1.32 | 1.25 |
| 1 | B | 667 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 1 | B | 1006 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 1 | A | 819 | GLU | CD-OE2 | 6.49 | 1.32 | 1.25 |
| 1 | A | 684 | GLU | CD-OE2 | 6.48 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 412 | GLU | CD-OE2 | 6.47 | 1.32 | 1.25 |
| 1 | A | 724 | GLU | CD-OE2 | 6.45 | 1.32 | 1.25 |
| 1 | C | 580 | GLU | CD-OE2 | 6.45 | 1.32 | 1.25 |
| 1 | B | 724 | GLU | CD-OE2 | 6.44 | 1.32 | 1.25 |
| 1 | B | 529 | GLU | CD-OE2 | 6.43 | 1.32 | 1.25 |
| 1 | B | 243 | GLU | CD-OE2 | 6.42 | 1.32 | 1.25 |
| 1 | D | 979 | GLU | CD-OE2 | 6.42 | 1.32 | 1.25 |
| 1 | A | 461 | GLU | CD-OE2 | 6.41 | 1.32 | 1.25 |
| 1 | B | 710 | GLU | CD-OE2 | 6.41 | 1.32 | 1.25 |
| 1 | B | 304 | GLU | CD-OE2 | 6.36 | 1.32 | 1.25 |
| 1 | A | 980 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | C | 667 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | D | 893 | GLU | CD-OE2 | 6.30 | 1.32 | 1.25 |
| 1 | C | 980 | GLU | CD-OE2 | 6.30 | 1.32 | 1.25 |
| 1 | C | 819 | GLU | CD-OE2 | 6.30 | 1.32 | 1.25 |
| 1 | B | 487 | GLU | CD-OE2 | 6.29 | 1.32 | 1.25 |
| 1 | B | 580 | GLU | CD-OE2 | 6.29 | 1.32 | 1.25 |
| 1 | C | 277 | GLU | CD-OE2 | 6.28 | 1.32 | 1.25 |
| 1 | A | 710 | GLU | CD-OE2 | 6.28 | 1.32 | 1.25 |
| 1 | B | 181 | GLU | CD-OE2 | 6.28 | 1.32 | 1.25 |
| 1 | C | 281 | GLU | CD-OE2 | 6.28 | 1.32 | 1.25 |
| 1 | A | 529 | GLU | CD-OE2 | 6.25 | 1.32 | 1.25 |
| 1 | B | 744 | GLU | CD-OE2 | 6.25 | 1.32 | 1.25 |
| 1 | D | 277 | GLU | CD-OE2 | 6.24 | 1.32 | 1.25 |
| 1 | C | 198 | GLU | CD-OE2 | 6.24 | 1.32 | 1.25 |
| 1 | B | 264 | GLU | CD-OE2 | 6.22 | 1.32 | 1.25 |
| 1 | D | 684 | GLU | CD-OE2 | 6.21 | 1.32 | 1.25 |
| 1 | B | 17 | GLU | CD-OE2 | 6.20 | 1.32 | 1.25 |
| 1 | B | 980 | GLU | CD-OE2 | 6.20 | 1.32 | 1.25 |
| 1 | C | 241 | GLU | CD-OE2 | 6.18 | 1.32 | 1.25 |
| 1 | A | 979 | GLU | CD-OE2 | 6.18 | 1.32 | 1.25 |
| 1 | D | 264 | GLU | CD-OE2 | 6.18 | 1.32 | 1.25 |
| 1 | C | 136 | GLU | CD-OE2 | 6.16 | 1.32 | 1.25 |
| 1 | C | 689 | GLU | CD-OE2 | 6.14 | 1.32 | 1.25 |
| 1 | C | 326 | GLU | CD-OE2 | 6.14 | 1.32 | 1.25 |
| 1 | D | 529 | GLU | CD-OE2 | 6.10 | 1.32 | 1.25 |
| 1 | B | 797 | GLU | CD-OE2 | 6.08 | 1.32 | 1.25 |
| 1 | D | 797 | GLU | CD-OE2 | 6.07 | 1.32 | 1.25 |
| 1 | C | 296 | GLU | CD-OE2 | 6.07 | 1.32 | 1.25 |
| 1 | B | 170 | GLU | CD-OE2 | 6.05 | 1.32 | 1.25 |
| 1 | D | 17 | GLU | CD-OE2 | 6.05 | 1.32 | 1.25 |
| 1 | A | 264 | GLU | CD-OE2 | 6.05 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 277 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | B | 904 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | C | 75 | GLU | CD-OE2 | 6.02 | 1.32 | 1.25 |
| 1 | D | 117 | GLU | CD-OE2 | 6.02 | 1.32 | 1.25 |
| 1 | A | 131 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | C | 650 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | A | 797 | GLU | CD-OE2 | 5.99 | 1.32 | 1.25 |
| 1 | D | 724 | GLU | CD-OE2 | 5.99 | 1.32 | 1.25 |
| 1 | B | 969 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |
| 1 | D | 438 | GLU | CD-OE2 | 5.94 | 1.32 | 1.25 |
| 1 | D | 943 | GLU | CD-OE2 | 5.93 | 1.32 | 1.25 |
| 1 | B | 117 | GLU | CD-OE2 | 5.89 | 1.32 | 1.25 |
| 1 | B | 241 | GLU | CD-OE2 | 5.88 | 1.32 | 1.25 |
| 1 | B | 57 | GLU | CD-OE2 | 5.86 | 1.32 | 1.25 |
| 1 | B | 537 | GLU | CD-OE2 | 5.86 | 1.32 | 1.25 |
| 1 | C | 338 | GLU | CD-OE2 | 5.86 | 1.32 | 1.25 |
| 1 | C | 681 | GLU | CD-OE2 | 5.82 | 1.32 | 1.25 |
| 1 | B | 893 | GLU | CD-OE2 | 5.79 | 1.32 | 1.25 |
| 1 | A | 641 | GLU | CD-OE1 | -5.78 | 1.19 | 1.25 |
| 1 | A | 338 | GLU | CD-OE2 | 5.74 | 1.31 | 1.25 |
| 1 | C | 324 | GLU | CD-OE2 | 5.71 | 1.31 | 1.25 |
| 1 | C | 724 | GLU | CD-OE2 | 5.71 | 1.31 | 1.25 |
| 1 | B | 416 | GLU | CD-OE2 | 5.69 | 1.31 | 1.25 |
| 1 | C | 750 | GLU | CD-OE2 | 5.67 | 1.31 | 1.25 |
| 1 | D | 131 | GLU | CD-OE2 | 5.66 | 1.31 | 1.25 |
| 1 | D | 334 | GLU | CD-OE2 | 5.64 | 1.31 | 1.25 |
| 1 | A | 637 | GLU | CD-OE2 | 5.64 | 1.31 | 1.25 |
| 1 | B | 80 | GLU | CD-OE2 | 5.63 | 1.31 | 1.25 |
| 1 | D | 249 | GLU | CD-OE2 | 5.63 | 1.31 | 1.25 |
| 1 | D | 241 | GLU | CD-OE2 | 5.60 | 1.31 | 1.25 |
| 1 | D | 281 | GLU | CD-OE2 | 5.60 | 1.31 | 1.25 |
| 1 | B | 131 | GLU | CD-OE2 | 5.59 | 1.31 | 1.25 |
| 1 | A | 304 | GLU | CD-OE2 | 5.58 | 1.31 | 1.25 |
| 1 | C | 57 | GLU | CD-OE2 | 5.56 | 1.31 | 1.25 |
| 1 | B | 249 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | B | 296 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | C | 249 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | B | 871 | GLU | CD-OE2 | 5.52 | 1.31 | 1.25 |
| 1 | D | 181 | GLU | CD-OE2 | 5.51 | 1.31 | 1.25 |
| 1 | D | 710 | GLU | CD-OE2 | 5.51 | 1.31 | 1.25 |
| 1 | D | 41 | GLU | CD-OE1 | -5.51 | 1.19 | 1.25 |
| 1 | A | 893 | GLU | CD-OE2 | 5.50 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 117 | GLU | CD-OE2 | 5.49 | 1.31 | 1.25 |
| 1 | A | 75 | GLU | CD-OE2 | 5.48 | 1.31 | 1.25 |
| 1 | D | 324 | GLU | CD-OE1 | -5.45 | 1.19 | 1.25 |
| 1 | C | 314 | GLU | CD-OE1 | -5.45 | 1.19 | 1.25 |
| 1 | C | 412 | GLU | CD-OE2 | 5.43 | 1.31 | 1.25 |
| 1 | D | 969 | GLU | CD-OE2 | 5.42 | 1.31 | 1.25 |
| 1 | C | 641 | GLU | CD-OE1 | -5.40 | 1.19 | 1.25 |
| 1 | C | 358 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | A | 650 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | D | 338 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | A | 57 | GLU | CD-OE2 | 5.30 | 1.31 | 1.25 |
| 1 | B | 75 | GLU | CD-OE2 | 5.28 | 1.31 | 1.25 |
| 1 | B | 41 | GLU | CD-OE2 | 5.28 | 1.31 | 1.25 |
| 1 | A | 667 | GLU | CD-OE2 | 5.27 | 1.31 | 1.25 |
| 1 | A | 438 | GLU | CD-OE2 | 5.25 | 1.31 | 1.25 |
| 1 | C | 243 | GLU | CD-OE1 | -5.24 | 1.19 | 1.25 |
| 1 | A | 198 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | B | 281 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | B | 681 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | C | 117 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | D | 296 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | A | 314 | GLU | CD-OE1 | -5.23 | 1.19 | 1.25 |
| 1 | C | 797 | GLU | CD-OE2 | 5.20 | 1.31 | 1.25 |
| 1 | D | 641 | GLU | CD-OE2 | 5.18 | 1.31 | 1.25 |
| 1 | C | 181 | GLU | CD-OE2 | 5.17 | 1.31 | 1.25 |
| 1 | A | 41 | GLU | CD-OE2 | 5.14 | 1.31 | 1.25 |
| 1 | C | 40 | GLU | CD-OE2 | 5.14 | 1.31 | 1.25 |
| 1 | A | 41 | GLU | CD-OE1 | -5.10 | 1.20 | 1.25 |
| 1 | C | 969 | GLU | CD-OE2 | 5.09 | 1.31 | 1.25 |
| 1 | B | 338 | GLU | CD-OE2 | 5.07 | 1.31 | 1.25 |
| 1 | D | 67 | GLU | CD-OE2 | 5.07 | 1.31 | 1.25 |
| 1 | D | 326 | GLU | CD-OE2 | 5.03 | 1.31 | 1.25 |
| 1 | C | 67 | GLU | CD-OE2 | 5.01 | 1.31 | 1.25 |
| 1 | C | 131 | GLU | CD-OE2 | 5.01 | 1.31 | 1.25 |
| 1 | C | 264 | GLU | CD-OE2 | 5.00 | 1.31 | 1.25 |

All (602) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 809 | ARG | NE-CZ-NH1 | 21.36 | 130.98 | 120.30 |
| 1 | B | 699 | ARG | NE-CZ-NH1 | 18.89 | 129.75 | 120.30 |
| 1 | C | 809 | ARG | NE-CZ-NH1 | 17.33 | 128.97 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 699 | ARG | NE-CZ-NH2 | -16.56 | 112.02 | 120.30 |
| 1 | B | 809 | ARG | NE-CZ-NH2 | -15.81 | 112.39 | 120.30 |
| 1 | B | 442 | ARG | NE-CZ-NH1 | 15.46 | 128.03 | 120.30 |
| 1 | B | 442 | ARG | NE-CZ-NH2 | -13.59 | 113.51 | 120.30 |
| 1 | C | 442 | ARG | NE-CZ-NH2 | -13.45 | 113.57 | 120.30 |
| 1 | A | 997 | ASP | CB-CG-OD2 | -13.45 | 106.19 | 118.30 |
| 1 | A | 442 | ARG | NE-CZ-NH2 | -12.50 | 114.05 | 120.30 |
| 1 | C | 431 | ARG | NE-CZ-NH2 | -12.42 | 114.09 | 120.30 |
| 1 | D | 781 | ARG | NE-CZ-NH1 | 12.35 | 126.48 | 120.30 |
| 1 | D | 431 | ARG | NE-CZ-NH2 | -12.25 | 114.17 | 120.30 |
| 1 | D | 699 | ARG | NE-CZ-NH1 | 11.91 | 126.25 | 120.30 |
| 1 | C | 721 | ARG | NE-CZ-NH1 | 11.84 | 126.22 | 120.30 |
| 1 | C | 809 | ARG | NE-CZ-NH2 | -11.49 | 114.56 | 120.30 |
| 1 | A | 442 | ARG | NE-CZ-NH1 | 11.28 | 125.94 | 120.30 |
| 1 | D | 439 | ARG | NE-CZ-NH2 | -11.14 | 114.73 | 120.30 |
| 1 | B | 252 | ASP | CB-CG-OD2 | -10.84 | 108.55 | 118.30 |
| 1 | C | 909 | ARG | NE-CZ-NH1 | 10.39 | 125.50 | 120.30 |
| 1 | A | 610 | ASP | CB-CG-OD1 | 10.26 | 127.53 | 118.30 |
| 1 | A | 224 | ASP | CB-CG-OD1 | 10.22 | 127.50 | 118.30 |
| 1 | A | 144 | ASP | CB-CG-OD1 | 10.08 | 127.37 | 118.30 |
| 1 | D | 336 | ARG | NE-CZ-NH1 | 10.07 | 125.34 | 120.30 |
| 1 | A | 172 | ASP | CB-CG-OD2 | -10.01 | 109.29 | 118.30 |
| 1 | A | 594 | ASP | CB-CG-OD1 | 9.97 | 127.27 | 118.30 |
| 1 | D | 429 | ASP | CB-CG-OD2 | -9.94 | 109.35 | 118.30 |
| 1 | D | 942 | ARG | NE-CZ-NH1 | 9.88 | 125.24 | 120.30 |
| 1 | A | 659 | ASP | CB-CG-OD2 | -9.73 | 109.54 | 118.30 |
| 1 | D | 429 | ASP | CB-CG-OD1 | 9.69 | 127.02 | 118.30 |
| 1 | C | 425 | ARG | NE-CZ-NH1 | 9.58 | 125.09 | 120.30 |
| 1 | B | 287 | ASP | CB-CG-OD1 | 9.58 | 126.92 | 118.30 |
| 1 | D | 446 | ARG | NE-CZ-NH2 | -9.54 | 115.53 | 120.30 |
| 1 | D | 746 | ASP | CB-CG-OD2 | -9.54 | 109.72 | 118.30 |
| 1 | A | 336 | ARG | NE-CZ-NH1 | 9.53 | 125.06 | 120.30 |
| 1 | D | 594 | ASP | CB-CG-OD2 | -9.53 | 109.72 | 118.30 |
| 1 | B | 648 | ASP | CB-CG-OD2 | -9.51 | 109.74 | 118.30 |
| 1 | A | 755 | ARG | NE-CZ-NH1 | 9.44 | 125.02 | 120.30 |
| 1 | C | 473 | ARG | NE-CZ-NH1 | 9.42 | 125.01 | 120.30 |
| 1 | D | 224 | ASP | CB-CG-OD1 | 9.42 | 126.78 | 118.30 |
| 1 | A | 166 | ARG | NE-CZ-NH2 | -9.37 | 115.61 | 120.30 |
| 1 | C | 199 | ASP | CB-CG-OD1 | 9.34 | 126.71 | 118.30 |
| 1 | B | 368 | ASP | CB-CG-OD2 | -9.34 | 109.90 | 118.30 |
| 1 | D | 388 | ARG | NE-CZ-NH2 | -9.34 | 115.63 | 120.30 |
| 1 | B | 557 | ARG | NE-CZ-NH2 | -9.27 | 115.66 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 425 | ARG | NE-CZ-NH1 | 9.27 | 124.94 | 120.30 |
| 1 | B | 13 | ARG | NE-CZ-NH2 | -9.26 | 115.67 | 120.30 |
| 1 | D | 952 | ARG | NE-CZ-NH1 | 9.26 | 124.93 | 120.30 |
| 1 | B | 388 | ARG | NE-CZ-NH2 | -9.26 | 115.67 | 120.30 |
| 1 | C | 13 | ARG | NE-CZ-NH2 | -9.21 | 115.69 | 120.30 |
| 1 | C | 224 | ASP | CB-CG-OD1 | 9.18 | 126.56 | 118.30 |
| 1 | D | 172 | ASP | CB-CG-OD2 | -9.18 | 110.04 | 118.30 |
| 1 | A | 130 | ASP | CB-CG-OD2 | -9.12 | 110.09 | 118.30 |
| 1 | D | 287 | ASP | CB-CG-OD1 | 9.04 | 126.44 | 118.30 |
| 1 | B | 368 | ASP | CB-CG-OD1 | 9.04 | 126.43 | 118.30 |
| 1 | B | 572 | ASP | CB-CG-OD2 | -9.00 | 110.20 | 118.30 |
| 1 | C | 961 | ARG | NE-CZ-NH1 | 8.98 | 124.79 | 120.30 |
| 1 | A | 997 | ASP | CB-CG-OD1 | 8.96 | 126.36 | 118.30 |
| 1 | B | 828 | ASP | CB-CG-OD2 | -8.96 | 110.24 | 118.30 |
| 1 | B | 425 | ARG | NE-CZ-NH2 | -8.88 | 115.86 | 120.30 |
| 1 | A | 233 | ASP | CB-CG-OD2 | -8.88 | 110.31 | 118.30 |
| 1 | D | 469 | ASP | CB-CG-OD1 | 8.86 | 126.28 | 118.30 |
| 1 | A | 172 | ASP | CB-CG-OD1 | 8.82 | 126.24 | 118.30 |
| 1 | D | 869 | ASP | CB-CG-OD1 | 8.81 | 126.22 | 118.30 |
| 1 | B | 505 | ARG | NE-CZ-NH1 | 8.80 | 124.70 | 120.30 |
| 1 | D | 786 | ARG | NE-CZ-NH2 | -8.78 | 115.91 | 120.30 |
| 1 | A | 431 | ARG | NE-CZ-NH2 | -8.71 | 115.94 | 120.30 |
| 1 | D | 987 | ASP | CB-CG-OD1 | 8.71 | 126.14 | 118.30 |
| 1 | B | 875 | ASP | CB-CG-OD1 | 8.71 | 126.14 | 118.30 |
| 1 | C | 43 | ARG | NE-CZ-NH1 | 8.71 | 124.66 | 120.30 |
| 1 | B | 448 | ARG | NE-CZ-NH2 | -8.71 | 115.95 | 120.30 |
| 1 | C | 802 | ASP | CB-CG-OD1 | 8.69 | 126.12 | 118.30 |
| 1 | C | 952 | ARG | NE-CZ-NH1 | 8.69 | 124.64 | 120.30 |
| 1 | D | 721 | ARG | NE-CZ-NH2 | -8.69 | 115.95 | 120.30 |
| 1 | C | 233 | ASP | CB-CG-OD1 | 8.69 | 126.12 | 118.30 |
| 1 | A | 908 | ASP | CB-CG-OD1 | 8.67 | 126.10 | 118.30 |
| 1 | D | 859 | ASP | CB-CG-OD1 | 8.65 | 126.09 | 118.30 |
| 1 | B | 809 | ARG | CD-NE-CZ | 8.65 | 135.70 | 123.60 |
| 1 | B | 909 | ARG | NE-CZ-NH2 | -8.62 | 115.99 | 120.30 |
| 1 | B | 942 | ARG | NE-CZ-NH1 | 8.62 | 124.61 | 120.30 |
| 1 | B | 367 | MET | CG-SD-CE | 8.60 | 113.95 | 100.20 |
| 1 | B | 594 | ASP | CB-CG-OD1 | 8.55 | 125.99 | 118.30 |
| 1 | C | 310 | ARG | NE-CZ-NH1 | 8.54 | 124.57 | 120.30 |
| 1 | D | 659 | ASP | CB-CG-OD1 | 8.53 | 125.98 | 118.30 |
| 1 | C | 579 | ASP | CB-CG-OD1 | 8.52 | 125.97 | 118.30 |
| 1 | A | 857 | ARG | NE-CZ-NH1 | 8.51 | 124.56 | 120.30 |
| 1 | D | 572 | ASP | CB-CG-OD1 | 8.50 | 125.95 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 233 | ASP | CB-CG-OD1 | 8.47 | 125.93 | 118.30 |
| 1 | C | 579 | ASP | CB-CG-OD2 | -8.47 | 110.68 | 118.30 |
| 1 | D | 746 | ASP | CB-CG-OD1 | 8.47 | 125.92 | 118.30 |
| 1 | A | 233 | ASP | CB-CG-OD1 | 8.43 | 125.88 | 118.30 |
| 1 | A | 755 | ARG | NE-CZ-NH2 | -8.41 | 116.09 | 120.30 |
| 1 | B | 859 | ASP | CB-CG-OD2 | -8.41 | 110.73 | 118.30 |
| 1 | D | 859 | ASP | CB-CG-OD2 | -8.41 | 110.73 | 118.30 |
| 1 | D | 144 | ASP | CB-CG-OD1 | 8.39 | 125.85 | 118.30 |
| 1 | B | 557 | ARG | NE-CZ-NH1 | 8.38 | 124.49 | 120.30 |
| 1 | A | 234 | ASP | CB-CG-OD2 | -8.36 | 110.78 | 118.30 |
| 1 | A | 634 | GLN | N-CA-CB | 8.36 | 125.65 | 110.60 |
| 1 | B | 356 | ARG | NE-CZ-NH2 | -8.34 | 116.13 | 120.30 |
| 1 | C | 442 | ARG | NE-CZ-NH1 | 8.33 | 124.46 | 120.30 |
| 1 | A | 509 | ASP | CB-CG-OD1 | 8.31 | 125.78 | 118.30 |
| 1 | A | 954 | ASP | CB-CG-OD2 | -8.28 | 110.85 | 118.30 |
| 1 | B | 671 | ASP | CB-CG-OD2 | -8.28 | 110.85 | 118.30 |
| 1 | A | 699 | ARG | NE-CZ-NH1 | 8.26 | 124.43 | 120.30 |
| 1 | C | 648 | ASP | CB-CG-OD2 | -8.24 | 110.89 | 118.30 |
| 1 | A | 447 | ASP | CB-CG-OD1 | 8.20 | 125.68 | 118.30 |
| 1 | C | 659 | ASP | CB-CG-OD2 | -8.18 | 110.94 | 118.30 |
| 1 | D | 828 | ASP | CB-CG-OD2 | -8.18 | 110.94 | 118.30 |
| 1 | D | 368 | ASP | CB-CG-OD2 | -8.18 | 110.94 | 118.30 |
| 1 | D | 37 | ARG | NE-CZ-NH2 | -8.15 | 116.22 | 120.30 |
| 1 | B | 469 | ASP | CB-CG-OD1 | 8.14 | 125.63 | 118.30 |
| 1 | C | 802 | ASP | CB-CG-OD2 | -8.12 | 110.99 | 118.30 |
| 1 | B | 356 | ARG | NE-CZ-NH1 | 8.11 | 124.36 | 120.30 |
| 1 | B | 859 | ASP | CB-CG-OD1 | 8.10 | 125.59 | 118.30 |
| 1 | C | 233 | ASP | CB-CG-OD2 | -8.09 | 111.02 | 118.30 |
| 1 | D | 15 | ASP | CB-CG-OD2 | -8.09 | 111.02 | 118.30 |
| 1 | D | 809 | ARG | NE-CZ-NH2 | 8.08 | 124.34 | 120.30 |
| 1 | A | 869 | ASP | CB-CG-OD1 | 8.07 | 125.56 | 118.30 |
| 1 | C | 908 | ASP | CB-CG-OD1 | 8.05 | 125.55 | 118.30 |
| 1 | A | 446 | ARG | NE-CZ-NH1 | 8.05 | 124.33 | 120.30 |
| 1 | C | 909 | ARG | NE-CZ-NH2 | -8.04 | 116.28 | 120.30 |
| 1 | D | 130 | ASP | CB-CG-OD2 | -8.04 | 111.07 | 118.30 |
| 1 | A | 987 | ASP | CB-CG-OD1 | 8.02 | 125.52 | 118.30 |
| 1 | C | 230 | ARG | NE-CZ-NH1 | 8.02 | 124.31 | 120.30 |
| 1 | B | 428 | ASP | CB-CG-OD1 | 8.00 | 125.50 | 118.30 |
| 1 | C | 594 | ASP | CB-CG-OD1 | 7.99 | 125.49 | 118.30 |
| 1 | D | 246 | MET | CG-SD-CE | -7.98 | 87.43 | 100.20 |
| 1 | A | 234 | ASP | CB-CG-OD1 | 7.96 | 125.46 | 118.30 |
| 1 | A | 439 | ARG | NE-CZ-NH2 | -7.93 | 116.33 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 630 | ARG | NE-CZ-NH1 | 7.93 | 124.26 | 120.30 |
| 1 | D | 659 | ASP | CB-CG-OD2 | -7.92 | 111.17 | 118.30 |
| 1 | A | 509 | ASP | CB-CG-OD2 | -7.92 | 111.17 | 118.30 |
| 1 | D | 802 | ASP | CB-CG-OD2 | -7.90 | 111.19 | 118.30 |
| 1 | D | 287 | ASP | CB-CG-OD2 | -7.90 | 111.19 | 118.30 |
| 1 | D | 201 | ASP | CB-CG-OD2 | -7.89 | 111.20 | 118.30 |
| 1 | A | 190 | ARG | NE-CZ-NH2 | -7.88 | 116.36 | 120.30 |
| 1 | A | 411 | ASP | CB-CG-OD2 | -7.88 | 111.21 | 118.30 |
| 1 | B | 363 | HIS | CA-CB-CG | -7.87 | 100.22 | 113.60 |
| 1 | B | 671 | ASP | CB-CG-OD1 | 7.87 | 125.38 | 118.30 |
| 1 | D | 802 | ASP | CB-CG-OD1 | 7.87 | 125.38 | 118.30 |
| 1 | B | 287 | ASP | CB-CG-OD2 | -7.86 | 111.22 | 118.30 |
| 1 | D | 52 | ARG | NE-CZ-NH1 | 7.85 | 124.22 | 120.30 |
| 1 | A | 648 | ASP | CB-CG-OD1 | 7.83 | 125.35 | 118.30 |
| 1 | D | 772 | ASP | CB-CG-OD2 | -7.83 | 111.25 | 118.30 |
| 1 | C | 310 | ARG | NE-CZ-NH2 | -7.81 | 116.39 | 120.30 |
| 1 | C | 659 | ASP | CB-CG-OD1 | 7.81 | 125.33 | 118.30 |
| 1 | D | 45 | ASP | CB-CG-OD1 | 7.80 | 125.32 | 118.30 |
| 1 | A | 469 | ASP | CB-CG-OD1 | 7.77 | 125.30 | 118.30 |
| 1 | B | 648 | ASP | CB-CG-OD1 | 7.75 | 125.27 | 118.30 |
| 1 | B | 996 | ASP | CB-CG-OD2 | -7.75 | 111.33 | 118.30 |
| 1 | D | 987 | ASP | CB-CG-OD2 | -7.72 | 111.35 | 118.30 |
| 1 | C | 431 | ARG | NE-CZ-NH1 | 7.71 | 124.15 | 120.30 |
| 1 | D | 938 | ARG | NE-CZ-NH2 | -7.70 | 116.45 | 120.30 |
| 1 | A | 987 | ASP | CB-CG-OD2 | -7.69 | 111.38 | 118.30 |
| 1 | C | 509 | ASP | CB-CG-OD1 | 7.69 | 125.22 | 118.30 |
| 1 | D | 403 | ASP | CB-CG-OD1 | 7.68 | 125.21 | 118.30 |
| 1 | A | 746 | ASP | CB-CG-OD2 | -7.64 | 111.42 | 118.30 |
| 1 | A | 224 | ASP | CB-CG-OD2 | -7.61 | 111.45 | 118.30 |
| 1 | C | 611 | ARG | NE-CZ-NH1 | 7.61 | 124.11 | 120.30 |
| 1 | D | 869 | ASP | CB-CG-OD2 | -7.61 | 111.45 | 118.30 |
| 1 | B | 828 | ASP | CB-CG-OD1 | 7.61 | 125.15 | 118.30 |
| 1 | A | 411 | ASP | CB-CG-OD1 | 7.56 | 125.10 | 118.30 |
| 1 | A | 403 | ASP | CB-CG-OD1 | 7.55 | 125.10 | 118.30 |
| 1 | C | 996 | ASP | CB-CG-OD1 | 7.54 | 125.09 | 118.30 |
| 1 | A | 859 | ASP | CB-CG-OD2 | -7.50 | 111.55 | 118.30 |
| 1 | C | 557 | ARG | NE-CZ-NH2 | -7.50 | 116.55 | 120.30 |
| 1 | D | 917 | ARG | NE-CZ-NH1 | -7.49 | 116.56 | 120.30 |
| 1 | C | 439 | ARG | NE-CZ-NH1 | 7.49 | 124.04 | 120.30 |
| 1 | B | 559 | TYR | CB-CG-CD2 | -7.48 | 116.51 | 121.00 |
| 1 | C | 610 | ASP | CB-CG-OD1 | 7.46 | 125.02 | 118.30 |
| 1 | D | 233 | ASP | CB-CG-OD1 | 7.45 | 125.00 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 572 | ASP | CB-CG-OD2 | -7.44 | 111.60 | 118.30 |
| 1 | A | 388 | ARG | NE-CZ-NH2 | -7.44 | 116.58 | 120.30 |
| 1 | B | 45 | ASP | CB-CG-OD1 | 7.43 | 124.99 | 118.30 |
| 1 | C | 875 | ASP | CB-CG-OD1 | 7.38 | 124.94 | 118.30 |
| 1 | B | 594 | ASP | CB-CG-OD2 | -7.37 | 111.67 | 118.30 |
| 1 | A | 210 | ARG | NE-CZ-NH2 | -7.35 | 116.63 | 120.30 |
| 1 | B | 699 | ARG | CD-NE-CZ | 7.33 | 133.87 | 123.60 |
| 1 | C | 961 | ARG | NE-CZ-NH2 | -7.33 | 116.64 | 120.30 |
| 1 | C | 997 | ASP | CB-CG-OD1 | 7.33 | 124.89 | 118.30 |
| 1 | A | 201 | ASP | CB-CG-OD2 | -7.33 | 111.71 | 118.30 |
| 1 | C | 144 | ASP | CB-CG-OD1 | 7.33 | 124.89 | 118.30 |
| 1 | C | 388 | ARG | NE-CZ-NH2 | -7.33 | 116.64 | 120.30 |
| 1 | B | 553 | TRP | CA-CB-CG | -7.32 | 99.79 | 113.70 |
| 1 | B | 561 | ARG | NE-CZ-NH1 | 7.30 | 123.95 | 120.30 |
| 1 | C | 439 | ARG | NE-CZ-NH2 | -7.29 | 116.65 | 120.30 |
| 1 | B | 469 | ASP | CB-CG-OD2 | -7.29 | 111.74 | 118.30 |
| 1 | D | 632 | SER | N-CA-CB | 7.25 | 121.38 | 110.50 |
| 1 | D | 469 | ASP | CB-CG-OD2 | -7.24 | 111.78 | 118.30 |
| 1 | B | 958 | ASN | N-CA-CB | 7.24 | 123.62 | 110.60 |
| 1 | B | 572 | ASP | CB-CG-OD1 | 7.23 | 124.80 | 118.30 |
| 1 | B | 319 | ASP | CB-CG-OD1 | 7.20 | 124.78 | 118.30 |
| 1 | C | 772 | ASP | CB-CG-OD2 | -7.19 | 111.83 | 118.30 |
| 1 | C | 828 | ASP | CB-CG-OD2 | -7.18 | 111.84 | 118.30 |
| 1 | C | 924 | ASP | CB-CG-OD1 | 7.18 | 124.76 | 118.30 |
| 1 | C | 509 | ASP | CB-CG-OD2 | -7.17 | 111.85 | 118.30 |
| 1 | D | 786 | ARG | NE-CZ-NH1 | 7.16 | 123.88 | 120.30 |
| 1 | C | 610 | ASP | CB-CG-OD2 | -7.16 | 111.86 | 118.30 |
| 1 | B | 429 | ASP | CB-CG-OD2 | -7.15 | 111.86 | 118.30 |
| 1 | C | 13 | ARG | NE-CZ-NH1 | 7.15 | 123.87 | 120.30 |
| 1 | C | 594 | ASP | CB-CG-OD2 | -7.14 | 111.88 | 118.30 |
| 1 | D | 59 | ARG | NE-CZ-NH2 | -7.13 | 116.73 | 120.30 |
| 1 | B | 792 | ASP | CB-CG-OD1 | 7.11 | 124.70 | 118.30 |
| 1 | B | 255 | ARG | NE-CZ-NH1 | 7.11 | 123.85 | 120.30 |
| 1 | D | 403 | ASP | CB-CG-OD2 | -7.10 | 111.91 | 118.30 |
| 1 | C | 375 | ASP | CB-CG-OD1 | 7.09 | 124.68 | 118.30 |
| 1 | C | 572 | ASP | CB-CG-OD2 | -7.07 | 111.93 | 118.30 |
| 1 | D | 172 | ASP | CB-CG-OD1 | 7.07 | 124.66 | 118.30 |
| 1 | A | 632 | SER | N-CA-CB | 7.07 | 121.10 | 110.50 |
| 1 | D | 237 | ARG | NE-CZ-NH1 | 7.07 | 123.83 | 120.30 |
| 1 | C | 505 | ARG | NE-CZ-NH2 | -7.04 | 116.78 | 120.30 |
| 1 | C | 246 | MET | CG-SD-CE | -7.04 | 88.94 | 100.20 |
| 1 | C | 561 | ARG | NE-CZ-NH2 | -7.02 | 116.79 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 594 | ASP | CB-CG-OD1 | 7.02 | 124.62 | 118.30 |
| 1 | D | 648 | ASP | CB-CG-OD2 | -7.02 | 111.98 | 118.30 |
| 1 | D | 431 | ARG | NE-CZ-NH1 | 6.97 | 123.78 | 120.30 |
| 1 | A | 594 | ASP | CB-CG-OD2 | -6.96 | 112.03 | 118.30 |
| 1 | C | 507 | ASP | CB-CG-OD1 | 6.96 | 124.56 | 118.30 |
| 1 | C | 473 | ARG | NE-CZ-NH2 | -6.96 | 116.82 | 120.30 |
| 1 | A | 610 | ASP | CB-CG-OD2 | -6.96 | 112.04 | 118.30 |
| 1 | D | 579 | ASP | CB-CG-OD2 | -6.96 | 112.04 | 118.30 |
| 1 | B | 802 | ASP | CB-CG-OD1 | 6.93 | 124.53 | 118.30 |
| 1 | C | 368 | ASP | CB-CG-OD2 | -6.92 | 112.07 | 118.30 |
| 1 | D | 447 | ASP | CB-CG-OD1 | 6.92 | 124.53 | 118.30 |
| 1 | C | 76 | CYS | N-CA-CB | -6.89 | 98.19 | 110.60 |
| 1 | B | 77 | ASP | CB-CG-OD2 | -6.88 | 112.10 | 118.30 |
| 1 | B | 233 | ASP | CB-CG-OD2 | -6.88 | 112.11 | 118.30 |
| 1 | B | 853 | ARG | NE-CZ-NH1 | 6.88 | 123.74 | 120.30 |
| 1 | B | 448 | ARG | NE-CZ-NH1 | 6.88 | 123.74 | 120.30 |
| 1 | A | 802 | ASP | CB-CG-OD1 | 6.83 | 124.45 | 118.30 |
| 1 | A | 247 | CYS | CA-CB-SG | -6.82 | 101.72 | 114.00 |
| 1 | B | 786 | ARG | NE-CZ-NH2 | -6.82 | 116.89 | 120.30 |
| 1 | D | 329 | ASP | CB-CG-OD2 | -6.81 | 112.17 | 118.30 |
| 1 | B | 319 | ASP | CB-CG-OD2 | -6.79 | 112.19 | 118.30 |
| 1 | A | 916 | ASP | CB-CG-OD1 | 6.78 | 124.40 | 118.30 |
| 1 | A | 857 | ARG | NE-CZ-NH2 | -6.78 | 116.91 | 120.30 |
| 1 | B | 869 | ASP | CB-CG-OD2 | -6.77 | 112.20 | 118.30 |
| 1 | C | 388 | ARG | NE-CZ-NH1 | 6.77 | 123.69 | 120.30 |
| 1 | C | 853 | ARG | NE-CZ-NH2 | -6.77 | 116.91 | 120.30 |
| 1 | D | 193 | ASP | CB-CG-OD2 | -6.76 | 112.22 | 118.30 |
| 1 | D | 13 | ARG | NE-CZ-NH2 | -6.73 | 116.93 | 120.30 |
| 1 | C | 77 | ASP | CB-CG-OD1 | 6.73 | 124.36 | 118.30 |
| 1 | D | 288 | ARG | NE-CZ-NH1 | 6.72 | 123.66 | 120.30 |
| 1 | D | 559 | TYR | CB-CG-CD2 | -6.71 | 116.97 | 121.00 |
| 1 | C | 43 | ARG | NE-CZ-NH2 | -6.71 | 116.95 | 120.30 |
| 1 | B | 569 | ASP | CB-CG-OD1 | 6.69 | 124.32 | 118.30 |
| 1 | C | 190 | ARG | NE-CZ-NH2 | -6.68 | 116.96 | 120.30 |
| 1 | C | 719 | GLN | CB-CA-C | -6.68 | 97.03 | 110.40 |
| 1 | C | 429 | ASP | CB-CG-OD1 | 6.68 | 124.31 | 118.30 |
| 1 | D | 233 | ASP | CB-CG-OD2 | -6.65 | 112.31 | 118.30 |
| 1 | D | 832 | ASP | CB-CG-OD2 | -6.64 | 112.32 | 118.30 |
| 1 | C | 553 | TRP | CA-CB-CG | -6.64 | 101.09 | 113.70 |
| 1 | A | 996 | ASP | CB-CG-OD1 | 6.63 | 124.27 | 118.30 |
| 1 | B | 166 | ARG | NE-CZ-NH2 | -6.63 | 116.99 | 120.30 |
| 1 | B | 832 | ASP | CB-CG-OD1 | 6.62 | 124.26 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 439 | ARG | NE-CZ-NH2 | -6.61 | 117.00 | 120.30 |
| 1 | D | 800 | ARG | NE-CZ-NH2 | -6.56 | 117.02 | 120.30 |
| 1 | D | 996 | ASP | CB-CG-OD1 | 6.56 | 124.20 | 118.30 |
| 1 | B | 611 | ARG | NE-CZ-NH1 | 6.56 | 123.58 | 120.30 |
| 1 | C | 853 | ARG | NE-CZ-NH1 | 6.56 | 123.58 | 120.30 |
| 1 | C | 199 | ASP | CB-CG-OD2 | -6.56 | 112.40 | 118.30 |
| 1 | C | 869 | ASP | CB-CG-OD1 | 6.55 | 124.20 | 118.30 |
| 1 | B | 439 | ARG | NE-CZ-NH1 | 6.54 | 123.57 | 120.30 |
| 1 | A | 428 | ASP | CB-CG-OD1 | 6.54 | 124.19 | 118.30 |
| 1 | A | 15 | ASP | CB-CG-OD2 | -6.54 | 112.42 | 118.30 |
| 1 | A | 439 | ARG | NE-CZ-NH1 | 6.53 | 123.56 | 120.30 |
| 1 | A | 746 | ASP | CB-CA-C | -6.52 | 97.36 | 110.40 |
| 1 | B | 721 | ARG | NE-CZ-NH1 | 6.51 | 123.56 | 120.30 |
| 1 | C | 630 | ARG | NE-CZ-NH2 | -6.51 | 117.04 | 120.30 |
| 1 | A | 809 | ARG | NE-CZ-NH1 | 6.51 | 123.56 | 120.30 |
| 1 | B | 497 | ASP | CB-CG-OD1 | 6.51 | 124.16 | 118.30 |
| 1 | B | 96 | ASP | CB-CG-OD2 | -6.51 | 112.44 | 118.30 |
| 1 | C | 411 | ASP | CB-CG-OD2 | -6.50 | 112.45 | 118.30 |
| 1 | A | 403 | ASP | CB-CG-OD2 | -6.50 | 112.45 | 118.30 |
| 1 | D | 252 | ASP | CB-CG-OD1 | 6.49 | 124.14 | 118.30 |
| 1 | B | 772 | ASP | CB-CG-OD2 | -6.48 | 112.47 | 118.30 |
| 1 | C | 404 | ARG | NE-CZ-NH2 | -6.47 | 117.06 | 120.30 |
| 1 | D | 336 | ARG | NE-CZ-NH2 | -6.47 | 117.06 | 120.30 |
| 1 | A | 659 | ASP | CB-CG-OD1 | 6.47 | 124.12 | 118.30 |
| 1 | C | 869 | ASP | CB-CG-OD2 | -6.47 | 112.48 | 118.30 |
| 1 | B | 595 | THR | CA-CB-CG2 | -6.46 | 103.35 | 112.40 |
| 1 | A | 469 | ASP | CB-CG-OD2 | -6.46 | 112.49 | 118.30 |
| 1 | D | 800 | ARG | NE-CZ-NH1 | 6.45 | 123.53 | 120.30 |
| 1 | A | 671 | ASP | CB-CG-OD2 | -6.45 | 112.50 | 118.30 |
| 1 | C | 924 | ASP | CB-CG-OD2 | -6.44 | 112.50 | 118.30 |
| 1 | C | 859 | ASP | CB-CG-OD1 | 6.42 | 124.08 | 118.30 |
| 1 | A | 909 | ARG | NE-CZ-NH2 | -6.42 | 117.09 | 120.30 |
| 1 | B | 792 | ASP | CB-CG-OD2 | -6.42 | 112.52 | 118.30 |
| 1 | D | 996 | ASP | CB-CG-OD2 | -6.42 | 112.53 | 118.30 |
| 1 | D | 442 | ARG | NE-CZ-NH2 | -6.41 | 117.09 | 120.30 |
| 1 | D | 919 | ASP | CB-CG-OD2 | -6.41 | 112.53 | 118.30 |
| 1 | B | 1018 | LEU | CB-CA-C | -6.41 | 98.03 | 110.20 |
| 1 | B | 473 | ARG | NE-CZ-NH1 | 6.40 | 123.50 | 120.30 |
| 1 | B | 579 | ASP | CB-CG-OD2 | -6.40 | 112.54 | 118.30 |
| 1 | B | 908 | ASP | CB-CG-OD1 | 6.40 | 124.06 | 118.30 |
| 1 | A | 772 | ASP | CB-CG-OD1 | 6.40 | 124.06 | 118.30 |
| 1 | B | 280 | ASP | CB-CG-OD1 | 6.40 | 124.06 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 130 | ASP | CB-CG-OD1 | 6.38 | 124.04 | 118.30 |
| 1 | C | 367 | MET | CB-CA-C | -6.38 | 97.64 | 110.40 |
| 1 | C | 193 | ASP | CB-CG-OD1 | 6.37 | 124.04 | 118.30 |
| 1 | A | 859 | ASP | CB-CG-OD1 | 6.37 | 124.03 | 118.30 |
| 1 | C | 859 | ASP | CB-CG-OD2 | -6.36 | 112.57 | 118.30 |
| 1 | C | 140 | ARG | NE-CZ-NH2 | -6.36 | 117.12 | 120.30 |
| 1 | D | 224 | ASP | CB-CG-OD2 | -6.35 | 112.58 | 118.30 |
| 1 | B | 832 | ASP | CB-CG-OD2 | -6.35 | 112.59 | 118.30 |
| 1 | C | 997 | ASP | CB-CG-OD2 | -6.33 | 112.60 | 118.30 |
| 1 | C | 856 | TYR | CB-CG-CD2 | -6.32 | 117.21 | 121.00 |
| 1 | B | 659 | ASP | CB-CG-OD2 | -6.32 | 112.61 | 118.30 |
| 1 | B | 375 | ASP | CB-CG-OD1 | 6.32 | 123.98 | 118.30 |
| 1 | D | 439 | ARG | NE-CZ-NH1 | 6.30 | 123.45 | 120.30 |
| 1 | A | 954 | ASP | CB-CG-OD1 | 6.29 | 123.96 | 118.30 |
| 1 | D | 329 | ASP | CB-CG-OD1 | 6.29 | 123.96 | 118.30 |
| 1 | A | 572 | ASP | CB-CG-OD2 | -6.29 | 112.64 | 118.30 |
| 1 | D | 630 | ARG | NE-CZ-NH1 | 6.29 | 123.44 | 120.30 |
| 1 | B | 429 | ASP | CB-CG-OD1 | 6.28 | 123.95 | 118.30 |
| 1 | A | 1021 | CYS | CA-CB-SG | -6.28 | 102.70 | 114.00 |
| 1 | C | 790 | ASP | CB-CG-OD1 | 6.25 | 123.93 | 118.30 |
| 1 | B | 632 | SER | N-CA-CB | 6.25 | 119.88 | 110.50 |
| 1 | C | 403 | ASP | CB-CG-OD2 | -6.25 | 112.67 | 118.30 |
| 1 | A | 924 | ASP | CB-CG-OD2 | -6.25 | 112.68 | 118.30 |
| 1 | B | 997 | ASP | N-CA-CB | 6.24 | 121.82 | 110.60 |
| 1 | A | 559 | TYR | CB-CG-CD2 | -6.23 | 117.26 | 121.00 |
| 1 | C | 987 | ASP | CB-CG-OD1 | 6.22 | 123.90 | 118.30 |
| 1 | B | 482 | ARG | NE-CZ-NH1 | 6.22 | 123.41 | 120.30 |
| 1 | C | 492 | ASP | CB-CG-OD2 | -6.22 | 112.70 | 118.30 |
| 1 | B | 996 | ASP | CB-CG-OD1 | 6.21 | 123.89 | 118.30 |
| 1 | B | 76 | CYS | CA-CB-SG | -6.20 | 102.84 | 114.00 |
| 1 | A | 579 | ASP | CB-CG-OD2 | -6.20 | 112.72 | 118.30 |
| 1 | D | 561 | ARG | NE-CZ-NH1 | 6.20 | 123.40 | 120.30 |
| 1 | C | 178 | ARG | NE-CZ-NH1 | 6.19 | 123.40 | 120.30 |
| 1 | D | 255 | ARG | NE-CZ-NH1 | 6.18 | 123.39 | 120.30 |
| 1 | D | 446 | ARG | NE-CZ-NH1 | 6.18 | 123.39 | 120.30 |
| 1 | B | 954 | ASP | CB-CG-OD2 | -6.17 | 112.75 | 118.30 |
| 1 | C | 184 | LEU | CB-CA-C | -6.17 | 98.48 | 110.20 |
| 1 | A | 832 | ASP | CB-CG-OD1 | 6.16 | 123.85 | 118.30 |
| 1 | A | 252 | ASP | CB-CG-OD2 | -6.16 | 112.75 | 118.30 |
| 1 | B | 13 | ARG | NE-CZ-NH1 | 6.16 | 123.38 | 120.30 |
| 1 | A | 46 | ARG | NE-CZ-NH1 | 6.15 | 123.38 | 120.30 |
| 1 | D | 15 | ASP | CB-CG-OD1 | 6.15 | 123.83 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 770 | ILE | CA-CB-CG1 | -6.15 | 99.32 | 111.00 |
| 1 | B | 579 | ASP | CB-CG-OD1 | 6.14 | 123.83 | 118.30 |
| 1 | D | 448 | ARG | NE-CZ-NH2 | -6.14 | 117.23 | 120.30 |
| 1 | C | 881 | ARG | NE-CZ-NH1 | -6.13 | 117.23 | 120.30 |
| 1 | C | 130 | ASP | CB-CG-OD1 | 6.12 | 123.81 | 118.30 |
| 1 | D | 509 | ASP | CB-CG-OD1 | 6.12 | 123.80 | 118.30 |
| 1 | B | 869 | ASP | CB-CG-OD1 | 6.11 | 123.80 | 118.30 |
| 1 | D | 411 | ASP | CB-CG-OD1 | 6.09 | 123.78 | 118.30 |
| 1 | D | 130 | ASP | CB-CG-OD1 | 6.06 | 123.76 | 118.30 |
| 1 | D | 699 | ARG | NE-CZ-NH2 | -6.06 | 117.27 | 120.30 |
| 1 | D | 1018 | LEU | CB-CA-C | -6.06 | 98.68 | 110.20 |
| 1 | A | 438 | GLU | CG-CD-OE2 | -6.06 | 106.18 | 118.30 |
| 1 | A | 82 | ASP | CB-CG-OD1 | 6.06 | 123.75 | 118.30 |
| 1 | C | 333 | ARG | NE-CZ-NH2 | -6.05 | 117.27 | 120.30 |
| 1 | C | 746 | ASP | CB-CG-OD2 | -6.05 | 112.85 | 118.30 |
| 1 | D | 193 | ASP | CB-CG-OD1 | 6.04 | 123.74 | 118.30 |
| 1 | B | 43 | ARG | NE-CZ-NH1 | 6.02 | 123.31 | 120.30 |
| 1 | B | 45 | ASP | CB-CG-OD2 | -6.00 | 112.90 | 118.30 |
| 1 | C | 429 | ASP | CB-CG-OD2 | -5.99 | 112.91 | 118.30 |
| 1 | D | 997 | ASP | N-CA-CB | 5.99 | 121.38 | 110.60 |
| 1 | A | 672 | VAL | CG1-CB-CG2 | 5.98 | 120.47 | 110.90 |
| 1 | A | 178 | ARG | NE-CZ-NH2 | -5.97 | 117.31 | 120.30 |
| 1 | B | 172 | ASP | CB-CG-OD1 | 5.97 | 123.67 | 118.30 |
| 1 | A | 648 | ASP | CB-CG-OD2 | -5.97 | 112.93 | 118.30 |
| 1 | A | 768 | MET | CA-CB-CG | 5.96 | 123.42 | 113.30 |
| 1 | B | 507 | ASP | CB-CG-OD1 | 5.95 | 123.66 | 118.30 |
| 1 | B | 509 | ASP | CB-CG-OD1 | 5.95 | 123.65 | 118.30 |
| 1 | A | 828 | ASP | CB-CG-OD2 | -5.94 | 112.95 | 118.30 |
| 1 | D | 199 | ASP | CB-CG-OD2 | -5.94 | 112.95 | 118.30 |
| 1 | D | 96 | ASP | CB-CG-OD1 | 5.94 | 123.65 | 118.30 |
| 1 | A | 280 | ASP | CB-CG-OD2 | -5.94 | 112.95 | 118.30 |
| 1 | D | 856 | TYR | CB-CG-CD2 | -5.94 | 117.44 | 121.00 |
| 1 | A | 211 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 1 | C | 234 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 1 | D | 199 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 1 | A | 96 | ASP | N-CA-CB | 5.92 | 121.26 | 110.60 |
| 1 | C | 958 | ASN | N-CA-CB | 5.92 | 121.25 | 110.60 |
| 1 | B | 77 | ASP | CB-CG-OD1 | 5.91 | 123.62 | 118.30 |
| 1 | C | 630 | ARG | NE-CZ-NH1 | 5.91 | 123.26 | 120.30 |
| 1 | A | 917 | ARG | NE-CZ-NH1 | -5.91 | 117.34 | 120.30 |
| 1 | D | 855 | THR | N-CA-CB | 5.91 | 121.53 | 110.30 |
| 1 | C | 147 | ASN | N-CA-CB | -5.89 | 100.00 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 403 | ASP | CB-CG-OD1 | 5.89 | 123.60 | 118.30 |
| 1 | A | 719 | GLN | CB-CA-C | -5.89 | 98.62 | 110.40 |
| 1 | D | 45 | ASP | CB-CG-OD2 | -5.88 | 113.00 | 118.30 |
| 1 | D | 288 | ARG | NE-CZ-NH2 | -5.88 | 117.36 | 120.30 |
| 1 | A | 782 | ASP | CB-CG-OD2 | -5.88 | 113.00 | 118.30 |
| 1 | C | 77 | ASP | CB-CG-OD2 | -5.88 | 113.01 | 118.30 |
| 1 | B | 723 | ALA | CB-CA-C | -5.87 | 101.30 | 110.10 |
| 1 | A | 497 | ASP | CB-CG-OD2 | -5.87 | 113.02 | 118.30 |
| 1 | C | 598 | ASP | CB-CG-OD2 | -5.85 | 113.03 | 118.30 |
| 1 | D | 234 | ASP | CB-CG-OD1 | 5.84 | 123.56 | 118.30 |
| 1 | A | 144 | ASP | CB-CG-OD2 | -5.84 | 113.05 | 118.30 |
| 1 | A | 890 | GLN | N-CA-CB | -5.84 | 100.09 | 110.60 |
| 1 | B | 280 | ASP | CB-CG-OD2 | -5.84 | 113.04 | 118.30 |
| 1 | A | 251 | ARG | NE-CZ-NH1 | 5.84 | 123.22 | 120.30 |
| 1 | A | 579 | ASP | CB-CG-OD1 | 5.83 | 123.55 | 118.30 |
| 1 | A | 832 | ASP | N-CA-CB | -5.83 | 100.10 | 110.60 |
| 1 | B | 246 | MET | CG-SD-CE | -5.83 | 90.86 | 100.20 |
| 1 | B | 193 | ASP | CB-CG-OD1 | 5.83 | 123.55 | 118.30 |
| 1 | C | 832 | ASP | CB-CG-OD1 | 5.83 | 123.55 | 118.30 |
| 1 | D | 980 | GLU | C-N-CA | -5.83 | 110.06 | 122.30 |
| 1 | C | 748 | CYS | CA-CB-SG | -5.82 | 103.52 | 114.00 |
| 1 | A | 46 | ARG | NE-CZ-NH2 | -5.82 | 117.39 | 120.30 |
| 1 | C | 648 | ASP | CB-CG-OD1 | 5.81 | 123.53 | 118.30 |
| 1 | C | 438 | GLU | CG-CD-OE2 | -5.81 | 106.68 | 118.30 |
| 1 | D | 52 | ARG | CB-CA-C | -5.81 | 98.78 | 110.40 |
| 1 | B | 505 | ARG | NE-CZ-NH2 | -5.80 | 117.40 | 120.30 |
| 1 | D | 653 | HIS | N-CA-CB | 5.79 | 121.02 | 110.60 |
| 1 | D | 96 | ASP | N-CA-CB | 5.78 | 121.00 | 110.60 |
| 1 | B | 237 | ARG | NE-CZ-NH2 | -5.77 | 117.41 | 120.30 |
| 1 | B | 172 | ASP | CB-CG-OD2 | -5.76 | 113.11 | 118.30 |
| 1 | A | 553 | TRP | CA-CB-CG | -5.75 | 102.77 | 113.70 |
| 1 | C | 906 | TYR | CB-CG-CD2 | -5.75 | 117.55 | 121.00 |
| 1 | A | 429 | ASP | CB-CG-OD2 | -5.75 | 113.12 | 118.30 |
| 1 | A | 477 | SER | N-CA-CB | 5.75 | 119.12 | 110.50 |
| 1 | D | 13 | ARG | NE-CZ-NH1 | 5.75 | 123.17 | 120.30 |
| 1 | D | 553 | TRP | CA-CB-CG | -5.75 | 102.78 | 113.70 |
| 1 | C | 782 | ASP | CB-CG-OD1 | 5.75 | 123.47 | 118.30 |
| 1 | C | 746 | ASP | CB-CG-OD1 | 5.74 | 123.47 | 118.30 |
| 1 | C | 792 | ASP | CB-CG-OD1 | 5.74 | 123.47 | 118.30 |
| 1 | B | 292 | ARG | NE-CZ-NH1 | 5.73 | 123.17 | 120.30 |
| 1 | D | 140 | ARG | NE-CZ-NH2 | -5.73 | 117.44 | 120.30 |
| 1 | D | 253 | TYR | CB-CG-CD1 | -5.73 | 117.56 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 772 | ASP | CB-CG-OD1 | 5.72 | 123.45 | 118.30 |
| 1 | B | 909 | ARG | NE-CZ-NH1 | 5.71 | 123.15 | 120.30 |
| 1 | C | 572 | ASP | CB-CG-OD1 | 5.71 | 123.44 | 118.30 |
| 1 | C | 996 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | B | 428 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | A | 140 | ARG | NE-CZ-NH2 | -5.69 | 117.45 | 120.30 |
| 1 | A | 867 | THR | CA-CB-CG2 | -5.69 | 104.43 | 112.40 |
| 1 | B | 279 | ILE | CA-CB-CG2 | 5.69 | 122.28 | 110.90 |
| 1 | D | 630 | ARG | NE-CZ-NH2 | -5.69 | 117.46 | 120.30 |
| 1 | C | 259 | SER | CB-CA-C | 5.68 | 120.90 | 110.10 |
| 1 | C | 721 | ARG | NE-CZ-NH2 | -5.67 | 117.46 | 120.30 |
| 1 | C | 890 | GLN | N-CA-CB | -5.67 | 100.39 | 110.60 |
| 1 | B | 201 | ASP | CB-CG-OD2 | -5.67 | 113.20 | 118.30 |
| 1 | C | 140 | ARG | NE-CZ-NH1 | 5.67 | 123.13 | 120.30 |
| 1 | D | 772 | ASP | CB-CG-OD1 | 5.65 | 123.38 | 118.30 |
| 1 | A | 193 | ASP | CB-CG-OD1 | 5.64 | 123.38 | 118.30 |
| 1 | B | 875 | ASP | CB-CG-OD2 | -5.64 | 113.22 | 118.30 |
| 1 | B | 329 | ASP | CB-CG-OD2 | -5.64 | 113.22 | 118.30 |
| 1 | C | 832 | ASP | CB-CG-OD2 | -5.63 | 113.23 | 118.30 |
| 1 | A | 43 | ARG | NE-CZ-NH1 | 5.63 | 123.12 | 120.30 |
| 1 | D | 559 | TYR | CB-CG-CD1 | 5.63 | 124.38 | 121.00 |
| 1 | D | 144 | ASP | CB-CG-OD2 | -5.62 | 113.24 | 118.30 |
| 1 | A | 147 | ASN | N-CA-CB | -5.61 | 100.50 | 110.60 |
| 1 | A | 15 | ASP | CB-CG-OD1 | 5.61 | 123.35 | 118.30 |
| 1 | B | 201 | ASP | CB-CG-OD1 | 5.61 | 123.34 | 118.30 |
| 1 | D | 587 | ALA | CB-CA-C | -5.61 | 101.69 | 110.10 |
| 1 | B | 329 | ASP | CB-CG-OD1 | 5.60 | 123.34 | 118.30 |
| 1 | B | 252 | ASP | CB-CG-OD1 | 5.60 | 123.34 | 118.30 |
| 1 | B | 82 | ASP | CB-CG-OD1 | 5.60 | 123.34 | 118.30 |
| 1 | C | 494 | THR | CA-CB-CG2 | -5.59 | 104.57 | 112.40 |
| 1 | B | 52 | ARG | CB-CA-C | -5.59 | 99.22 | 110.40 |
| 1 | C | 252 | ASP | CB-CG-OD2 | -5.58 | 113.27 | 118.30 |
| 1 | D | 234 | ASP | CB-CG-OD2 | -5.58 | 113.28 | 118.30 |
| 1 | A | 800 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 1 | B | 908 | ASP | CB-CG-OD2 | -5.58 | 113.28 | 118.30 |
| 1 | A | 741 | THR | CA-CB-CG2 | -5.57 | 104.61 | 112.40 |
| 1 | B | 924 | ASP | CB-CG-OD1 | 5.56 | 123.30 | 118.30 |
| 1 | C | 302 | SER | N-CA-CB | 5.55 | 118.83 | 110.50 |
| 1 | A | 924 | ASP | CB-CG-OD1 | 5.55 | 123.30 | 118.30 |
| 1 | A | 908 | ASP | CB-CG-OD2 | -5.55 | 113.31 | 118.30 |
| 1 | B | 916 | ASP | CB-CG-OD1 | 5.53 | 123.28 | 118.30 |
| 1 | A | 329 | ASP | CB-CG-OD1 | 5.53 | 123.28 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 138 | GLN | N-CA-CB | -5.53 | 100.64 | 110.60 |
| 1 | A | 61 | ALA | N-CA-CB | 5.51 | 117.82 | 110.10 |
| 1 | C | 671 | ASP | CB-CG-OD2 | -5.51 | 113.34 | 118.30 |
| 1 | B | 116 | THR | CA-CB-CG2 | -5.51 | 104.69 | 112.40 |
| 1 | A | 546 | LEU | N-CA-CB | 5.50 | 121.41 | 110.40 |
| 1 | A | 952 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 1 | A | 771 | GLY | C-N-CA | -5.49 | 107.96 | 121.70 |
| 1 | B | 772 | ASP | CB-CG-OD1 | 5.48 | 123.23 | 118.30 |
| 1 | D | 781 | ARG | CD-NE-CZ | 5.48 | 131.28 | 123.60 |
| 1 | A | 782 | ASP | CB-CG-OD1 | 5.48 | 123.23 | 118.30 |
| 1 | A | 431 | ARG | NE-CZ-NH1 | 5.48 | 123.04 | 120.30 |
| 1 | A | 310 | ARG | NE-CZ-NH2 | -5.47 | 117.56 | 120.30 |
| 1 | C | 599 | ARG | NE-CZ-NH1 | 5.47 | 123.03 | 120.30 |
| 1 | A | 14 | ARG | N-CA-CB | -5.47 | 100.76 | 110.60 |
| 1 | A | 356 | ARG | NE-CZ-NH1 | 5.47 | 123.03 | 120.30 |
| 1 | C | 411 | ASP | CB-CG-OD1 | 5.47 | 123.22 | 118.30 |
| 1 | A | 280 | ASP | CB-CG-OD1 | 5.45 | 123.21 | 118.30 |
| 1 | D | 442 | ARG | NE-CZ-NH1 | 5.45 | 123.02 | 120.30 |
| 1 | A | 329 | ASP | CB-CG-OD2 | -5.45 | 113.40 | 118.30 |
| 1 | D | 610 | ASP | CB-CG-OD1 | 5.43 | 123.19 | 118.30 |
| 1 | C | 95 | TYR | CB-CG-CD2 | -5.43 | 117.74 | 121.00 |
| 1 | C | 96 | ASP | N-CA-CB | 5.42 | 120.36 | 110.60 |
| 1 | C | 447 | ASP | CB-CG-OD2 | -5.42 | 113.42 | 118.30 |
| 1 | A | 909 | ARG | NE-CZ-NH1 | 5.42 | 123.01 | 120.30 |
| 1 | C | 234 | ASP | CB-CG-OD2 | -5.41 | 113.43 | 118.30 |
| 1 | D | 569 | ASP | CB-CG-OD2 | -5.41 | 113.43 | 118.30 |
| 1 | C | 329 | ASP | CB-CG-OD2 | -5.41 | 113.43 | 118.30 |
| 1 | D | 579 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 1 | C | 201 | ASP | CB-CG-OD2 | -5.41 | 113.44 | 118.30 |
| 1 | B | 610 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | D | 770 | ILE | N-CA-C | -5.40 | 96.42 | 111.00 |
| 1 | A | 201 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | C | 699 | ARG | CB-CA-C | -5.38 | 99.63 | 110.40 |
| 1 | A | 13 | ARG | NE-CZ-NH1 | 5.37 | 122.99 | 120.30 |
| 1 | D | 505 | ARG | NE-CZ-NH1 | 5.37 | 122.98 | 120.30 |
| 1 | C | 247 | CYS | CA-CB-SG | -5.36 | 104.35 | 114.00 |
| 1 | D | 388 | ARG | NE-CZ-NH1 | 5.36 | 122.98 | 120.30 |
| 1 | C | 403 | ASP | CB-CG-OD1 | 5.36 | 123.12 | 118.30 |
| 1 | B | 919 | ASP | CB-CG-OD2 | -5.35 | 113.48 | 118.30 |
| 1 | C | 15 | ASP | CB-CG-OD1 | 5.34 | 123.11 | 118.30 |
| 1 | A | 225 | PHE | N-CA-CB | 5.34 | 120.21 | 110.60 |
| 1 | B | 659 | ASP | CB-CG-OD1 | 5.34 | 123.10 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 919 | ASP | CB-CG-OD1 | 5.33 | 123.10 | 118.30 |
| 1 | A | 287 | ASP | CB-CG-OD1 | 5.33 | 123.09 | 118.30 |
| 1 | B | 392 | TYR | CG-CD2-CE2 | 5.33 | 125.56 | 121.30 |
| 1 | D | 538 | TYR | CB-CG-CD2 | 5.33 | 124.20 | 121.00 |
| 1 | C | 126 | THR | CA-CB-CG2 | -5.32 | 104.95 | 112.40 |
| 1 | D | 324 | GLU | N-CA-CB | 5.32 | 120.18 | 110.60 |
| 1 | B | 954 | ASP | CB-CG-OD1 | 5.32 | 123.09 | 118.30 |
| 1 | D | 252 | ASP | CB-CG-OD2 | -5.32 | 113.51 | 118.30 |
| 1 | A | 369 | GLU | CG-CD-OE2 | -5.31 | 107.68 | 118.30 |
| 1 | B | 224 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 1 | B | 224 | ASP | CB-CG-OD2 | -5.30 | 113.53 | 118.30 |
| 1 | C | 230 | ARG | CD-NE-CZ | 5.30 | 131.02 | 123.60 |
| 1 | A | 1018 | LEU | CB-CA-C | -5.29 | 100.15 | 110.20 |
| 1 | B | 438 | GLU | CG-CD-OE2 | -5.29 | 107.73 | 118.30 |
| 1 | B | 144 | ASP | CB-CG-OD1 | 5.28 | 123.06 | 118.30 |
| 1 | A | 185 | ALA | N-CA-CB | 5.28 | 117.49 | 110.10 |
| 1 | B | 157 | ARG | NE-CZ-NH2 | 5.28 | 122.94 | 120.30 |
| 1 | D | 472 | TYR | CB-CG-CD1 | 5.28 | 124.17 | 121.00 |
| 1 | D | 591 | ASP | CB-CG-OD1 | 5.27 | 123.04 | 118.30 |
| 1 | B | 509 | ASP | CB-CG-OD2 | -5.26 | 113.56 | 118.30 |
| 1 | B | 598 | ASP | CB-CG-OD2 | -5.26 | 113.57 | 118.30 |
| 1 | D | 80 | GLU | OE1-CD-OE2 | 5.26 | 129.61 | 123.30 |
| 1 | D | 591 | ASP | CB-CG-OD2 | -5.25 | 113.57 | 118.30 |
| 1 | A | 45 | ASP | CB-CG-OD1 | 5.24 | 123.02 | 118.30 |
| 1 | A | 634 | GLN | CB-CA-C | 5.24 | 120.88 | 110.40 |
| 1 | C | 130 | ASP | CB-CG-OD2 | -5.24 | 113.58 | 118.30 |
| 1 | A | 942 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 1 | C | 368 | ASP | CB-CG-OD1 | 5.23 | 123.01 | 118.30 |
| 1 | B | 144 | ASP | CB-CG-OD2 | -5.23 | 113.59 | 118.30 |
| 1 | A | 997 | ASP | N-CA-CB | 5.23 | 120.01 | 110.60 |
| 1 | B | 598 | ASP | CB-CG-OD1 | 5.22 | 123.00 | 118.30 |
| 1 | C | 255 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 1 | A | 251 | ARG | NE-CZ-NH2 | -5.21 | 117.69 | 120.30 |
| 1 | D | 645 | ARG | NE-CZ-NH1 | -5.21 | 117.69 | 120.30 |
| 1 | D | 916 | ASP | CB-CG-OD1 | 5.21 | 122.99 | 118.30 |
| 1 | A | 714 | ILE | CA-CB-CG1 | -5.21 | 101.10 | 111.00 |
| 1 | B | 164 | ASP | CB-CG-OD1 | 5.20 | 122.98 | 118.30 |
| 1 | C | 287 | ASP | CB-CG-OD1 | 5.20 | 122.98 | 118.30 |
| 1 | A | 497 | ASP | CB-CG-OD1 | 5.20 | 122.98 | 118.30 |
| 1 | A | 1019 | VAL | CA-CB-CG2 | -5.18 | 103.12 | 110.90 |
| 1 | C | 906 | TYR | CB-CG-CD1 | 5.18 | 124.11 | 121.00 |
| 1 | A | 672 | VAL | CA-CB-CG1 | 5.18 | 118.67 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 782 | ASP | CB-CG-OD2 | -5.18 | 113.64 | 118.30 |
| 1 | C | 280 | ASP | CB-CG-OD1 | 5.17 | 122.96 | 118.30 |
| 1 | C | 601 | PHE | CB-CG-CD2 | -5.17 | 117.18 | 120.80 |
| 1 | A | 519 | SER | N-CA-CB | -5.17 | 102.74 | 110.50 |
| 1 | A | 869 | ASP | CB-CG-OD2 | -5.17 | 113.65 | 118.30 |
| 1 | C | 855 | THR | N-CA-CB | 5.15 | 120.09 | 110.30 |
| 1 | A | 319 | ASP | CB-CG-OD2 | -5.15 | 113.67 | 118.30 |
| 1 | D | 280 | ASP | CB-CG-OD1 | 5.15 | 122.93 | 118.30 |
| 1 | C | 319 | ASP | CB-CG-OD2 | -5.15 | 113.67 | 118.30 |
| 1 | B | 1020 | TRP | CB-CA-C | -5.14 | 100.11 | 110.40 |
| 1 | D | 319 | ASP | CB-CG-OD2 | -5.14 | 113.67 | 118.30 |
| 1 | C | 519 | SER | N-CA-CB | -5.14 | 102.79 | 110.50 |
| 1 | C | 569 | ASP | CB-CG-OD1 | 5.14 | 122.92 | 118.30 |
| 1 | D | 645 | ARG | NE-CZ-NH2 | 5.13 | 122.87 | 120.30 |
| 1 | B | 403 | ASP | CB-CG-OD2 | -5.13 | 113.68 | 118.30 |
| 1 | A | 721 | ARG | NE-CZ-NH2 | -5.13 | 117.74 | 120.30 |
| 1 | B | 161 | TYR | CB-CG-CD1 | -5.13 | 117.92 | 121.00 |
| 1 | C | 344 | LEU | CA-CB-CG | -5.13 | 103.51 | 115.30 |
| 1 | A | 991 | MET | CG-SD-CE | 5.12 | 108.40 | 100.20 |
| 1 | D | 829 | THR | N-CA-CB | 5.12 | 120.03 | 110.30 |
| 1 | B | 95 | TYR | CB-CG-CD1 | -5.12 | 117.93 | 121.00 |
| 1 | C | 448 | ARG | NE-CZ-NH2 | -5.12 | 117.74 | 120.30 |
| 1 | A | 288 | ARG | NE-CZ-NH2 | -5.12 | 117.74 | 120.30 |
| 1 | A | 958 | ASN | N-CA-CB | 5.12 | 119.81 | 110.60 |
| 1 | C | 842 | TRP | CA-CB-CG | -5.12 | 103.98 | 113.70 |
| 1 | D | 954 | ASP | CB-CG-OD2 | -5.11 | 113.70 | 118.30 |
| 1 | C | 840 | HIS | CB-CA-C | -5.11 | 100.18 | 110.40 |
| 1 | A | 447 | ASP | CB-CG-OD2 | -5.11 | 113.70 | 118.30 |
| 1 | A | 368 | ASP | CB-CG-OD2 | -5.10 | 113.71 | 118.30 |
| 1 | D | 77 | ASP | CB-CG-OD2 | -5.10 | 113.71 | 118.30 |
| 1 | B | 292 | ARG | NE-CZ-NH2 | -5.09 | 117.75 | 120.30 |
| 1 | D | 719 | GLN | CB-CA-C | -5.09 | 100.21 | 110.40 |
| 1 | C | 545 | SER | N-CA-CB | -5.09 | 102.86 | 110.50 |
| 1 | D | 14 | ARG | N-CA-CB | -5.09 | 101.44 | 110.60 |
| 1 | A | 96 | ASP | CB-CG-OD1 | 5.08 | 122.88 | 118.30 |
| 1 | B | 497 | ASP | CB-CG-OD2 | -5.08 | 113.72 | 118.30 |
| 1 | D | 832 | ASP | CB-CG-OD1 | 5.08 | 122.87 | 118.30 |
| 1 | C | 681 | GLU | C-N-CA | -5.08 | 109.00 | 121.70 |
| 1 | C | 838 | THR | CA-CB-CG2 | -5.07 | 105.30 | 112.40 |
| 1 | D | 809 | ARG | NH1-CZ-NH2 | -5.07 | 113.82 | 119.40 |
| 1 | B | 924 | ASP | CB-CG-OD2 | -5.07 | 113.74 | 118.30 |
| 1 | D | 477 | SER | N-CA-CB | 5.07 | 118.10 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 809 | ARG | CD-NE-CZ | 5.06 | 130.68 | 123.60 |
| 1 | B | 987 | ASP | CB-CG-OD1 | 5.05 | 122.85 | 118.30 |
| 1 | D | 411 | ASP | CB-CG-OD2 | -5.05 | 113.75 | 118.30 |
| 1 | B | 26 | ARG | NE-CZ-NH1 | -5.04 | 117.78 | 120.30 |
| 1 | B | 140 | ARG | NE-CZ-NH2 | -5.03 | 117.78 | 120.30 |
| 1 | C | 172 | ASP | CB-CG-OD2 | -5.02 | 113.78 | 118.30 |
| 1 | C | 388 | ARG | CG-CD-NE | 5.01 | 122.33 | 111.80 |
| 1 | C | 629 | PHE | CB-CA-C | -5.01 | 100.38 | 110.40 |
| 1 | D | 319 | ASP | CB-CG-OD1 | 5.01 | 122.81 | 118.30 |
| 1 | B | 221 | GLN | N-CA-CB | -5.01 | 101.59 | 110.60 |
| 1 | A | 285 | TYR | CB-CG-CD2 | -5.00 | 118.00 | 121.00 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 1 | A | 634 | GLN | CA |

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 | 8125 | 0 | 7716 | 105 | 0 |
| 1 | B | 8131 | 0 | 7721 | 88 | 0 |
| 1 | C | 8125 | 0 | 7716 | 105 | 0 |
| 1 | D | 8125 | 0 | 7716 | 105 | 0 |
| 2 | A | 10 | 0 | 9 | 0 | 0 |
| 2 | B | 10 | 0 | 9 | 0 | 0 |
| 2 | C | 10 | 0 | 9 | 0 | 0 |
| 2 | D | 10 | 0 | 10 | 0 | 0 |
| 3 | A | 4 | 0 | 0 | 0 | 0 |
| 3 | B | 3 | 0 | 0 | 0 | 0 |
| 3 | C | 6 | 0 | 0 | 0 | 0 |
| 3 | D | 4 | 0 | 0 | 0 | 0 |
| 4 | A | 4 | 0 | 0 | 0 | 0 |
| 4 | B | 4 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 4 | C | 4 | 0 | 0 | 0 | 0 |
| 4 | D | 4 | 0 | 0 | 0 | 0 |
| 5 | A | 14 | 0 | 19 | 0 | 0 |
| 5 | B | 14 | 0 | 19 | 0 | 0 |
| 5 | C | 14 | 0 | 19 | 1 | 0 |
| 5 | D | 14 | 0 | 19 | 1 | 0 |
| 6 | A | 108 | 0 | 162 | 9 | 0 |
| 6 | B | 108 | 0 | 162 | 7 | 0 |
| 6 | C | 112 | 0 | 168 | 10 | 0 |
| 6 | D | 112 | 0 | 168 | 9 | 0 |
| 7 | A | 1090 | 0 | 0 | 17 | 1 |
| 7 | B | 1091 | 0 | 0 | 9 | 1 |
| 7 | C | 1034 | 0 | 0 | 14 | 0 |
| 7 | D | 1079 | 0 | 0 | 19 | 0 |
| All | All | 37369 | 0 | 31642 | 415 | 1 |

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 6.

All (415) 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) |
|---|---|---|---|
| 6:B:8508:DMS:C1 | 6:B:8508:DMS:S | 2.06 | 1.42 |
| 6:B:8407:DMS:C2 | 6:B:8407:DMS:S | 2.10 | 1.39 |
| 1:C:634:GLN:H | 1:C:634:GLN:NE2 | 1.37 | 1.21 |
| 1:D:804:ASN:HD22 | 1:D:809:ARG:NH2 | 1.41 | 1.16 |
| 1:D:804:ASN:ND2 | 1:D:809:ARG:HH21 | 1.41 | 1.16 |
| 1:B:655:MET:HE2 | 1:B:665:SER:HB3 | 1.31 | 1.08 |
| 1:A:237:ARG:HH11 | 1:A:237:ARG:HB3 | 1.25 | 1.02 |
| 1:A:1022:GLN:HG2 | 1:A:1023:LYS:H | 1.25 | 0.97 |
| 1:C:356:ARG:HD2 | 1:C:379:MET:HE1 | 1.49 | 0.94 |
| 1:A:473:ARG:NH1 | 1:A:476:LYS:HB2 | 1.84 | 0.92 |
| 1:D:809:ARG:HH11 | 1:D:809:ARG:HG2 | 1.34 | 0.90 |
| 1:A:804:ASN:HA | 1:A:809:ARG:NH1 | 1.87 | 0.89 |
| 1:A:777:LEU:CD1 | 1:A:980:GLU:HG2 | 2.04 | 0.88 |
| 1:B:600:GLN:H | 1:B:600:GLN:HE21 | 1.18 | 0.87 |
| 1:B:655:MET:CE | 1:B:665:SER:HB3 | 2.04 | 0.87 |
| 1:C:634:GLN:NE2 | 1:C:634:GLN:N | 2.22 | 0.87 |
| 1:C:687:GLN:HG3 | 1:C:688:PRO:HD2 | 1.57 | 0.86 |
| 1:B:599:ARG:HG3 | 1:B:599:ARG:HH11 | 1.40 | 0.82 |
| 1:D:237:ARG:HH11 | 1:D:237:ARG:HG2 | 1.44 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:658:LEU:O | 1:D:661:LYS:HG3 | 1.81 | 0.81 |
| 1:A:787:ALA:HA | 1:A:968:MET:HG3 | 1.63 | 0.81 |
| 1:C:703:PRO:HG2 | 6:C:8425:DMS:H13 | 1.63 | 0.80 |
| 1:B:797:GLU:HG2 | 1:B:799:THR:HG23 | 1.62 | 0.80 |
| 1:D:663:LEU:CD1 | 1:D:686:PRO:HG2 | 2.11 | 0.80 |
| 1:A:237:ARG:HB3 | 1:A:237:ARG:NH1 | 1.97 | 0.80 |
| 1:A:797:GLU:O | 1:A:801:ILE:HD13 | 1.83 | 0.77 |
| 1:B:651:LEU:O | 1:B:651:LEU:HD23 | 1.83 | 0.77 |
| 1:B:651:LEU:HD21 | 1:B:701:VAL:HB | 1.65 | 0.77 |
| 1:D:663:LEU:HD13 | 1:D:686:PRO:HG2 | 1.66 | 0.77 |
| 1:A:237:ARG:HH11 | 1:A:237:ARG:CB | 1.98 | 0.77 |
| 1:A:1022:GLN:HG2 | 1:A:1023:LYS:N | 1.99 | 0.77 |
| 6:A:8503:DMS:H23 | 7:A:8976:HOH:O | 1.85 | 0.77 |
| 1:A:797:GLU:HB3 | 1:A:799:THR:HG23 | 1.66 | 0.76 |
| 1:C:634:GLN:H | 1:C:634:GLN:HE21 | 1.27 | 0.76 |
| 1:D:629:PHE:O | 1:D:630:ARG:HD3 | 1.86 | 0.75 |
| 1:A:777:LEU:HD13 | 1:A:980:GLU:HG2 | 1.68 | 0.75 |
| 1:C:737:ILE:HD12 | 1:C:738:PRO:HD2 | 1.67 | 0.74 |
| 1:D:887:GLN:NE2 | 1:D:980:GLU:O | 2.20 | 0.74 |
| 1:B:737:ILE:HD11 | 7:B:9591:HOH:O | 1.88 | 0.74 |
| 1:A:600:GLN:H | 1:A:600:GLN:HE21 | 1.35 | 0.73 |
| 1:C:230:ARG:HD2 | 7:C:8959:HOH:O | 1.89 | 0.71 |
| 1:A:685:LEU:HB3 | 1:A:686:PRO:HD2 | 1.72 | 0.70 |
| 1:C:824:GLN:HG2 | 1:C:825:CYS:N | 2.05 | 0.70 |
| 1:C:651:LEU:HD11 | 1:C:653:HIS:CE1 | 2.27 | 0.70 |
| 1:C:703:PRO:HG2 | 6:C:8425:DMS:C1 | 2.20 | 0.70 |
| 1:D:748:CYS:C | 1:D:749:ILE:HD12 | 2.13 | 0.69 |
| 1:A:777:LEU:HD11 | 1:A:980:GLU:HG2 | 1.72 | 0.69 |
| 1:D:653:HIS:ND1 | 1:D:701:VAL:HG21 | 2.08 | 0.69 |
| 6:A:8420:DMS:H21 | 7:D:9523:HOH:O | 1.92 | 0.69 |
| 1:A:800:ARG:HB3 | 7:A:9395:HOH:O | 1.92 | 0.68 |
| 1:A:832:ASP:OD1 | 1:A:832:ASP:N | 2.27 | 0.68 |
| 1:D:749:ILE:HD12 | 1:D:749:ILE:N | 2.08 | 0.68 |
| 1:C:685:LEU:HB3 | 1:C:686:PRO:HD2 | 1.75 | 0.68 |
| 1:B:262:GLN:HE21 | 1:B:263:GLY:N | 1.92 | 0.68 |
| 1:B:651:LEU:CD2 | 1:B:701:VAL:HB | 2.24 | 0.68 |
| 1:B:878:HIS:HD2 | 7:B:8695:HOH:O | 1.76 | 0.68 |
| 1:C:237:ARG:NH1 | 1:C:237:ARG:HB3 | 2.08 | 0.68 |
| 1:D:133:TRP:HE1 | 6:D:8703:DMS:H23 | 1.59 | 0.67 |
| 1:C:749:ILE:N | 1:C:749:ILE:HD12 | 2.10 | 0.67 |
| 6:B:8410:DMS:H13 | 7:B:9151:HOH:O | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:878:HIS:HD2 | 7:C:8695:HOH:O | 1.76 | 0.67 |
| 1:B:845:GLN:OE1 | 1:B:845:GLN:HA | 1.95 | 0.66 |
| 1:D:237:ARG:HH11 | 1:D:237:ARG:CG | 2.07 | 0.66 |
| 1:A:878:HIS:HD2 | 7:A:8674:HOH:O | 1.78 | 0.66 |
| 1:D:128:ASN:HB3 | 1:D:180:GLY:O | 1.95 | 0.66 |
| 1:B:494:THR:HB | 1:C:473:ARG:NH2 | 2.11 | 0.66 |
| 1:C:356:ARG:HD2 | 1:C:379:MET:CE | 2.23 | 0.66 |
| 1:C:690:SER:HB2 | 7:C:9380:HOH:O | 1.95 | 0.66 |
| 1:D:804:ASN:HA | 1:D:809:ARG:CZ | 2.26 | 0.66 |
| 1:D:804:ASN:HA | 1:D:809:ARG:NH2 | 2.11 | 0.66 |
| 1:D:237:ARG:NH1 | 7:D:9273:HOH:O | 2.28 | 0.66 |
| 6:D:8703:DMS:H23 | 7:D:9706:HOH:O | 1.96 | 0.66 |
| 1:A:473:ARG:HH11 | 1:A:476:LYS:HB2 | 1.60 | 0.65 |
| 1:A:754:LYS:NZ | 7:A:9527:HOH:O | 2.30 | 0.65 |
| 1:D:685:LEU:HB3 | 1:D:686:PRO:HD2 | 1.77 | 0.65 |
| 1:D:651:LEU:HD11 | 1:D:653:HIS:CE1 | 2.31 | 0.65 |
| 1:A:887:GLN:NE2 | 1:A:980:GLU:O | 2.29 | 0.65 |
| 1:B:434:PRO:HB3 | 1:C:434:PRO:HB3 | 1.77 | 0.65 |
| 1:D:653:HIS:CE1 | 1:D:701:VAL:HG21 | 2.32 | 0.64 |
| 1:C:748:CYS:C | 1:C:749:ILE:HD12 | 2.17 | 0.64 |
| 1:D:237:ARG:HG2 | 1:D:237:ARG:NH1 | 2.08 | 0.64 |
| 1:A:277:GLU:H | 1:A:277:GLU:CD | 1.99 | 0.64 |
| 6:D:8421:DMS:H11 | 7:D:9361:HOH:O | 1.97 | 0.64 |
| 1:C:651:LEU:HD12 | 1:C:651:LEU:C | 2.17 | 0.64 |
| 1:A:655:MET:HE2 | 1:A:656:VAL:N | 2.12 | 0.64 |
| 1:C:651:LEU:HD12 | 1:C:651:LEU:O | 1.98 | 0.64 |
| 1:D:254:LEU:HD12 | 7:D:9641:HOH:O | 1.97 | 0.63 |
| 1:D:292:ARG:HH12 | 6:D:8412:DMS:C2 | 2.11 | 0.63 |
| 1:A:431:ARG:HG3 | 7:A:9378:HOH:O | 1.97 | 0.63 |
| 1:A:648:ASP:OD2 | 7:A:9548:HOH:O | 2.15 | 0.63 |
| 1:B:262:GLN:HE21 | 1:B:262:GLN:C | 2.01 | 0.62 |
| 1:C:278:ILE:HD13 | 1:C:278:ILE:N | 2.13 | 0.62 |
| 1:B:634:GLN:HG3 | 1:B:682:LEU:HB2 | 1.80 | 0.62 |
| 1:B:797:GLU:CG | 1:B:799:THR:HG23 | 2.28 | 0.62 |
| 1:B:637:GLU:OE2 | 1:B:677:LYS:HE3 | 2.00 | 0.62 |
| 1:B:377:LEU:HD22 | 1:B:708:TRP:HA | 1.80 | 0.62 |
| 1:D:725:ASN:HB2 | 7:D:9581:HOH:O | 1.99 | 0.61 |
| 1:A:804:ASN:OD1 | 1:A:809:ARG:NH2 | 2.33 | 0.61 |
| 1:A:976:LEU:HB2 | 6:A:8423:DMS:H11 | 1.82 | 0.61 |
| 1:D:1022:GLN:O | 1:D:1022:GLN:HG3 | 1.98 | 0.61 |
| 1:A:658:LEU:O | 1:A:661:LYS:HG3 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:88:SER:HA | 1:C:366:VAL:HG21 | 1.82 | 0.61 |
| 1:D:878:HIS:HD2 | 7:D:8814:HOH:O | 1.83 | 0.61 |
| 1:D:135:GLN:C | 1:D:136:GLU:HG2 | 2.22 | 0.60 |
| 1:C:730:LEU:N | 1:C:730:LEU:HD23 | 2.16 | 0.60 |
| 1:B:863:GLN:HG2 | 1:B:1021:CYS:HB3 | 1.83 | 0.60 |
| 1:C:237:ARG:HH11 | 1:C:237:ARG:CB | 2.13 | 0.60 |
| 1:A:241:GLU:OE2 | 1:A:292:ARG:NE | 2.28 | 0.60 |
| 1:A:809:ARG:HH11 | 1:A:809:ARG:CG | 2.15 | 0.60 |
| 1:D:292:ARG:HH12 | 6:D:8412:DMS:H21 | 1.66 | 0.60 |
| 1:D:663:LEU:HD13 | 1:D:686:PRO:CG | 2.32 | 0.59 |
| 1:C:682:LEU:HB3 | 1:C:683:PRO:HD2 | 1.85 | 0.59 |
| 1:D:618:THR:HG21 | 7:D:9054:HOH:O | 2.02 | 0.59 |
| 1:D:809:ARG:HG2 | 1:D:809:ARG:NH1 | 2.09 | 0.59 |
| 1:C:890:GLN:HG3 | 1:C:891:VAL:N | 2.18 | 0.59 |
| 1:C:703:PRO:HD2 | 6:C:8425:DMS:H11 | 1.84 | 0.59 |
| 1:B:599:ARG:NH1 | 1:B:601[A]:PHE:CD1 | 2.71 | 0.59 |
| 1:A:687:GLN:HG3 | 7:A:9467:HOH:O | 2.02 | 0.59 |
| 1:C:595:THR:HA | 1:C:596:PRO:C | 2.23 | 0.58 |
| 1:B:890:GLN:OE1 | 1:B:947:GLY:HA3 | 2.03 | 0.58 |
| 6:C:8427:DMS:H21 | 7:C:9057:HOH:O | 2.02 | 0.58 |
| 1:A:699:ARG:NH2 | 7:A:9471:HOH:O | 2.35 | 0.57 |
| 1:C:646:HIS:CE1 | 1:C:673:ALA:HB2 | 2.39 | 0.57 |
| 1:D:809:ARG:HH11 | 1:D:809:ARG:CG | 2.14 | 0.57 |
| 1:C:240:LEU:C | 1:C:240:LEU:HD23 | 2.25 | 0.57 |
| 1:C:806:TRP:CE2 | 1:C:809:ARG:NH2 | 2.73 | 0.57 |
| 1:A:237:ARG:NH1 | 7:A:9138:HOH:O | 2.29 | 0.57 |
| 1:C:687:GLN:HE21 | 1:C:687:GLN:HA | 1.69 | 0.57 |
| 1:C:730:LEU:HD23 | 1:C:730:LEU:H | 1.67 | 0.57 |
| 1:D:595:THR:HA | 1:D:596:PRO:C | 2.25 | 0.56 |
| 1:C:730:LEU:H | 1:C:730:LEU:CD2 | 2.18 | 0.56 |
| 5:C:2002:BTB:O8 | 5:C:2002:BTB:H62 | 2.05 | 0.56 |
| 1:D:799:THR:OG1 | 1:D:800:ARG:N | 2.38 | 0.56 |
| 1:A:789:LEU:HD11 | 1:A:993:ILE:HG22 | 1.88 | 0.56 |
| 1:A:651:LEU:C | 1:A:651:LEU:HD12 | 2.26 | 0.56 |
| 1:B:654:TRP:CZ3 | 1:B:665:SER:HA | 2.39 | 0.56 |
| 1:C:866:ILE:O | 1:C:1017:GLN:NE2 | 2.36 | 0.56 |
| 1:C:499:ILE:HG22 | 1:C:501:PRO:HD3 | 1.88 | 0.56 |
| 1:D:802:ASP:OD1 | 1:D:803:PRO:HD2 | 2.06 | 0.56 |
| 1:A:803:PRO:O | 1:A:809:ARG:NH1 | 2.38 | 0.55 |
| 1:A:473:ARG:HH12 | 1:A:476:LYS:HB2 | 1.71 | 0.55 |
| 1:B:157:ARG:HD3 | 7:B:9476:HOH:O | 2.05 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:75:GLU:HA | 1:B:75:GLU:OE1 | 2.06 | 0.55 |
| 1:A:595:THR:HA | 1:A:596:PRO:C | 2.27 | 0.55 |
| 1:C:70:PRO:HG2 | 1:C:78:LEU:HD21 | 1.88 | 0.55 |
| 1:C:649:ASN:HA | 6:C:8425:DMS:C1 | 2.37 | 0.55 |
| 1:B:950:GLN:OE1 | 1:B:952:ARG:HD3 | 2.07 | 0.55 |
| 1:A:735:HIS:O | 1:A:736:ALA:HB2 | 2.07 | 0.54 |
| 1:B:615:PRO:O | 1:B:618:THR:HG22 | 2.08 | 0.54 |
| 1:B:646:HIS:CE1 | 1:B:673:ALA:HA | 2.43 | 0.54 |
| 1:A:178:ARG:HD2 | 7:A:9497:HOH:O | 2.07 | 0.54 |
| 1:D:133:TRP:HE1 | 6:D:8703:DMS:C2 | 2.20 | 0.54 |
| 1:D:653:HIS:CD2 | 1:D:667:GLU:HB3 | 2.42 | 0.54 |
| 1:B:79:PRO:HD2 | 1:B:80:GLU:OE2 | 2.07 | 0.54 |
| 1:D:878:HIS:HE1 | 7:D:9399:HOH:O | 1.91 | 0.54 |
| 1:B:320:GLY:O | 6:B:8406:DMS:O | 2.26 | 0.54 |
| 1:B:595:THR:HA | 1:B:596:PRO:C | 2.28 | 0.54 |
| 1:D:135:GLN:O | 1:D:136:GLU:HG2 | 2.07 | 0.54 |
| 1:D:473:ARG:HH11 | 1:D:476:LYS:HB2 | 1.73 | 0.54 |
| 1:A:88:SER:HA | 1:A:366:VAL:HG21 | 1.90 | 0.54 |
| 1:D:847:LYS:HG3 | 1:D:848:THR:N | 2.17 | 0.54 |
| 1:A:718:GLN:CD | 6:A:8503:DMS:H13 | 2.28 | 0.53 |
| 1:B:178:ARG:HG3 | 1:B:178:ARG:O | 2.08 | 0.53 |
| 1:C:649:ASN:HA | 6:C:8425:DMS:H12 | 1.90 | 0.53 |
| 1:A:764:PHE:CE1 | 1:A:781:ARG:NH1 | 2.76 | 0.53 |
| 1:C:745:MET:HE3 | 1:C:745:MET:HA | 1.91 | 0.53 |
| 1:A:768:MET:CE | 1:A:1020:TRP:CZ2 | 2.92 | 0.53 |
| 1:C:241:GLU:OE1 | 1:C:292:ARG:NE | 2.41 | 0.53 |
| 1:D:685:LEU:HB3 | 1:D:686:PRO:CD | 2.39 | 0.52 |
| 1:A:1017:GLN:HG3 | 1:A:1018:LEU:N | 2.16 | 0.52 |
| 6:A:8423:DMS:H13 | 7:A:9155:HOH:O | 2.09 | 0.52 |
| 1:C:266:GLN:O | 6:C:8602:DMS:H22 | 2.09 | 0.52 |
| 1:B:651:LEU:HD23 | 1:B:651:LEU:C | 2.29 | 0.52 |
| 1:C:1011:ALA:HB3 | 1:C:1014:TYR:CZ | 2.44 | 0.52 |
| 1:A:1022:GLN:C | 1:A:1023:LYS:HG3 | 2.30 | 0.52 |
| 1:C:178:ARG:HD2 | 7:C:9553:HOH:O | 2.09 | 0.52 |
| 1:D:554:GLN:NE2 | 7:D:9666:HOH:O | 2.24 | 0.52 |
| 1:B:634:GLN:HG2 | 1:B:682:LEU:O | 2.10 | 0.52 |
| 1:B:596:PRO:HB3 | 7:B:9423:HOH:O | 2.09 | 0.52 |
| 6:C:8407:DMS:H21 | 7:C:9561:HOH:O | 2.08 | 0.52 |
| 1:B:599:ARG:HH11 | 1:B:599:ARG:CG | 2.16 | 0.51 |
| 1:C:46:ARG:HG2 | 7:C:9538:HOH:O | 2.10 | 0.51 |
| 1:A:768:MET:HE3 | 1:A:1020:TRP:CZ2 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:615:PRO:O | 1:A:618:THR:HG22 | 2.11 | 0.51 |
| 1:B:797:GLU:HG2 | 1:B:799:THR:CG2 | 2.38 | 0.51 |
| 1:C:673:ALA:HB1 | 1:C:674:PRO:HD2 | 1.92 | 0.51 |
| 1:D:749:ILE:N | 1:D:749:ILE:CD1 | 2.73 | 0.51 |
| 6:B:8407:DMS:C2 | 6:B:8407:DMS:C1 | 2.88 | 0.51 |
| 1:A:264:GLU:HG3 | 7:A:9518:HOH:O | 2.11 | 0.51 |
| 1:B:127:PHE:CE2 | 1:B:184:LEU:HG | 2.46 | 0.51 |
| 1:B:599:ARG:HH12 | 1:B:601[A]:PHE:HE1 | 1.50 | 0.50 |
| 1:D:584:PRO:HD2 | 7:D:9453:HOH:O | 2.11 | 0.50 |
| 1:D:754:LYS:HE2 | 1:D:1022:GLN:HG2 | 1.92 | 0.50 |
| 1:C:630:ARG:HH11 | 1:C:630:ARG:CB | 2.25 | 0.50 |
| 1:D:651:LEU:O | 1:D:651:LEU:HD12 | 2.11 | 0.50 |
| 1:A:863:GLN:NE2 | 1:A:952:ARG:HH22 | 2.09 | 0.50 |
| 1:C:736:ALA:O | 1:C:860:GLY:HA3 | 2.12 | 0.50 |
| 1:D:363:HIS:HD2 | 7:D:9324:HOH:O | 1.93 | 0.50 |
| 1:C:13:ARG:O | 1:C:14:ARG:C | 2.50 | 0.49 |
| 1:C:16:TRP:CG | 1:C:189:LEU:HD13 | 2.47 | 0.49 |
| 1:C:759:ASN:OD1 | 1:C:761:GLN:N | 2.44 | 0.49 |
| 1:B:13:ARG:HG3 | 1:C:13:ARG:CZ | 2.42 | 0.49 |
| 1:C:608:PHE:CE1 | 1:C:614:HIS:HD2 | 2.30 | 0.49 |
| 1:D:131:GLU:O | 1:D:131:GLU:OE2 | 2.30 | 0.49 |
| 1:D:651:LEU:HD12 | 1:D:651:LEU:C | 2.33 | 0.49 |
| 1:D:859:ASP:OD1 | 1:D:861:SER:HB2 | 2.12 | 0.49 |
| 1:A:433:LEU:HB3 | 1:A:434:PRO:HD3 | 1.95 | 0.49 |
| 1:B:689:GLU:O | 1:B:690:SER:OG | 2.29 | 0.49 |
| 1:D:797:GLU:HB3 | 1:D:799:THR:HG23 | 1.95 | 0.49 |
| 1:D:844:HIS:O | 1:D:845:GLN:HB2 | 2.13 | 0.49 |
| 1:B:74:LEU:HD22 | 1:B:153:TRP:CG | 2.47 | 0.49 |
| 1:B:232:ASN:ND2 | 1:B:237:ARG:HG3 | 2.28 | 0.49 |
| 1:D:237:ARG:CG | 1:D:237:ARG:NH1 | 2.73 | 0.49 |
| 1:C:634:GLN:H | 1:C:634:GLN:CD | 2.08 | 0.49 |
| 1:A:680:ILE:HG12 | 7:A:9249:HOH:O | 2.13 | 0.48 |
| 1:C:728:VAL:O | 1:C:730:LEU:HD23 | 2.13 | 0.48 |
| 1:C:824:GLN:CG | 1:C:825:CYS:N | 2.75 | 0.48 |
| 1:D:809:ARG:NH1 | 1:D:809:ARG:CG | 2.75 | 0.48 |
| 1:C:651:LEU:CD1 | 1:C:653:HIS:CE1 | 2.95 | 0.48 |
| 1:D:795:VAL:HG12 | 6:D:8506:DMS:C1 | 2.43 | 0.48 |
| 1:D:1022:GLN:O | 1:D:1023:LYS:HB2 | 2.14 | 0.48 |
| 1:B:88:SER:HA | 1:B:366:VAL:HG21 | 1.95 | 0.48 |
| 1:D:441:THR:O | 1:D:445:GLN:HG3 | 2.13 | 0.48 |
| 1:D:843:GLN:HB3 | 1:D:847:LYS:O | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:890:GLN:OE1 | 1:C:948:PRO:HD3 | 2.13 | 0.48 |
| 1:D:634:GLN:NE2 | 1:D:682:LEU:O | 2.46 | 0.48 |
| 1:B:411:ASP:OD2 | 1:B:447:ASP:OD2 | 2.32 | 0.48 |
| 1:B:381:GLN:O | 1:B:621:LYS:HE3 | 2.14 | 0.48 |
| 1:C:671:ASP:N | 1:C:678:GLN:OE1 | 2.28 | 0.48 |
| 1:A:809:ARG:HH11 | 1:A:809:ARG:HG3 | 1.79 | 0.48 |
| 1:A:890:GLN:HG3 | 1:A:891:VAL:N | 2.28 | 0.48 |
| 1:C:44:THR:OG1 | 1:C:46:ARG:HD3 | 2.14 | 0.47 |
| 1:D:739:HIS:HB2 | 7:D:9753:HOH:O | 2.15 | 0.47 |
| 1:D:795:VAL:HG12 | 6:D:8506:DMS:H13 | 1.96 | 0.47 |
| 1:A:599:ARG:HD2 | 1:A:600:GLN:HE22 | 1.79 | 0.47 |
| 1:A:768:MET:HE1 | 1:A:1020:TRP:CH2 | 2.49 | 0.47 |
| 1:B:573:GLN:HB2 | 1:B:602:CYS:O | 2.13 | 0.47 |
| 1:C:878:HIS:CE1 | 1:C:1010:SER:HB3 | 2.49 | 0.47 |
| 1:B:1022:GLN:CG | 1:B:1023:LYS:N | 2.77 | 0.47 |
| 1:D:890:GLN:HG3 | 1:D:891:VAL:N | 2.30 | 0.47 |
| 1:A:372:MET:HE1 | 1:A:395:HIS:HB3 | 1.97 | 0.47 |
| 1:A:668:VAL:HG12 | 1:A:669:PRO:O | 2.14 | 0.47 |
| 1:B:1017:GLN:HB2 | 7:B:9592:HOH:O | 2.14 | 0.47 |
| 1:C:615:PRO:O | 1:C:618:THR:HG22 | 2.14 | 0.47 |
| 1:C:651:LEU:CD1 | 1:C:653:HIS:ND1 | 2.77 | 0.47 |
| 1:D:340:GLY:O | 1:D:561:ARG:HG2 | 2.15 | 0.47 |
| 1:A:147:ASN:HA | 1:A:148:SER:HA | 1.58 | 0.47 |
| 1:A:685:LEU:HB3 | 1:A:686:PRO:CD | 2.43 | 0.47 |
| 1:B:499:ILE:HG22 | 1:B:501:PRO:HD3 | 1.95 | 0.47 |
| 1:C:86:VAL:HG13 | 1:C:87:PRO:HA | 1.97 | 0.47 |
| 1:C:237:ARG:NH1 | 1:C:237:ARG:CB | 2.73 | 0.47 |
| 1:C:749:ILE:N | 1:C:749:ILE:CD1 | 2.77 | 0.47 |
| 1:A:654:TRP:CZ3 | 1:A:665:SER:HA | 2.49 | 0.47 |
| 1:A:599:ARG:HD2 | 1:A:600:GLN:NE2 | 2.30 | 0.46 |
| 6:A:8409:DMS:O | 7:A:9110:HOH:O | 2.20 | 0.46 |
| 1:C:746:ASP:HA | 1:C:760:ARG:HG3 | 1.97 | 0.46 |
| 1:B:127:PHE:CD2 | 1:B:127:PHE:N | 2.83 | 0.46 |
| 1:A:167:LEU:HB3 | 1:A:168:PRO:HD2 | 1.98 | 0.46 |
| 1:B:730:LEU:H | 1:B:730:LEU:HG | 1.27 | 0.46 |
| 1:A:809:ARG:NH1 | 1:A:809:ARG:CG | 2.78 | 0.46 |
| 1:B:595:THR:HG23 | 1:B:595:THR:O | 2.15 | 0.46 |
| 1:A:86:VAL:HG13 | 1:A:87:PRO:HA | 1.97 | 0.46 |
| 1:C:610:ASP:O | 1:C:611:ARG:HB2 | 2.16 | 0.46 |
| 1:D:653:HIS:ND1 | 1:D:701:VAL:CG2 | 2.77 | 0.46 |
| 1:D:696:LEU:HB2 | 1:D:722:LEU:HD11 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1022:GLN:CG | 1:A:1023:LYS:N | 2.75 | 0.46 |
| 1:B:494:THR:HB | 1:C:473:ARG:HH21 | 1.81 | 0.46 |
| 1:B:670:LEU:HA | 1:B:670:LEU:HD23 | 1.66 | 0.46 |
| 1:C:16:TRP:CG | 1:C:189:LEU:CD1 | 2.98 | 0.46 |
| 1:C:751:LEU:HD21 | 1:C:860:GLY:O | 2.16 | 0.46 |
| 1:D:250:LEU:O | 1:D:251:ARG:HG2 | 2.17 | 0.45 |
| 1:C:745:MET:HE3 | 1:C:745:MET:CA | 2.45 | 0.45 |
| 1:D:147:ASN:HA | 1:D:148:SER:HA | 1.75 | 0.45 |
| 1:A:663:LEU:HD11 | 1:A:688:PRO:HG3 | 1.96 | 0.45 |
| 1:B:777:LEU:HG | 1:B:889:ALA:HA | 1.99 | 0.45 |
| 1:D:411:ASP:OD2 | 1:D:447:ASP:OD2 | 2.34 | 0.45 |
| 1:A:178:ARG:HG3 | 7:A:9497:HOH:O | 2.16 | 0.45 |
| 1:B:147:ASN:HA | 1:B:148:SER:HA | 1.59 | 0.45 |
| 1:D:688:PRO:C | 1:D:690:SER:H | 2.20 | 0.45 |
| 1:A:128:ASN:HB2 | 7:A:9543:HOH:O | 2.17 | 0.45 |
| 1:A:251:ARG:HH11 | 6:A:8416:DMS:H11 | 1.82 | 0.45 |
| 1:C:646:HIS:HB3 | 7:C:9488:HOH:O | 2.17 | 0.45 |
| 1:A:58:TRP:CD1 | 1:A:86:VAL:HB | 2.52 | 0.45 |
| 1:B:377:LEU:O | 1:B:381:GLN:HG3 | 2.16 | 0.45 |
| 1:C:755:ARG:HG2 | 1:C:769:TRP:CE3 | 2.52 | 0.45 |
| 1:A:243:GLU:OE2 | 1:A:245:GLN:NE2 | 2.43 | 0.45 |
| 1:B:599:ARG:NH1 | 1:B:601[A]:PHE:CE1 | 2.74 | 0.45 |
| 1:C:253:TYR:CD1 | 1:C:317:THR:HG22 | 2.52 | 0.45 |
| 1:D:545:SER:O | 1:D:909:ARG:HD3 | 2.17 | 0.45 |
| 1:A:361:PRO:HB2 | 1:A:576:ILE:HG12 | 1.99 | 0.44 |
| 1:C:114:VAL:HB | 1:C:115:PRO:CD | 2.47 | 0.44 |
| 1:C:237:ARG:HB3 | 1:C:237:ARG:HH11 | 1.72 | 0.44 |
| 1:A:742:THR:HG22 | 1:A:743:SER:N | 2.31 | 0.44 |
| 1:C:147:ASN:HA | 1:C:148:SER:HA | 1.60 | 0.44 |
| 1:C:433:LEU:O | 1:C:437:SER:HB3 | 2.17 | 0.44 |
| 1:D:808:GLU:OE2 | 1:D:811:LYS:NZ | 2.49 | 0.44 |
| 1:B:262:GLN:CA | 1:B:262:GLN:NE2 | 2.80 | 0.44 |
| 1:C:577:LYS:HB3 | 1:C:577:LYS:HE3 | 1.88 | 0.44 |
| 1:C:667:GLU:C | 1:C:668:VAL:HG23 | 2.38 | 0.44 |
| 1:D:668:VAL:HG11 | 1:D:680:ILE:HG12 | 1.99 | 0.44 |
| 1:B:360:HIS:CE1 | 1:B:362:LEU:HB2 | 2.52 | 0.44 |
| 1:D:133:TRP:NE1 | 6:D:8703:DMS:H23 | 2.30 | 0.44 |
| 1:A:84:VAL:HA | 6:A:8414:DMS:O | 2.17 | 0.44 |
| 1:A:685:LEU:HD23 | 1:A:686:PRO:HD3 | 1.99 | 0.44 |
| 6:C:8410:DMS:H13 | 7:C:8966:HOH:O | 2.17 | 0.44 |
| 1:C:844:HIS:HD2 | 7:C:9471:HOH:O | 2.01 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:687:GLN:HE21 | 1:B:687:GLN:N | 2.15 | 0.44 |
| 1:D:651:LEU:CD1 | 1:D:653:HIS:CE1 | 3.00 | 0.44 |
| 1:D:663:LEU:HD11 | 1:D:686:PRO:HG2 | 1.96 | 0.44 |
| 1:B:599:ARG:NH1 | 1:B:601[A]:PHE:HD1 | 2.16 | 0.43 |
| 7:B:9403:HOH:O | 6:C:8420:DMS:H21 | 2.17 | 0.43 |
| 1:B:630:ARG:HH21 | 1:B:637:GLU:CD | 2.21 | 0.43 |
| 1:C:569:ASP:O | 1:C:605:GLY:HA2 | 2.19 | 0.43 |
| 1:C:768:MET:HE1 | 1:C:1020:TRP:CH2 | 2.54 | 0.43 |
| 1:D:802:ASP:O | 1:D:808:GLU:HG3 | 2.18 | 0.43 |
| 1:C:549:PHE:CE2 | 1:C:620:ALA:HA | 2.54 | 0.43 |
| 1:D:659:ASP:HB3 | 1:D:898:LEU:HD21 | 2.01 | 0.43 |
| 1:A:127:PHE:N | 1:A:127:PHE:CD2 | 2.86 | 0.43 |
| 1:A:843:GLN:HA | 1:A:847:LYS:O | 2.18 | 0.43 |
| 1:B:114:VAL:HB | 1:B:115:PRO:HD2 | 2.01 | 0.43 |
| 1:B:890:GLN:OE1 | 1:B:948:PRO:HD2 | 2.18 | 0.43 |
| 1:B:128:ASN:HA | 1:B:180:GLY:O | 2.19 | 0.43 |
| 1:D:576:ILE:HD13 | 1:D:576:ILE:HA | 1.86 | 0.43 |
| 1:D:829:THR:O | 1:D:830:LEU:HD23 | 2.19 | 0.43 |
| 1:C:375:ASP:O | 1:C:379:MET:HG3 | 2.18 | 0.43 |
| 1:C:568:TRP:CD2 | 1:C:569:ASP:HB3 | 2.54 | 0.43 |
| 1:D:651:LEU:C | 1:D:651:LEU:CD1 | 2.87 | 0.43 |
| 1:A:433:LEU:N | 1:A:434:PRO:CD | 2.82 | 0.43 |
| 1:A:600:GLN:HE21 | 1:A:600:GLN:N | 2.09 | 0.42 |
| 1:B:745:MET:N | 1:B:745:MET:SD | 2.75 | 0.42 |
| 1:D:843:GLN:HA | 1:D:847:LYS:O | 2.19 | 0.42 |
| 1:D:873:ALA:O | 1:D:876:THR:HG22 | 2.19 | 0.42 |
| 1:C:49:GLN:HG2 | 7:C:9326:HOH:O | 2.18 | 0.42 |
| 1:C:230:ARG:HB3 | 7:C:9557:HOH:O | 2.18 | 0.42 |
| 1:A:568:TRP:CD2 | 1:A:569:ASP:HB3 | 2.54 | 0.42 |
| 1:A:658:LEU:O | 1:A:659:ASP:C | 2.55 | 0.42 |
| 1:B:13:ARG:O | 1:B:14:ARG:C | 2.57 | 0.42 |
| 1:B:233:ASP:HA | 6:B:8417:DMS:C1 | 2.49 | 0.42 |
| 1:D:88:SER:HA | 1:D:366:VAL:HG21 | 2.01 | 0.42 |
| 1:B:663:LEU:HD22 | 1:B:663:LEU:HA | 1.60 | 0.42 |
| 1:D:646:HIS:ND1 | 7:D:9585:HOH:O | 2.37 | 0.42 |
| 1:A:873:ALA:O | 1:A:876:THR:HG22 | 2.20 | 0.42 |
| 1:A:685:LEU:CB | 1:A:686:PRO:HD2 | 2.45 | 0.42 |
| 1:A:701:VAL:O | 1:A:703:PRO:HD3 | 2.20 | 0.42 |
| 1:C:682:LEU:HA | 1:C:683:PRO:HD3 | 1.84 | 0.42 |
| 1:C:785:THR:O | 1:C:881:ARG:HD2 | 2.19 | 0.42 |
| 1:C:930:VAL:HA | 1:C:973:ARG:HD3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:251:ARG:HH11 | 6:A:8416:DMS:C1 | 2.33 | 0.42 |
| 1:B:246:MET:HE1 | 1:B:254:LEU:HD13 | 2.02 | 0.42 |
| 1:D:372:MET:HE1 | 1:D:395:HIS:HB3 | 2.01 | 0.42 |
| 1:D:681:GLU:HG2 | 7:D:9468:HOH:O | 2.19 | 0.42 |
| 1:B:297:ASN:N | 1:B:298:PRO:CD | 2.83 | 0.42 |
| 1:D:619:GLU:HG2 | 1:D:909:ARG:HG3 | 2.02 | 0.42 |
| 5:D:2002:BTB:H31 | 5:D:2002:BTB:H51 | 1.73 | 0.42 |
| 1:A:781:ARG:NH1 | 7:A:9346:HOH:O | 2.53 | 0.42 |
| 1:B:433:LEU:N | 1:B:434:PRO:CD | 2.83 | 0.42 |
| 1:C:580:GLU:H | 1:C:580:GLU:HG3 | 1.26 | 0.42 |
| 1:D:622:HIS:O | 1:D:625:GLN:HG3 | 2.20 | 0.42 |
| 1:A:685:LEU:HD23 | 1:A:685:LEU:HA | 1.84 | 0.41 |
| 1:A:685:LEU:HD22 | 1:A:686:PRO:HD2 | 2.01 | 0.41 |
| 1:B:46:ARG:HH11 | 1:B:46:ARG:HD2 | 1.57 | 0.41 |
| 1:C:285:TYR:HB3 | 1:C:288:ARG:HG3 | 2.01 | 0.41 |
| 1:D:377:LEU:HD22 | 1:D:708:TRP:HA | 2.02 | 0.41 |
| 1:A:742:THR:CG2 | 1:A:743:SER:N | 2.84 | 0.41 |
| 1:D:499:ILE:HG22 | 1:D:501:PRO:HD3 | 2.02 | 0.41 |
| 1:D:682:LEU:HD23 | 1:D:682:LEU:HA | 1.77 | 0.41 |
| 1:C:653:HIS:ND1 | 1:C:667:GLU:HG2 | 2.35 | 0.41 |
| 1:A:990:HIS:HD2 | 1:A:991:MET:O | 2.03 | 0.41 |
| 1:B:966:GLN:HG3 | 7:B:9663:HOH:O | 2.20 | 0.41 |
| 1:A:685:LEU:CD2 | 1:A:686:PRO:HD3 | 2.51 | 0.41 |
| 1:A:753:ASN:OD1 | 1:A:753:ASN:N | 2.53 | 0.41 |
| 1:C:670:LEU:HD23 | 1:C:670:LEU:HA | 1.89 | 0.41 |
| 1:D:568:TRP:CD2 | 1:D:569:ASP:HB3 | 2.55 | 0.41 |
| 1:D:876:THR:OG1 | 1:D:877:PRO:HD2 | 2.20 | 0.41 |
| 1:A:745:MET:HB3 | 1:A:745:MET:HE2 | 1.75 | 0.41 |
| 1:C:279:ILE:HD13 | 1:C:279:ILE:HA | 1.87 | 0.41 |
| 1:C:625:GLN:NE2 | 7:C:8824:HOH:O | 2.50 | 0.41 |
| 1:D:654:TRP:CZ2 | 1:D:683:PRO:HG2 | 2.56 | 0.41 |
| 1:D:781:ARG:NH1 | 7:D:9479:HOH:O | 2.36 | 0.41 |
| 1:A:16:TRP:CG | 1:A:189:LEU:HD13 | 2.55 | 0.41 |
| 1:A:753:ASN:OD1 | 1:A:754:LYS:HG3 | 2.20 | 0.41 |
| 1:B:890:GLN:HB3 | 7:B:9443:HOH:O | 2.21 | 0.41 |
| 1:C:655:MET:SD | 1:C:656:VAL:N | 2.93 | 0.41 |
| 1:D:240:LEU:C | 1:D:240:LEU:HD23 | 2.41 | 0.41 |
| 1:D:618:THR:HG23 | 7:D:9070:HOH:O | 2.20 | 0.41 |
| 1:D:651:LEU:CD1 | 1:D:701:VAL:HB | 2.50 | 0.41 |
| 1:A:427:THR:HG21 | 1:A:462:SER:HB3 | 2.02 | 0.41 |
| 1:B:961:ARG:HG3 | 6:B:8508:DMS:H23 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:685:LEU:CD2 | 1:A:686:PRO:CD | 2.99 | 0.41 |
| 1:A:804:ASN:HA | 1:A:809:ARG:CZ | 2.50 | 0.41 |
| 1:C:730:LEU:N | 1:C:730:LEU:CD2 | 2.78 | 0.41 |
| 1:C:883:GLY:HA3 | 1:C:987:ASP:HA | 2.03 | 0.41 |
| 1:D:143:PHE:O | 1:D:168:PRO:HA | 2.20 | 0.41 |
| 1:D:472:TYR:O | 1:D:476:LYS:HG2 | 2.20 | 0.41 |
| 1:A:473:ARG:HA | 1:A:473:ARG:HD2 | 1.85 | 0.41 |
| 1:B:658:LEU:O | 1:B:659:ASP:C | 2.58 | 0.41 |
| 1:B:1023:LYS:HE3 | 1:B:1023:LYS:HB3 | 1.66 | 0.41 |
| 1:C:71:GLU:N | 7:C:9383:HOH:O | 2.53 | 0.40 |
| 1:A:635:THR:OG1 | 1:A:681:GLU:HG3 | 2.21 | 0.40 |
| 1:A:337:ILE:HA | 1:A:341:LEU:O | 2.21 | 0.40 |
| 1:B:301:TRP:CH2 | 1:B:452:SER:HA | 2.56 | 0.40 |
| 1:B:355:ASN:OD1 | 1:B:388:ARG:HD3 | 2.21 | 0.40 |
| 1:B:562:LEU:HD23 | 1:B:562:LEU:HA | 1.83 | 0.40 |
| 1:B:655:MET:HE2 | 1:B:664:ALA:O | 2.22 | 0.40 |
| 1:B:930:VAL:HA | 1:B:973:ARG:HD3 | 2.03 | 0.40 |
| 1:C:471:LEU:HD23 | 1:C:471:LEU:HA | 1.95 | 0.40 |
| 1:B:111:PRO:HA | 1:B:112:PRO:HA | 1.86 | 0.40 |
| 1:B:142:ILE:HG12 | 1:B:170:GLU:HG2 | 2.02 | 0.40 |
| 1:B:457:SER:HA | 1:B:485:GLN:O | 2.22 | 0.40 |
| 1:A:557:ARG:HH11 | 1:A:557:ARG:HD2 | 1.72 | 0.40 |
| 1:A:685:LEU:CB | 1:A:686:PRO:CD | 2.99 | 0.40 |
| 1:A:861:SER:OG | 1:A:863:GLN:HG3 | 2.22 | 0.40 |
| 1:D:431:ARG:HD2 | 7:D:9514:HOH:O | 2.21 | 0.40 |
| 1:D:583:ASN:HB3 | 7:D:9453:HOH:O | 2.20 | 0.40 |
| 1:D:759:ASN:OD1 | 1:D:761:GLN:N | 2.47 | 0.40 |

All (1) 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) |
|---|---|---|---|
| 7:A:9544:HOH:O | 7:B:9658:HOH:O[2_454] | 2.18 | 0.02 |

## 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 | 1009/1023 (99%) | 974 (96%) | 34 (3%) | 1 (0%) | 51 | 33 |
| 1 | B | 1010/1023 (99%) | 969 (96%) | 36 (4%) | 5 (0%) | 29 | 12 |
| 1 | C | 1009/1023 (99%) | 975 (97%) | 34 (3%) | 0 | 100 | 100 |
| 1 | D | 1009/1023 (99%) | 970 (96%) | 38 (4%) | 1 (0%) | 51 | 33 |
| All | All | 4037/4092 (99%) | 3888 (96%) | 142 (4%) | 7 (0%) | 47 | 29 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 731 | PRO |
| 1 | B | 732 | ALA |
| 1 | D | 688 | PRO |
| 1 | B | 690 | SER |
| 1 | A | 164 | ASP |
| 1 | B | 164 | ASP |
| 1 | B | 688 | PRO |

### 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 | 864/875 (99%) | 834 (96%) | 30 (4%) | 36 | 13 |
| 1 | B | 865/875 (99%) | 835 (96%) | 30 (4%) | 36 | 13 |
| 1 | C | 864/875 (99%) | 824 (95%) | 40 (5%) | 27 | 8 |
| 1 | D | 864/875 (99%) | 825 (96%) | 39 (4%) | 27 | 8 |
| All | All | 3457/3500 (99%) | 3318 (96%) | 139 (4%) | 31 | 10 |

All (139) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 237 | ARG |
| 1 | A | 333 | ARG |
| 1 | A | 370 | GLN |
| 1 | A | 394 | ASN |
| 1 | A | 519 | SER |
| 1 | A | 600 | GLN |
| 1 | A | 632 | SER |
| 1 | A | 634 | GLN |
| 1 | A | 655 | MET |
| 1 | A | 661 | LYS |
| 1 | A | 663 | LEU |
| 1 | A | 667 | GLU |
| 1 | A | 684 | GLU |
| 1 | A | 729 | THR |
| 1 | A | 730 | LEU |
| 1 | A | 735 | HIS |
| 1 | A | 737 | ILE |
| 1 | A | 773 | LYS |
| 1 | A | 796 | SER |
| 1 | A | 797 | GLU |
| 1 | A | 799 | THR |
| 1 | A | 800 | ARG |
| 1 | A | 801 | ILE |
| 1 | A | 809 | ARG |
| 1 | A | 817 | GLN |
| 1 | A | 885 | ASN |
| 1 | A | 956 | GLN |
| 1 | A | 986 | ILE |
| 1 | A | 1017 | GLN |
| 1 | A | 1023 | LYS |
| 1 | B | 237 | ARG |
| 1 | B | 246 | MET |
| 1 | B | 262 | GLN |
| 1 | B | 333 | ARG |
| 1 | B | 344 | LEU |
| 1 | B | 362 | LEU |
| 1 | B | 370 | GLN |
| 1 | B | 394 | ASN |
| 1 | B | 546 | LEU |
| 1 | B | 554 | GLN |
| 1 | B | 580 | GLU |
| 1 | B | 599 | ARG |
| 1 | B | 600 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 651 | LEU |
| 1 | B | 655 | MET |
| 1 | B | 661 | LYS |
| 1 | B | 663 | LEU |
| 1 | B | 687 | GLN |
| 1 | B | 699 | ARG |
| 1 | B | 730 | LEU |
| 1 | B | 737 | ILE |
| 1 | B | 745 | MET |
| 1 | B | 797 | GLU |
| 1 | B | 799 | THR |
| 1 | B | 800 | ARG |
| 1 | B | 819 | GLU |
| 1 | B | 845 | GLN |
| 1 | B | 885 | ASN |
| 1 | B | 956 | GLN |
| 1 | B | 1023 | LYS |
| 1 | C | 71 | GLU |
| 1 | C | 80 | GLU |
| 1 | C | 135 | GLN |
| 1 | C | 178 | ARG |
| 1 | C | 230 | ARG |
| 1 | C | 251 | ARG |
| 1 | C | 262 | GLN |
| 1 | C | 264 | GLU |
| 1 | C | 278 | ILE |
| 1 | C | 333 | ARG |
| 1 | C | 370 | GLN |
| 1 | C | 394 | ASN |
| 1 | C | 437 | SER |
| 1 | C | 519 | SER |
| 1 | C | 546 | LEU |
| 1 | C | 580 | GLU |
| 1 | C | 595 | THR |
| 1 | C | 634 | GLN |
| 1 | C | 653 | HIS |
| 1 | C | 655 | MET |
| 1 | C | 663 | LEU |
| 1 | C | 681 | GLU |
| 1 | C | 684 | GLU |
| 1 | C | 685 | LEU |
| 1 | C | 687 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 699 | ARG |
| 1 | C | 729 | THR |
| 1 | C | 730 | LEU |
| 1 | C | 734 | SER |
| 1 | C | 735 | HIS |
| 1 | C | 737 | ILE |
| 1 | C | 773 | LYS |
| 1 | C | 796 | SER |
| 1 | C | 799 | THR |
| 1 | C | 819 | GLU |
| 1 | C | 829 | THR |
| 1 | C | 893 | GLU |
| 1 | C | 986 | ILE |
| 1 | C | 1017 | GLN |
| 1 | C | 1023 | LYS |
| 1 | D | 13 | ARG |
| 1 | D | 80 | GLU |
| 1 | D | 237 | ARG |
| 1 | D | 277 | GLU |
| 1 | D | 299 | LYS |
| 1 | D | 333 | ARG |
| 1 | D | 344 | LEU |
| 1 | D | 370 | GLN |
| 1 | D | 394 | ASN |
| 1 | D | 480 | PRO |
| 1 | D | 519 | SER |
| 1 | D | 581 | ASN |
| 1 | D | 594 | ASP |
| 1 | D | 595 | THR |
| 1 | D | 632 | SER |
| 1 | D | 634 | GLN |
| 1 | D | 651 | LEU |
| 1 | D | 655 | MET |
| 1 | D | 661 | LYS |
| 1 | D | 663 | LEU |
| 1 | D | 667 | GLU |
| 1 | D | 681 | GLU |
| 1 | D | 684 | GLU |
| 1 | D | 687 | GLN |
| 1 | D | 689 | GLU |
| 1 | D | 735 | HIS |
| 1 | D | 737 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 755 | ARG |
| 1 | D | 772 | ASP |
| 1 | D | 773 | LYS |
| 1 | D | 796 | SER |
| 1 | D | 799 | THR |
| 1 | D | 800 | ARG |
| 1 | D | 845 | GLN |
| 1 | D | 885 | ASN |
| 1 | D | 893 | GLU |
| 1 | D | 986 | ILE |
| 1 | D | 1013 | ARG |
| 1 | D | 1022 | GLN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 600 | GLN |
| 1 | A | 624 | GLN |
| 1 | A | 675 | GLN |
| 1 | A | 817 | GLN |
| 1 | A | 844 | HIS |
| 1 | A | 863 | GLN |
| 1 | A | 878 | HIS |
| 1 | B | 262 | GLN |
| 1 | B | 363 | HIS |
| 1 | B | 583 | ASN |
| 1 | B | 600 | GLN |
| 1 | B | 624 | GLN |
| 1 | B | 628 | GLN |
| 1 | B | 646 | HIS |
| 1 | B | 687 | GLN |
| 1 | B | 863 | GLN |
| 1 | B | 878 | HIS |
| 1 | B | 977 | HIS |
| 1 | C | 163 | GLN |
| 1 | C | 266 | GLN |
| 1 | C | 614 | HIS |
| 1 | C | 624 | GLN |
| 1 | C | 634 | GLN |
| 1 | C | 646 | HIS |
| 1 | C | 687 | GLN |
| 1 | C | 817 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 878 | HIS |
| 1 | D | 135 | GLN |
| 1 | D | 363 | HIS |
| 1 | D | 624 | GLN |
| 1 | D | 628 | GLN |
| 1 | D | 704 | ASN |
| 1 | D | 804 | ASN |
| 1 | D | 878 | HIS |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 151 ligands modelled in this entry, 33 are monoatomic - leaving 118 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 | $\#\|Z\| > 2$ |
| 6 | DMS | B | 8416 | - | 3,3,3 | 1.45 | 1 (33%) | 3,3,3 | 0.52 | 0 |
| 6 | DMS | A | 8414 | - | 3,3,3 | 1.12 | 0 | 3,3,3 | 0.23 | 0 |
| 2 | 2DG | C | 2001 | 1,4 | 10,10,11 | 1.01 | 1 (10%) | 13,13,15 | 2.25 | 3 (23%) |
| 6 | DMS | A | 8502 | - | 3,3,3 | 1.97 | 1 (33%) | 3,3,3 | 1.08 | 0 |
| 6 | DMS | A | 8405 | - | 3,3,3 | 0.51 | 0 | 3,3,3 | 0.49 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 6 | DMS | D | 8417 | - | 3,3,3 | 1.66 | 1 (33%) | 3,3,3 | 0.60 | 0 |
| 6 | DMS | B | 8406 | - | 3,3,3 | 1.19 | 0 | 3,3,3 | 0.44 | 0 |
| 6 | DMS | B | 8502 | - | 3,3,3 | 0.77 | 0 | 3,3,3 | 1.28 | 1 (33%) |
| 6 | DMS | C | 8403 | - | 3,3,3 | 0.86 | 0 | 3,3,3 | 0.66 | 0 |
| 6 | DMS | C | 8416 | - | 3,3,3 | 0.59 | 0 | 3,3,3 | 0.37 | 0 |
| 6 | DMS | D | 8423 | - | 3,3,3 | 1.32 | 0 | 3,3,3 | 0.33 | 0 |
| 6 | DMS | B | 8427 | - | 3,3,3 | 0.74 | 0 | 3,3,3 | 0.16 | 0 |
| 6 | DMS | D | 8703 | - | 3,3,3 | 1.60 | 1 (33%) | 3,3,3 | 0.29 | 0 |
| 6 | DMS | C | 8504 | - | 3,3,3 | 0.54 | 0 | 3,3,3 | 0.20 | 0 |
| 6 | DMS | D | 8705 | - | 3,3,3 | 1.91 | 1 (33%) | 3,3,3 | 0.61 | 0 |
| 6 | DMS | A | 8501 | - | 3,3,3 | 1.16 | 0 | 3,3,3 | 0.12 | 0 |
| 6 | DMS | D | 8407 | - | 3,3,3 | 0.80 | 0 | 3,3,3 | 0.63 | 0 |
| 5 | BTB | A | 2002 | - | 13,13,13 | 1.52 | 4 (30%) | 7,16,16 | 1.15 | 1 (14%) |
| 6 | DMS | B | 8407 | - | 3,3,3 | 2.94 | 2 (66%) | 3,3,3 | 0.31 | 0 |
| 2 | 2DG | A | 2001 | 1,4 | 10,10,11 | 0.82 | 0 | 13,13,15 | 1.85 | 2 (15%) |
| 6 | DMS | C | 8408 | - | 3,3,3 | 0.62 | 0 | 3,3,3 | 0.72 | 0 |
| 6 | DMS | C | 8420 | - | 3,3,3 | 1.28 | 1 (33%) | 3,3,3 | 0.34 | 0 |
| 6 | DMS | D | 8503 | - | 3,3,3 | 0.63 | 0 | 3,3,3 | 0.96 | 0 |
| 6 | DMS | B | 8408 | - | 3,3,3 | 0.45 | 0 | 3,3,3 | 0.06 | 0 |
| 6 | DMS | C | 8602 | - | 3,3,3 | 0.92 | 0 | 3,3,3 | 0.15 | 0 |
| 6 | DMS | A | 8421 | - | 3,3,3 | 0.79 | 0 | 3,3,3 | 0.50 | 0 |
| 6 | DMS | C | 8501 | - | 3,3,3 | 0.89 | 0 | 3,3,3 | 0.85 | 0 |
| 6 | DMS | A | 8425 | 4 | 3,3,3 | 1.39 | 1 (33%) | 3,3,3 | 0.56 | 0 |
| 6 | DMS | D | 8411 | - | 3,3,3 | 0.48 | 0 | 3,3,3 | 0.22 | 0 |
| 6 | DMS | A | 8602 | - | 3,3,3 | 0.67 | 0 | 3,3,3 | 0.29 | 0 |
| 6 | DMS | D | 8421 | - | 3,3,3 | 0.29 | 0 | 3,3,3 | 0.15 | 0 |
| 6 | DMS | D | 8506 | - | 3,3,3 | 1.02 | 0 | 3,3,3 | 0.17 | 0 |
| 6 | DMS | A | 8413 | - | 3,3,3 | 1.58 | 0 | 3,3,3 | 0.09 | 0 |
| 6 | DMS | B | 8504 | - | 3,3,3 | 0.67 | 0 | 3,3,3 | 0.68 | 0 |
| 6 | DMS | B | 8425 | 4 | 3,3,3 | 2.29 | 2 (66%) | 3,3,3 | 0.33 | 0 |
| 5 | BTB | C | 2002 | - | 13,13,13 | 1.69 | 3 (23%) | 7,16,16 | 1.00 | 1 (14%) |
| 6 | DMS | C | 8409 | - | 3,3,3 | 1.34 | 1 (33%) | 3,3,3 | 1.26 | 1 (33%) |
| 6 | DMS | D | 8415 | - | 3,3,3 | 2.86 | 1 (33%) | 3,3,3 | 0.32 | 0 |
| 6 | DMS | C | 8423 | - | 3,3,3 | 0.67 | 0 | 3,3,3 | 0.10 | 0 |
| 6 | DMS | A | 8412 | - | 3,3,3 | 0.39 | 0 | 3,3,3 | 0.26 | 0 |
| 6 | DMS | B | 8417 | - | 3,3,3 | 0.47 | 0 | 3,3,3 | 0.49 | 0 |
| 6 | DMS | B | 8423 | - | 3,3,3 | 0.56 | 0 | 3,3,3 | 0.59 | 0 |
| 6 | DMS | D | 8410 | - | 3,3,3 | 0.94 | 0 | 3,3,3 | 0.22 | 0 |
| 6 | DMS | A | 8409 | - | 3,3,3 | 2.37 | 1 (33%) | 3,3,3 | 0.20 | 0 |
| 6 | DMS | B | 8404 | - | 3,3,3 | 0.77 | 0 | 3,3,3 | 0.22 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 6 | DMS | B | 8410 | - | 3,3,3 | 0.60 | 0 | 3,3,3 | 0.47 | 0 |
| 6 | DMS | D | 8413 | - | 3,3,3 | 0.95 | 0 | 3,3,3 | 0.25 | 0 |
| 6 | DMS | D | 8419 | - | 3,3,3 | 0.94 | 0 | 3,3,3 | 0.10 | 0 |
| 6 | DMS | A | 8503 | - | 3,3,3 | 0.47 | 0 | 3,3,3 | 0.31 | 0 |
| 6 | DMS | B | 8413 | - | 3,3,3 | 1.86 | 1 (33%) | 3,3,3 | 0.43 | 0 |
| 6 | DMS | B | 8403 | - | 3,3,3 | 1.04 | 0 | 3,3,3 | 0.24 | 0 |
| 6 | DMS | B | 8506 | - | 3,3,3 | 1.01 | 0 | 3,3,3 | 0.49 | 0 |
| 6 | DMS | B | 8421 | - | 3,3,3 | 0.27 | 0 | 3,3,3 | 0.45 | 0 |
| 6 | DMS | B | 8601 | - | 3,3,3 | 1.54 | 1 (33%) | 3,3,3 | 0.47 | 0 |
| 6 | DMS | C | 8404 | - | 3,3,3 | 0.49 | 0 | 3,3,3 | 1.06 | 0 |
| 6 | DMS | C | 8410 | - | 3,3,3 | 1.07 | 0 | 3,3,3 | 0.20 | 0 |
| 6 | DMS | C | 8417 | - | 3,3,3 | 0.77 | 0 | 3,3,3 | 0.30 | 0 |
| 6 | DMS | D | 8403 | - | 3,3,3 | 0.58 | 0 | 3,3,3 | 0.20 | 0 |
| 6 | DMS | A | 8402 | - | 3,3,3 | 1.00 | 0 | 3,3,3 | 0.50 | 0 |
| 6 | DMS | C | 8413 | - | 3,3,3 | 2.28 | 1 (33%) | 3,3,3 | 0.13 | 0 |
| 6 | DMS | C | 8421 | - | 3,3,3 | 0.59 | 0 | 3,3,3 | 0.56 | 0 |
| 6 | DMS | D | 8402 | - | 3,3,3 | 1.08 | 0 | 3,3,3 | 0.21 | 0 |
| 6 | DMS | C | 8414 | - | 3,3,3 | 0.51 | 0 | 3,3,3 | 0.78 | 0 |
| 6 | DMS | C | 8415 | - | 3,3,3 | 1.10 | 0 | 3,3,3 | 0.37 | 0 |
| 6 | DMS | C | 8402 | - | 3,3,3 | 1.40 | 1 (33%) | 3,3,3 | 0.14 | 0 |
| 6 | DMS | A | 8401 | - | 3,3,3 | 0.73 | 0 | 3,3,3 | 0.48 | 0 |
| 6 | DMS | D | 8401 | - | 3,3,3 | 1.02 | 0 | 3,3,3 | 0.15 | 0 |
| 6 | DMS | D | 8425 | 4 | 3,3,3 | 0.26 | 0 | 3,3,3 | 0.37 | 0 |
| 6 | DMS | C | 8503 | - | 3,3,3 | 0.88 | 0 | 3,3,3 | 0.55 | 0 |
| 6 | DMS | D | 8412 | - | 3,3,3 | 0.60 | 0 | 3,3,3 | 0.76 | 0 |
| 6 | DMS | A | 8420 | - | 3,3,3 | 0.80 | 0 | 3,3,3 | 1.07 | 0 |
| 6 | DMS | D | 8501 | - | 3,3,3 | 0.55 | 0 | 3,3,3 | 0.41 | 0 |
| 6 | DMS | B | 8405 | - | 3,3,3 | 1.36 | 1 (33%) | 3,3,3 | 0.54 | 0 |
| 6 | DMS | B | 8411 | - | 3,3,3 | 1.23 | 0 | 3,3,3 | 0.57 | 0 |
| 5 | BTB | B | 2002 | - | 13,13,13 | 1.32 | 2 (15%) | 7,16,16 | 0.82 | 0 |
| 6 | DMS | B | 8409 | - | 3,3,3 | 1.45 | 1 (33%) | 3,3,3 | 0.77 | 0 |
| 6 | DMS | C | 8401 | - | 3,3,3 | 0.70 | 0 | 3,3,3 | 0.14 | 0 |
| 6 | DMS | C | 8405 | - | 3,3,3 | 1.06 | 0 | 3,3,3 | 0.61 | 0 |
| 6 | DMS | A | 8403 | - | 3,3,3 | 2.04 | 2 (66%) | 3,3,3 | 0.48 | 0 |
| 6 | DMS | A | 8419 | - | 3,3,3 | 0.58 | 0 | 3,3,3 | 0.32 | 0 |
| 5 | BTB | D | 2002 | - | 13,13,13 | 1.33 | 3 (23%) | 7,16,16 | 1.05 | 0 |
| 6 | DMS | B | 8401 | - | 3,3,3 | 0.35 | 0 | 3,3,3 | 0.36 | 0 |
| 6 | DMS | D | 8409 | - | 3,3,3 | 1.39 | 1 (33%) | 3,3,3 | 0.60 | 0 |
| 6 | DMS | C | 8411 | - | 3,3,3 | 0.96 | 0 | 3,3,3 | 0.34 | 0 |
| 6 | DMS | A | 8417 | - | 3,3,3 | 1.27 | 0 | 3,3,3 | 0.13 | 0 |
| 6 | DMS | C | 8419 | - | 3,3,3 | 0.71 | 0 | 3,3,3 | 0.25 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 6 | DMS | A | 8423 | - | 3,3,3 | 1.29 | 1 (33%) | 3,3,3 | 0.26 | 0 |
| 6 | DMS | D | 8508 | - | 3,3,3 | 1.70 | 1 (33%) | 3,3,3 | 0.53 | 0 |
| 6 | DMS | D | 8414 | - | 3,3,3 | 0.25 | 0 | 3,3,3 | 0.34 | 0 |
| 6 | DMS | D | 8404 | - | 3,3,3 | 1.42 | 1 (33%) | 3,3,3 | 0.28 | 0 |
| 6 | DMS | B | 8414 | - | 3,3,3 | 0.95 | 0 | 3,3,3 | 0.34 | 0 |
| 6 | DMS | C | 8506 | - | 3,3,3 | 1.19 | 0 | 3,3,3 | 0.45 | 0 |
| 6 | DMS | C | 8601 | - | 3,3,3 | 1.42 | 1 (33%) | 3,3,3 | 0.78 | 0 |
| 6 | DMS | D | 8406 | - | 3,3,3 | 0.98 | 0 | 3,3,3 | 0.67 | 0 |
| 6 | DMS | B | 8420 | - | 3,3,3 | 1.67 | 1 (33%) | 3,3,3 | 0.80 | 0 |
| 6 | DMS | A | 8410 | - | 3,3,3 | 0.74 | 0 | 3,3,3 | 0.85 | 0 |
| 6 | DMS | B | 8412 | - | 3,3,3 | 0.91 | 0 | 3,3,3 | 0.28 | 0 |
| 6 | DMS | D | 8416 | - | 3,3,3 | 0.58 | 0 | 3,3,3 | 0.48 | 0 |
| 6 | DMS | A | 8404 | - | 3,3,3 | 1.11 | 0 | 3,3,3 | 0.18 | 0 |
| 6 | DMS | B | 8415 | - | 3,3,3 | 2.00 | 1 (33%) | 3,3,3 | 1.20 | 0 |
| 6 | DMS | B | 8402 | - | 3,3,3 | 0.98 | 0 | 3,3,3 | 0.71 | 0 |
| 6 | DMS | B | 8508 | - | 3,3,3 | 2.64 | 1 (33%) | 3,3,3 | 0.60 | 0 |
| 6 | DMS | C | 8412 | - | 3,3,3 | 0.88 | 0 | 3,3,3 | 0.58 | 0 |
| 6 | DMS | A | 8407 | - | 3,3,3 | 1.56 | 0 | 3,3,3 | 0.66 | 0 |
| 6 | DMS | A | 8406 | - | 3,3,3 | 0.62 | 0 | 3,3,3 | 0.87 | 0 |
| 6 | DMS | A | 8416 | - | 3,3,3 | 0.49 | 0 | 3,3,3 | 0.36 | 0 |
| 6 | DMS | C | 8427 | - | 3,3,3 | 0.42 | 0 | 3,3,3 | 0.22 | 0 |
| 6 | DMS | D | 8701 | - | 3,3,3 | 2.24 | 2 (66%) | 3,3,3 | 0.46 | 0 |
| 6 | DMS | D | 8408 | - | 3,3,3 | 1.20 | 0 | 3,3,3 | 0.31 | 0 |
| 6 | DMS | C | 8407 | - | 3,3,3 | 1.38 | 0 | 3,3,3 | 0.05 | 0 |
| 6 | DMS | A | 8506 | - | 3,3,3 | 1.04 | 0 | 3,3,3 | 0.42 | 0 |
| 6 | DMS | A | 8408 | - | 3,3,3 | 0.67 | 0 | 3,3,3 | 0.45 | 0 |
| 6 | DMS | D | 8405 | - | 3,3,3 | 0.70 | 0 | 3,3,3 | 0.83 | 0 |
| 2 | 2DG | B | 2001 | 1,4 | 10,10,11 | 0.93 | 0 | 13,13,15 | 1.08 | 0 |
| 2 | 2DG | D | 2001 | 1,4 | 10,10,11 | 0.73 | 0 | 13,13,15 | 2.09 | 3 (23%) |
| 6 | DMS | C | 8425 | 4 | 3,3,3 | 1.42 | 1 (33%) | 3,3,3 | 0.23 | 0 |
| 6 | DMS | A | 8504 | - | 3,3,3 | 0.61 | 0 | 3,3,3 | 0.27 | 0 |
| 6 | DMS | A | 8411 | - | 3,3,3 | 0.92 | 0 | 3,3,3 | 0.39 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | 2DG | D | 2001 | 1,4 | - | 1/2/16/18 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 5 | BTB | B | 2002 | - | - | 2/21/21/21 | - |
| 5 | BTB | C | 2002 | - | - | 2/21/21/21 | - |
| 2 | 2DG | A | 2001 | 1,4 | - | 1/2/16/18 | 0/1/1/1 |
| 2 | 2DG | C | 2001 | 1,4 | - | 1/2/16/18 | 0/1/1/1 |
| 5 | BTB | D | 2002 | - | - | 3/21/21/21 | - |
| 5 | BTB | A | 2002 | - | - | 3/21/21/21 | - |
| 2 | 2DG | B | 2001 | 1,4 | - | 1/2/16/18 | 0/1/1/1 |

All (46) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | B | 8407 | DMS | C2-S | 4.65 | 2.10 | 1.75 |
| 6 | D | 8415 | DMS | O-S | 4.54 | 1.80 | 1.50 |
| 6 | B | 8508 | DMS | C1-S | 4.06 | 2.06 | 1.75 |
| 5 | C | 2002 | BTB | C1-C2 | -3.91 | 1.48 | 1.53 |
| 6 | A | 8409 | DMS | O-S | 3.77 | 1.75 | 1.50 |
| 6 | C | 8413 | DMS | O-S | 3.42 | 1.73 | 1.50 |
| 6 | B | 8425 | DMS | O-S | 3.29 | 1.72 | 1.50 |
| 6 | D | 8705 | DMS | O-S | 2.87 | 1.69 | 1.50 |
| 5 | A | 2002 | BTB | C1-C2 | -2.86 | 1.49 | 1.53 |
| 6 | A | 8403 | DMS | O-S | 2.75 | 1.68 | 1.50 |
| 6 | B | 8420 | DMS | C2-S | 2.74 | 1.96 | 1.75 |
| 6 | A | 8502 | DMS | C1-S | 2.73 | 1.96 | 1.75 |
| 5 | A | 2002 | BTB | C5-N | 2.73 | 1.51 | 1.48 |
| 6 | D | 8701 | DMS | O-S | 2.71 | 1.68 | 1.50 |
| 5 | D | 2002 | BTB | C1-C2 | -2.68 | 1.49 | 1.53 |
| 6 | D | 8508 | DMS | O-S | 2.68 | 1.68 | 1.50 |
| 5 | C | 2002 | BTB | C3-C2 | 2.66 | 1.57 | 1.53 |
| 5 | B | 2002 | BTB | C1-C2 | -2.55 | 1.50 | 1.53 |
| 6 | B | 8416 | DMS | O-S | 2.44 | 1.66 | 1.50 |
| 5 | C | 2002 | BTB | C7-N | 2.42 | 1.51 | 1.48 |
| 6 | C | 8402 | DMS | C2-S | 2.42 | 1.93 | 1.75 |
| 6 | B | 8409 | DMS | O-S | 2.40 | 1.66 | 1.50 |
| 6 | C | 8601 | DMS | C2-S | 2.32 | 1.93 | 1.75 |
| 6 | D | 8701 | DMS | C1-S | 2.27 | 1.92 | 1.75 |
| 6 | C | 8409 | DMS | O-S | 2.25 | 1.65 | 1.50 |
| 2 | C | 2001 | 2DG | C3-C4 | 2.24 | 1.55 | 1.52 |
| 6 | C | 8425 | DMS | O-S | 2.24 | 1.65 | 1.50 |
| 6 | A | 8403 | DMS | C2-S | 2.20 | 1.92 | 1.75 |
| 6 | B | 8425 | DMS | C2-S | 2.19 | 1.92 | 1.75 |
| 6 | D | 8404 | DMS | C2-S | 2.18 | 1.92 | 1.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | B | 2002 | BTB | C3-C2 | 2.18 | 1.56 | 1.53 |
| 6 | B | 8405 | DMS | O-S | 2.17 | 1.64 | 1.50 |
| 6 | B | 8601 | DMS | C2-S | 2.16 | 1.91 | 1.75 |
| 6 | A | 8423 | DMS | C1-S | 2.15 | 1.91 | 1.75 |
| 6 | B | 8415 | DMS | C2-S | 2.13 | 1.91 | 1.75 |
| 6 | D | 8409 | DMS | O-S | 2.13 | 1.64 | 1.50 |
| 6 | C | 8420 | DMS | O-S | 2.13 | 1.64 | 1.50 |
| 5 | A | 2002 | BTB | C2-N | 2.11 | 1.52 | 1.48 |
| 6 | D | 8703 | DMS | O-S | 2.10 | 1.64 | 1.50 |
| 6 | B | 8413 | DMS | O-S | 2.10 | 1.64 | 1.50 |
| 5 | D | 2002 | BTB | C7-N | 2.08 | 1.51 | 1.48 |
| 6 | B | 8407 | DMS | O-S | 2.08 | 1.64 | 1.50 |
| 5 | A | 2002 | BTB | C3-C2 | 2.06 | 1.56 | 1.53 |
| 6 | D | 8417 | DMS | O-S | 2.05 | 1.64 | 1.50 |
| 5 | D | 2002 | BTB | C5-N | 2.05 | 1.50 | 1.48 |
| 6 | A | 8425 | DMS | O-S | 2.01 | 1.63 | 1.50 |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 2001 | 2DG | C3-C4-C5 | -6.80 | 103.19 | 109.97 |
| 2 | D | 2001 | 2DG | C3-C4-C5 | -4.70 | 105.28 | 109.97 |
| 2 | D | 2001 | 2DG | C1-O5-C5 | 4.53 | 119.89 | 112.01 |
| 2 | A | 2001 | 2DG | C3-C4-C5 | -4.33 | 105.65 | 109.97 |
| 2 | A | 2001 | 2DG | O5-C5-C6 | -3.61 | 101.55 | 107.20 |
| 2 | C | 2001 | 2DG | C1-O5-C5 | 2.53 | 116.41 | 112.01 |
| 6 | B | 8502 | DMS | C2-S-C1 | 2.18 | 109.66 | 98.44 |
| 2 | D | 2001 | 2DG | O5-C5-C6 | -2.11 | 103.90 | 107.20 |
| 2 | C | 2001 | 2DG | C6-C5-C4 | -2.07 | 108.16 | 113.00 |
| 6 | C | 8409 | DMS | C2-S-C1 | 2.06 | 109.02 | 98.44 |
| 5 | C | 2002 | BTB | O1-C1-C2 | -2.05 | 105.82 | 111.44 |
| 5 | A | 2002 | BTB | O3-C3-C2 | -2.03 | 105.88 | 111.44 |

There are no chirality outliers.

All (14) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | A | 2002 | BTB | C1-C2-C3-O3 |
| 5 | A | 2002 | BTB | C4-C2-C3-O3 |
| 5 | C | 2002 | BTB | N-C7-C8-O8 |
| 2 | A | 2001 | 2DG | O5-C5-C6-O6 |
| 2 | B | 2001 | 2DG | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | D | 2002 | BTB | N-C7-C8-O8 |
| 2 | C | 2001 | 2DG | O5-C5-C6-O6 |
| 2 | D | 2001 | 2DG | O5-C5-C6-O6 |
| 5 | B | 2002 | BTB | N-C7-C8-O8 |
| 5 | A | 2002 | BTB | N-C2-C3-O3 |
| 5 | B | 2002 | BTB | N-C2-C3-O3 |
| 5 | C | 2002 | BTB | N-C2-C3-O3 |
| 5 | D | 2002 | BTB | N-C2-C3-O3 |
| 5 | D | 2002 | BTB | C1-C2-C3-O3 |

There are no ring outliers.

23 monomers are involved in 37 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 6 | A | 8414 | DMS | 1 | 0 |
| 6 | B | 8406 | DMS | 1 | 0 |
| 6 | D | 8703 | DMS | 4 | 0 |
| 6 | B | 8407 | DMS | 2 | 0 |
| 6 | C | 8420 | DMS | 1 | 0 |
| 6 | C | 8602 | DMS | 1 | 0 |
| 6 | D | 8421 | DMS | 1 | 0 |
| 6 | D | 8506 | DMS | 2 | 0 |
| 5 | C | 2002 | BTB | 1 | 0 |
| 6 | B | 8417 | DMS | 1 | 0 |
| 6 | A | 8409 | DMS | 1 | 0 |
| 6 | B | 8410 | DMS | 1 | 0 |
| 6 | A | 8503 | DMS | 2 | 0 |
| 6 | C | 8410 | DMS | 1 | 0 |
| 6 | D | 8412 | DMS | 2 | 0 |
| 6 | A | 8420 | DMS | 1 | 0 |
| 5 | D | 2002 | BTB | 1 | 0 |
| 6 | A | 8423 | DMS | 2 | 0 |
| 6 | B | 8508 | DMS | 2 | 0 |
| 6 | A | 8416 | DMS | 2 | 0 |
| 6 | C | 8427 | DMS | 1 | 0 |
| 6 | C | 8407 | DMS | 1 | 0 |
| 6 | C | 8425 | DMS | 5 | 0 |

## 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

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, $95^{th}$ 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$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 1011/1023 (98%) | 0.00 | 32 (3%) | 47 | 54 | 11, 18, 46, 98 | 0 |
| 1 | B | 1011/1023 (98%) | 0.03 | 31 (3%) | 49 | 55 | 10, 18, 47, 97 | 0 |
| 1 | C | 1011/1023 (98%) | 0.06 | 34 (3%) | 45 | 51 | 11, 19, 49, 100 | 0 |
| 1 | D | 1011/1023 (98%) | 0.05 | 43 (4%) | 35 | 41 | 10, 18, 50, 100 | 0 |
| All | All | 4044/4092 (98%) | 0.04 | 140 (3%) | 44 | 50 | 10, 18, 48, 100 | 0 |

All (140) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 735 | HIS | 11.4 |
| 1 | D | 735 | HIS | 11.0 |
| 1 | C | 732 | ALA | 10.4 |
| 1 | D | 798 | ALA | 10.3 |
| 1 | A | 686 | PRO | 9.9 |
| 1 | D | 732 | ALA | 9.4 |
| 1 | C | 731 | PRO | 9.4 |
| 1 | B | 799 | THR | 8.3 |
| 1 | D | 799 | THR | 8.2 |
| 1 | B | 730 | LEU | 7.9 |
| 1 | B | 731 | PRO | 7.8 |
| 1 | C | 730 | LEU | 7.7 |
| 1 | A | 799 | THR | 7.6 |
| 1 | A | 687 | GLN | 7.5 |
| 1 | B | 689 | GLU | 7.5 |
| 1 | B | 733 | ALA | 7.5 |
| 1 | D | 800 | ARG | 7.4 |
| 1 | B | 685 | LEU | 7.2 |
| 1 | C | 689 | GLU | 7.0 |
| 1 | B | 798 | ALA | 6.9 |
| 1 | D | 734 | SER | 6.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 735 | HIS | 6.6 |
| 1 | D | 730 | LEU | 6.5 |
| 1 | A | 732 | ALA | 6.4 |
| 1 | A | 730 | LEU | 6.1 |
| 1 | A | 689 | GLU | 5.8 |
| 1 | B | 732 | ALA | 5.6 |
| 1 | C | 799 | THR | 5.5 |
| 1 | D | 731 | PRO | 5.5 |
| 1 | D | 689 | GLU | 5.5 |
| 1 | C | 686 | PRO | 5.4 |
| 1 | B | 686 | PRO | 5.4 |
| 1 | C | 800 | ARG | 5.3 |
| 1 | C | 798 | ALA | 5.3 |
| 1 | A | 685 | LEU | 5.3 |
| 1 | C | 733 | ALA | 5.2 |
| 1 | A | 731 | PRO | 5.2 |
| 1 | D | 686 | PRO | 4.8 |
| 1 | C | 687 | GLN | 4.8 |
| 1 | D | 771 | GLY | 4.6 |
| 1 | C | 729 | THR | 4.6 |
| 1 | D | 733 | ALA | 4.6 |
| 1 | A | 800 | ARG | 4.5 |
| 1 | A | 733 | ALA | 4.5 |
| 1 | D | 684 | GLU | 4.4 |
| 1 | A | 1023 | LYS | 4.3 |
| 1 | D | 685 | LEU | 4.3 |
| 1 | A | 801 | ILE | 4.3 |
| 1 | C | 772 | ASP | 4.2 |
| 1 | A | 736 | ALA | 4.1 |
| 1 | D | 581 | ASN | 4.1 |
| 1 | A | 580 | GLU | 4.1 |
| 1 | D | 687 | GLN | 4.1 |
| 1 | A | 729 | THR | 4.0 |
| 1 | A | 845 | GLN | 4.0 |
| 1 | D | 797 | GLU | 3.9 |
| 1 | C | 633 | GLY | 3.8 |
| 1 | C | 634 | GLN | 3.8 |
| 1 | D | 845 | GLN | 3.8 |
| 1 | D | 580 | GLU | 3.8 |
| 1 | C | 685 | LEU | 3.7 |
| 1 | B | 800 | ARG | 3.7 |
| 1 | B | 684 | GLU | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 729 | THR | 3.6 |
| 1 | B | 581 | ASN | 3.6 |
| 1 | D | 688 | PRO | 3.5 |
| 1 | A | 582 | GLY | 3.5 |
| 1 | C | 745 | MET | 3.4 |
| 1 | D | 663 | LEU | 3.4 |
| 1 | D | 683 | PRO | 3.4 |
| 1 | D | 664 | ALA | 3.3 |
| 1 | D | 633 | GLY | 3.3 |
| 1 | A | 798 | ALA | 3.3 |
| 1 | B | 797 | GLU | 3.3 |
| 1 | D | 682 | LEU | 3.2 |
| 1 | D | 772 | ASP | 3.2 |
| 1 | B | 687 | GLN | 3.1 |
| 1 | B | 734 | SER | 3.1 |
| 1 | C | 71 | GLU | 3.1 |
| 1 | D | 801 | ILE | 3.1 |
| 1 | C | 770 | ILE | 3.0 |
| 1 | A | 734 | SER | 3.0 |
| 1 | B | 801 | ILE | 3.0 |
| 1 | B | 1018 | LEU | 3.0 |
| 1 | D | 79 | PRO | 3.0 |
| 1 | B | 745 | MET | 3.0 |
| 1 | C | 737 | ILE | 2.9 |
| 1 | B | 79 | PRO | 2.9 |
| 1 | C | 684 | GLU | 2.9 |
| 1 | A | 632 | SER | 2.8 |
| 1 | C | 734 | SER | 2.8 |
| 1 | D | 632 | SER | 2.8 |
| 1 | A | 668 | VAL | 2.8 |
| 1 | A | 688 | PRO | 2.8 |
| 1 | A | 684 | GLU | 2.8 |
| 1 | C | 736 | ALA | 2.8 |
| 1 | B | 580 | GLU | 2.8 |
| 1 | A | 846 | GLY | 2.8 |
| 1 | D | 1023 | LYS | 2.8 |
| 1 | B | 632 | SER | 2.7 |
| 1 | D | 582 | GLY | 2.6 |
| 1 | A | 682 | LEU | 2.6 |
| 1 | C | 831 | ALA | 2.6 |
| 1 | D | 71 | GLU | 2.6 |
| 1 | B | 728 | VAL | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 683 | PRO | 2.5 |
| 1 | C | 1023 | LYS | 2.4 |
| 1 | D | 736 | ALA | 2.4 |
| 1 | D | 830 | LEU | 2.4 |
| 1 | A | 829 | THR | 2.4 |
| 1 | D | 179 | ALA | 2.4 |
| 1 | C | 761 | GLN | 2.4 |
| 1 | A | 581 | ASN | 2.3 |
| 1 | B | 663 | LEU | 2.3 |
| 1 | A | 71 | GLU | 2.3 |
| 1 | C | 688 | PRO | 2.3 |
| 1 | C | 861 | SER | 2.3 |
| 1 | B | 582 | GLY | 2.3 |
| 1 | C | 743 | SER | 2.3 |
| 1 | D | 796 | SER | 2.3 |
| 1 | D | 1022 | GLN | 2.3 |
| 1 | A | 79 | PRO | 2.2 |
| 1 | B | 845 | GLN | 2.2 |
| 1 | B | 688 | PRO | 2.2 |
| 1 | C | 830 | LEU | 2.2 |
| 1 | C | 728 | VAL | 2.2 |
| 1 | C | 845 | GLN | 2.2 |
| 1 | A | 179 | ALA | 2.2 |
| 1 | D | 669 | PRO | 2.1 |
| 1 | B | 71 | GLU | 2.1 |
| 1 | B | 735 | HIS | 2.1 |
| 1 | D | 752 | GLY | 2.1 |
| 1 | C | 581 | ASN | 2.1 |
| 1 | D | 84 | VAL | 2.1 |
| 1 | D | 795 | VAL | 2.1 |
| 1 | B | 47 | PRO | 2.1 |
| 1 | B | 690 | SER | 2.1 |
| 1 | D | 831 | ALA | 2.1 |
| 1 | C | 690 | SER | 2.0 |
| 1 | B | 583 | ASN | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

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, $95^{th}$ 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$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | DMS | D | 8407 | 4/4 | 0.73 | 0.15 | 21,34,71,100 | 0 |
| 3 | MG | C | 3105 | 1/1 | 0.76 | 0.34 | 47,47,47,47 | 1 |
| 3 | MG | C | 3004 | 1/1 | 0.77 | 0.15 | 51,51,51,51 | 0 |
| 6 | DMS | B | 8413 | 4/4 | 0.85 | 0.15 | 50,55,58,70 | 0 |
| 6 | DMS | B | 8406 | 4/4 | 0.85 | 0.20 | 32,40,52,59 | 0 |
| 6 | DMS | C | 8419 | 4/4 | 0.86 | 0.15 | 38,51,67,78 | 0 |
| 6 | DMS | D | 8415 | 4/4 | 0.86 | 0.16 | 29,37,68,100 | 0 |
| 6 | DMS | A | 8413 | 4/4 | 0.87 | 0.15 | 36,70,79,100 | 0 |
| 6 | DMS | C | 8427 | 4/4 | 0.87 | 0.18 | 42,55,62,70 | 0 |
| 6 | DMS | D | 8417 | 4/4 | 0.87 | 0.15 | 27,29,72,94 | 0 |
| 3 | MG | B | 3003 | 1/1 | 0.88 | 0.17 | 25,25,25,25 | 1 |
| 6 | DMS | D | 8503 | 4/4 | 0.88 | 0.20 | 41,57,72,74 | 0 |
| 5 | BTB | A | 2002 | 14/14 | 0.89 | 0.16 | 11,20,31,34 | 14 |
| 3 | MG | A | 3003 | 1/1 | 0.89 | 0.35 | 26,26,26,26 | 1 |
| 6 | DMS | B | 8415 | 4/4 | 0.89 | 0.12 | 27,28,42,56 | 0 |
| 6 | DMS | C | 8417 | 4/4 | 0.89 | 0.13 | 27,37,45,68 | 0 |
| 6 | DMS | D | 8423 | 4/4 | 0.89 | 0.19 | 39,55,62,70 | 0 |
| 6 | DMS | A | 8423 | 4/4 | 0.89 | 0.19 | 39,68,81,100 | 0 |
| 6 | DMS | D | 8703 | 4/4 | 0.89 | 0.20 | 31,48,50,51 | 0 |
| 6 | DMS | B | 8508 | 4/4 | 0.90 | 0.18 | 30,40,45,49 | 0 |
| 6 | DMS | B | 8407 | 4/4 | 0.90 | 0.23 | 34,34,41,47 | 0 |
| 6 | DMS | C | 8423 | 4/4 | 0.91 | 0.15 | 39,39,54,61 | 0 |
| 6 | DMS | D | 8404 | 4/4 | 0.91 | 0.14 | 24,24,49,100 | 0 |
| 6 | DMS | C | 8504 | 4/4 | 0.92 | 0.11 | 30,39,48,58 | 0 |
| 6 | DMS | B | 8420 | 4/4 | 0.92 | 0.17 | 52,54,69,77 | 0 |
| 6 | DMS | B | 8425 | 4/4 | 0.92 | 0.13 | 23,34,44,50 | 0 |
| 6 | DMS | A | 8407 | 4/4 | 0.92 | 0.19 | 29,40,41,45 | 0 |
| 6 | DMS | D | 8416 | 4/4 | 0.92 | 0.19 | 28,30,51,100 | 0 |
| 6 | DMS | B | 8410 | 4/4 | 0.92 | 0.15 | 34,36,57,82 | 0 |
| 6 | DMS | A | 8501 | 4/4 | 0.92 | 0.15 | 20,32,36,41 | 0 |
| 3 | MG | C | 3003 | 1/1 | 0.92 | 0.19 | 24,24,24,24 | 1 |
| 6 | DMS | B | 8416 | 4/4 | 0.92 | 0.17 | 36,45,53,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | DMS | C | 8506 | 4/4 | 0.93 | 0.12 | 22,30,37,38 | 0 |
| 6 | DMS | A | 8420 | 4/4 | 0.93 | 0.12 | 37,43,45,66 | 0 |
| 6 | DMS | A | 8421 | 4/4 | 0.93 | 0.24 | 54,67,79,94 | 0 |
| 5 | BTB | C | 2002 | 14/14 | 0.93 | 0.10 | 14,25,38,98 | 14 |
| 6 | DMS | A | 8406 | 4/4 | 0.93 | 0.12 | 23,33,65,73 | 0 |
| 6 | DMS | A | 8502 | 4/4 | 0.93 | 0.14 | 23,31,54,67 | 0 |
| 6 | DMS | A | 8417 | 4/4 | 0.93 | 0.19 | 32,34,90,100 | 0 |
| 6 | DMS | C | 8501 | 4/4 | 0.93 | 0.14 | 20,30,36,46 | 0 |
| 6 | DMS | D | 8508 | 4/4 | 0.93 | 0.11 | 37,39,45,47 | 0 |
| 6 | DMS | B | 8423 | 4/4 | 0.93 | 0.14 | 34,35,59,100 | 0 |
| 6 | DMS | D | 8705 | 4/4 | 0.93 | 0.13 | 21,33,40,43 | 0 |
| 6 | DMS | C | 8413 | 4/4 | 0.94 | 0.16 | 30,41,52,95 | 0 |
| 6 | DMS | C | 8415 | 4/4 | 0.94 | 0.14 | 26,38,38,46 | 0 |
| 6 | DMS | D | 8413 | 4/4 | 0.94 | 0.19 | 39,44,45,83 | 0 |
| 5 | BTB | B | 2002 | 14/14 | 0.94 | 0.10 | 13,23,30,99 | 14 |
| 6 | DMS | B | 8421 | 4/4 | 0.94 | 0.16 | 28,56,60,67 | 0 |
| 3 | MG | D | 3003 | 1/1 | 0.94 | 0.30 | 30,30,30,30 | 1 |
| 5 | BTB | D | 2002 | 14/14 | 0.94 | 0.11 | 15,22,29,95 | 14 |
| 6 | DMS | D | 8501 | 4/4 | 0.94 | 0.10 | 23,35,42,54 | 0 |
| 6 | DMS | B | 8427 | 4/4 | 0.94 | 0.09 | 35,38,53,66 | 0 |
| 6 | DMS | C | 8503 | 4/4 | 0.94 | 0.14 | 36,58,65,76 | 0 |
| 6 | DMS | B | 8504 | 4/4 | 0.94 | 0.10 | 27,44,46,47 | 0 |
| 6 | DMS | A | 8416 | 4/4 | 0.94 | 0.18 | 23,38,47,100 | 0 |
| 3 | MG | A | 3005 | 1/1 | 0.95 | 0.13 | 30,30,30,30 | 0 |
| 6 | DMS | C | 8408 | 4/4 | 0.95 | 0.11 | 25,34,39,40 | 0 |
| 6 | DMS | B | 8408 | 4/4 | 0.95 | 0.17 | 28,34,40,90 | 0 |
| 2 | 2DG | C | 2001 | 10/11 | 0.95 | 0.10 | 8,15,17,18 | 0 |
| 6 | DMS | D | 8425 | 4/4 | 0.95 | 0.21 | 21,31,44,76 | 4 |
| 6 | DMS | C | 8416 | 4/4 | 0.95 | 0.29 | 59,65,71,72 | 0 |
| 6 | DMS | C | 8602 | 4/4 | 0.95 | 0.10 | 39,45,60,72 | 0 |
| 6 | DMS | A | 8503 | 4/4 | 0.95 | 0.27 | 26,100,100,100 | 0 |
| 6 | DMS | A | 8506 | 4/4 | 0.95 | 0.12 | 35,35,36,38 | 0 |
| 6 | DMS | A | 8425 | 4/4 | 0.95 | 0.15 | 31,38,42,43 | 0 |
| 6 | DMS | A | 8404 | 4/4 | 0.96 | 0.10 | 23,27,36,37 | 0 |
| 6 | DMS | C | 8425 | 4/4 | 0.96 | 0.16 | 34,43,58,100 | 0 |
| 6 | DMS | A | 8602 | 4/4 | 0.96 | 0.31 | 41,45,100,100 | 0 |
| 6 | DMS | B | 8404 | 4/4 | 0.96 | 0.08 | 22,22,32,36 | 0 |
| 2 | 2DG | B | 2001 | 10/11 | 0.96 | 0.10 | 5,9,12,13 | 10 |
| 3 | MG | C | 3006 | 1/1 | 0.96 | 0.20 | 43,43,43,43 | 0 |
| 6 | DMS | B | 8502 | 4/4 | 0.96 | 0.15 | 25,30,42,46 | 0 |
| 6 | DMS | C | 8601 | 4/4 | 0.96 | 0.17 | 28,47,53,57 | 0 |
| 6 | DMS | A | 8409 | 4/4 | 0.96 | 0.12 | 26,37,45,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | DMS | B | 8506 | 4/4 | 0.96 | 0.12 | 31,32,33,47 | 0 |
| 6 | DMS | D | 8406 | 4/4 | 0.96 | 0.11 | 24,26,26,28 | 0 |
| 6 | DMS | B | 8409 | 4/4 | 0.96 | 0.12 | 29,31,35,39 | 0 |
| 6 | DMS | D | 8409 | 4/4 | 0.96 | 0.12 | 30,32,36,36 | 0 |
| 6 | DMS | C | 8407 | 4/4 | 0.96 | 0.15 | 29,32,44,100 | 0 |
| 6 | DMS | A | 8410 | 4/4 | 0.96 | 0.14 | 25,30,46,55 | 0 |
| 6 | DMS | C | 8409 | 4/4 | 0.96 | 0.12 | 30,32,39,39 | 0 |
| 6 | DMS | C | 8410 | 4/4 | 0.96 | 0.17 | 30,37,45,45 | 0 |
| 6 | DMS | D | 8421 | 4/4 | 0.96 | 0.19 | 43,48,50,100 | 0 |
| 4 | NA | B | 3104 | 1/1 | 0.96 | 0.11 | 33,33,33,33 | 0 |
| 6 | DMS | B | 8414 | 4/4 | 0.96 | 0.14 | 30,32,51,100 | 0 |
| 6 | DMS | A | 8414 | 4/4 | 0.96 | 0.12 | 31,43,51,100 | 0 |
| 4 | NA | D | 3104 | 1/1 | 0.96 | 0.07 | 35,35,35,35 | 0 |
| 6 | DMS | D | 8506 | 4/4 | 0.96 | 0.08 | 19,25,31,40 | 0 |
| 6 | DMS | B | 8417 | 4/4 | 0.96 | 0.09 | 25,34,62,100 | 0 |
| 6 | DMS | C | 8420 | 4/4 | 0.96 | 0.14 | 44,46,79,100 | 0 |
| 6 | DMS | C | 8421 | 4/4 | 0.96 | 0.13 | 38,48,94,100 | 0 |
| 6 | DMS | A | 8419 | 4/4 | 0.97 | 0.11 | 43,46,51,56 | 0 |
| 6 | DMS | D | 8419 | 4/4 | 0.97 | 0.07 | 23,41,52,62 | 0 |
| 6 | DMS | A | 8408 | 4/4 | 0.97 | 0.08 | 19,31,40,59 | 0 |
| 6 | DMS | B | 8402 | 4/4 | 0.97 | 0.08 | 17,17,23,25 | 0 |
| 6 | DMS | A | 8412 | 4/4 | 0.97 | 0.11 | 31,33,39,100 | 0 |
| 6 | DMS | B | 8405 | 4/4 | 0.97 | 0.12 | 27,29,32,32 | 0 |
| 2 | 2DG | D | 2001 | 10/11 | 0.97 | 0.09 | 9,11,17,18 | 0 |
| 6 | DMS | D | 8410 | 4/4 | 0.97 | 0.14 | 33,35,39,44 | 0 |
| 6 | DMS | B | 8601 | 4/4 | 0.97 | 0.10 | 29,36,40,48 | 0 |
| 6 | DMS | C | 8402 | 4/4 | 0.97 | 0.08 | 18,28,30,32 | 0 |
| 6 | DMS | C | 8404 | 4/4 | 0.97 | 0.08 | 19,24,25,31 | 0 |
| 6 | DMS | C | 8403 | 4/4 | 0.98 | 0.11 | 20,21,24,28 | 0 |
| 6 | DMS | D | 8408 | 4/4 | 0.98 | 0.12 | 24,31,32,40 | 0 |
| 6 | DMS | B | 8401 | 4/4 | 0.98 | 0.07 | 15,17,21,21 | 0 |
| 6 | DMS | C | 8405 | 4/4 | 0.98 | 0.07 | 24,24,25,29 | 0 |
| 6 | DMS | D | 8411 | 4/4 | 0.98 | 0.07 | 20,27,28,55 | 0 |
| 6 | DMS | D | 8412 | 4/4 | 0.98 | 0.09 | 27,30,31,37 | 0 |
| 2 | 2DG | A | 2001 | 10/11 | 0.98 | 0.10 | 9,13,20,23 | 0 |
| 6 | DMS | D | 8414 | 4/4 | 0.98 | 0.17 | 27,45,89,100 | 0 |
| 6 | DMS | B | 8411 | 4/4 | 0.98 | 0.07 | 27,30,30,87 | 0 |
| 6 | DMS | B | 8412 | 4/4 | 0.98 | 0.07 | 28,34,34,36 | 0 |
| 6 | DMS | B | 8403 | 4/4 | 0.98 | 0.07 | 18,24,26,26 | 0 |
| 6 | DMS | C | 8412 | 4/4 | 0.98 | 0.09 | 32,35,36,100 | 0 |
| 4 | NA | C | 3104 | 1/1 | 0.98 | 0.10 | 30,30,30,30 | 0 |
| 6 | DMS | A | 8405 | 4/4 | 0.98 | 0.09 | 18,25,28,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 6 | DMS | A | 8504 | 4/4 | 0.98 | 0.07 | 18,38,53,89 | 0 |
| 6 | DMS | D | 8401 | 4/4 | 0.98 | 0.08 | 16,18,19,23 | 0 |
| 6 | DMS | D | 8402 | 4/4 | 0.98 | 0.07 | 18,22,23,24 | 0 |
| 6 | DMS | D | 8403 | 4/4 | 0.98 | 0.08 | 19,29,29,37 | 0 |
| 3 | MG | D | 3005 | 1/1 | 0.98 | 0.10 | 25,25,25,25 | 0 |
| 6 | DMS | D | 8701 | 4/4 | 0.98 | 0.08 | 14,17,20,31 | 0 |
| 6 | DMS | D | 8405 | 4/4 | 0.98 | 0.08 | 23,26,31,52 | 0 |
| 6 | DMS | A | 8411 | 4/4 | 0.98 | 0.07 | 28,29,31,45 | 0 |
| 4 | NA | D | 3102 | 1/1 | 0.99 | 0.06 | 15,15,15,15 | 0 |
| 4 | NA | D | 3103 | 1/1 | 0.99 | 0.06 | 30,30,30,30 | 0 |
| 3 | MG | B | 3002 | 1/1 | 0.99 | 0.05 | 19,19,19,19 | 0 |
| 6 | DMS | C | 8411 | 4/4 | 0.99 | 0.10 | 24,29,35,45 | 0 |
| 3 | MG | A | 3001 | 1/1 | 0.99 | 0.05 | 16,16,16,16 | 0 |
| 3 | MG | D | 3001 | 1/1 | 0.99 | 0.06 | 15,15,15,15 | 0 |
| 6 | DMS | C | 8414 | 4/4 | 0.99 | 0.07 | 21,40,71,100 | 0 |
| 3 | MG | D | 3002 | 1/1 | 0.99 | 0.06 | 17,17,17,17 | 0 |
| 3 | MG | C | 3001 | 1/1 | 0.99 | 0.04 | 15,15,15,15 | 0 |
| 6 | DMS | A | 8401 | 4/4 | 0.99 | 0.09 | 14,15,17,19 | 0 |
| 6 | DMS | A | 8402 | 4/4 | 0.99 | 0.07 | 16,18,23,29 | 0 |
| 6 | DMS | A | 8403 | 4/4 | 0.99 | 0.07 | 21,22,25,28 | 0 |
| 3 | MG | C | 3002 | 1/1 | 0.99 | 0.07 | 15,15,15,15 | 0 |
| 4 | NA | A | 3101 | 1/1 | 0.99 | 0.06 | 16,16,16,16 | 0 |
| 4 | NA | A | 3102 | 1/1 | 0.99 | 0.05 | 14,14,14,14 | 0 |
| 4 | NA | A | 3103 | 1/1 | 0.99 | 0.07 | 28,28,28,28 | 0 |
| 4 | NA | A | 3104 | 1/1 | 0.99 | 0.08 | 25,25,25,25 | 0 |
| 4 | NA | B | 3101 | 1/1 | 0.99 | 0.07 | 15,15,15,15 | 0 |
| 4 | NA | B | 3102 | 1/1 | 0.99 | 0.05 | 16,16,16,16 | 0 |
| 6 | DMS | C | 8401 | 4/4 | 0.99 | 0.06 | 16,16,21,22 | 0 |
| 4 | NA | B | 3103 | 1/1 | 0.99 | 0.06 | 23,23,23,23 | 0 |
| 3 | MG | A | 3002 | 1/1 | 0.99 | 0.07 | 17,17,17,17 | 0 |
| 4 | NA | C | 3102 | 1/1 | 0.99 | 0.06 | 17,17,17,17 | 0 |
| 4 | NA | C | 3103 | 1/1 | 0.99 | 0.06 | 24,24,24,24 | 0 |
| 3 | MG | B | 3001 | 1/1 | 0.99 | 0.06 | 15,15,15,15 | 0 |
| 4 | NA | D | 3101 | 1/1 | 1.00 | 0.06 | 16,16,16,16 | 0 |
| 4 | NA | C | 3101 | 1/1 | 1.00 | 0.09 | 15,15,15,15 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.