



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 11:48 PM EDT

PDB ID : 1PX3
Title : E. COLI (LACZ) BETA-GALACTOSIDASE (G794A)
Authors : Juers, D.H.; Hakda, S.; Matthews, B.W.; Huber, R.E.
Deposited on : 2003-07-02
Resolution : 1.60 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.23.2
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) : 2.23.2

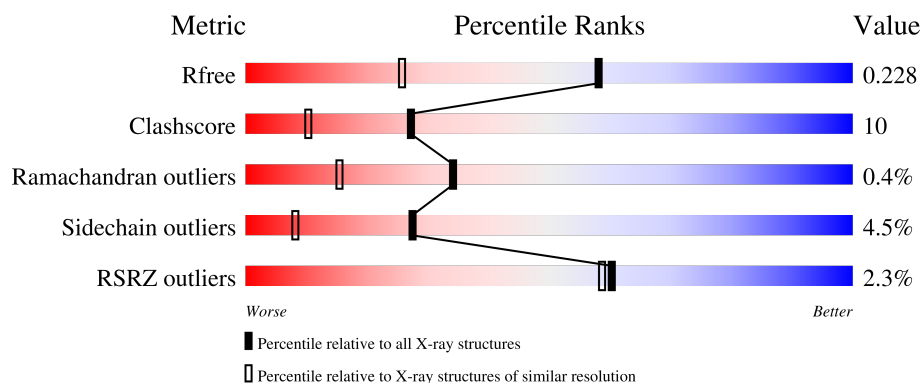
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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 | 3398 (1.60-1.60) |
| Clashscore | 141614 | 3665 (1.60-1.60) |
| Ramachandran outliers | 138981 | 3564 (1.60-1.60) |
| Sidechain outliers | 138945 | 3563 (1.60-1.60) |
| RSRZ outliers | 127900 | 3321 (1.60-1.60) |

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 1023 | <div> <div>3%</div> <div>69%</div> <div>25%</div> <div>5%</div> <div>.</div> </div> |
| 1 | B | 1023 | <div> <div>2%</div> <div>68%</div> <div>25%</div> <div>6%</div> <div>..</div> </div> |
| 1 | C | 1023 | <div> <div>2%</div> <div>69%</div> <div>25%</div> <div>.</div> <div>..</div> </div> |
| 1 | D | 1023 | <div> <div>2%</div> <div>68%</div> <div>24%</div> <div>5%</div> <div>..</div> </div> |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4 | DMS | A | 8404 | - | - | X | - |
| 4 | DMS | C | 8425 | - | - | X | - |
| 4 | DMS | D | 8703 | - | - | X | - |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36619 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 |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 1010 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8119 | 5135 | 1439 | 1507 | 38 | | | |
| 1 | B | 1009 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8114 | 5132 | 1438 | 1506 | 38 | | | |
| 1 | C | 1007 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8095 | 5120 | 1433 | 1504 | 38 | | | |
| 1 | D | 1008 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8103 | 5126 | 1434 | 1505 | 38 | | | |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 1 | GLY | - | cloning artifact | UNP P00722 |
| A | 2 | SER | - | cloning artifact | UNP P00722 |
| A | 3 | HIS | - | cloning artifact | UNP P00722 |
| A | 4 | MET | - | cloning artifact | UNP P00722 |
| A | 5 | LEU | - | cloning artifact | UNP P00722 |
| A | 6 | GLU | - | cloning artifact | UNP P00722 |
| A | 7 | ASP | - | cloning artifact | UNP P00722 |
| A | 8 | PRO | - | cloning artifact | UNP P00722 |
| A | 794 | ALA | GLY | engineered mutation | UNP P00722 |
| B | 1 | GLY | - | cloning artifact | UNP P00722 |
| B | 2 | SER | - | cloning artifact | UNP P00722 |
| B | 3 | HIS | - | cloning artifact | UNP P00722 |
| B | 4 | MET | - | cloning artifact | UNP P00722 |
| B | 5 | LEU | - | cloning artifact | UNP P00722 |
| B | 6 | GLU | - | cloning artifact | UNP P00722 |
| B | 7 | ASP | - | cloning artifact | UNP P00722 |
| B | 8 | PRO | - | cloning artifact | UNP P00722 |
| B | 794 | ALA | GLY | engineered mutation | UNP P00722 |
| C | 1 | GLY | - | cloning artifact | UNP P00722 |
| C | 2 | SER | - | cloning artifact | UNP P00722 |
| C | 3 | HIS | - | cloning artifact | UNP P00722 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| C | 4 | MET | - | cloning artifact | UNP P00722 |
| C | 5 | LEU | - | cloning artifact | UNP P00722 |
| C | 6 | GLU | - | cloning artifact | UNP P00722 |
| C | 7 | ASP | - | cloning artifact | UNP P00722 |
| C | 8 | PRO | - | cloning artifact | UNP P00722 |
| C | 794 | ALA | GLY | engineered mutation | UNP P00722 |
| D | 1 | GLY | - | cloning artifact | UNP P00722 |
| D | 2 | SER | - | cloning artifact | UNP P00722 |
| D | 3 | HIS | - | cloning artifact | UNP P00722 |
| D | 4 | MET | - | cloning artifact | UNP P00722 |
| D | 5 | LEU | - | cloning artifact | UNP P00722 |
| D | 6 | GLU | - | cloning artifact | UNP P00722 |
| D | 7 | ASP | - | cloning artifact | UNP P00722 |
| D | 8 | PRO | - | cloning artifact | UNP P00722 |
| D | 794 | ALA | GLY | engineered mutation | UNP P00722 |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2 | A | 3 | Total Mg 3 3 | 0 | 0 |
| 2 | B | 2 | Total Mg 2 2 | 0 | 0 |
| 2 | C | 4 | Total Mg 4 4 | 0 | 0 |
| 2 | D | 3 | Total Mg 3 3 | 0 | 0 |

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

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

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

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

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

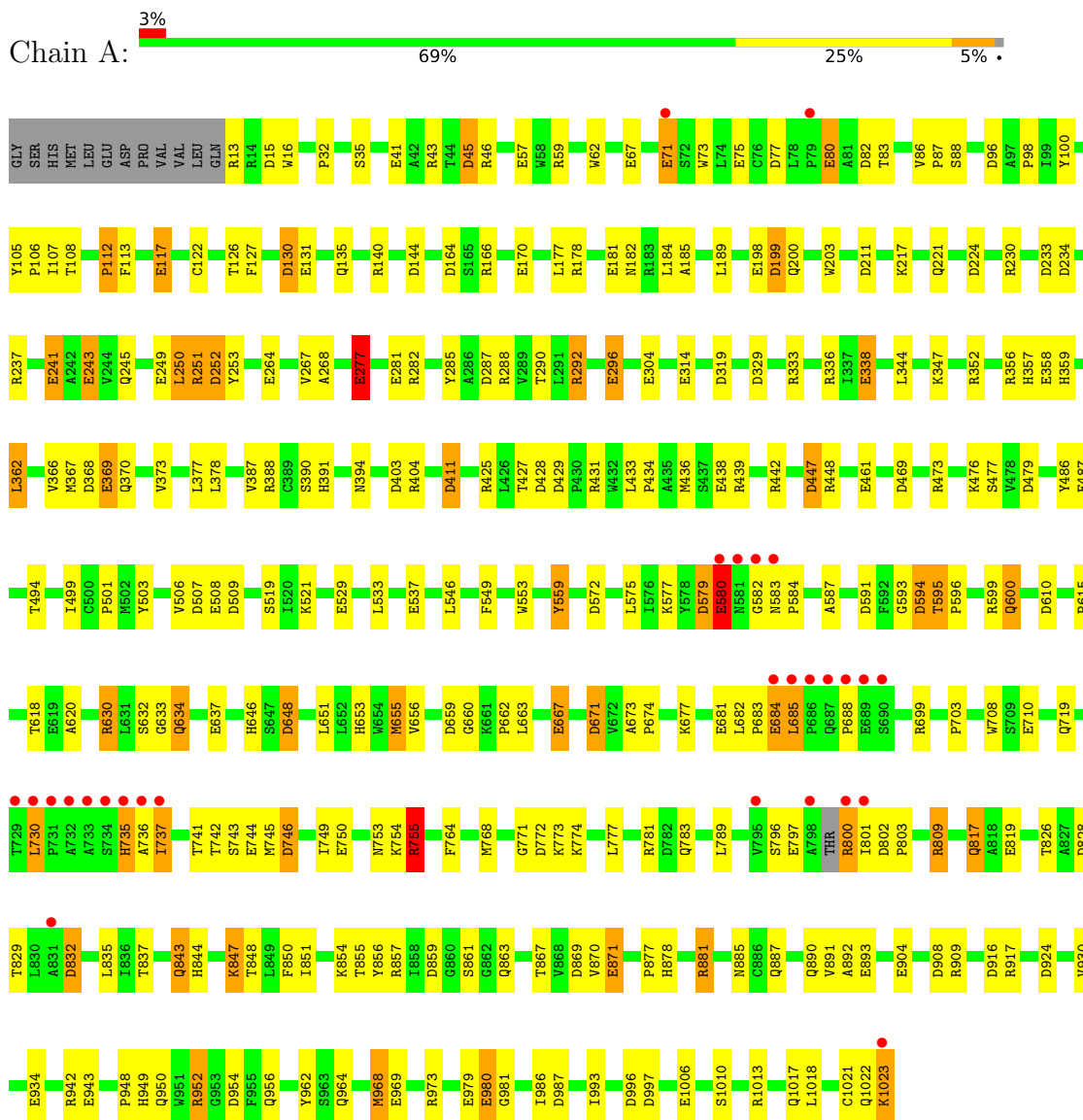
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5 | A | 916 | Total 916 | O 916 | 0 | 0 |
| 5 | B | 985 | Total 985 | O 985 | 0 | 0 |
| 5 | C | 935 | Total 935 | O 935 | 0 | 0 |
| 5 | D | 984 | Total 984 | O 984 | 0 | 0 |

3 Residue-property plots

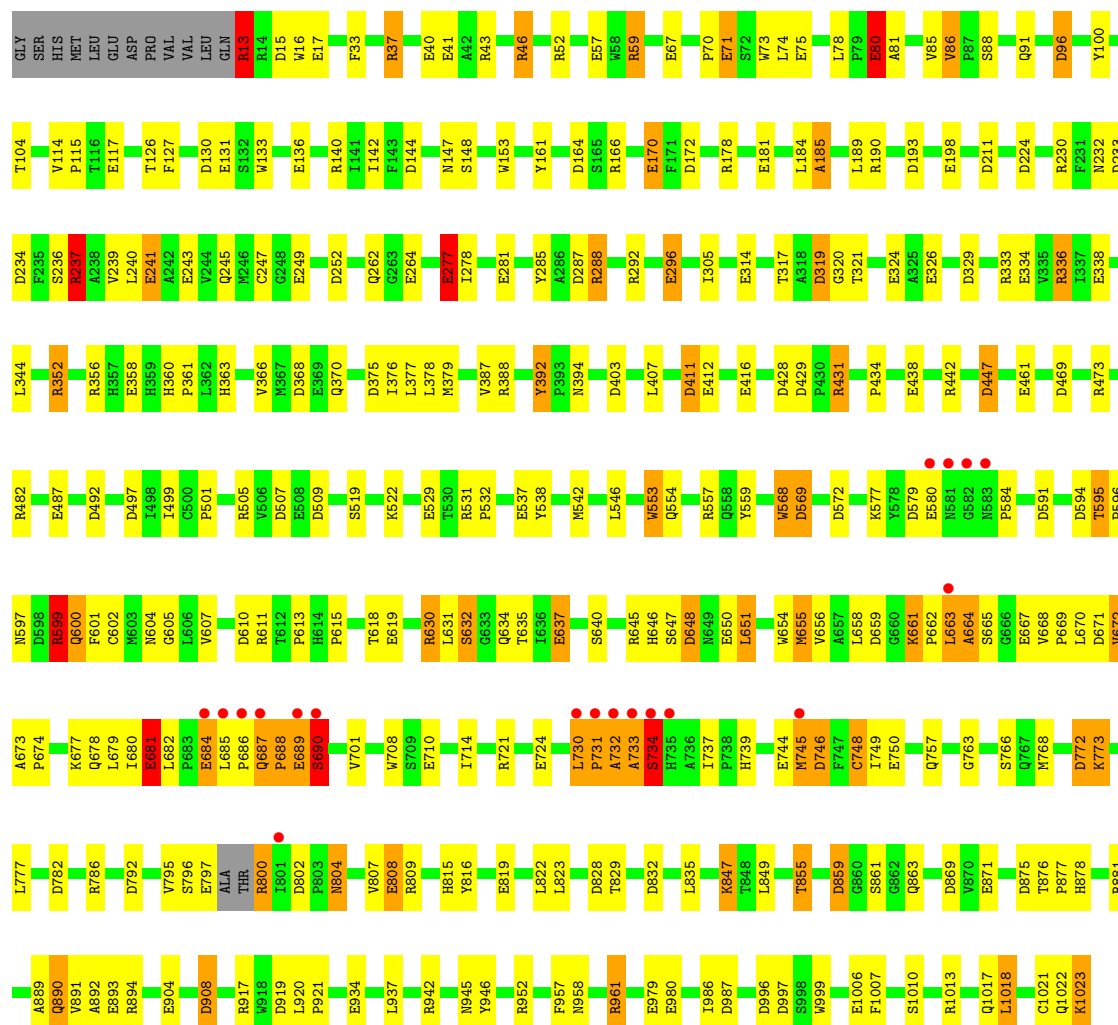
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



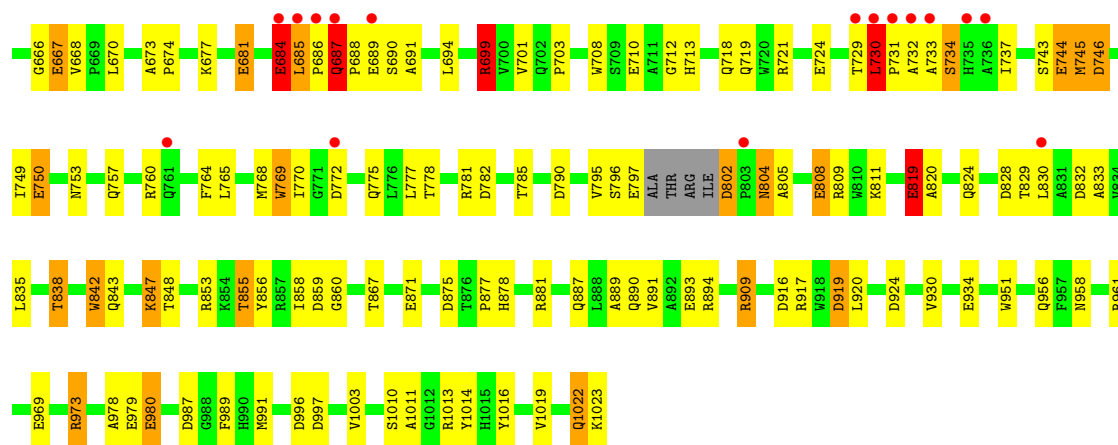
- Molecule 1: beta-galactosidase



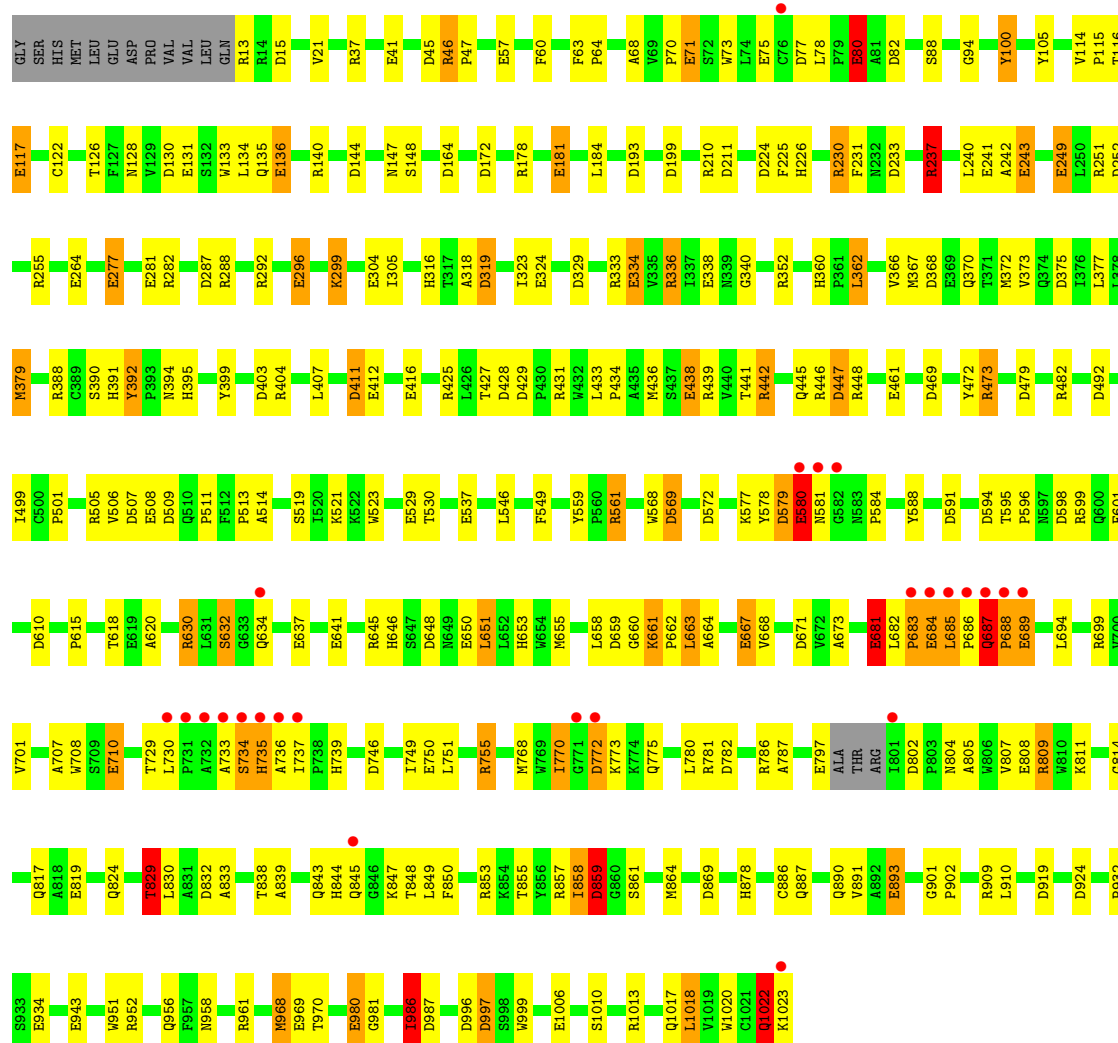


• Molecule 1: beta-galactosidase





• Molecule 1: beta-galactosidase



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 149.70Å 168.59Å 200.99Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 21.70 – 1.60 21.69 – 1.60 | Depositor EDS |
| % Data completeness (in resolution range) | 92.1 (21.70-1.60) 88.2 (21.69-1.60) | Depositor EDS |
| R_{merge} | 0.05 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.03 (at 1.60Å) | Xtrriage |
| Refinement program | TNT | Depositor |
| R, R_{free} | 0.192 , 0.243 0.180 , 0.228 | Depositor DCC |
| R_{free} test set | 8858 reflections (1.45%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 14.1 | Xtrriage |
| Anisotropy | 0.138 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.34 , 83.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.96 | EDS |
| Total number of atoms | 36619 | wwPDB-VP |
| Average B, all atoms (Å ²) | 22.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.46 % 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 5.8122e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DMS, MG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 1.12 | 44/8360 (0.5%) | 1.67 | 159/11404 (1.4%) |
| 1 | B | 1.15 | 55/8355 (0.7%) | 1.64 | 152/11397 (1.3%) |
| 1 | C | 1.13 | 50/8336 (0.6%) | 1.66 | 162/11372 (1.4%) |
| 1 | D | 1.13 | 45/8344 (0.5%) | 1.68 | 172/11383 (1.5%) |
| All | All | 1.13 | 194/33395 (0.6%) | 1.66 | 645/45556 (1.4%) |

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 | C | 1 | 0 |

All (194) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | D | 537 | GLU | CD-OE2 | 9.86 | 1.36 | 1.25 |
| 1 | A | 249 | GLU | CD-OE2 | 9.72 | 1.36 | 1.25 |
| 1 | D | 136 | GLU | CD-OE2 | 8.94 | 1.35 | 1.25 |
| 1 | D | 893 | GLU | CD-OE2 | 8.89 | 1.35 | 1.25 |
| 1 | C | 650 | GLU | CD-OE2 | 8.83 | 1.35 | 1.25 |
| 1 | D | 681 | GLU | CD-OE2 | 8.80 | 1.35 | 1.25 |
| 1 | C | 684 | GLU | CD-OE2 | 8.73 | 1.35 | 1.25 |
| 1 | B | 980 | GLU | CD-OE2 | 8.60 | 1.35 | 1.25 |
| 1 | C | 170 | GLU | CD-OE2 | 8.51 | 1.35 | 1.25 |
| 1 | D | 650 | GLU | CD-OE2 | 8.40 | 1.34 | 1.25 |
| 1 | C | 969 | GLU | CD-OE2 | 8.40 | 1.34 | 1.25 |
| 1 | A | 537 | GLU | CD-OE2 | 8.21 | 1.34 | 1.25 |
| 1 | A | 296 | GLU | CD-OE2 | 8.05 | 1.34 | 1.25 |
| 1 | D | 281 | GLU | CD-OE2 | 7.99 | 1.34 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1 | B | 580 | GLU | CD-OE2 | 7.86 | 1.34 | 1.25 |
| 1 | A | 1006 | GLU | CD-OE2 | 7.86 | 1.34 | 1.25 |
| 1 | A | 487 | GLU | CD-OE2 | 7.81 | 1.34 | 1.25 |
| 1 | C | 819 | GLU | CD-OE2 | 7.64 | 1.34 | 1.25 |
| 1 | B | 71 | GLU | CD-OE2 | 7.59 | 1.34 | 1.25 |
| 1 | D | 71 | GLU | CD-OE2 | 7.58 | 1.33 | 1.25 |
| 1 | A | 304 | GLU | CD-OE2 | 7.55 | 1.33 | 1.25 |
| 1 | D | 41 | GLU | CD-OE2 | 7.53 | 1.33 | 1.25 |
| 1 | B | 1006 | GLU | CD-OE2 | 7.52 | 1.33 | 1.25 |
| 1 | A | 71 | GLU | CD-OE2 | 7.51 | 1.33 | 1.25 |
| 1 | D | 296 | GLU | CD-OE2 | 7.51 | 1.33 | 1.25 |
| 1 | C | 934 | GLU | CD-OE2 | 7.49 | 1.33 | 1.25 |
| 1 | D | 710 | GLU | CD-OE2 | 7.47 | 1.33 | 1.25 |
| 1 | C | 75 | GLU | CD-OE2 | 7.42 | 1.33 | 1.25 |
| 1 | A | 281 | GLU | CD-OE2 | 7.40 | 1.33 | 1.25 |
| 1 | B | 281 | GLU | CD-OE2 | 7.39 | 1.33 | 1.25 |
| 1 | A | 980 | GLU | CD-OE2 | 7.36 | 1.33 | 1.25 |
| 1 | D | 819 | GLU | CD-OE2 | 7.30 | 1.33 | 1.25 |
| 1 | B | 681 | GLU | CD-OE2 | 7.29 | 1.33 | 1.25 |
| 1 | B | 461 | GLU | CD-OE2 | 7.27 | 1.33 | 1.25 |
| 1 | C | 641 | GLU | CD-OE1 | -7.26 | 1.17 | 1.25 |
| 1 | A | 681 | GLU | CD-OE2 | 7.21 | 1.33 | 1.25 |
| 1 | D | 943 | GLU | CD-OE2 | 7.20 | 1.33 | 1.25 |
| 1 | B | 689 | GLU | CD-OE2 | 7.15 | 1.33 | 1.25 |
| 1 | A | 131 | GLU | CD-OE2 | 7.13 | 1.33 | 1.25 |
| 1 | A | 979 | GLU | CD-OE2 | 7.11 | 1.33 | 1.25 |
| 1 | A | 667 | GLU | CD-OE2 | 7.09 | 1.33 | 1.25 |
| 1 | A | 80 | GLU | CD-OE2 | 7.09 | 1.33 | 1.25 |
| 1 | D | 808 | GLU | CD-OE2 | 7.04 | 1.33 | 1.25 |
| 1 | D | 243 | GLU | CD-OE2 | 6.97 | 1.33 | 1.25 |
| 1 | C | 529 | GLU | CD-OE2 | 6.95 | 1.33 | 1.25 |
| 1 | B | 893 | GLU | CD-OE2 | 6.95 | 1.33 | 1.25 |
| 1 | B | 243 | GLU | CD-OE2 | 6.94 | 1.33 | 1.25 |
| 1 | C | 80 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | D | 75 | GLU | CD-OE2 | 6.86 | 1.33 | 1.25 |
| 1 | C | 667 | GLU | CD-OE2 | 6.84 | 1.33 | 1.25 |
| 1 | C | 750 | GLU | CD-OE2 | 6.83 | 1.33 | 1.25 |
| 1 | C | 314 | GLU | CD-OE1 | -6.80 | 1.18 | 1.25 |
| 1 | A | 969 | GLU | CD-OE2 | 6.80 | 1.33 | 1.25 |
| 1 | A | 241 | GLU | CD-OE2 | 6.79 | 1.33 | 1.25 |
| 1 | C | 744 | GLU | CD-OE2 | 6.79 | 1.33 | 1.25 |
| 1 | C | 980 | GLU | CD-OE2 | 6.79 | 1.33 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | B | 744 | GLU | CD-OE2 | 6.78 | 1.33 | 1.25 |
| 1 | D | 438 | GLU | CD-OE2 | 6.78 | 1.33 | 1.25 |
| 1 | C | 131 | GLU | CD-OE2 | 6.77 | 1.33 | 1.25 |
| 1 | C | 710 | GLU | CD-OE2 | 6.73 | 1.33 | 1.25 |
| 1 | D | 969 | GLU | CD-OE2 | 6.73 | 1.33 | 1.25 |
| 1 | A | 508 | GLU | CD-OE2 | 6.73 | 1.33 | 1.25 |
| 1 | C | 71 | GLU | CD-OE2 | 6.73 | 1.33 | 1.25 |
| 1 | D | 667 | GLU | CD-OE2 | 6.72 | 1.33 | 1.25 |
| 1 | B | 170 | GLU | CD-OE2 | 6.66 | 1.32 | 1.25 |
| 1 | C | 277 | GLU | CD-OE2 | 6.64 | 1.32 | 1.25 |
| 1 | A | 943 | GLU | CD-OE2 | 6.63 | 1.32 | 1.25 |
| 1 | D | 338 | GLU | CD-OE2 | 6.63 | 1.32 | 1.25 |
| 1 | C | 537 | GLU | CD-OE2 | 6.62 | 1.32 | 1.25 |
| 1 | C | 304 | GLU | CD-OE2 | 6.59 | 1.32 | 1.25 |
| 1 | A | 684 | GLU | CD-OE2 | 6.58 | 1.32 | 1.25 |
| 1 | D | 797 | GLU | CD-OE2 | 6.57 | 1.32 | 1.25 |
| 1 | D | 980 | GLU | CD-OE2 | 6.56 | 1.32 | 1.25 |
| 1 | A | 710 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 1 | B | 75 | GLU | CD-OE2 | 6.53 | 1.32 | 1.25 |
| 1 | D | 750 | GLU | CD-OE2 | 6.47 | 1.32 | 1.25 |
| 1 | C | 893 | GLU | CD-OE2 | 6.45 | 1.32 | 1.25 |
| 1 | D | 117 | GLU | CD-OE2 | 6.43 | 1.32 | 1.25 |
| 1 | C | 296 | GLU | CD-OE2 | 6.43 | 1.32 | 1.25 |
| 1 | A | 819 | GLU | CD-OE2 | 6.42 | 1.32 | 1.25 |
| 1 | B | 667 | GLU | CD-OE2 | 6.39 | 1.32 | 1.25 |
| 1 | A | 243 | GLU | CD-OE2 | 6.39 | 1.32 | 1.25 |
| 1 | D | 684 | GLU | CD-OE2 | 6.37 | 1.32 | 1.25 |
| 1 | B | 17 | GLU | CD-OE2 | 6.37 | 1.32 | 1.25 |
| 1 | B | 338 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | C | 681 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | A | 170 | GLU | CD-OE2 | 6.33 | 1.32 | 1.25 |
| 1 | A | 438 | GLU | CD-OE2 | 6.32 | 1.32 | 1.25 |
| 1 | C | 797 | GLU | CD-OE2 | 6.31 | 1.32 | 1.25 |
| 1 | B | 619 | GLU | CD-OE2 | 6.29 | 1.32 | 1.25 |
| 1 | A | 277 | GLU | CD-OE2 | 6.28 | 1.32 | 1.25 |
| 1 | D | 304 | GLU | CD-OE2 | 6.27 | 1.32 | 1.25 |
| 1 | B | 871 | GLU | CD-OE2 | 6.26 | 1.32 | 1.25 |
| 1 | C | 281 | GLU | CD-OE2 | 6.24 | 1.32 | 1.25 |
| 1 | D | 241 | GLU | CD-OE2 | 6.23 | 1.32 | 1.25 |
| 1 | A | 41 | GLU | CD-OE2 | 6.23 | 1.32 | 1.25 |
| 1 | B | 904 | GLU | CD-OE1 | -6.22 | 1.18 | 1.25 |
| 1 | D | 689 | GLU | CD-OE2 | 6.21 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 744 | GLU | CD-OE2 | 6.20 | 1.32 | 1.25 |
| 1 | C | 181 | GLU | CD-OE2 | 6.20 | 1.32 | 1.25 |
| 1 | B | 117 | GLU | CD-OE2 | 6.19 | 1.32 | 1.25 |
| 1 | D | 131 | GLU | CD-OE2 | 6.16 | 1.32 | 1.25 |
| 1 | B | 684 | GLU | CD-OE2 | 6.15 | 1.32 | 1.25 |
| 1 | B | 808 | GLU | CD-OE2 | 6.15 | 1.32 | 1.25 |
| 1 | A | 117 | GLU | CD-OE2 | 6.15 | 1.32 | 1.25 |
| 1 | C | 198 | GLU | CD-OE2 | 6.14 | 1.32 | 1.25 |
| 1 | D | 249 | GLU | CD-OE2 | 6.14 | 1.32 | 1.25 |
| 1 | C | 41 | GLU | CD-OE2 | 6.13 | 1.32 | 1.25 |
| 1 | B | 314 | GLU | CD-OE1 | -6.13 | 1.19 | 1.25 |
| 1 | C | 871 | GLU | CD-OE2 | 6.12 | 1.32 | 1.25 |
| 1 | D | 277 | GLU | CD-OE2 | 6.12 | 1.32 | 1.25 |
| 1 | B | 296 | GLU | CD-OE2 | 6.11 | 1.32 | 1.25 |
| 1 | D | 508 | GLU | CD-OE1 | -6.10 | 1.19 | 1.25 |
| 1 | D | 580 | GLU | CD-OE2 | 6.08 | 1.32 | 1.25 |
| 1 | C | 619 | GLU | CD-OE2 | 6.04 | 1.32 | 1.25 |
| 1 | B | 724 | GLU | CD-OE2 | 6.04 | 1.32 | 1.25 |
| 1 | D | 181 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | B | 487 | GLU | CD-OE2 | 6.02 | 1.32 | 1.25 |
| 1 | C | 580 | GLU | CD-OE2 | 6.02 | 1.32 | 1.25 |
| 1 | B | 416 | GLU | CD-OE2 | 6.01 | 1.32 | 1.25 |
| 1 | A | 264 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | C | 689 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | C | 117 | GLU | CD-OE2 | 5.99 | 1.32 | 1.25 |
| 1 | B | 438 | GLU | CD-OE2 | 5.99 | 1.32 | 1.25 |
| 1 | D | 934 | GLU | CD-OE2 | 5.96 | 1.32 | 1.25 |
| 1 | A | 934 | GLU | CD-OE2 | 5.96 | 1.32 | 1.25 |
| 1 | A | 750 | GLU | CD-OE2 | 5.93 | 1.32 | 1.25 |
| 1 | B | 934 | GLU | CD-OE2 | 5.93 | 1.32 | 1.25 |
| 1 | A | 904 | GLU | CD-OE2 | 5.91 | 1.32 | 1.25 |
| 1 | C | 17 | GLU | CD-OE1 | -5.89 | 1.19 | 1.25 |
| 1 | B | 131 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | A | 580 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | D | 529 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | D | 57 | GLU | CD-OE2 | 5.82 | 1.32 | 1.25 |
| 1 | C | 241 | GLU | CD-OE2 | 5.79 | 1.32 | 1.25 |
| 1 | C | 249 | GLU | CD-OE2 | 5.79 | 1.32 | 1.25 |
| 1 | B | 40 | GLU | CD-OE2 | 5.79 | 1.32 | 1.25 |
| 1 | B | 277 | GLU | CD-OE2 | 5.76 | 1.31 | 1.25 |
| 1 | C | 136 | GLU | CD-OE2 | 5.75 | 1.31 | 1.25 |
| 1 | D | 264 | GLU | CD-OE2 | 5.75 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | D | 80 | GLU | CD-OE2 | 5.74 | 1.31 | 1.25 |
| 1 | B | 650 | GLU | CD-OE2 | 5.73 | 1.31 | 1.25 |
| 1 | B | 412 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |
| 1 | D | 324 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |
| 1 | B | 819 | GLU | CD-OE2 | 5.68 | 1.31 | 1.25 |
| 1 | D | 641 | GLU | CD-OE2 | 5.68 | 1.31 | 1.25 |
| 1 | A | 67 | GLU | CD-OE2 | 5.68 | 1.31 | 1.25 |
| 1 | D | 637 | GLU | CD-OE2 | 5.66 | 1.31 | 1.25 |
| 1 | B | 80 | GLU | CD-OE2 | 5.62 | 1.31 | 1.25 |
| 1 | B | 136 | GLU | CD-OE2 | 5.62 | 1.31 | 1.25 |
| 1 | C | 482 | ARG | CZ-NH1 | 5.62 | 1.40 | 1.33 |
| 1 | A | 893 | GLU | CD-OE2 | 5.58 | 1.31 | 1.25 |
| 1 | B | 537 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | C | 724 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | B | 979 | GLU | CD-OE2 | 5.54 | 1.31 | 1.25 |
| 1 | B | 264 | GLU | CD-OE2 | 5.52 | 1.31 | 1.25 |
| 1 | C | 338 | GLU | CD-OE2 | 5.50 | 1.31 | 1.25 |
| 1 | A | 871 | GLU | CD-OE2 | 5.49 | 1.31 | 1.25 |
| 1 | B | 324 | GLU | CD-OE2 | 5.49 | 1.31 | 1.25 |
| 1 | B | 249 | GLU | CD-OE2 | 5.47 | 1.31 | 1.25 |
| 1 | C | 57 | GLU | CD-OE2 | 5.45 | 1.31 | 1.25 |
| 1 | C | 324 | GLU | CD-OE2 | 5.45 | 1.31 | 1.25 |
| 1 | B | 797 | GLU | CD-OE2 | 5.44 | 1.31 | 1.25 |
| 1 | A | 797 | GLU | CD-OE2 | 5.43 | 1.31 | 1.25 |
| 1 | D | 334 | GLU | CD-OE2 | 5.41 | 1.31 | 1.25 |
| 1 | A | 369 | GLU | CD-OE2 | 5.40 | 1.31 | 1.25 |
| 1 | B | 326 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 |
| 1 | C | 243 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | A | 358 | GLU | CD-OE2 | 5.34 | 1.31 | 1.25 |
| 1 | B | 334 | GLU | CD-OE1 | -5.31 | 1.19 | 1.25 |
| 1 | B | 241 | GLU | CD-OE2 | 5.29 | 1.31 | 1.25 |
| 1 | C | 461 | GLU | CD-OE1 | -5.27 | 1.19 | 1.25 |
| 1 | C | 438 | GLU | CD-OE2 | 5.26 | 1.31 | 1.25 |
| 1 | B | 710 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | B | 41 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | B | 67 | GLU | CD-OE1 | -5.24 | 1.19 | 1.25 |
| 1 | B | 637 | GLU | CD-OE2 | 5.22 | 1.31 | 1.25 |
| 1 | B | 198 | GLU | CD-OE2 | 5.20 | 1.31 | 1.25 |
| 1 | B | 57 | GLU | CD-OE2 | 5.19 | 1.31 | 1.25 |
| 1 | D | 461 | GLU | CD-OE2 | 5.19 | 1.31 | 1.25 |
| 1 | C | 442 | ARG | CZ-NH1 | 5.17 | 1.39 | 1.33 |
| 1 | A | 181 | GLU | CD-OE2 | 5.17 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 1 | A | 198 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 1 | B | 314 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 1 | B | 529 | GLU | CD-OE2 | 5.15 | 1.31 | 1.25 |
| 1 | A | 529 | GLU | CD-OE2 | 5.12 | 1.31 | 1.25 |
| 1 | C | 979 | GLU | CD-OE2 | 5.11 | 1.31 | 1.25 |
| 1 | C | 637 | GLU | CD-OE2 | 5.10 | 1.31 | 1.25 |
| 1 | A | 461 | GLU | CD-OE2 | 5.09 | 1.31 | 1.25 |
| 1 | D | 412 | GLU | CD-OE2 | 5.06 | 1.31 | 1.25 |
| 1 | C | 808 | GLU | CD-OE2 | 5.03 | 1.31 | 1.25 |
| 1 | B | 358 | GLU | CD-OE2 | 5.02 | 1.31 | 1.25 |
| 1 | D | 1006 | GLU | CD-OE2 | 5.01 | 1.31 | 1.25 |
| 1 | A | 338 | GLU | CD-OE2 | 5.01 | 1.31 | 1.25 |

All (645) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | C | 699 | ARG | NE-CZ-NH1 | 24.71 | 132.65 | 120.30 |
| 1 | C | 699 | ARG | NE-CZ-NH2 | -20.33 | 110.14 | 120.30 |
| 1 | C | 599 | ARG | NE-CZ-NH1 | 16.78 | 128.69 | 120.30 |
| 1 | D | 630 | ARG | NE-CZ-NH1 | 16.23 | 128.41 | 120.30 |
| 1 | C | 473 | ARG | NE-CZ-NH1 | 16.07 | 128.33 | 120.30 |
| 1 | A | 431 | ARG | NE-CZ-NH2 | -16.02 | 112.29 | 120.30 |
| 1 | A | 431 | ARG | NE-CZ-NH1 | 15.68 | 128.14 | 120.30 |
| 1 | C | 442 | ARG | NE-CZ-NH2 | -15.01 | 112.80 | 120.30 |
| 1 | B | 557 | ARG | NE-CZ-NH2 | -14.83 | 112.89 | 120.30 |
| 1 | D | 431 | ARG | NE-CZ-NH1 | 14.75 | 127.67 | 120.30 |
| 1 | B | 599 | ARG | NE-CZ-NH1 | 14.44 | 127.52 | 120.30 |
| 1 | B | 473 | ARG | NE-CZ-NH1 | 13.91 | 127.25 | 120.30 |
| 1 | D | 781 | ARG | NE-CZ-NH1 | 13.68 | 127.14 | 120.30 |
| 1 | D | 439 | ARG | NE-CZ-NH2 | -13.64 | 113.48 | 120.30 |
| 1 | A | 166 | ARG | NE-CZ-NH2 | -13.23 | 113.68 | 120.30 |
| 1 | D | 630 | ARG | NE-CZ-NH2 | -13.21 | 113.70 | 120.30 |
| 1 | D | 446 | ARG | NE-CZ-NH1 | 13.01 | 126.81 | 120.30 |
| 1 | A | 233 | ASP | CB-CG-OD2 | -12.96 | 106.63 | 118.30 |
| 1 | B | 599 | ARG | NE-CZ-NH2 | -12.83 | 113.89 | 120.30 |
| 1 | A | 251 | ARG | NE-CZ-NH1 | 12.71 | 126.65 | 120.30 |
| 1 | C | 233 | ASP | CB-CG-OD2 | -12.70 | 106.87 | 118.30 |
| 1 | D | 172 | ASP | CB-CG-OD2 | -12.58 | 106.98 | 118.30 |
| 1 | B | 356 | ARG | NE-CZ-NH1 | 12.57 | 126.58 | 120.30 |
| 1 | A | 13 | ARG | NE-CZ-NH2 | -12.22 | 114.19 | 120.30 |
| 1 | D | 439 | ARG | NE-CZ-NH1 | 12.13 | 126.36 | 120.30 |
| 1 | D | 15 | ASP | CB-CG-OD2 | -12.07 | 107.43 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | A | 233 | ASP | CB-CG-OD1 | 12.05 | 129.14 | 118.30 |
| 1 | D | 857 | ARG | NE-CZ-NH1 | 11.93 | 126.26 | 120.30 |
| 1 | D | 473 | ARG | NE-CZ-NH1 | 11.91 | 126.25 | 120.30 |
| 1 | C | 853 | ARG | NE-CZ-NH2 | -11.88 | 114.36 | 120.30 |
| 1 | B | 557 | ARG | NE-CZ-NH1 | 11.83 | 126.21 | 120.30 |
| 1 | B | 746 | ASP | CB-CG-OD2 | -11.71 | 107.76 | 118.30 |
| 1 | B | 166 | ARG | NE-CZ-NH2 | -11.68 | 114.46 | 120.30 |
| 1 | A | 442 | ARG | NE-CZ-NH2 | -11.49 | 114.56 | 120.30 |
| 1 | A | 13 | ARG | NE-CZ-NH1 | 11.46 | 126.03 | 120.30 |
| 1 | D | 687 | GLN | C-N-CD | -11.41 | 95.50 | 120.60 |
| 1 | C | 721 | ARG | NE-CZ-NH1 | 11.39 | 125.99 | 120.30 |
| 1 | C | 43 | ARG | NE-CZ-NH1 | 11.36 | 125.98 | 120.30 |
| 1 | C | 224 | ASP | CB-CG-OD1 | 11.11 | 128.29 | 118.30 |
| 1 | D | 13 | ARG | NE-CZ-NH2 | -10.96 | 114.82 | 120.30 |
| 1 | D | 431 | ARG | NE-CZ-NH2 | -10.88 | 114.86 | 120.30 |
| 1 | D | 996 | ASP | CB-CG-OD1 | 10.82 | 128.04 | 118.30 |
| 1 | B | 285 | TYR | CB-CG-CD2 | -10.79 | 114.52 | 121.00 |
| 1 | D | 13 | ARG | NE-CZ-NH1 | 10.78 | 125.69 | 120.30 |
| 1 | D | 15 | ASP | CB-CG-OD1 | 10.76 | 127.99 | 118.30 |
| 1 | D | 594 | ASP | CB-CG-OD2 | -10.72 | 108.66 | 118.30 |
| 1 | D | 172 | ASP | CB-CG-OD1 | 10.66 | 127.89 | 118.30 |
| 1 | B | 952 | ARG | NE-CZ-NH1 | 10.62 | 125.61 | 120.30 |
| 1 | C | 13 | ARG | NE-CZ-NH2 | -10.62 | 114.99 | 120.30 |
| 1 | C | 233 | ASP | CB-CG-OD1 | 10.58 | 127.82 | 118.30 |
| 1 | C | 721 | ARG | NE-CZ-NH2 | -10.56 | 115.02 | 120.30 |
| 1 | C | 599 | ARG | NE-CZ-NH2 | -10.49 | 115.05 | 120.30 |
| 1 | A | 166 | ARG | NE-CZ-NH1 | 10.48 | 125.54 | 120.30 |
| 1 | B | 329 | ASP | CB-CG-OD2 | -10.47 | 108.88 | 118.30 |
| 1 | A | 1013 | ARG | NE-CZ-NH1 | 10.18 | 125.39 | 120.30 |
| 1 | B | 388 | ARG | NE-CZ-NH2 | -10.02 | 115.29 | 120.30 |
| 1 | A | 352 | ARG | NE-CZ-NH1 | 9.94 | 125.27 | 120.30 |
| 1 | A | 224 | ASP | CB-CG-OD1 | 9.93 | 127.24 | 118.30 |
| 1 | C | 917 | ARG | NE-CZ-NH2 | 9.89 | 125.24 | 120.30 |
| 1 | A | 336 | ARG | NE-CZ-NH1 | 9.84 | 125.22 | 120.30 |
| 1 | A | 46 | ARG | NE-CZ-NH1 | 9.83 | 125.21 | 120.30 |
| 1 | B | 368 | ASP | CB-CG-OD1 | 9.79 | 127.11 | 118.30 |
| 1 | A | 987 | ASP | CB-CG-OD2 | -9.78 | 109.50 | 118.30 |
| 1 | B | 224 | ASP | CB-CG-OD1 | 9.70 | 127.03 | 118.30 |
| 1 | B | 336 | ARG | NE-CZ-NH1 | 9.70 | 125.15 | 120.30 |
| 1 | A | 439 | ARG | NE-CZ-NH2 | -9.59 | 115.50 | 120.30 |
| 1 | A | 428 | ASP | CB-CG-OD2 | -9.57 | 109.68 | 118.30 |
| 1 | A | 292 | ARG | NE-CZ-NH1 | 9.48 | 125.04 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 442 | ARG | NE-CZ-NH1 | 9.46 | 125.03 | 120.30 |
| 1 | B | 233 | ASP | CB-CG-OD1 | 9.46 | 126.81 | 118.30 |
| 1 | A | 996 | ASP | CB-CG-OD2 | -9.42 | 109.82 | 118.30 |
| 1 | D | 473 | ARG | NE-CZ-NH2 | -9.41 | 115.59 | 120.30 |
| 1 | D | 230 | ARG | NE-CZ-NH1 | 9.40 | 125.00 | 120.30 |
| 1 | B | 572 | ASP | CB-CG-OD2 | -9.40 | 109.84 | 118.30 |
| 1 | A | 439 | ARG | NE-CZ-NH1 | 9.34 | 124.97 | 120.30 |
| 1 | C | 482 | ARG | NE-CZ-NH1 | 9.33 | 124.97 | 120.30 |
| 1 | B | 772 | ASP | CB-CG-OD2 | -9.24 | 109.99 | 118.30 |
| 1 | C | 973 | ARG | NE-CZ-NH1 | 9.19 | 124.89 | 120.30 |
| 1 | C | 473 | ARG | NE-CZ-NH2 | -9.18 | 115.71 | 120.30 |
| 1 | A | 509 | ASP | CB-CG-OD2 | -9.17 | 110.05 | 118.30 |
| 1 | B | 875 | ASP | CB-CG-OD1 | 9.17 | 126.55 | 118.30 |
| 1 | C | 473 | ARG | CD-NE-CZ | 9.15 | 136.41 | 123.60 |
| 1 | C | 431 | ARG | NE-CZ-NH2 | -9.13 | 115.74 | 120.30 |
| 1 | B | 996 | ASP | CB-CG-OD2 | -9.11 | 110.10 | 118.30 |
| 1 | A | 425 | ARG | NE-CZ-NH1 | 9.09 | 124.84 | 120.30 |
| 1 | B | 319 | ASP | CB-CG-OD1 | 9.09 | 126.48 | 118.30 |
| 1 | A | 292 | ARG | NE-CZ-NH2 | -9.07 | 115.77 | 120.30 |
| 1 | A | 828 | ASP | CB-CG-OD2 | -9.01 | 110.19 | 118.30 |
| 1 | B | 411 | ASP | CB-CG-OD2 | -8.96 | 110.24 | 118.30 |
| 1 | D | 699 | ARG | NE-CZ-NH1 | 8.96 | 124.78 | 120.30 |
| 1 | A | 997 | ASP | CB-CG-OD2 | -8.94 | 110.25 | 118.30 |
| 1 | C | 859 | ASP | CB-CG-OD2 | -8.92 | 110.27 | 118.30 |
| 1 | A | 509 | ASP | CB-CG-OD1 | 8.92 | 126.33 | 118.30 |
| 1 | D | 144 | ASP | CB-CG-OD1 | 8.90 | 126.31 | 118.30 |
| 1 | C | 832 | ASP | CB-CG-OD2 | -8.86 | 110.33 | 118.30 |
| 1 | A | 610 | ASP | CB-CG-OD1 | 8.85 | 126.27 | 118.30 |
| 1 | C | 199 | ASP | CB-CG-OD1 | 8.84 | 126.26 | 118.30 |
| 1 | A | 909 | ARG | NE-CZ-NH1 | 8.84 | 124.72 | 120.30 |
| 1 | D | 336 | ARG | NE-CZ-NH1 | 8.84 | 124.72 | 120.30 |
| 1 | D | 594 | ASP | CB-CG-OD1 | 8.84 | 126.25 | 118.30 |
| 1 | C | 482 | ARG | NE-CZ-NH2 | -8.82 | 115.89 | 120.30 |
| 1 | C | 961 | ARG | NE-CZ-NH2 | -8.81 | 115.89 | 120.30 |
| 1 | B | 572 | ASP | CB-CG-OD1 | 8.80 | 126.22 | 118.30 |
| 1 | D | 233 | ASP | CB-CG-OD2 | -8.77 | 110.41 | 118.30 |
| 1 | A | 336 | ARG | NE-CZ-NH2 | -8.74 | 115.93 | 120.30 |
| 1 | A | 917 | ARG | NE-CZ-NH1 | -8.73 | 115.94 | 120.30 |
| 1 | B | 630 | ARG | NE-CZ-NH1 | 8.72 | 124.66 | 120.30 |
| 1 | B | 429 | ASP | CB-CG-OD2 | -8.71 | 110.46 | 118.30 |
| 1 | B | 594 | ASP | CB-CG-OD2 | -8.71 | 110.46 | 118.30 |
| 1 | D | 282 | ARG | NE-CZ-NH2 | -8.69 | 115.95 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | C | 310 | ARG | NE-CZ-NH2 | -8.67 | 115.97 | 120.30 |
| 1 | C | 996 | ASP | CB-CG-OD1 | 8.67 | 126.10 | 118.30 |
| 1 | D | 210 | ARG | NE-CZ-NH1 | -8.67 | 115.97 | 120.30 |
| 1 | B | 13 | ARG | NE-CZ-NH1 | 8.60 | 124.60 | 120.30 |
| 1 | B | 442 | ARG | NE-CZ-NH2 | -8.56 | 116.02 | 120.30 |
| 1 | A | 869 | ASP | CB-CG-OD1 | 8.52 | 125.97 | 118.30 |
| 1 | B | 952 | ARG | NE-CZ-NH2 | -8.50 | 116.05 | 120.30 |
| 1 | D | 482 | ARG | NE-CZ-NH2 | -8.50 | 116.05 | 120.30 |
| 1 | B | 329 | ASP | CB-CG-OD1 | 8.50 | 125.95 | 118.30 |
| 1 | A | 428 | ASP | CB-CG-OD1 | 8.49 | 125.94 | 118.30 |
| 1 | B | 746 | ASP | CB-CG-OD1 | 8.49 | 125.94 | 118.30 |
| 1 | B | 287 | ASP | CB-CG-OD2 | -8.47 | 110.67 | 118.30 |
| 1 | A | 771 | GLY | N-CA-C | -8.46 | 91.96 | 113.10 |
| 1 | D | 996 | ASP | CB-CG-OD2 | -8.41 | 110.73 | 118.30 |
| 1 | C | 428 | ASP | CB-CG-OD1 | 8.41 | 125.87 | 118.30 |
| 1 | D | 579 | ASP | CB-CG-OD2 | -8.39 | 110.75 | 118.30 |
| 1 | D | 428 | ASP | CB-CG-OD1 | 8.38 | 125.84 | 118.30 |
| 1 | B | 569 | ASP | CB-CG-OD2 | -8.38 | 110.76 | 118.30 |
| 1 | C | 287 | ASP | CB-CG-OD2 | -8.36 | 110.77 | 118.30 |
| 1 | C | 772 | ASP | CB-CG-OD2 | -8.35 | 110.79 | 118.30 |
| 1 | D | 869 | ASP | CB-CG-OD1 | 8.34 | 125.81 | 118.30 |
| 1 | B | 648 | ASP | CB-CG-OD2 | -8.34 | 110.80 | 118.30 |
| 1 | B | 233 | ASP | CB-CG-OD2 | -8.33 | 110.80 | 118.30 |
| 1 | B | 43 | ARG | NE-CZ-NH1 | 8.33 | 124.46 | 120.30 |
| 1 | A | 954 | ASP | CB-CG-OD1 | 8.32 | 125.79 | 118.30 |
| 1 | A | 671 | ASP | CB-CG-OD2 | -8.31 | 110.82 | 118.30 |
| 1 | A | 144 | ASP | CB-CG-OD2 | -8.31 | 110.82 | 118.30 |
| 1 | B | 130 | ASP | CB-CG-OD1 | 8.29 | 125.76 | 118.30 |
| 1 | A | 755 | ARG | NE-CZ-NH1 | 8.25 | 124.42 | 120.30 |
| 1 | A | 144 | ASP | CB-CG-OD1 | 8.24 | 125.71 | 118.30 |
| 1 | D | 909 | ARG | NE-CZ-NH1 | 8.22 | 124.41 | 120.30 |
| 1 | A | 942 | ARG | NE-CZ-NH2 | -8.21 | 116.19 | 120.30 |
| 1 | C | 375 | ASP | CB-CG-OD1 | 8.18 | 125.66 | 118.30 |
| 1 | D | 442 | ARG | NE-CZ-NH2 | -8.18 | 116.21 | 120.30 |
| 1 | D | 507 | ASP | CB-CG-OD1 | 8.17 | 125.66 | 118.30 |
| 1 | D | 388 | ARG | NE-CZ-NH2 | -8.16 | 116.22 | 120.30 |
| 1 | B | 368 | ASP | CB-CG-OD2 | -8.13 | 110.98 | 118.30 |
| 1 | D | 446 | ARG | NE-CZ-NH2 | -8.10 | 116.25 | 120.30 |
| 1 | B | 809 | ARG | NE-CZ-NH2 | -8.09 | 116.25 | 120.30 |
| 1 | A | 954 | ASP | CB-CG-OD2 | -8.09 | 111.02 | 118.30 |
| 1 | A | 828 | ASP | CB-CG-OD1 | 8.08 | 125.57 | 118.30 |
| 1 | D | 997 | ASP | CB-CG-OD2 | -8.07 | 111.04 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 987 | ASP | CB-CG-OD1 | 8.04 | 125.54 | 118.30 |
| 1 | B | 786 | ARG | NE-CZ-NH2 | -8.03 | 116.28 | 120.30 |
| 1 | D | 482 | ARG | NE-CZ-NH1 | 8.01 | 124.31 | 120.30 |
| 1 | D | 987 | ASP | CB-CG-OD1 | 8.01 | 125.51 | 118.30 |
| 1 | C | 909 | ARG | NE-CZ-NH2 | -8.00 | 116.30 | 120.30 |
| 1 | C | 802 | ASP | CB-CG-OD2 | -7.99 | 111.11 | 118.30 |
| 1 | B | 509 | ASP | CB-CG-OD1 | 7.99 | 125.49 | 118.30 |
| 1 | A | 507 | ASP | CB-CG-OD2 | -7.98 | 111.11 | 118.30 |
| 1 | C | 924 | ASP | CB-CG-OD2 | -7.97 | 111.13 | 118.30 |
| 1 | D | 469 | ASP | CB-CG-OD1 | 7.94 | 125.45 | 118.30 |
| 1 | B | 431 | ARG | NE-CZ-NH1 | 7.94 | 124.27 | 120.30 |
| 1 | D | 572 | ASP | CB-CG-OD2 | -7.93 | 111.16 | 118.30 |
| 1 | B | 832 | ASP | CB-CG-OD2 | -7.93 | 111.16 | 118.30 |
| 1 | D | 352 | ARG | NE-CZ-NH1 | 7.91 | 124.25 | 120.30 |
| 1 | D | 648 | ASP | CB-CG-OD2 | -7.91 | 111.18 | 118.30 |
| 1 | A | 140 | ARG | NE-CZ-NH2 | -7.90 | 116.35 | 120.30 |
| 1 | D | 45 | ASP | CB-CG-OD1 | 7.90 | 125.41 | 118.30 |
| 1 | C | 557 | ARG | NE-CZ-NH2 | -7.89 | 116.36 | 120.30 |
| 1 | A | 288 | ARG | NE-CZ-NH1 | 7.88 | 124.24 | 120.30 |
| 1 | D | 591 | ASP | CB-CG-OD1 | 7.86 | 125.37 | 118.30 |
| 1 | C | 802 | ASP | CB-CG-OD1 | 7.81 | 125.33 | 118.30 |
| 1 | A | 211 | ASP | CB-CG-OD1 | 7.79 | 125.31 | 118.30 |
| 1 | A | 411 | ASP | CB-CG-OD2 | -7.76 | 111.32 | 118.30 |
| 1 | C | 832 | ASP | CB-CG-OD1 | 7.76 | 125.28 | 118.30 |
| 1 | C | 772 | ASP | CB-CG-OD1 | 7.74 | 125.27 | 118.30 |
| 1 | B | 469 | ASP | CB-CG-OD1 | 7.74 | 125.27 | 118.30 |
| 1 | C | 859 | ASP | CB-CG-OD1 | 7.74 | 125.27 | 118.30 |
| 1 | A | 659 | ASP | CB-CG-OD2 | -7.69 | 111.38 | 118.30 |
| 1 | D | 251 | ARG | NE-CZ-NH1 | 7.69 | 124.14 | 120.30 |
| 1 | B | 442 | ARG | NE-CZ-NH1 | 7.68 | 124.14 | 120.30 |
| 1 | C | 352 | ARG | NE-CZ-NH1 | 7.68 | 124.14 | 120.30 |
| 1 | A | 908 | ASP | CB-CG-OD1 | 7.68 | 125.21 | 118.30 |
| 1 | C | 961 | ARG | NE-CZ-NH1 | 7.62 | 124.11 | 120.30 |
| 1 | B | 648 | ASP | CB-CG-OD1 | 7.58 | 125.12 | 118.30 |
| 1 | C | 183 | ARG | NE-CZ-NH1 | 7.57 | 124.09 | 120.30 |
| 1 | C | 287 | ASP | CB-CG-OD1 | 7.57 | 125.11 | 118.30 |
| 1 | A | 809 | ARG | NE-CZ-NH2 | -7.56 | 116.52 | 120.30 |
| 1 | C | 352 | ARG | NE-CZ-NH2 | -7.52 | 116.54 | 120.30 |
| 1 | D | 224 | ASP | CB-CG-OD1 | 7.52 | 125.06 | 118.30 |
| 1 | A | 856 | TYR | CB-CG-CD2 | -7.51 | 116.49 | 121.00 |
| 1 | D | 116 | THR | CA-CB-CG2 | -7.51 | 101.88 | 112.40 |
| 1 | D | 288 | ARG | NE-CZ-NH1 | 7.51 | 124.05 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 630 | ARG | NE-CZ-NH2 | -7.50 | 116.55 | 120.30 |
| 1 | B | 130 | ASP | CB-CG-OD2 | -7.50 | 111.55 | 118.30 |
| 1 | B | 287 | ASP | CB-CG-OD1 | 7.50 | 125.05 | 118.30 |
| 1 | C | 750 | GLU | N-CA-CB | 7.49 | 124.08 | 110.60 |
| 1 | C | 599 | ARG | CD-NE-CZ | 7.49 | 134.09 | 123.60 |
| 1 | C | 996 | ASP | CB-CG-OD2 | -7.49 | 111.56 | 118.30 |
| 1 | A | 388 | ARG | NE-CZ-NH2 | -7.48 | 116.56 | 120.30 |
| 1 | D | 507 | ASP | CB-CG-OD2 | -7.48 | 111.57 | 118.30 |
| 1 | B | 569 | ASP | CB-CG-OD1 | 7.47 | 125.02 | 118.30 |
| 1 | C | 699 | ARG | CD-NE-CZ | 7.45 | 134.03 | 123.60 |
| 1 | D | 252 | ASP | CB-CG-OD2 | -7.45 | 111.60 | 118.30 |
| 1 | D | 659 | ASP | CB-CG-OD2 | -7.44 | 111.60 | 118.30 |
| 1 | B | 919 | ASP | CB-CG-OD2 | -7.44 | 111.61 | 118.30 |
| 1 | B | 859 | ASP | CB-CG-OD2 | -7.42 | 111.62 | 118.30 |
| 1 | B | 252 | ASP | CB-CG-OD2 | -7.41 | 111.63 | 118.30 |
| 1 | D | 130 | ASP | CB-CG-OD2 | -7.41 | 111.63 | 118.30 |
| 1 | C | 611 | ARG | NE-CZ-NH1 | 7.41 | 124.00 | 120.30 |
| 1 | D | 579 | ASP | CB-CG-OD1 | 7.41 | 124.97 | 118.30 |
| 1 | B | 288 | ARG | NE-CZ-NH2 | -7.39 | 116.61 | 120.30 |
| 1 | B | 804 | ASN | N-CA-CB | 7.38 | 123.89 | 110.60 |
| 1 | C | 853 | ARG | NE-CZ-NH1 | 7.36 | 123.98 | 120.30 |
| 1 | C | 411 | ASP | CB-CG-OD1 | 7.34 | 124.91 | 118.30 |
| 1 | B | 428 | ASP | CB-CG-OD1 | 7.33 | 124.90 | 118.30 |
| 1 | C | 329 | ASP | CB-CG-OD2 | -7.33 | 111.70 | 118.30 |
| 1 | A | 77 | ASP | CB-CG-OD2 | -7.32 | 111.72 | 118.30 |
| 1 | B | 15 | ASP | CB-CG-OD2 | -7.30 | 111.73 | 118.30 |
| 1 | A | 282 | ARG | NE-CZ-NH2 | -7.29 | 116.66 | 120.30 |
| 1 | C | 234 | ASP | CB-CG-OD2 | -7.29 | 111.74 | 118.30 |
| 1 | C | 630 | ARG | NE-CZ-NH1 | 7.28 | 123.94 | 120.30 |
| 1 | C | 659 | ASP | CB-CG-OD2 | -7.27 | 111.75 | 118.30 |
| 1 | D | 561 | ARG | NE-CZ-NH2 | -7.27 | 116.66 | 120.30 |
| 1 | C | 594 | ASP | CB-CG-OD2 | -7.24 | 111.79 | 118.30 |
| 1 | D | 193 | ASP | CB-CG-OD1 | 7.23 | 124.81 | 118.30 |
| 1 | A | 469 | ASP | CB-CG-OD1 | 7.22 | 124.80 | 118.30 |
| 1 | D | 857 | ARG | NE-CZ-NH2 | -7.22 | 116.69 | 120.30 |
| 1 | D | 919 | ASP | CB-CG-OD2 | -7.22 | 111.80 | 118.30 |
| 1 | B | 828 | ASP | CB-CG-OD1 | 7.21 | 124.78 | 118.30 |
| 1 | B | 832 | ASP | CB-CG-OD1 | 7.20 | 124.78 | 118.30 |
| 1 | C | 267 | VAL | CA-CB-CG2 | -7.20 | 100.11 | 110.90 |
| 1 | D | 469 | ASP | CB-CG-OD2 | -7.19 | 111.83 | 118.30 |
| 1 | C | 77 | ASP | CB-CG-OD1 | 7.17 | 124.75 | 118.30 |
| 1 | D | 233 | ASP | CB-CG-OD1 | 7.17 | 124.75 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | D | 980 | GLU | C-N-CA | -7.17 | 107.25 | 122.30 |
| 1 | A | 45 | ASP | CB-CG-OD1 | 7.16 | 124.74 | 118.30 |
| 1 | D | 403 | ASP | CB-CG-OD1 | 7.15 | 124.73 | 118.30 |
| 1 | A | 224 | ASP | CB-CG-OD2 | -7.13 | 111.88 | 118.30 |
| 1 | C | 579 | ASP | CB-CG-OD1 | 7.13 | 124.72 | 118.30 |
| 1 | B | 13 | ARG | NE-CZ-NH2 | -7.11 | 116.75 | 120.30 |
| 1 | A | 130 | ASP | CB-CG-OD2 | -7.09 | 111.92 | 118.30 |
| 1 | A | 997 | ASP | N-CA-CB | 7.09 | 123.37 | 110.60 |
| 1 | D | 428 | ASP | CB-CG-OD2 | -7.08 | 111.93 | 118.30 |
| 1 | A | 610 | ASP | CB-CG-OD2 | -7.08 | 111.93 | 118.30 |
| 1 | D | 429 | ASP | CB-CG-OD2 | -7.07 | 111.94 | 118.30 |
| 1 | B | 610 | ASP | CB-CG-OD2 | -7.07 | 111.94 | 118.30 |
| 1 | D | 559 | TYR | CB-CG-CD2 | -7.06 | 116.77 | 121.00 |
| 1 | C | 958 | ASN | N-CA-CB | 7.05 | 123.30 | 110.60 |
| 1 | C | 411 | ASP | CB-CG-OD2 | -7.05 | 111.95 | 118.30 |
| 1 | A | 96 | ASP | CB-CG-OD1 | 7.05 | 124.65 | 118.30 |
| 1 | C | 178 | ARG | NE-CZ-NH1 | 7.05 | 123.83 | 120.30 |
| 1 | B | 828 | ASP | CB-CG-OD2 | -7.04 | 111.96 | 118.30 |
| 1 | D | 287 | ASP | CB-CG-OD1 | 7.03 | 124.63 | 118.30 |
| 1 | B | 473 | ARG | CD-NE-CZ | 7.02 | 133.43 | 123.60 |
| 1 | D | 448 | ARG | NE-CZ-NH2 | -7.02 | 116.79 | 120.30 |
| 1 | D | 659 | ASP | CB-CG-OD1 | 7.01 | 124.61 | 118.30 |
| 1 | C | 782 | ASP | CB-CG-OD1 | 7.00 | 124.60 | 118.30 |
| 1 | D | 509 | ASP | CB-CG-OD1 | 7.00 | 124.59 | 118.30 |
| 1 | B | 1018 | LEU | CB-CA-C | -6.99 | 96.92 | 110.20 |
| 1 | C | 368 | ASP | CB-CG-OD2 | -6.99 | 112.01 | 118.30 |
| 1 | A | 579 | ASP | CB-CG-OD1 | 6.97 | 124.58 | 118.30 |
| 1 | B | 875 | ASP | CB-CG-OD2 | -6.97 | 112.03 | 118.30 |
| 1 | B | 859 | ASP | CB-CG-OD1 | 6.96 | 124.56 | 118.30 |
| 1 | C | 1016 | TYR | CB-CG-CD2 | -6.95 | 116.83 | 121.00 |
| 1 | A | 579 | ASP | CB-CG-OD2 | -6.94 | 112.05 | 118.30 |
| 1 | A | 404 | ARG | NE-CZ-NH2 | -6.94 | 116.83 | 120.30 |
| 1 | B | 447 | ASP | CB-CG-OD1 | 6.93 | 124.54 | 118.30 |
| 1 | D | 319 | ASP | CB-CG-OD2 | -6.93 | 112.06 | 118.30 |
| 1 | A | 942 | ARG | NE-CZ-NH1 | 6.93 | 123.76 | 120.30 |
| 1 | C | 255 | ARG | NE-CZ-NH1 | 6.93 | 123.76 | 120.30 |
| 1 | C | 987 | ASP | CB-CG-OD1 | 6.91 | 124.52 | 118.30 |
| 1 | B | 190 | ARG | NE-CZ-NH2 | -6.89 | 116.85 | 120.30 |
| 1 | C | 252 | ASP | CB-CG-OD2 | -6.89 | 112.10 | 118.30 |
| 1 | D | 388 | ARG | NE-CZ-NH1 | 6.88 | 123.74 | 120.30 |
| 1 | C | 172 | ASP | CB-CG-OD2 | -6.88 | 112.11 | 118.30 |
| 1 | C | 404 | ARG | NE-CZ-NH2 | -6.87 | 116.87 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | D | 193 | ASP | CB-CG-OD2 | -6.84 | 112.14 | 118.30 |
| 1 | C | 190 | ARG | NE-CZ-NH2 | -6.83 | 116.89 | 120.30 |
| 1 | B | 772 | ASP | CB-CG-OD1 | 6.80 | 124.42 | 118.30 |
| 1 | C | 561 | ARG | NE-CZ-NH2 | -6.80 | 116.90 | 120.30 |
| 1 | B | 579 | ASP | CB-CG-OD1 | 6.79 | 124.41 | 118.30 |
| 1 | B | 829 | THR | CA-CB-CG2 | -6.77 | 102.92 | 112.40 |
| 1 | B | 881 | ARG | NE-CZ-NH1 | 6.77 | 123.68 | 120.30 |
| 1 | A | 671 | ASP | CB-CG-OD1 | 6.77 | 124.39 | 118.30 |
| 1 | D | 802 | ASP | CB-CG-OD2 | -6.76 | 112.22 | 118.30 |
| 1 | A | 319 | ASP | CB-CG-OD2 | -6.76 | 112.22 | 118.30 |
| 1 | D | 829 | THR | N-CA-CB | 6.75 | 123.13 | 110.30 |
| 1 | D | 997 | ASP | N-CA-CB | 6.75 | 122.75 | 110.60 |
| 1 | B | 492 | ASP | CB-CG-OD2 | -6.75 | 112.23 | 118.30 |
| 1 | B | 559 | TYR | CD1-CE1-CZ | -6.74 | 113.74 | 119.80 |
| 1 | C | 557 | ARG | NE-CZ-NH1 | 6.72 | 123.66 | 120.30 |
| 1 | A | 253 | TYR | CB-CG-CD2 | -6.72 | 116.97 | 121.00 |
| 1 | D | 392 | TYR | CB-CG-CD2 | 6.72 | 125.03 | 121.00 |
| 1 | C | 894 | ARG | NE-CZ-NH1 | 6.72 | 123.66 | 120.30 |
| 1 | B | 469 | ASP | CB-CG-OD2 | -6.69 | 112.28 | 118.30 |
| 1 | D | 429 | ASP | CB-CG-OD1 | 6.68 | 124.31 | 118.30 |
| 1 | B | 509 | ASP | CB-CG-OD2 | -6.67 | 112.30 | 118.30 |
| 1 | B | 59 | ARG | NE-CZ-NH2 | -6.67 | 116.97 | 120.30 |
| 1 | D | 404 | ARG | NE-CZ-NH2 | -6.65 | 116.97 | 120.30 |
| 1 | A | 916 | ASP | CB-CG-OD1 | 6.65 | 124.28 | 118.30 |
| 1 | C | 76 | CYS | N-CA-CB | -6.65 | 98.63 | 110.60 |
| 1 | C | 288 | ARG | NE-CZ-NH1 | 6.65 | 123.62 | 120.30 |
| 1 | D | 140 | ARG | NE-CZ-NH1 | 6.65 | 123.62 | 120.30 |
| 1 | A | 108 | THR | CA-CB-CG2 | -6.64 | 103.11 | 112.40 |
| 1 | B | 958 | ASN | N-CA-CB | 6.64 | 122.55 | 110.60 |
| 1 | A | 252 | ASP | CB-CG-OD2 | -6.64 | 112.33 | 118.30 |
| 1 | B | 388 | ARG | NE-CZ-NH1 | 6.62 | 123.61 | 120.30 |
| 1 | C | 569 | ASP | CB-CG-OD1 | 6.61 | 124.25 | 118.30 |
| 1 | C | 875 | ASP | CB-CG-OD1 | 6.60 | 124.24 | 118.30 |
| 1 | D | 1022 | GLN | N-CA-CB | 6.60 | 122.48 | 110.60 |
| 1 | D | 144 | ASP | CB-CG-OD2 | -6.59 | 112.37 | 118.30 |
| 1 | C | 425 | ARG | NE-CZ-NH1 | 6.59 | 123.59 | 120.30 |
| 1 | B | 782 | ASP | CB-CG-OD1 | 6.57 | 124.21 | 118.30 |
| 1 | B | 611 | ARG | NE-CZ-NH2 | -6.57 | 117.02 | 120.30 |
| 1 | D | 781 | ARG | CD-NE-CZ | 6.57 | 132.79 | 123.60 |
| 1 | B | 288 | ARG | NE-CZ-NH1 | 6.56 | 123.58 | 120.30 |
| 1 | D | 632 | SER | N-CA-CB | 6.55 | 120.32 | 110.50 |
| 1 | A | 82 | ASP | CB-CG-OD1 | 6.54 | 124.19 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 411 | ASP | CB-CG-OD1 | 6.54 | 124.19 | 118.30 |
| 1 | C | 43 | ARG | NE-CZ-NH2 | -6.53 | 117.04 | 120.30 |
| 1 | D | 375 | ASP | CB-CG-OD2 | -6.52 | 112.43 | 118.30 |
| 1 | B | 239 | VAL | CA-CB-CG2 | -6.52 | 101.12 | 110.90 |
| 1 | A | 594 | ASP | CB-CG-OD1 | 6.50 | 124.16 | 118.30 |
| 1 | D | 986 | ILE | CG1-CB-CG2 | -6.50 | 97.10 | 111.40 |
| 1 | C | 909 | ARG | NE-CZ-NH1 | 6.49 | 123.55 | 120.30 |
| 1 | D | 569 | ASP | CB-CG-OD2 | -6.49 | 112.46 | 118.30 |
| 1 | C | 733 | ALA | N-CA-CB | 6.49 | 119.18 | 110.10 |
| 1 | B | 172 | ASP | CB-CG-OD1 | 6.48 | 124.13 | 118.30 |
| 1 | D | 809 | ARG | NE-CZ-NH2 | -6.48 | 117.06 | 120.30 |
| 1 | D | 1013 | ARG | NE-CZ-NH1 | 6.48 | 123.54 | 120.30 |
| 1 | A | 952 | ARG | NE-CZ-NH1 | 6.47 | 123.54 | 120.30 |
| 1 | A | 559 | TYR | CB-CG-CD2 | -6.47 | 117.12 | 121.00 |
| 1 | C | 199 | ASP | CB-CG-OD2 | -6.46 | 112.48 | 118.30 |
| 1 | D | 598 | ASP | CB-CG-OD2 | -6.46 | 112.49 | 118.30 |
| 1 | D | 569 | ASP | CB-CG-OD1 | 6.46 | 124.11 | 118.30 |
| 1 | D | 591 | ASP | CB-CG-OD2 | -6.45 | 112.49 | 118.30 |
| 1 | B | 96 | ASP | CB-CG-OD2 | -6.45 | 112.50 | 118.30 |
| 1 | D | 838 | THR | CA-CB-CG2 | -6.45 | 103.37 | 112.40 |
| 1 | B | 482 | ARG | NE-CZ-NH2 | -6.44 | 117.08 | 120.30 |
| 1 | D | 425 | ARG | NE-CZ-NH1 | 6.43 | 123.52 | 120.30 |
| 1 | A | 234 | ASP | CB-CG-OD1 | 6.42 | 124.08 | 118.30 |
| 1 | A | 178 | ARG | NE-CZ-NH2 | -6.41 | 117.09 | 120.30 |
| 1 | D | 336 | ARG | NE-CZ-NH2 | -6.40 | 117.10 | 120.30 |
| 1 | C | 439 | ARG | NE-CZ-NH1 | 6.38 | 123.49 | 120.30 |
| 1 | B | 671 | ASP | CB-CG-OD2 | -6.37 | 112.57 | 118.30 |
| 1 | D | 237 | ARG | NE-CZ-NH1 | 6.36 | 123.48 | 120.30 |
| 1 | D | 368 | ASP | CB-CG-OD2 | -6.36 | 112.58 | 118.30 |
| 1 | A | 448 | ARG | NE-CZ-NH1 | 6.35 | 123.48 | 120.30 |
| 1 | C | 442 | ARG | NE-CZ-NH1 | 6.33 | 123.47 | 120.30 |
| 1 | B | 507 | ASP | CB-CG-OD2 | -6.33 | 112.60 | 118.30 |
| 1 | A | 648 | ASP | CB-CG-OD1 | 6.33 | 124.00 | 118.30 |
| 1 | D | 255 | ARG | NE-CZ-NH1 | 6.32 | 123.46 | 120.30 |
| 1 | A | 199 | ASP | CB-CG-OD1 | 6.32 | 123.99 | 118.30 |
| 1 | B | 594 | ASP | CB-CG-OD1 | 6.32 | 123.98 | 118.30 |
| 1 | B | 816 | TYR | CB-CG-CD2 | -6.31 | 117.21 | 121.00 |
| 1 | C | 164 | ASP | CB-CG-OD1 | 6.31 | 123.98 | 118.30 |
| 1 | A | 859 | ASP | CB-CG-OD2 | -6.31 | 112.62 | 118.30 |
| 1 | C | 280 | ASP | CB-CG-OD2 | -6.30 | 112.63 | 118.30 |
| 1 | D | 352 | ARG | NE-CZ-NH2 | -6.30 | 117.15 | 120.30 |
| 1 | C | 531 | ARG | NE-CZ-NH1 | 6.30 | 123.45 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | D | 578 | TYR | CB-CG-CD2 | -6.29 | 117.22 | 121.00 |
| 1 | C | 492 | ASP | CB-CG-OD2 | -6.27 | 112.65 | 118.30 |
| 1 | A | 869 | ASP | CB-CG-OD2 | -6.27 | 112.66 | 118.30 |
| 1 | B | 285 | TYR | CB-CG-CD1 | 6.27 | 124.76 | 121.00 |
| 1 | B | 997 | ASP | CB-CG-OD2 | -6.26 | 112.66 | 118.30 |
| 1 | A | 996 | ASP | CB-CG-OD1 | 6.26 | 123.94 | 118.30 |
| 1 | A | 968 | MET | N-CA-CB | -6.26 | 99.33 | 110.60 |
| 1 | B | 507 | ASP | CB-CG-OD1 | 6.25 | 123.93 | 118.30 |
| 1 | B | 792 | ASP | CB-CG-OD2 | -6.25 | 112.67 | 118.30 |
| 1 | A | 43 | ARG | NE-CZ-NH1 | 6.25 | 123.42 | 120.30 |
| 1 | A | 768 | MET | CA-CB-CG | 6.24 | 123.92 | 113.30 |
| 1 | A | 429 | ASP | CB-CG-OD2 | -6.24 | 112.69 | 118.30 |
| 1 | D | 509 | ASP | CB-CG-OD2 | -6.23 | 112.69 | 118.30 |
| 1 | C | 917 | ARG | CD-NE-CZ | -6.23 | 114.88 | 123.60 |
| 1 | B | 579 | ASP | CB-CG-OD2 | -6.22 | 112.70 | 118.30 |
| 1 | B | 247 | CYS | CA-CB-SG | -6.22 | 102.80 | 114.00 |
| 1 | D | 802 | ASP | CB-CG-OD1 | 6.22 | 123.90 | 118.30 |
| 1 | B | 591 | ASP | CB-CG-OD1 | 6.22 | 123.90 | 118.30 |
| 1 | D | 630 | ARG | CD-NE-CZ | 6.21 | 132.30 | 123.60 |
| 1 | A | 178 | ARG | NE-CZ-NH1 | 6.20 | 123.40 | 120.30 |
| 1 | C | 26 | ARG | NE-CZ-NH2 | -6.20 | 117.20 | 120.30 |
| 1 | A | 772 | ASP | CB-CG-OD1 | 6.20 | 123.88 | 118.30 |
| 1 | B | 497 | ASP | CB-CG-OD1 | 6.17 | 123.85 | 118.30 |
| 1 | A | 184 | LEU | CB-CA-C | -6.16 | 98.49 | 110.20 |
| 1 | C | 553 | TRP | CA-CB-CG | -6.16 | 101.99 | 113.70 |
| 1 | B | 178 | ARG | NE-CZ-NH1 | 6.15 | 123.38 | 120.30 |
| 1 | C | 130 | ASP | CB-CG-OD2 | -6.15 | 112.76 | 118.30 |
| 1 | A | 594 | ASP | CB-CG-OD2 | -6.14 | 112.77 | 118.30 |
| 1 | D | 130 | ASP | CB-CG-OD1 | 6.12 | 123.81 | 118.30 |
| 1 | C | 404 | ARG | NE-CZ-NH1 | 6.12 | 123.36 | 120.30 |
| 1 | C | 319 | ASP | CB-CG-OD1 | 6.11 | 123.80 | 118.30 |
| 1 | B | 15 | ASP | CB-CG-OD1 | 6.10 | 123.79 | 118.30 |
| 1 | B | 319 | ASP | CB-CG-OD2 | -6.10 | 112.81 | 118.30 |
| 1 | D | 987 | ASP | CB-CG-OD2 | -6.10 | 112.81 | 118.30 |
| 1 | A | 881 | ARG | NE-CZ-NH1 | 6.10 | 123.35 | 120.30 |
| 1 | D | 448 | ARG | NE-CZ-NH1 | 6.09 | 123.34 | 120.30 |
| 1 | D | 100 | TYR | CB-CG-CD1 | -6.07 | 117.36 | 121.00 |
| 1 | D | 997 | ASP | CB-CG-OD1 | 6.07 | 123.76 | 118.30 |
| 1 | D | 287 | ASP | CB-CG-OD2 | -6.06 | 112.84 | 118.30 |
| 1 | C | 507 | ASP | CB-CG-OD1 | 6.05 | 123.74 | 118.30 |
| 1 | D | 224 | ASP | CB-CG-OD2 | -6.05 | 112.86 | 118.30 |
| 1 | D | 199 | ASP | CB-CG-OD1 | 6.04 | 123.74 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 82 | ASP | CB-CG-OD2 | -6.04 | 112.86 | 118.30 |
| 1 | A | 429 | ASP | CB-CG-OD1 | 6.03 | 123.73 | 118.30 |
| 1 | C | 594 | ASP | CB-CG-OD1 | 6.03 | 123.72 | 118.30 |
| 1 | A | 431 | ARG | CD-NE-CZ | 6.02 | 132.03 | 123.60 |
| 1 | A | 730 | LEU | CB-CA-C | 6.01 | 121.61 | 110.20 |
| 1 | C | 598 | ASP | CB-CG-OD1 | 6.00 | 123.70 | 118.30 |
| 1 | D | 505 | ARG | NE-CZ-NH1 | 6.00 | 123.30 | 120.30 |
| 1 | D | 230 | ARG | NE-CZ-NH2 | -5.99 | 117.30 | 120.30 |
| 1 | A | 447 | ASP | CB-CG-OD2 | -5.99 | 112.91 | 118.30 |
| 1 | D | 251 | ARG | NE-CZ-NH2 | -5.99 | 117.31 | 120.30 |
| 1 | D | 832 | ASP | CB-CG-OD2 | -5.98 | 112.92 | 118.30 |
| 1 | C | 13 | ARG | NE-CZ-NH1 | 5.98 | 123.29 | 120.30 |
| 1 | D | 319 | ASP | CB-CG-OD1 | 5.98 | 123.68 | 118.30 |
| 1 | C | 610 | ASP | CB-CG-OD1 | 5.97 | 123.68 | 118.30 |
| 1 | B | 144 | ASP | CB-CG-OD1 | 5.96 | 123.67 | 118.30 |
| 1 | C | 431 | ARG | NE-CZ-NH1 | 5.96 | 123.28 | 120.30 |
| 1 | A | 719 | GLN | CB-CA-C | -5.92 | 98.56 | 110.40 |
| 1 | C | 828 | ASP | CB-CG-OD1 | 5.91 | 123.62 | 118.30 |
| 1 | B | 997 | ASP | N-CA-CB | 5.91 | 121.24 | 110.60 |
| 1 | D | 958 | ASN | N-CA-CB | 5.91 | 121.23 | 110.60 |
| 1 | C | 782 | ASP | CB-CG-OD2 | -5.90 | 112.99 | 118.30 |
| 1 | D | 850 | PHE | CB-CA-C | -5.90 | 98.60 | 110.40 |
| 1 | A | 553 | TRP | CA-CB-CG | -5.90 | 102.50 | 113.70 |
| 1 | A | 997 | ASP | CB-CG-OD1 | 5.89 | 123.60 | 118.30 |
| 1 | D | 772 | ASP | CB-CG-OD1 | 5.89 | 123.60 | 118.30 |
| 1 | B | 942 | ARG | NE-CZ-NH1 | 5.89 | 123.24 | 120.30 |
| 1 | D | 37 | ARG | NE-CZ-NH2 | -5.89 | 117.36 | 120.30 |
| 1 | B | 908 | ASP | CB-CG-OD2 | -5.88 | 113.01 | 118.30 |
| 1 | A | 15 | ASP | CB-CG-OD2 | -5.88 | 113.01 | 118.30 |
| 1 | C | 369 | GLU | CG-CD-OE2 | -5.87 | 106.56 | 118.30 |
| 1 | A | 648 | ASP | CB-CG-OD2 | -5.87 | 113.02 | 118.30 |
| 1 | A | 164 | ASP | CB-CG-OD1 | 5.86 | 123.58 | 118.30 |
| 1 | A | 469 | ASP | CB-CG-OD2 | -5.85 | 113.04 | 118.30 |
| 1 | C | 867 | THR | CA-CB-CG2 | -5.85 | 104.21 | 112.40 |
| 1 | A | 1018 | LEU | CB-CA-C | -5.85 | 99.09 | 110.20 |
| 1 | B | 211 | ASP | CB-CG-OD2 | -5.84 | 113.04 | 118.30 |
| 1 | C | 997 | ASP | N-CA-CB | 5.83 | 121.10 | 110.60 |
| 1 | A | 15 | ASP | CB-CG-OD1 | 5.83 | 123.55 | 118.30 |
| 1 | B | 1013 | ARG | NE-CZ-NH1 | 5.83 | 123.21 | 120.30 |
| 1 | D | 804 | ASN | CA-CB-CG | -5.83 | 100.58 | 113.40 |
| 1 | D | 699 | ARG | NE-CZ-NH2 | -5.81 | 117.40 | 120.30 |
| 1 | D | 416 | GLU | CG-CD-OE1 | 5.80 | 129.91 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | D | 782 | ASP | CB-CG-OD2 | -5.80 | 113.08 | 118.30 |
| 1 | C | 659 | ASP | CB-CG-OD1 | 5.80 | 123.52 | 118.30 |
| 1 | C | 508 | GLU | N-CA-CB | -5.79 | 100.17 | 110.60 |
| 1 | C | 255 | ARG | NE-CZ-NH2 | -5.79 | 117.41 | 120.30 |
| 1 | B | 802 | ASP | CB-CG-OD1 | 5.79 | 123.51 | 118.30 |
| 1 | B | 671 | ASP | CB-CG-OD1 | 5.78 | 123.50 | 118.30 |
| 1 | C | 997 | ASP | CB-CG-OD1 | 5.78 | 123.50 | 118.30 |
| 1 | B | 33 | PHE | CB-CA-C | -5.78 | 98.84 | 110.40 |
| 1 | C | 201 | ASP | CB-CG-OD2 | -5.78 | 113.10 | 118.30 |
| 1 | B | 224 | ASP | CB-CG-OD2 | -5.77 | 113.10 | 118.30 |
| 1 | B | 869 | ASP | CB-CG-OD1 | 5.77 | 123.49 | 118.30 |
| 1 | D | 610 | ASP | CB-CG-OD1 | 5.77 | 123.49 | 118.30 |
| 1 | B | 664 | ALA | CB-CA-C | -5.76 | 101.47 | 110.10 |
| 1 | D | 598 | ASP | CB-CG-OD1 | 5.75 | 123.48 | 118.30 |
| 1 | D | 329 | ASP | CB-CG-OD2 | -5.75 | 113.12 | 118.30 |
| 1 | A | 796 | SER | N-CA-CB | 5.75 | 119.12 | 110.50 |
| 1 | C | 856 | TYR | CB-CG-CD2 | -5.75 | 117.55 | 121.00 |
| 1 | D | 588 | TYR | CZ-CE2-CD2 | -5.75 | 114.63 | 119.80 |
| 1 | B | 568 | TRP | CA-CB-CG | -5.75 | 102.78 | 113.70 |
| 1 | A | 741 | THR | CA-CB-CG2 | -5.74 | 104.36 | 112.40 |
| 1 | D | 859 | ASP | CB-CG-OD2 | -5.74 | 113.14 | 118.30 |
| 1 | C | 224 | ASP | CB-CG-OD2 | -5.72 | 113.15 | 118.30 |
| 1 | A | 287 | ASP | CB-CG-OD1 | 5.71 | 123.44 | 118.30 |
| 1 | A | 112 | PRO | N-CA-CB | -5.69 | 96.34 | 102.60 |
| 1 | B | 352 | ARG | NE-CZ-NH2 | -5.69 | 117.46 | 120.30 |
| 1 | D | 46 | ARG | NE-CZ-NH1 | -5.69 | 117.46 | 120.30 |
| 1 | D | 1013 | ARG | NE-CZ-NH2 | -5.68 | 117.46 | 120.30 |
| 1 | C | 691 | ALA | CB-CA-C | -5.68 | 101.58 | 110.10 |
| 1 | A | 285 | TYR | CB-CG-CD2 | -5.67 | 117.59 | 121.00 |
| 1 | C | 997 | ASP | CB-CG-OD2 | -5.67 | 113.19 | 118.30 |
| 1 | D | 178 | ARG | NE-CZ-NH1 | 5.66 | 123.13 | 120.30 |
| 1 | A | 803 | PRO | N-CA-CB | 5.66 | 110.09 | 103.30 |
| 1 | D | 919 | ASP | CB-CG-OD1 | 5.66 | 123.39 | 118.30 |
| 1 | C | 790 | ASP | CB-CG-OD1 | 5.64 | 123.38 | 118.30 |
| 1 | C | 842 | TRP | CG-CD2-CE3 | -5.64 | 128.82 | 133.90 |
| 1 | B | 46 | ARG | NE-CZ-NH2 | -5.64 | 117.48 | 120.30 |
| 1 | B | 505 | ARG | NE-CZ-NH1 | 5.63 | 123.12 | 120.30 |
| 1 | C | 280 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |
| 1 | A | 832 | ASP | CB-CG-OD2 | -5.62 | 113.24 | 118.30 |
| 1 | C | 919 | ASP | CB-CG-OD1 | 5.62 | 123.36 | 118.30 |
| 1 | B | 429 | ASP | CB-CG-OD1 | 5.61 | 123.35 | 118.30 |
| 1 | C | 388 | ARG | NE-CZ-NH2 | -5.61 | 117.49 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | B | 161 | TYR | N-CA-CB | -5.61 | 100.51 | 110.60 |
| 1 | C | 733 | ALA | CB-CA-C | 5.60 | 118.50 | 110.10 |
| 1 | B | 961 | ARG | NE-CZ-NH2 | -5.60 | 117.50 | 120.30 |
| 1 | B | 919 | ASP | CB-CG-OD1 | 5.59 | 123.33 | 118.30 |
| 1 | A | 344 | LEU | CA-CB-CG | -5.58 | 102.46 | 115.30 |
| 1 | C | 85 | VAL | CA-CB-CG2 | -5.58 | 102.53 | 110.90 |
| 1 | C | 126 | THR | CA-CB-CG2 | -5.58 | 104.58 | 112.40 |
| 1 | A | 75 | GLU | CB-CA-C | 5.58 | 121.56 | 110.40 |
| 1 | B | 721 | ARG | NE-CZ-NH2 | -5.57 | 117.51 | 120.30 |
| 1 | C | 428 | ASP | CB-CG-OD2 | -5.57 | 113.29 | 118.30 |
| 1 | A | 314 | GLU | OE1-CD-OE2 | -5.57 | 116.62 | 123.30 |
| 1 | A | 599 | ARG | NE-CZ-NH2 | -5.56 | 117.52 | 120.30 |
| 1 | B | 908 | ASP | CB-CG-OD1 | 5.56 | 123.30 | 118.30 |
| 1 | B | 519 | SER | N-CA-CB | -5.56 | 102.17 | 110.50 |
| 1 | A | 486 | TYR | CG-CD2-CE2 | -5.54 | 116.86 | 121.30 |
| 1 | B | 403 | ASP | CB-CG-OD1 | 5.54 | 123.29 | 118.30 |
| 1 | A | 403 | ASP | CB-CG-OD2 | -5.54 | 113.31 | 118.30 |
| 1 | C | 164 | ASP | CB-CG-OD2 | -5.54 | 113.31 | 118.30 |
| 1 | A | 368 | ASP | CB-CG-OD2 | -5.54 | 113.32 | 118.30 |
| 1 | D | 968 | MET | N-CA-CB | -5.54 | 100.63 | 110.60 |
| 1 | D | 770 | ILE | N-CA-C | -5.53 | 96.06 | 111.00 |
| 1 | D | 772 | ASP | CB-CG-OD2 | -5.53 | 113.32 | 118.30 |
| 1 | B | 126 | THR | CA-CB-CG2 | -5.52 | 104.67 | 112.40 |
| 1 | C | 1013 | ARG | NE-CZ-NH1 | 5.51 | 123.06 | 120.30 |
| 1 | D | 299 | LYS | CA-CB-CG | -5.51 | 101.28 | 113.40 |
| 1 | D | 681 | GLU | CB-CA-C | 5.51 | 121.42 | 110.40 |
| 1 | C | 204 | ARG | NE-CZ-NH1 | 5.51 | 123.05 | 120.30 |
| 1 | A | 634 | GLN | CB-CG-CD | 5.50 | 125.91 | 111.60 |
| 1 | C | 234 | ASP | CB-CG-OD1 | 5.49 | 123.24 | 118.30 |
| 1 | C | 15 | ASP | CB-CG-OD1 | 5.49 | 123.24 | 118.30 |
| 1 | A | 962 | TYR | CB-CG-CD2 | 5.49 | 124.29 | 121.00 |
| 1 | D | 673 | ALA | N-CA-CB | -5.48 | 102.43 | 110.10 |
| 1 | B | 52 | ARG | NE-CZ-NH2 | 5.47 | 123.04 | 120.30 |
| 1 | B | 86 | VAL | CG1-CB-CG2 | -5.47 | 102.14 | 110.90 |
| 1 | C | 653 | HIS | N-CA-CB | 5.46 | 120.44 | 110.60 |
| 1 | D | 379 | MET | CG-SD-CE | -5.46 | 91.46 | 100.20 |
| 1 | D | 746 | ASP | CB-CG-OD2 | -5.46 | 113.38 | 118.30 |
| 1 | A | 486 | TYR | CZ-CE2-CD2 | 5.46 | 124.71 | 119.80 |
| 1 | B | 193 | ASP | CB-CG-OD1 | 5.46 | 123.21 | 118.30 |
| 1 | C | 425 | ARG | NE-CZ-NH2 | -5.46 | 117.57 | 120.30 |
| 1 | D | 77 | ASP | CB-CG-OD2 | -5.46 | 113.39 | 118.30 |
| 1 | D | 395 | HIS | N-CA-CB | -5.45 | 100.79 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 100 | TYR | N-CA-CB | 5.45 | 120.40 | 110.60 |
| 1 | A | 924 | ASP | CB-CG-OD1 | 5.45 | 123.20 | 118.30 |
| 1 | B | 234 | ASP | CB-CG-OD2 | -5.44 | 113.41 | 118.30 |
| 1 | B | 659 | ASP | CB-CG-OD1 | 5.43 | 123.19 | 118.30 |
| 1 | D | 855 | THR | N-CA-CB | 5.43 | 120.62 | 110.30 |
| 1 | D | 479 | ASP | CB-CG-OD2 | -5.43 | 113.41 | 118.30 |
| 1 | B | 553 | TRP | CA-CB-CG | -5.42 | 103.39 | 113.70 |
| 1 | C | 96 | ASP | N-CA-CB | 5.42 | 120.35 | 110.60 |
| 1 | B | 782 | ASP | CB-CG-OD2 | -5.40 | 113.44 | 118.30 |
| 1 | B | 987 | ASP | CB-CG-OD2 | -5.40 | 113.44 | 118.30 |
| 1 | A | 503 | TYR | CG-CD1-CE1 | 5.40 | 125.62 | 121.30 |
| 1 | C | 172 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | A | 479 | ASP | CB-CG-OD2 | -5.40 | 113.44 | 118.30 |
| 1 | D | 909 | ARG | NE-CZ-NH2 | -5.39 | 117.60 | 120.30 |
| 1 | C | 368 | ASP | CB-CG-OD1 | 5.39 | 123.15 | 118.30 |
| 1 | B | 37 | ARG | NE-CZ-NH1 | 5.38 | 122.99 | 120.30 |
| 1 | C | 15 | ASP | CB-CG-OD2 | -5.38 | 113.46 | 118.30 |
| 1 | D | 411 | ASP | CB-CG-OD1 | 5.38 | 123.14 | 118.30 |
| 1 | A | 62 | TRP | CB-CG-CD2 | 5.37 | 133.59 | 126.60 |
| 1 | A | 861 | SER | CB-CA-C | -5.37 | 99.90 | 110.10 |
| 1 | A | 802 | ASP | CB-CG-OD1 | 5.36 | 123.12 | 118.30 |
| 1 | B | 996 | ASP | CB-CG-OD1 | 5.36 | 123.12 | 118.30 |
| 1 | A | 352 | ARG | NE-CZ-NH2 | -5.35 | 117.62 | 120.30 |
| 1 | D | 329 | ASP | CB-CG-OD1 | 5.35 | 123.11 | 118.30 |
| 1 | D | 755 | ARG | N-CA-CB | 5.35 | 120.23 | 110.60 |
| 1 | A | 251 | ARG | NH1-CZ-NH2 | -5.35 | 113.52 | 119.40 |
| 1 | C | 730 | LEU | C-N-CD | -5.34 | 108.86 | 120.60 |
| 1 | A | 802 | ASP | CB-CG-OD2 | -5.34 | 113.50 | 118.30 |
| 1 | D | 399 | TYR | CD1-CE1-CZ | -5.34 | 115.00 | 119.80 |
| 1 | C | 729 | THR | N-CA-CB | 5.33 | 120.43 | 110.30 |
| 1 | C | 651 | LEU | N-CA-CB | 5.32 | 121.03 | 110.40 |
| 1 | D | 492 | ASP | CB-CG-OD2 | -5.32 | 113.52 | 118.30 |
| 1 | A | 329 | ASP | CB-CG-OD2 | -5.31 | 113.53 | 118.30 |
| 1 | D | 211 | ASP | CB-CG-OD2 | -5.30 | 113.53 | 118.30 |
| 1 | B | 140 | ARG | NE-CZ-NH2 | -5.30 | 117.65 | 120.30 |
| 1 | A | 572 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |
| 1 | C | 746 | ASP | CB-CA-C | -5.29 | 99.82 | 110.40 |
| 1 | B | 894 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 1 | B | 237 | ARG | NE-CZ-NH1 | 5.27 | 122.94 | 120.30 |
| 1 | D | 472 | TYR | CB-CG-CD2 | -5.27 | 117.84 | 121.00 |
| 1 | A | 221 | GLN | N-CA-CB | -5.27 | 101.11 | 110.60 |
| 1 | B | 640 | SER | CB-CA-C | -5.26 | 100.11 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | C | 721 | ARG | CD-NE-CZ | 5.25 | 130.96 | 123.60 |
| 1 | D | 853 | ARG | NE-CZ-NH2 | 5.25 | 122.93 | 120.30 |
| 1 | B | 505 | ARG | NE-CZ-NH2 | -5.25 | 117.67 | 120.30 |
| 1 | A | 632 | SER | CB-CA-C | 5.25 | 120.07 | 110.10 |
| 1 | A | 477 | SER | N-CA-CB | 5.25 | 118.37 | 110.50 |
| 1 | C | 431 | ARG | CA-CB-CG | -5.24 | 101.87 | 113.40 |
| 1 | C | 408 | TYR | CD1-CE1-CZ | -5.24 | 115.09 | 119.80 |
| 1 | C | 855 | THR | N-CA-CB | 5.24 | 120.25 | 110.30 |
| 1 | A | 96 | ASP | N-CA-CB | 5.24 | 120.03 | 110.60 |
| 1 | C | 211 | ASP | CB-CG-OD2 | -5.23 | 113.60 | 118.30 |
| 1 | C | 1013 | ARG | NE-CZ-NH2 | -5.22 | 117.69 | 120.30 |
| 1 | C | 136 | GLU | CB-CA-C | -5.22 | 99.96 | 110.40 |
| 1 | B | 185 | ALA | N-CA-CB | 5.21 | 117.40 | 110.10 |
| 1 | C | 336 | ARG | NE-CZ-NH1 | 5.21 | 122.91 | 120.30 |
| 1 | C | 769 | TRP | CB-CA-C | -5.21 | 99.98 | 110.40 |
| 1 | D | 288 | ARG | NE-CZ-NH2 | -5.21 | 117.70 | 120.30 |
| 1 | A | 277 | GLU | CG-CD-OE1 | 5.21 | 128.71 | 118.30 |
| 1 | A | 211 | ASP | CB-CG-OD2 | -5.20 | 113.62 | 118.30 |
| 1 | B | 748 | CYS | CA-CB-SG | -5.20 | 104.65 | 114.00 |
| 1 | B | 591 | ASP | CB-CG-OD2 | -5.19 | 113.63 | 118.30 |
| 1 | D | 416 | GLU | CG-CD-OE2 | -5.19 | 107.92 | 118.30 |
| 1 | D | 184 | LEU | CB-CA-C | -5.18 | 100.35 | 110.20 |
| 1 | B | 632 | SER | N-CA-CB | 5.18 | 118.26 | 110.50 |
| 1 | C | 13 | ARG | N-CA-CB | 5.17 | 119.90 | 110.60 |
| 1 | C | 719 | GLN | CB-CA-C | -5.17 | 100.07 | 110.40 |
| 1 | C | 978 | ALA | CB-CA-C | -5.17 | 102.35 | 110.10 |
| 1 | B | 538 | TYR | CG-CD2-CE2 | 5.17 | 125.43 | 121.30 |
| 1 | D | 924 | ASP | CB-CG-OD1 | 5.16 | 122.95 | 118.30 |
| 1 | B | 855 | THR | N-CA-CB | 5.16 | 120.10 | 110.30 |
| 1 | C | 384 | PHE | CB-CG-CD1 | -5.16 | 117.19 | 120.80 |
| 1 | B | 952 | ARG | CD-NE-CZ | 5.15 | 130.81 | 123.60 |
| 1 | C | 477 | SER | N-CA-CB | -5.14 | 102.78 | 110.50 |
| 1 | D | 403 | ASP | CB-CG-OD2 | -5.14 | 113.67 | 118.30 |
| 1 | A | 857 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 1 | A | 746 | ASP | CB-CG-OD1 | 5.13 | 122.92 | 118.30 |
| 1 | A | 185 | ALA | N-CA-CB | 5.13 | 117.28 | 110.10 |
| 1 | B | 392 | TYR | CG-CD2-CE2 | 5.12 | 125.39 | 121.30 |
| 1 | A | 329 | ASP | CB-CG-OD1 | 5.12 | 122.90 | 118.30 |
| 1 | C | 210 | ARG | N-CA-CB | 5.11 | 119.80 | 110.60 |
| 1 | C | 916 | ASP | CB-CG-OD1 | 5.11 | 122.90 | 118.30 |
| 1 | D | 523 | TRP | CE3-CZ3-CH2 | -5.10 | 115.59 | 121.20 |
| 1 | A | 177 | LEU | CB-CG-CD1 | -5.10 | 102.33 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | C | 170 | GLU | OE1-CD-OE2 | 5.10 | 129.42 | 123.30 |
| 1 | A | 447 | ASP | CB-CG-OD1 | 5.10 | 122.89 | 118.30 |
| 1 | D | 431 | ARG | CD-NE-CZ | 5.09 | 130.73 | 123.60 |
| 1 | D | 21 | VAL | CA-CB-CG2 | -5.07 | 103.30 | 110.90 |
| 1 | C | 610 | ASP | CB-CG-OD2 | -5.07 | 113.74 | 118.30 |
| 1 | D | 782 | ASP | CB-CG-OD1 | 5.07 | 122.86 | 118.30 |
| 1 | B | 746 | ASP | CB-CA-C | -5.06 | 100.28 | 110.40 |
| 1 | A | 772 | ASP | CB-CG-OD2 | -5.06 | 113.75 | 118.30 |
| 1 | A | 230 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 1 | A | 356 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 1 | C | 319 | ASP | CB-CG-OD2 | -5.06 | 113.75 | 118.30 |
| 1 | D | 786 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 1 | B | 234 | ASP | CB-CG-OD1 | 5.06 | 122.85 | 118.30 |
| 1 | D | 707 | ALA | CB-CA-C | -5.05 | 102.52 | 110.10 |
| 1 | C | 663 | LEU | CB-CA-C | -5.05 | 100.60 | 110.20 |
| 1 | D | 869 | ASP | CB-CG-OD2 | -5.05 | 113.76 | 118.30 |
| 1 | A | 282 | ARG | NE-CZ-NH1 | 5.05 | 122.82 | 120.30 |
| 1 | D | 447 | ASP | CB-CG-OD1 | 5.05 | 122.84 | 118.30 |
| 1 | A | 962 | TYR | CB-CG-CD1 | -5.04 | 117.97 | 121.00 |
| 1 | A | 892 | ALA | CB-CA-C | 5.04 | 117.66 | 110.10 |
| 1 | C | 509 | ASP | CB-CG-OD1 | 5.03 | 122.83 | 118.30 |
| 1 | D | 82 | ASP | CB-CG-OD1 | 5.03 | 122.83 | 118.30 |
| 1 | D | 324 | GLU | N-CA-CB | 5.03 | 119.66 | 110.60 |
| 1 | A | 267 | VAL | CG1-CB-CG2 | -5.02 | 102.86 | 110.90 |
| 1 | A | 746 | ASP | CB-CG-OD2 | -5.02 | 113.78 | 118.30 |
| 1 | C | 448 | ARG | NE-CZ-NH2 | -5.02 | 117.79 | 120.30 |
| 1 | B | 334 | GLU | OE1-CD-OE2 | -5.01 | 117.28 | 123.30 |
| 1 | B | 659 | ASP | CB-CG-OD2 | -5.01 | 113.79 | 118.30 |
| 1 | D | 559 | TYR | CB-CG-CD1 | 5.01 | 124.01 | 121.00 |
| 1 | C | 838 | THR | CA-CB-CG2 | -5.01 | 105.39 | 112.40 |
| 1 | D | 100 | TYR | N-CA-CB | 5.00 | 119.61 | 110.60 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | C | 733 | ALA | CA |

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 8119 | 0 | 7710 | 160 | 0 |
| 1 | B | 8114 | 0 | 7705 | 173 | 0 |
| 1 | C | 8095 | 0 | 7681 | 156 | 0 |
| 1 | D | 8103 | 0 | 7692 | 154 | 0 |
| 2 | A | 3 | 0 | 0 | 0 | 0 |
| 2 | B | 2 | 0 | 0 | 0 | 0 |
| 2 | C | 4 | 0 | 0 | 0 | 0 |
| 2 | D | 3 | 0 | 0 | 0 | 0 |
| 3 | A | 4 | 0 | 0 | 0 | 0 |
| 3 | B | 4 | 0 | 0 | 0 | 0 |
| 3 | C | 4 | 0 | 0 | 0 | 0 |
| 3 | D | 4 | 0 | 0 | 0 | 0 |
| 4 | A | 88 | 0 | 132 | 19 | 0 |
| 4 | B | 72 | 0 | 108 | 7 | 0 |
| 4 | C | 84 | 0 | 126 | 17 | 0 |
| 4 | D | 96 | 0 | 144 | 15 | 0 |
| 5 | A | 916 | 0 | 0 | 20 | 0 |
| 5 | B | 985 | 0 | 0 | 15 | 0 |
| 5 | C | 935 | 0 | 0 | 14 | 0 |
| 5 | D | 984 | 0 | 0 | 17 | 0 |
| All | All | 36619 | 0 | 31298 | 645 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (645) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 4:B:8601:DMS:C2 | 4:B:8601:DMS:S | 2.03 | 1.47 |
| 1:B:376:ILE:HA | 1:B:379:MET:HE2 | 1.26 | 1.12 |
| 1:C:649:ASN:HA | 4:C:8425:DMS:H12 | 1.37 | 1.06 |
| 1:B:232:ASN:ND2 | 1:B:237:ARG:HG3 | 1.84 | 0.92 |
| 1:B:651:LEU:CD2 | 1:B:701:VAL:HB | 2.01 | 0.91 |
| 1:B:599:ARG:HG3 | 1:B:599:ARG:HH11 | 1.39 | 0.88 |
| 1:B:684:GLU:O | 1:B:686:PRO:HD3 | 1.74 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:755:ARG:HD2 | 5:A:9418:HOH:O | 1.75 | 0.86 |
| 1:D:1017:GLN:HG2 | 1:D:1018:LEU:N | 1.90 | 0.86 |
| 1:B:376:ILE:HA | 1:B:379:MET:CE | 2.07 | 0.84 |
| 1:C:808:GLU:HA | 1:C:811:LYS:HZ3 | 1.42 | 0.84 |
| 1:D:829:THR:O | 1:D:830:LEU:HD23 | 1.78 | 0.84 |
| 1:A:600:GLN:H | 1:A:600:GLN:HE21 | 1.26 | 0.83 |
| 1:B:13:ARG:HG3 | 1:C:13:ARG:CZ | 2.08 | 0.83 |
| 1:B:13:ARG:HG3 | 1:C:13:ARG:NH2 | 1.92 | 0.83 |
| 1:B:600:GLN:H | 1:B:600:GLN:HE21 | 1.24 | 0.83 |
| 1:C:687:GLN:HB3 | 1:C:688:PRO:HD2 | 1.60 | 0.82 |
| 1:D:858:ILE:CD1 | 1:D:864:MET:HG3 | 2.09 | 0.82 |
| 1:B:847:LYS:HD3 | 1:B:849:LEU:HD23 | 1.63 | 0.81 |
| 1:C:367:MET:HB3 | 1:C:372:MET:HE2 | 1.62 | 0.81 |
| 1:D:807:VAL:O | 1:D:811:LYS:HD3 | 1.79 | 0.81 |
| 1:B:599:ARG:HG3 | 1:B:599:ARG:NH1 | 1.89 | 0.81 |
| 1:D:316:HIS:HA | 1:D:323:ILE:HD12 | 1.63 | 0.80 |
| 1:C:703:PRO:HG2 | 4:C:8425:DMS:H13 | 1.64 | 0.80 |
| 1:D:787:ALA:HA | 1:D:968:MET:HE2 | 1.64 | 0.80 |
| 1:A:655:MET:HE2 | 1:A:662:PRO:HA | 1.62 | 0.80 |
| 1:A:653:HIS:CD2 | 1:A:667:GLU:HG3 | 2.17 | 0.79 |
| 1:B:651:LEU:O | 1:B:651:LEU:HD23 | 1.82 | 0.79 |
| 1:A:843:GLN:HG3 | 1:A:848:THR:HA | 1.63 | 0.79 |
| 1:D:843:GLN:HG2 | 1:D:848:THR:HA | 1.64 | 0.79 |
| 1:C:808:GLU:HA | 1:C:811:LYS:NZ | 1.96 | 0.79 |
| 1:D:634:GLN:HB2 | 1:D:682:LEU:HB2 | 1.64 | 0.78 |
| 1:C:765:LEU:HD21 | 1:C:768:MET:CE | 2.13 | 0.78 |
| 1:C:809:ARG:NH1 | 1:C:877:PRO:HB3 | 1.99 | 0.78 |
| 1:A:930:VAL:HA | 1:A:973:ARG:HD3 | 1.66 | 0.78 |
| 1:B:379:MET:HE3 | 1:B:407:LEU:HD11 | 1.66 | 0.77 |
| 1:B:1022:GLN:HG3 | 1:B:1023:LYS:O | 1.85 | 0.77 |
| 1:A:863:GLN:CG | 1:A:1021:CYS:HB3 | 2.14 | 0.77 |
| 1:B:678:GLN:NE2 | 1:B:680:ILE:HD11 | 1.99 | 0.77 |
| 1:C:745:MET:HG2 | 5:C:9388:HOH:O | 1.83 | 0.77 |
| 1:C:746:ASP:HA | 1:C:760:ARG:HG3 | 1.67 | 0.77 |
| 1:C:703:PRO:HD2 | 4:C:8425:DMS:H11 | 1.66 | 0.76 |
| 1:C:599:ARG:HG3 | 1:C:600:GLN:OE1 | 1.85 | 0.76 |
| 1:A:634:GLN:HB3 | 1:A:682:LEU:HB2 | 1.66 | 0.76 |
| 1:C:78:LEU:HD22 | 1:C:80:GLU:OE1 | 1.86 | 0.76 |
| 1:D:858:ILE:HD11 | 1:D:864:MET:HG3 | 1.65 | 0.76 |
| 4:A:8416:DMS:H11 | 5:A:9210:HOH:O | 1.86 | 0.75 |
| 5:C:9488:HOH:O | 1:D:530:THR:HG22 | 1.87 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:679:LEU:C | 1:B:680:ILE:HD12 | 2.07 | 0.75 |
| 1:B:651:LEU:HD21 | 1:B:701:VAL:HB | 1.69 | 0.75 |
| 1:B:986:ILE:CD1 | 1:B:1018:LEU:HD21 | 2.17 | 0.75 |
| 1:D:685:LEU:HD23 | 1:D:686:PRO:HD2 | 1.68 | 0.74 |
| 1:C:684:GLU:OE2 | 1:C:686:PRO:HB3 | 1.88 | 0.74 |
| 1:C:649:ASN:HA | 4:C:8425:DMS:C1 | 2.17 | 0.74 |
| 1:C:599:ARG:NH2 | 1:C:795:VAL:HB | 2.03 | 0.73 |
| 1:C:835:LEU:HD11 | 1:C:855:THR:HB | 1.70 | 0.73 |
| 1:B:679:LEU:O | 1:B:680:ILE:HD12 | 1.89 | 0.73 |
| 1:A:277:GLU:H | 1:A:277:GLU:CD | 1.90 | 0.73 |
| 1:B:687:GLN:HE21 | 1:B:687:GLN:N | 1.85 | 0.73 |
| 1:A:243:GLU:OE2 | 1:A:245:GLN:NE2 | 2.21 | 0.73 |
| 1:A:241:GLU:OE1 | 1:A:292:ARG:NE | 2.21 | 0.73 |
| 1:D:360:HIS:CE1 | 1:D:362:LEU:HB2 | 2.24 | 0.73 |
| 1:B:658:LEU:O | 1:B:661:LYS:HD2 | 1.88 | 0.73 |
| 1:B:745:MET:H | 1:B:745:MET:CE | 2.02 | 0.73 |
| 1:A:32:PRO:HB2 | 4:A:8404:DMS:H13 | 1.71 | 0.72 |
| 1:A:583:ASN:OD1 | 1:A:584:PRO:HD2 | 1.89 | 0.72 |
| 1:B:634:GLN:HG3 | 1:B:682:LEU:HB2 | 1.71 | 0.72 |
| 1:B:890:GLN:HG3 | 1:B:891:VAL:N | 2.03 | 0.71 |
| 1:C:770:ILE:HD12 | 1:C:775:GLN:CD | 2.10 | 0.71 |
| 1:D:664:ALA:HB3 | 1:D:685:LEU:HD21 | 1.71 | 0.71 |
| 1:C:745:MET:HA | 1:C:745:MET:CE | 2.20 | 0.71 |
| 4:D:8421:DMS:H11 | 5:D:9329:HOH:O | 1.90 | 0.71 |
| 1:C:802:ASP:OD1 | 1:C:804:ASN:HB2 | 1.90 | 0.71 |
| 1:D:651:LEU:HD13 | 1:D:651:LEU:C | 2.11 | 0.71 |
| 1:A:746:ASP:HB2 | 5:A:9486:HOH:O | 1.90 | 0.71 |
| 1:B:278:ILE:HD12 | 5:B:9153:HOH:O | 1.92 | 0.70 |
| 1:C:765:LEU:HD21 | 1:C:768:MET:HE2 | 1.72 | 0.70 |
| 1:B:1022:GLN:HG3 | 1:B:1023:LYS:N | 2.04 | 0.70 |
| 1:D:843:GLN:CG | 1:D:848:THR:HA | 2.22 | 0.70 |
| 1:B:319:ASP:OD1 | 1:B:321:THR:N | 2.22 | 0.70 |
| 1:A:651:LEU:CD1 | 1:A:667:GLU:HG2 | 2.22 | 0.69 |
| 1:B:772:ASP:OD1 | 1:B:773:LYS:HD3 | 1.92 | 0.69 |
| 1:B:655:MET:CE | 1:B:662:PRO:HB3 | 2.22 | 0.69 |
| 1:A:737:ILE:O | 1:A:737:ILE:HD13 | 1.91 | 0.69 |
| 4:C:8410:DMS:H13 | 5:C:8970:HOH:O | 1.91 | 0.69 |
| 1:A:80:GLU:OE1 | 1:A:80:GLU:N | 2.23 | 0.69 |
| 1:A:863:GLN:HG3 | 1:A:1021:CYS:HB3 | 1.74 | 0.69 |
| 4:C:8413:DMS:H12 | 5:C:9181:HOH:O | 1.93 | 0.68 |
| 1:B:739:HIS:ND1 | 1:B:750:GLU:OE1 | 2.26 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:8411:DMS:H21 | 5:B:9552:HOH:O | 1.92 | 0.68 |
| 1:D:634:GLN:NE2 | 1:D:682:LEU:O | 2.26 | 0.68 |
| 1:D:134:LEU:HA | 4:D:8705:DMS:H22 | 1.74 | 0.68 |
| 1:D:952:ARG:O | 1:D:1018:LEU:HD22 | 1.93 | 0.68 |
| 1:D:360:HIS:HE1 | 1:D:362:LEU:HB2 | 1.58 | 0.68 |
| 1:D:595:THR:HA | 1:D:596:PRO:C | 2.13 | 0.68 |
| 1:C:684:GLU:O | 1:C:684:GLU:HG3 | 1.94 | 0.68 |
| 1:D:135:GLN:C | 1:D:136:GLU:HG2 | 2.13 | 0.68 |
| 1:D:133:TRP:HE1 | 4:D:8703:DMS:H23 | 1.57 | 0.68 |
| 1:B:654:TRP:CZ3 | 1:B:665:SER:HA | 2.29 | 0.68 |
| 1:A:749:ILE:HD12 | 1:A:749:ILE:N | 2.09 | 0.67 |
| 1:C:703:PRO:HG2 | 4:C:8425:DMS:C1 | 2.24 | 0.67 |
| 1:B:634:GLN:HG2 | 1:B:682:LEU:O | 1.94 | 0.67 |
| 1:B:687:GLN:N | 1:B:687:GLN:NE2 | 2.43 | 0.67 |
| 1:C:730:LEU:N | 1:C:730:LEU:HD23 | 2.09 | 0.67 |
| 1:A:494:THR:HB | 1:D:473:ARG:NH2 | 2.10 | 0.67 |
| 1:A:32:PRO:HB2 | 4:A:8404:DMS:C1 | 2.25 | 0.66 |
| 1:A:473:ARG:NH1 | 1:A:476:LYS:HB2 | 2.11 | 0.66 |
| 1:D:887:GLN:NE2 | 1:D:980:GLU:O | 2.28 | 0.66 |
| 1:A:1022:GLN:HG2 | 1:A:1023:LYS:H | 1.60 | 0.66 |
| 1:D:230:ARG:HD3 | 5:D:9609:HOH:O | 1.95 | 0.66 |
| 1:A:887:GLN:NE2 | 1:A:980:GLU:O | 2.26 | 0.66 |
| 1:D:687:GLN:OE1 | 1:D:688:PRO:HD2 | 1.95 | 0.66 |
| 1:C:890:GLN:HG3 | 1:C:891:VAL:N | 2.11 | 0.65 |
| 1:D:117:GLU:HB2 | 5:D:9146:HOH:O | 1.96 | 0.65 |
| 1:A:847:LYS:NZ | 5:A:9292:HOH:O | 2.30 | 0.65 |
| 1:B:678:GLN:HE21 | 1:B:680:ILE:HD11 | 1.61 | 0.65 |
| 1:D:237:ARG:NH1 | 5:D:9254:HOH:O | 2.29 | 0.65 |
| 1:D:658:LEU:O | 1:D:661:LYS:HG3 | 1.96 | 0.64 |
| 1:D:579:ASP:HA | 5:D:9220:HOH:O | 1.97 | 0.64 |
| 1:A:863:GLN:HG2 | 1:A:1021:CYS:HB3 | 1.78 | 0.64 |
| 1:B:986:ILE:HD13 | 1:B:1018:LEU:HD21 | 1.78 | 0.64 |
| 1:C:599:ARG:NH1 | 5:C:8969:HOH:O | 2.30 | 0.64 |
| 1:C:599:ARG:HH21 | 1:C:795:VAL:CG1 | 2.11 | 0.64 |
| 1:A:106:PRO:O | 4:A:8410:DMS:H22 | 1.99 | 0.63 |
| 1:A:630:ARG:HA | 4:A:8503:DMS:O | 1.98 | 0.63 |
| 1:B:847:LYS:HD3 | 1:B:849:LEU:CD2 | 2.27 | 0.63 |
| 1:D:858:ILE:HD12 | 1:D:864:MET:HG3 | 1.79 | 0.63 |
| 1:A:579:ASP:O | 1:A:582:GLY:N | 2.26 | 0.63 |
| 1:C:878:HIS:HD2 | 5:C:8701:HOH:O | 1.79 | 0.63 |
| 1:A:832:ASP:OD1 | 1:A:832:ASP:N | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:334:GLU:OE1 | 1:D:336:ARG:NH1 | 2.29 | 0.63 |
| 1:D:859:ASP:CG | 1:D:861:SER:H | 2.02 | 0.62 |
| 1:B:730:LEU:CB | 1:B:731:PRO:HD2 | 2.29 | 0.62 |
| 1:C:367:MET:HB3 | 1:C:372:MET:CE | 2.28 | 0.62 |
| 1:D:859:ASP:OD2 | 1:D:861:SER:N | 2.29 | 0.62 |
| 1:B:655:MET:HE3 | 1:B:662:PRO:HB3 | 1.80 | 0.62 |
| 1:D:878:HIS:HD2 | 5:D:8818:HOH:O | 1.83 | 0.62 |
| 1:A:112:PRO:HD2 | 1:A:113:PHE:CE1 | 2.33 | 0.62 |
| 1:C:360:HIS:CE1 | 1:C:362:LEU:HB2 | 2.35 | 0.62 |
| 1:C:830:LEU:N | 1:C:830:LEU:HD23 | 2.14 | 0.61 |
| 1:A:777:LEU:CD1 | 1:A:980:GLU:HG2 | 2.30 | 0.61 |
| 1:B:746:ASP:OD1 | 1:B:757:GLN:NE2 | 2.34 | 0.61 |
| 1:A:800:ARG:HD3 | 1:A:801:ILE:N | 2.15 | 0.61 |
| 1:B:730:LEU:HB2 | 1:B:731:PRO:HD2 | 1.83 | 0.61 |
| 1:D:577:LYS:O | 1:D:584:PRO:HA | 2.01 | 0.61 |
| 1:B:434:PRO:HB3 | 1:C:434:PRO:HB3 | 1.82 | 0.61 |
| 1:B:890:GLN:CG | 1:B:891:VAL:N | 2.63 | 0.61 |
| 1:D:829:THR:C | 1:D:830:LEU:HD23 | 2.20 | 0.61 |
| 1:D:46:ARG:HB3 | 1:D:47:PRO:HD2 | 1.82 | 0.60 |
| 1:B:986:ILE:HD11 | 1:B:1018:LEU:HD21 | 1.82 | 0.60 |
| 1:D:681:GLU:HG2 | 5:D:9421:HOH:O | 1.99 | 0.60 |
| 1:D:237:ARG:HH11 | 1:D:237:ARG:HG2 | 1.66 | 0.60 |
| 1:A:660:GLY:O | 1:A:662:PRO:HD3 | 2.02 | 0.60 |
| 1:B:277:GLU:HG2 | 5:B:9401:HOH:O | 2.01 | 0.60 |
| 1:D:438:GLU:HG2 | 1:D:442:ARG:HD2 | 1.83 | 0.60 |
| 1:C:651:LEU:HD12 | 1:C:701:VAL:O | 2.01 | 0.60 |
| 1:B:685:LEU:O | 1:B:687:GLN:NE2 | 2.35 | 0.60 |
| 1:C:684:GLU:O | 1:C:686:PRO:HD3 | 2.01 | 0.60 |
| 1:C:743:SER:O | 1:C:760:ARG:NH1 | 2.27 | 0.60 |
| 1:B:379:MET:CE | 1:B:407:LEU:HD11 | 2.32 | 0.60 |
| 1:A:135:GLN:NE2 | 5:A:9437:HOH:O | 2.35 | 0.59 |
| 1:D:126:THR:CG2 | 1:D:181:GLU:HG2 | 2.32 | 0.59 |
| 1:D:133:TRP:HE1 | 4:D:8703:DMS:C2 | 2.15 | 0.59 |
| 1:B:878:HIS:HD2 | 5:B:8690:HOH:O | 1.85 | 0.59 |
| 1:D:73:TRP:CE2 | 1:D:122:CYS:HB3 | 2.37 | 0.59 |
| 1:A:878:HIS:CE1 | 1:A:1010:SER:HB3 | 2.38 | 0.59 |
| 4:D:8703:DMS:H23 | 5:D:9600:HOH:O | 2.03 | 0.59 |
| 1:A:655:MET:HE1 | 1:A:662:PRO:HB3 | 1.85 | 0.59 |
| 1:A:890:GLN:HG3 | 1:A:891:VAL:N | 2.18 | 0.59 |
| 1:B:387:VAL:HG22 | 5:B:9493:HOH:O | 2.02 | 0.59 |
| 1:D:373:VAL:O | 1:D:377:LEU:HG | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:795:VAL:HG12 | 5:B:9500:HOH:O | 2.03 | 0.58 |
| 1:D:379:MET:HE1 | 1:D:407:LEU:HD13 | 1.84 | 0.58 |
| 1:D:770:ILE:HD12 | 1:D:775:GLN:CD | 2.23 | 0.58 |
| 1:A:655:MET:HG2 | 5:A:8968:HOH:O | 2.01 | 0.58 |
| 1:D:237:ARG:HH11 | 1:D:237:ARG:CG | 2.16 | 0.58 |
| 1:C:278:ILE:HD13 | 1:C:278:ILE:N | 2.16 | 0.58 |
| 1:C:595:THR:HA | 1:C:596:PRO:C | 2.24 | 0.58 |
| 1:C:296:GLU:HA | 1:C:296:GLU:OE1 | 2.02 | 0.58 |
| 1:B:597:ASN:OD1 | 1:B:599:ARG:HD3 | 2.04 | 0.58 |
| 1:D:68:ALA:O | 1:D:70:PRO:HD3 | 2.03 | 0.58 |
| 1:C:599:ARG:HH21 | 1:C:795:VAL:HB | 1.68 | 0.58 |
| 1:D:859:ASP:OD2 | 1:D:861:SER:HB3 | 2.03 | 0.58 |
| 1:C:599:ARG:HG3 | 1:C:600:GLN:H | 1.69 | 0.57 |
| 1:C:734:SER:CB | 1:C:860:GLY:HA3 | 2.34 | 0.57 |
| 1:D:126:THR:HG23 | 1:D:181:GLU:HG2 | 1.86 | 0.57 |
| 1:A:347:LYS:HE3 | 5:A:9435:HOH:O | 2.04 | 0.57 |
| 1:A:683:PRO:O | 1:A:685:LEU:HG | 2.04 | 0.57 |
| 1:C:745:MET:HA | 1:C:745:MET:HE3 | 1.86 | 0.57 |
| 1:C:824:GLN:O | 1:C:838:THR:HA | 2.04 | 0.57 |
| 1:C:688:PRO:HG3 | 1:C:694:LEU:HD11 | 1.86 | 0.57 |
| 1:A:473:ARG:HH11 | 1:A:476:LYS:HB2 | 1.69 | 0.57 |
| 1:A:494:THR:CB | 1:D:473:ARG:HH22 | 2.17 | 0.57 |
| 1:B:245:GLN:HG2 | 1:B:288:ARG:HG2 | 1.86 | 0.57 |
| 1:A:777:LEU:HD11 | 1:A:980:GLU:HG2 | 1.85 | 0.57 |
| 1:D:805:ALA:O | 1:D:809:ARG:HG3 | 2.05 | 0.57 |
| 1:C:765:LEU:HD21 | 1:C:768:MET:HE1 | 1.85 | 0.57 |
| 1:B:236:SER:C | 1:B:237:ARG:HG2 | 2.25 | 0.56 |
| 1:D:710:GLU:HG2 | 5:D:9085:HOH:O | 2.05 | 0.56 |
| 1:A:730:LEU:HD21 | 1:B:823:LEU:HB3 | 1.87 | 0.56 |
| 1:B:431:ARG:HG2 | 5:C:9420:HOH:O | 2.05 | 0.56 |
| 1:B:678:GLN:HG2 | 1:B:680:ILE:CD1 | 2.34 | 0.56 |
| 1:C:240:LEU:C | 1:C:240:LEU:HD23 | 2.25 | 0.56 |
| 1:C:615:PRO:O | 1:C:618:THR:HG22 | 2.05 | 0.56 |
| 1:C:730:LEU:CB | 1:C:731:PRO:HD2 | 2.35 | 0.56 |
| 1:A:595:THR:HA | 1:A:596:PRO:C | 2.24 | 0.56 |
| 1:B:377:LEU:HD22 | 1:B:708:TRP:HA | 1.88 | 0.56 |
| 1:B:876:THR:OG1 | 1:B:877:PRO:HD2 | 2.06 | 0.56 |
| 1:C:757:GLN:OE1 | 1:C:769:TRP:HH2 | 1.87 | 0.56 |
| 1:B:637:GLU:CD | 1:B:677:LYS:HE2 | 2.25 | 0.55 |
| 1:C:317:THR:OG1 | 1:C:319:ASP:OD1 | 2.24 | 0.55 |
| 1:D:890:GLN:HG3 | 1:D:891:VAL:N | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1022:GLN:HG3 | 1:D:1023:LYS:N | 2.01 | 0.55 |
| 1:B:78:LEU:HB3 | 1:B:80:GLU:CG | 2.36 | 0.55 |
| 1:C:805:ALA:HB3 | 1:C:808:GLU:HG2 | 1.89 | 0.55 |
| 1:B:655:MET:HE1 | 1:B:662:PRO:HB3 | 1.88 | 0.55 |
| 1:B:890:GLN:HG2 | 5:B:9553:HOH:O | 2.06 | 0.55 |
| 1:C:991:MET:HE2 | 1:C:1003:VAL:HG21 | 1.89 | 0.55 |
| 1:B:363:HIS:HD2 | 5:B:9171:HOH:O | 1.89 | 0.55 |
| 1:C:809:ARG:CZ | 1:C:877:PRO:HB3 | 2.36 | 0.54 |
| 4:D:8406:DMS:O | 5:D:9596:HOH:O | 2.18 | 0.54 |
| 1:A:32:PRO:HB3 | 4:A:8404:DMS:H11 | 1.88 | 0.54 |
| 1:C:745:MET:HA | 1:C:745:MET:HE2 | 1.88 | 0.54 |
| 1:D:433:LEU:HB3 | 1:D:434:PRO:HD3 | 1.89 | 0.54 |
| 1:A:494:THR:HB | 1:D:473:ARG:HH22 | 1.72 | 0.54 |
| 1:C:646:HIS:CE1 | 1:C:673:ALA:HB2 | 2.42 | 0.54 |
| 1:D:292:ARG:HH12 | 4:D:8412:DMS:C2 | 2.19 | 0.54 |
| 1:B:655:MET:SD | 1:B:656:VAL:N | 2.80 | 0.54 |
| 1:C:360:HIS:HE1 | 1:C:362:LEU:HB2 | 1.71 | 0.54 |
| 1:A:32:PRO:CB | 4:A:8404:DMS:H11 | 2.37 | 0.54 |
| 1:A:703:PRO:HG2 | 4:A:8425:DMS:H11 | 1.90 | 0.54 |
| 1:A:878:HIS:HD2 | 5:A:8676:HOH:O | 1.90 | 0.54 |
| 1:D:114:VAL:HB | 1:D:115:PRO:HD2 | 1.90 | 0.54 |
| 1:A:648:ASP:OD2 | 5:A:9405:HOH:O | 2.19 | 0.54 |
| 1:A:817:GLN:HG2 | 5:A:8938:HOH:O | 2.08 | 0.54 |
| 4:A:8502:DMS:H12 | 5:A:9284:HOH:O | 2.07 | 0.54 |
| 1:D:951:TRP:HB3 | 1:D:1018:LEU:HD11 | 1.89 | 0.54 |
| 1:B:859:ASP:OD1 | 1:B:861:SER:OG | 2.23 | 0.54 |
| 1:D:843:GLN:HG2 | 1:D:848:THR:CA | 2.36 | 0.53 |
| 1:A:237:ARG:HG2 | 1:A:296:GLU:OE1 | 2.08 | 0.53 |
| 1:A:863:GLN:HG3 | 1:A:1021:CYS:CB | 2.38 | 0.53 |
| 1:B:945:ASN:HB3 | 1:B:1023:LYS:HE2 | 1.89 | 0.53 |
| 1:B:687:GLN:HE21 | 1:B:687:GLN:H | 1.53 | 0.53 |
| 1:C:778:THR:HG23 | 1:C:887:GLN:HB3 | 1.90 | 0.53 |
| 1:D:237:ARG:NH1 | 1:D:237:ARG:HG2 | 2.23 | 0.53 |
| 1:B:615:PRO:O | 1:B:618:THR:HG22 | 2.08 | 0.53 |
| 1:D:379:MET:HE2 | 1:D:407:LEU:HD11 | 1.91 | 0.53 |
| 1:B:70:PRO:HG2 | 1:B:78:LEU:HD21 | 1.91 | 0.53 |
| 1:B:673:ALA:HB1 | 1:B:674:PRO:HD2 | 1.90 | 0.53 |
| 1:C:513:PRO:HG2 | 5:C:8615:HOH:O | 2.08 | 0.53 |
| 1:D:46:ARG:HB3 | 1:D:47:PRO:CD | 2.38 | 0.53 |
| 1:D:292:ARG:HH12 | 4:D:8412:DMS:H21 | 1.74 | 0.53 |
| 1:D:615:PRO:O | 1:D:618:THR:HG22 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:733:ALA:O | 1:B:734:SER:O | 2.28 | 0.52 |
| 1:D:580:GLU:O | 1:D:580:GLU:OE1 | 2.27 | 0.52 |
| 1:D:687:GLN:CD | 1:D:688:PRO:HD2 | 2.30 | 0.52 |
| 1:A:783:GLN:HG2 | 1:A:881:ARG:HD2 | 1.90 | 0.52 |
| 1:A:809:ARG:HH21 | 1:A:877:PRO:HB3 | 1.74 | 0.52 |
| 1:B:78:LEU:HB3 | 1:B:80:GLU:HG3 | 1.92 | 0.52 |
| 1:D:237:ARG:NH1 | 1:D:296:GLU:OE1 | 2.43 | 0.52 |
| 1:A:107:ILE:HG22 | 4:A:8410:DMS:H22 | 1.91 | 0.52 |
| 1:B:317:THR:OG1 | 1:B:319:ASP:OD1 | 2.27 | 0.52 |
| 1:B:658:LEU:HD21 | 1:B:690:SER:HB3 | 1.92 | 0.52 |
| 1:B:748:CYS:C | 1:B:749:ILE:HD12 | 2.31 | 0.52 |
| 1:C:599:ARG:NH2 | 1:C:795:VAL:CB | 2.72 | 0.52 |
| 1:C:730:LEU:HB3 | 1:C:731:PRO:HD2 | 1.91 | 0.52 |
| 1:D:708:TRP:CZ2 | 4:D:8403:DMS:H12 | 2.45 | 0.52 |
| 1:C:930:VAL:HA | 1:C:973:ARG:HD3 | 1.91 | 0.52 |
| 1:C:703:PRO:CD | 4:C:8425:DMS:H11 | 2.40 | 0.51 |
| 1:A:32:PRO:CB | 4:A:8404:DMS:C1 | 2.88 | 0.51 |
| 1:B:595:THR:HA | 1:B:596:PRO:C | 2.31 | 0.51 |
| 1:D:299:LYS:NZ | 5:D:9387:HOH:O | 2.23 | 0.51 |
| 1:A:533:LEU:C | 1:A:533:LEU:HD23 | 2.30 | 0.51 |
| 1:B:749:ILE:HD12 | 1:B:749:ILE:N | 2.25 | 0.51 |
| 1:A:637:GLU:OE2 | 1:A:677:LYS:HE3 | 2.10 | 0.51 |
| 1:B:59:ARG:NH2 | 1:B:81:ALA:HB3 | 2.25 | 0.51 |
| 1:B:240:LEU:C | 1:B:240:LEU:HD23 | 2.30 | 0.51 |
| 1:A:742:THR:HG22 | 1:A:743:SER:N | 2.24 | 0.51 |
| 1:B:632:SER:O | 1:B:635:THR:N | 2.37 | 0.51 |
| 1:D:729:THR:HG23 | 5:D:9324:HOH:O | 2.11 | 0.51 |
| 1:B:296:GLU:OE1 | 1:B:296:GLU:HA | 2.11 | 0.51 |
| 1:D:773:LYS:HG2 | 1:D:775:GLN:NE2 | 2.26 | 0.51 |
| 1:B:631:LEU:HD12 | 1:B:635:THR:O | 2.11 | 0.50 |
| 1:C:637:GLU:OE2 | 1:C:677:LYS:NZ | 2.42 | 0.50 |
| 1:D:653:HIS:ND1 | 1:D:701:VAL:HG21 | 2.26 | 0.50 |
| 1:B:542:MET:HA | 1:B:604:ASN:HA | 1.93 | 0.50 |
| 1:D:1022:GLN:HG3 | 1:D:1023:LYS:HG2 | 1.91 | 0.50 |
| 1:A:252:ASP:OD1 | 4:A:8416:DMS:H11 | 2.11 | 0.50 |
| 1:A:378:LEU:HD11 | 5:A:8867:HOH:O | 2.11 | 0.50 |
| 1:C:764:PHE:CE1 | 1:C:781:ARG:NH1 | 2.80 | 0.50 |
| 1:A:673:ALA:HB1 | 1:A:674:PRO:HD2 | 1.92 | 0.50 |
| 1:C:833:ALA:HB1 | 1:C:858:ILE:O | 2.11 | 0.50 |
| 1:D:114:VAL:HB | 1:D:115:PRO:CD | 2.42 | 0.50 |
| 1:A:890:GLN:CG | 1:A:891:VAL:N | 2.75 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:375:ASP:O | 1:B:379:MET:HG3 | 2.12 | 0.50 |
| 1:C:127:PHE:CE2 | 1:C:184:LEU:HG | 2.47 | 0.50 |
| 1:A:86:VAL:HG13 | 1:A:87:PRO:HA | 1.93 | 0.50 |
| 1:A:88:SER:HA | 1:A:366:VAL:HG21 | 1.94 | 0.50 |
| 1:B:763:GLY:HA3 | 1:B:822:LEU:HD13 | 1.94 | 0.50 |
| 1:C:88:SER:HA | 1:C:366:VAL:HG21 | 1.92 | 0.50 |
| 1:A:45:ASP:OD2 | 5:A:9168:HOH:O | 2.20 | 0.50 |
| 1:C:673:ALA:HB1 | 1:C:674:PRO:HD2 | 1.94 | 0.50 |
| 1:C:699:ARG:NH2 | 5:C:9404:HOH:O | 2.45 | 0.50 |
| 1:A:662:PRO:O | 1:A:663:LEU:HD23 | 2.12 | 0.50 |
| 1:B:16:TRP:CG | 1:B:189:LEU:CD1 | 2.94 | 0.50 |
| 1:A:559:TYR:CE2 | 1:B:522:LYS:HA | 2.47 | 0.49 |
| 1:A:737:ILE:HD13 | 1:A:737:ILE:C | 2.31 | 0.49 |
| 1:A:764:PHE:CE1 | 1:A:781:ARG:NH1 | 2.80 | 0.49 |
| 1:B:777:LEU:HG | 1:B:889:ALA:HA | 1.94 | 0.49 |
| 1:A:655:MET:CE | 1:A:662:PRO:HA | 2.37 | 0.49 |
| 1:A:1022:GLN:CG | 1:A:1023:LYS:H | 2.24 | 0.49 |
| 1:D:318:ALA:HB3 | 5:D:9568:HOH:O | 2.12 | 0.49 |
| 1:A:703:PRO:HG2 | 4:A:8425:DMS:C1 | 2.43 | 0.49 |
| 1:D:411:ASP:OD2 | 1:D:447:ASP:OD2 | 2.30 | 0.49 |
| 1:A:851:ILE:O | 1:A:870:VAL:HA | 2.13 | 0.49 |
| 1:C:777:LEU:HG | 1:C:889:ALA:HA | 1.95 | 0.49 |
| 1:C:847:LYS:HE2 | 5:C:9333:HOH:O | 2.12 | 0.49 |
| 1:D:651:LEU:HD12 | 1:D:653:HIS:CE1 | 2.47 | 0.49 |
| 1:B:807:VAL:CG1 | 1:B:808:GLU:N | 2.75 | 0.49 |
| 1:A:633:GLY:O | 1:A:634:GLN:OE1 | 2.30 | 0.49 |
| 1:B:499:ILE:HG22 | 1:B:501:PRO:HD3 | 1.95 | 0.48 |
| 1:D:73:TRP:CZ2 | 1:D:122:CYS:HB3 | 2.47 | 0.48 |
| 1:D:240:LEU:HD23 | 1:D:240:LEU:C | 2.33 | 0.48 |
| 1:D:379:MET:HE1 | 1:D:407:LEU:CD1 | 2.42 | 0.48 |
| 1:D:651:LEU:CD1 | 1:D:653:HIS:CE1 | 2.97 | 0.48 |
| 1:C:734:SER:HB3 | 1:C:860:GLY:HA3 | 1.96 | 0.48 |
| 1:C:599:ARG:HH21 | 1:C:795:VAL:CB | 2.25 | 0.48 |
| 1:C:819:GLU:H | 1:C:819:GLU:HG2 | 1.45 | 0.48 |
| 1:D:687:GLN:CG | 1:D:688:PRO:HD2 | 2.43 | 0.48 |
| 1:A:59:ARG:HG2 | 4:A:8502:DMS:C1 | 2.43 | 0.48 |
| 1:D:60:PHE:HA | 1:D:122:CYS:O | 2.14 | 0.48 |
| 1:A:16:TRP:CG | 1:A:189:LEU:HD13 | 2.49 | 0.48 |
| 1:C:79:PRO:HD2 | 1:C:80:GLU:OE2 | 2.14 | 0.48 |
| 1:C:811:LYS:NZ | 1:C:811:LYS:HB2 | 2.29 | 0.48 |
| 1:D:682:LEU:C | 1:D:683:PRO:O | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:340:GLY:O | 1:D:561:ARG:HG2 | 2.14 | 0.48 |
| 1:B:730:LEU:H | 1:B:730:LEU:HG | 1.50 | 0.48 |
| 1:B:878:HIS:CE1 | 1:B:1010:SER:HB3 | 2.49 | 0.48 |
| 1:C:887:GLN:NE2 | 1:C:980:GLU:O | 2.46 | 0.48 |
| 1:C:919:ASP:O | 1:C:920:LEU:HD23 | 2.14 | 0.48 |
| 1:D:660:GLY:O | 1:D:662:PRO:HD3 | 2.14 | 0.48 |
| 1:A:600:GLN:HE21 | 1:A:600:GLN:N | 2.03 | 0.48 |
| 1:A:735:HIS:CD2 | 1:A:735:HIS:N | 2.81 | 0.48 |
| 1:C:651:LEU:HD12 | 1:C:651:LEU:N | 2.28 | 0.48 |
| 1:D:568:TRP:CD2 | 1:D:569:ASP:HB3 | 2.49 | 0.47 |
| 1:B:114:VAL:HB | 1:B:115:PRO:HD2 | 1.95 | 0.47 |
| 1:C:387:VAL:HG22 | 5:C:9470:HOH:O | 2.13 | 0.47 |
| 1:C:651:LEU:HD13 | 1:C:653:HIS:CE1 | 2.50 | 0.47 |
| 1:D:893:GLU:O | 1:D:893:GLU:HG2 | 2.13 | 0.47 |
| 1:C:687:GLN:CB | 1:C:688:PRO:HD2 | 2.32 | 0.47 |
| 1:A:754:LYS:NZ | 5:A:9390:HOH:O | 2.47 | 0.47 |
| 1:A:835:LEU:HD11 | 1:A:855:THR:HB | 1.95 | 0.47 |
| 1:B:645:ARG:NH2 | 1:B:648:ASP:OD1 | 2.47 | 0.47 |
| 1:C:655:MET:O | 1:C:655:MET:HG3 | 2.14 | 0.47 |
| 1:D:379:MET:CE | 1:D:407:LEU:HD11 | 2.45 | 0.47 |
| 1:B:663:LEU:C | 1:B:663:LEU:HD22 | 2.35 | 0.47 |
| 1:C:147:ASN:HA | 1:C:148:SER:HA | 1.64 | 0.47 |
| 1:D:63:PHE:HB3 | 1:D:64:PRO:HD2 | 1.96 | 0.47 |
| 1:A:433:LEU:N | 1:A:434:PRO:CD | 2.77 | 0.47 |
| 1:A:844:HIS:HD2 | 5:A:9350:HOH:O | 1.98 | 0.47 |
| 1:B:568:TRP:CD2 | 1:B:569:ASP:HB3 | 2.49 | 0.47 |
| 1:C:989:PHE:CD1 | 1:C:989:PHE:N | 2.83 | 0.47 |
| 1:D:513:PRO:O | 1:D:514:ALA:HB3 | 2.14 | 0.47 |
| 1:A:241:GLU:OE2 | 1:A:292:ARG:NH2 | 2.48 | 0.47 |
| 1:A:506:VAL:CG1 | 1:A:521:LYS:HE3 | 2.45 | 0.47 |
| 1:A:521:LYS:HE2 | 5:A:9021:HOH:O | 2.13 | 0.47 |
| 1:A:826:THR:OG1 | 1:A:837:THR:HB | 2.15 | 0.47 |
| 1:C:292:ARG:HH12 | 4:C:8412:DMS:C2 | 2.27 | 0.47 |
| 1:C:356:ARG:HD2 | 1:C:379:MET:CE | 2.45 | 0.47 |
| 1:C:568:TRP:CD2 | 1:C:569:ASP:HB3 | 2.50 | 0.47 |
| 1:C:634:GLN:CD | 1:C:634:GLN:H | 2.13 | 0.47 |
| 1:C:778:THR:HG23 | 1:C:887:GLN:OE1 | 2.15 | 0.47 |
| 1:D:664:ALA:HB3 | 1:D:685:LEU:CD2 | 2.40 | 0.47 |
| 1:B:241:GLU:OE1 | 1:B:292:ARG:HG2 | 2.15 | 0.47 |
| 1:C:70:PRO:HG2 | 1:C:78:LEU:HD21 | 1.96 | 0.47 |
| 1:A:369:GLU:O | 1:A:373:VAL:HG23 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:91:GLN:HG3 | 1:B:96:ASP:OD1 | 2.15 | 0.46 |
| 1:B:319:ASP:OD1 | 1:B:320:GLY:N | 2.47 | 0.46 |
| 1:D:133:TRP:NE1 | 4:D:8703:DMS:C2 | 2.78 | 0.46 |
| 1:D:231:PHE:O | 4:D:8417:DMS:H22 | 2.14 | 0.46 |
| 1:B:127:PHE:CE2 | 1:B:184:LEU:HG | 2.50 | 0.46 |
| 1:B:305:ILE:HD11 | 1:B:645:ARG:HB3 | 1.97 | 0.46 |
| 1:B:796:SER:HB3 | 1:B:999:TRP:HB3 | 1.97 | 0.46 |
| 1:D:521:LYS:HE2 | 5:D:9164:HOH:O | 2.15 | 0.46 |
| 1:A:126:THR:HA | 1:A:182:ASN:O | 2.15 | 0.46 |
| 1:A:434:PRO:HB3 | 1:D:434:PRO:HB3 | 1.97 | 0.46 |
| 4:B:8409:DMS:O | 5:B:9107:HOH:O | 2.21 | 0.46 |
| 1:C:599:ARG:NH2 | 1:C:795:VAL:CG1 | 2.78 | 0.46 |
| 1:C:829:THR:C | 1:C:830:LEU:HD23 | 2.35 | 0.46 |
| 1:A:73:TRP:CE2 | 1:A:122:CYS:HB3 | 2.50 | 0.46 |
| 1:C:78:LEU:HB3 | 1:C:80:GLU:CD | 2.35 | 0.46 |
| 1:A:387:VAL:HG22 | 5:A:9450:HOH:O | 2.15 | 0.46 |
| 1:A:809:ARG:NH2 | 1:A:877:PRO:HB3 | 2.30 | 0.46 |
| 1:C:296:GLU:HG2 | 4:C:8601:DMS:C1 | 2.46 | 0.46 |
| 1:C:610:ASP:O | 1:C:611:ARG:HB2 | 2.16 | 0.46 |
| 1:D:843:GLN:HA | 1:D:847:LYS:O | 2.15 | 0.46 |
| 1:D:133:TRP:NE1 | 4:D:8703:DMS:H23 | 2.27 | 0.46 |
| 1:D:858:ILE:CD1 | 1:D:858:ILE:N | 2.79 | 0.46 |
| 1:D:961:ARG:NE | 1:D:981:GLY:O | 2.49 | 0.46 |
| 1:A:59:ARG:HG2 | 4:A:8502:DMS:H11 | 1.97 | 0.46 |
| 1:A:774:LYS:HB2 | 1:A:774:LYS:HE2 | 1.61 | 0.46 |
| 1:B:892:ALA:HB3 | 1:B:946:TYR:CE1 | 2.51 | 0.46 |
| 1:C:718:GLN:HG2 | 4:C:8503:DMS:H11 | 1.98 | 0.46 |
| 1:A:127:PHE:N | 1:A:127:PHE:CD2 | 2.81 | 0.46 |
| 1:A:593:GLY:O | 1:A:595:THR:HG22 | 2.14 | 0.46 |
| 1:C:619:GLU:HG2 | 1:C:909:ARG:HG3 | 1.98 | 0.46 |
| 1:C:651:LEU:HD12 | 1:C:651:LEU:H | 1.80 | 0.46 |
| 1:C:843:GLN:HA | 1:C:847:LYS:O | 2.16 | 0.46 |
| 1:D:986:ILE:HD12 | 1:D:986:ILE:HG21 | 1.49 | 0.46 |
| 1:A:107:ILE:HG22 | 4:A:8410:DMS:C2 | 2.45 | 0.46 |
| 1:A:890:GLN:OE1 | 1:A:948:PRO:HD3 | 2.16 | 0.46 |
| 1:B:637:GLU:OE2 | 1:B:677:LYS:HE2 | 2.15 | 0.46 |
| 1:C:843:GLN:HG2 | 1:C:848:THR:HA | 1.97 | 0.46 |
| 1:D:682:LEU:O | 1:D:683:PRO:O | 2.34 | 0.46 |
| 1:D:736:ALA:HB3 | 1:D:751:LEU:HD11 | 1.98 | 0.46 |
| 1:C:730:LEU:HD23 | 1:C:730:LEU:H | 1.78 | 0.46 |
| 1:A:634:GLN:HE21 | 1:A:685:LEU:HD11 | 1.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:890:GLN:HG3 | 1:A:891:VAL:H | 1.78 | 0.45 |
| 1:B:376:ILE:CA | 1:B:379:MET:HE2 | 2.19 | 0.45 |
| 1:C:266:GLN:NE2 | 4:C:8602:DMS:S | 2.90 | 0.45 |
| 1:D:88:SER:HA | 1:D:366:VAL:HG21 | 1.98 | 0.45 |
| 1:A:290:THR:HB | 4:A:8412:DMS:H22 | 1.98 | 0.45 |
| 1:A:362:LEU:HA | 1:A:362:LEU:HD22 | 1.68 | 0.45 |
| 1:C:16:TRP:CG | 1:C:189:LEU:CD1 | 2.99 | 0.45 |
| 1:C:703:PRO:HD2 | 4:C:8425:DMS:C1 | 2.42 | 0.45 |
| 1:D:80:GLU:H | 1:D:80:GLU:HG3 | 1.58 | 0.45 |
| 1:A:651:LEU:HD13 | 1:A:667:GLU:HG2 | 1.96 | 0.45 |
| 1:A:843:GLN:HG3 | 1:A:848:THR:CA | 2.38 | 0.45 |
| 1:A:580:GLU:O | 1:A:580:GLU:OE1 | 2.35 | 0.45 |
| 1:A:730:LEU:HD12 | 1:A:730:LEU:N | 2.32 | 0.45 |
| 1:A:789:LEU:HD11 | 1:A:993:ILE:HG22 | 1.98 | 0.45 |
| 1:B:100:TYR:CE1 | 1:B:602:CYS:HB3 | 2.51 | 0.45 |
| 1:B:655:MET:SD | 1:B:664:ALA:O | 2.74 | 0.45 |
| 1:C:687:GLN:CB | 1:C:688:PRO:CD | 2.94 | 0.45 |
| 1:D:770:ILE:HD12 | 1:D:775:GLN:NE2 | 2.31 | 0.45 |
| 1:A:268:ALA:HA | 4:A:8602:DMS:H22 | 1.99 | 0.45 |
| 1:A:411:ASP:OD2 | 1:A:447:ASP:OD2 | 2.33 | 0.45 |
| 1:A:646:HIS:NE2 | 1:A:671:ASP:OD2 | 2.44 | 0.45 |
| 1:B:292:ARG:NH1 | 4:B:8412:DMS:C2 | 2.79 | 0.45 |
| 1:B:701:VAL:HG22 | 1:B:714:ILE:HG12 | 1.98 | 0.45 |
| 1:B:731:PRO:HB2 | 1:B:732:ALA:H | 1.64 | 0.45 |
| 1:B:796:SER:OG | 1:B:800:ARG:NH2 | 2.49 | 0.45 |
| 1:C:749:ILE:N | 1:C:749:ILE:HD12 | 2.31 | 0.45 |
| 1:D:105:TYR:O | 4:D:8419:DMS:O | 2.34 | 0.45 |
| 1:D:878:HIS:CE1 | 1:D:1010:SER:HB3 | 2.51 | 0.45 |
| 1:B:85:VAL:HG12 | 1:B:86:VAL:N | 2.28 | 0.45 |
| 1:C:377:LEU:CD2 | 1:C:708:TRP:HA | 2.47 | 0.45 |
| 1:D:441:THR:O | 1:D:445:GLN:HG3 | 2.17 | 0.45 |
| 1:D:833:ALA:HB1 | 1:D:858:ILE:O | 2.16 | 0.45 |
| 1:B:651:LEU:HD23 | 1:B:651:LEU:C | 2.36 | 0.45 |
| 1:D:824:GLN:HB3 | 1:D:839:ALA:HB3 | 1.98 | 0.45 |
| 1:D:844:HIS:O | 1:D:845:GLN:HB2 | 2.17 | 0.45 |
| 1:A:843:GLN:HA | 1:A:847:LYS:O | 2.17 | 0.45 |
| 1:B:379:MET:HE3 | 1:B:407:LEU:CD1 | 2.41 | 0.45 |
| 1:C:100:TYR:CZ | 1:C:602:CYS:HB3 | 2.51 | 0.45 |
| 1:B:678:GLN:HG2 | 1:B:680:ILE:HD11 | 1.99 | 0.45 |
| 1:B:745:MET:N | 1:B:745:MET:SD | 2.88 | 0.45 |
| 1:C:250:LEU:O | 1:C:251:ARG:HD3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:499:ILE:HG22 | 1:C:501:PRO:HD3 | 1.98 | 0.45 |
| 1:B:731:PRO:O | 1:B:732:ALA:HB2 | 2.16 | 0.45 |
| 1:C:569:ASP:O | 1:C:605:GLY:HA2 | 2.17 | 0.45 |
| 1:D:549:PHE:CE2 | 1:D:620:ALA:HA | 2.52 | 0.45 |
| 1:A:338:GLU:OE1 | 5:A:9270:HOH:O | 2.21 | 0.44 |
| 1:B:352:ARG:HG2 | 1:B:553:TRP:CH2 | 2.52 | 0.44 |
| 1:B:668:VAL:HG12 | 1:B:669:PRO:O | 2.17 | 0.44 |
| 1:C:656:VAL:O | 1:C:663:LEU:HB2 | 2.18 | 0.44 |
| 1:D:147:ASN:HA | 1:D:148:SER:HA | 1.68 | 0.44 |
| 1:C:601:PHE:CD1 | 1:C:796:SER:HA | 2.51 | 0.44 |
| 1:C:785:THR:O | 1:C:881:ARG:HD2 | 2.16 | 0.44 |
| 1:D:859:ASP:OD1 | 1:D:861:SER:OG | 2.26 | 0.44 |
| 1:C:651:LEU:HD13 | 1:C:653:HIS:HE1 | 1.82 | 0.44 |
| 1:D:932:PRO:HD2 | 1:D:970:THR:O | 2.17 | 0.44 |
| 1:B:142:ILE:HG12 | 1:B:170:GLU:HG2 | 2.00 | 0.44 |
| 1:C:78:LEU:HB3 | 1:C:80:GLU:OE2 | 2.18 | 0.44 |
| 1:B:80:GLU:H | 1:B:80:GLU:HG2 | 1.18 | 0.44 |
| 1:B:680:ILE:HD12 | 1:B:680:ILE:N | 2.31 | 0.44 |
| 1:B:745:MET:CE | 1:B:745:MET:N | 2.77 | 0.44 |
| 1:B:863:GLN:HG2 | 1:B:1021:CYS:HB3 | 2.00 | 0.44 |
| 1:A:549:PHE:CE2 | 1:A:620:ALA:HA | 2.53 | 0.44 |
| 1:B:835:LEU:HD11 | 1:B:855:THR:HB | 1.98 | 0.44 |
| 1:A:250:LEU:C | 1:A:251:ARG:HG2 | 2.38 | 0.44 |
| 1:B:88:SER:HA | 1:B:366:VAL:HG21 | 2.00 | 0.44 |
| 1:B:360:HIS:ND1 | 1:B:361:PRO:HD2 | 2.33 | 0.44 |
| 1:A:98:PRO:HB2 | 1:A:203:TRP:CE3 | 2.53 | 0.44 |
| 1:A:577:LYS:O | 1:A:584:PRO:HA | 2.18 | 0.44 |
| 1:B:920:LEU:HB3 | 1:B:921:PRO:HD2 | 2.00 | 0.44 |
| 1:A:742:THR:CG2 | 1:A:743:SER:N | 2.81 | 0.44 |
| 1:A:850:PHE:HA | 1:A:871:GLU:O | 2.18 | 0.44 |
| 1:C:744:GLU:O | 1:C:760:ARG:HD3 | 2.18 | 0.44 |
| 1:C:951:TRP:HA | 1:C:1019:VAL:O | 2.18 | 0.44 |
| 1:A:499:ILE:HG22 | 1:A:501:PRO:HD3 | 1.98 | 0.43 |
| 1:A:745:MET:HE2 | 1:A:745:MET:HB3 | 1.71 | 0.43 |
| 1:B:600:GLN:HE21 | 1:B:600:GLN:N | 2.03 | 0.43 |
| 1:C:835:LEU:CD1 | 1:C:855:THR:HB | 2.44 | 0.43 |
| 1:B:654:TRP:CE3 | 1:B:665:SER:HA | 2.54 | 0.43 |
| 4:D:8503:DMS:O | 5:D:8975:HOH:O | 2.20 | 0.43 |
| 1:B:745:MET:H | 1:B:745:MET:HE1 | 1.79 | 0.43 |
| 1:B:687:GLN:HA | 1:B:688:PRO:HD3 | 1.69 | 0.43 |
| 1:C:628:GLN:NE2 | 4:C:8402:DMS:O | 2.45 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:362:LEU:O | 1:A:362:LEU:HD13 | 2.18 | 0.43 |
| 1:A:735:HIS:O | 1:A:736:ALA:HB2 | 2.18 | 0.43 |
| 1:D:100:TYR:OH | 1:D:601:PHE:HB3 | 2.19 | 0.43 |
| 1:D:845:GLN:OE1 | 1:D:845:GLN:HA | 2.18 | 0.43 |
| 1:A:105:TYR:CE2 | 1:A:199:ASP:HB2 | 2.54 | 0.43 |
| 1:A:433:LEU:HB3 | 1:A:434:PRO:HD3 | 2.01 | 0.43 |
| 1:B:73:TRP:CZ2 | 1:B:185:ALA:HB1 | 2.54 | 0.43 |
| 1:B:961:ARG:NH1 | 5:B:9162:HOH:O | 2.33 | 0.43 |
| 1:D:433:LEU:N | 1:D:434:PRO:CD | 2.82 | 0.43 |
| 1:B:147:ASN:HA | 1:B:148:SER:HA | 1.54 | 0.43 |
| 1:B:601:PHE:CD1 | 1:B:796:SER:HA | 2.54 | 0.43 |
| 1:B:670:LEU:HA | 1:B:670:LEU:HD23 | 1.35 | 0.43 |
| 1:B:773:LYS:N | 1:B:773:LYS:CD | 2.79 | 0.43 |
| 1:C:651:LEU:HD13 | 1:C:701:VAL:HB | 2.01 | 0.43 |
| 1:A:587:ALA:HB1 | 1:A:591:ASP:HB2 | 2.01 | 0.43 |
| 1:A:682:LEU:HD23 | 1:A:682:LEU:HA | 1.83 | 0.43 |
| 1:B:74:LEU:HD22 | 1:B:153:TRP:CG | 2.54 | 0.43 |
| 1:B:730:LEU:CB | 1:B:731:PRO:CD | 2.97 | 0.43 |
| 1:A:427:THR:HG22 | 1:A:436:MET:SD | 2.59 | 0.43 |
| 1:A:655:MET:CE | 1:A:662:PRO:HB3 | 2.47 | 0.43 |
| 1:B:647:SER:OG | 1:B:672:VAL:HG23 | 2.18 | 0.43 |
| 1:B:669:PRO:CB | 5:B:9418:HOH:O | 2.66 | 0.43 |
| 1:D:94:GLY:HA3 | 4:D:8421:DMS:H22 | 2.01 | 0.43 |
| 1:D:237:ARG:NH1 | 1:D:237:ARG:CG | 2.79 | 0.43 |
| 1:D:581:ASN:N | 1:D:581:ASN:OD1 | 2.51 | 0.43 |
| 1:D:901:GLY:HA3 | 1:D:902:PRO:HA | 1.83 | 0.43 |
| 1:D:986:ILE:HG23 | 1:D:986:ILE:HD13 | 1.47 | 0.43 |
| 1:D:305:ILE:HD11 | 1:D:645:ARG:HB3 | 2.01 | 0.42 |
| 1:A:949:HIS:O | 1:A:1023:LYS:NZ | 2.53 | 0.42 |
| 1:C:730:LEU:N | 1:C:730:LEU:CD2 | 2.81 | 0.42 |
| 1:C:820:ALA:HB2 | 1:C:842:TRP:CE2 | 2.54 | 0.42 |
| 1:D:226:HIS:O | 1:D:242:ALA:HA | 2.18 | 0.42 |
| 1:D:427:THR:HG22 | 1:D:436:MET:SD | 2.59 | 0.42 |
| 1:A:494:THR:CB | 1:D:473:ARG:NH2 | 2.75 | 0.42 |
| 1:A:749:ILE:N | 1:A:749:ILE:CD1 | 2.79 | 0.42 |
| 1:B:336:ARG:HD3 | 5:B:9199:HOH:O | 2.19 | 0.42 |
| 1:C:367:MET:CB | 1:C:372:MET:HE2 | 2.39 | 0.42 |
| 1:C:545:SER:O | 1:C:909:ARG:HD3 | 2.19 | 0.42 |
| 1:D:379:MET:CE | 1:D:407:LEU:CD1 | 2.97 | 0.42 |
| 1:A:655:MET:HE3 | 1:A:656:VAL:O | 2.18 | 0.42 |
| 1:B:577:LYS:O | 1:B:584:PRO:HA | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:815:HIS:CD2 | 1:B:849:LEU:HD13 | 2.55 | 0.42 |
| 1:A:854:LYS:HA | 1:A:867:THR:O | 2.19 | 0.42 |
| 1:B:661:LYS:HA | 1:B:662:PRO:HD3 | 1.52 | 0.42 |
| 1:C:655:MET:SD | 1:C:657:ALA:HB2 | 2.60 | 0.42 |
| 1:C:658:LEU:O | 1:C:659:ASP:C | 2.55 | 0.42 |
| 1:A:781:ARG:NH1 | 5:A:9274:HOH:O | 2.53 | 0.42 |
| 1:B:104:THR:HB | 5:B:9533:HOH:O | 2.19 | 0.42 |
| 1:B:773:LYS:HD3 | 1:B:773:LYS:N | 2.35 | 0.42 |
| 1:C:49:GLN:HG2 | 5:C:9432:HOH:O | 2.19 | 0.42 |
| 1:D:780:LEU:HA | 1:D:886:CYS:HB3 | 2.02 | 0.42 |
| 1:A:57:GLU:HB3 | 1:A:83:THR:CG2 | 2.50 | 0.42 |
| 1:A:357:HIS:CD2 | 5:A:9479:HOH:O | 2.72 | 0.42 |
| 1:B:127:PHE:CD2 | 1:B:127:PHE:N | 2.88 | 0.42 |
| 1:B:569:ASP:O | 1:B:605:GLY:HA2 | 2.19 | 0.42 |
| 4:B:8403:DMS:H23 | 5:B:8899:HOH:O | 2.19 | 0.42 |
| 1:D:646:HIS:NE2 | 1:D:671:ASP:OD1 | 2.51 | 0.42 |
| 1:D:814:GLY:HA3 | 1:D:844:HIS:CG | 2.55 | 0.42 |
| 1:A:390:SER:HA | 1:A:391:HIS:HA | 1.85 | 0.42 |
| 1:A:473:ARG:HD3 | 5:D:8713:HOH:O | 2.18 | 0.42 |
| 1:A:950:GLN:OE1 | 1:A:952:ARG:NE | 2.37 | 0.42 |
| 1:D:78:LEU:HD23 | 1:D:78:LEU:HA | 1.75 | 0.42 |
| 1:D:664:ALA:CB | 1:D:685:LEU:HD21 | 2.44 | 0.42 |
| 1:A:35:SER:HB2 | 1:A:217:LYS:HD3 | 2.02 | 0.42 |
| 1:C:387:VAL:HG13 | 5:C:9470:HOH:O | 2.19 | 0.42 |
| 1:C:718:GLN:HG2 | 4:C:8503:DMS:C1 | 2.50 | 0.42 |
| 1:D:667:GLU:C | 1:D:668:VAL:HG23 | 2.39 | 0.42 |
| 1:D:739:HIS:O | 1:D:749:ILE:HA | 2.19 | 0.42 |
| 1:D:768:MET:HE1 | 1:D:1020:TRP:CE2 | 2.54 | 0.42 |
| 1:A:753:ASN:OD1 | 1:A:753:ASN:N | 2.51 | 0.41 |
| 1:B:937:LEU:HA | 1:B:957:PHE:O | 2.20 | 0.41 |
| 1:A:1022:GLN:CG | 1:A:1023:LYS:N | 2.83 | 0.41 |
| 1:B:379:MET:HE2 | 1:B:379:MET:HB2 | 1.93 | 0.41 |
| 1:B:607:VAL:HG12 | 1:B:613:PRO:HA | 2.02 | 0.41 |
| 1:B:908:ASP:HB3 | 1:B:1007:PHE:CD1 | 2.55 | 0.41 |
| 1:C:59:ARG:NH2 | 1:C:81:ALA:HB3 | 2.34 | 0.41 |
| 1:C:770:ILE:HD12 | 1:C:775:GLN:CG | 2.50 | 0.41 |
| 1:D:390:SER:HA | 1:D:391:HIS:HA | 1.94 | 0.41 |
| 1:A:843:GLN:HG2 | 1:A:847:LYS:C | 2.41 | 0.41 |
| 1:C:363:HIS:HD2 | 5:C:9179:HOH:O | 2.02 | 0.41 |
| 1:D:379:MET:HE3 | 1:D:379:MET:HB3 | 1.46 | 0.41 |
| 1:B:181:GLU:OE2 | 5:B:9427:HOH:O | 2.22 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:411:ASP:OD2 | 1:B:447:ASP:OD2 | 2.39 | 0.41 |
| 1:C:433:LEU:HB3 | 1:C:434:PRO:HD3 | 2.02 | 0.41 |
| 1:C:685:LEU:HA | 1:C:686:PRO:HD3 | 1.52 | 0.41 |
| 1:C:745:MET:CE | 1:C:745:MET:CA | 2.96 | 0.41 |
| 1:D:499:ILE:HG22 | 1:D:501:PRO:HD3 | 2.02 | 0.41 |
| 1:D:599:ARG:HH11 | 1:D:599:ARG:HD2 | 1.66 | 0.41 |
| 1:D:663:LEU:HD22 | 1:D:694:LEU:HD21 | 2.02 | 0.41 |
| 1:B:531:ARG:HB3 | 1:B:532:PRO:HD2 | 2.01 | 0.41 |
| 1:C:472:TYR:OH | 1:C:476:LYS:HE2 | 2.21 | 0.41 |
| 1:C:515:VAL:N | 1:C:516:PRO:CD | 2.83 | 0.41 |
| 1:D:878:HIS:HE1 | 5:D:9360:HOH:O | 2.02 | 0.41 |
| 1:B:687:GLN:NE2 | 1:B:687:GLN:CA | 2.83 | 0.41 |
| 1:B:777:LEU:HD23 | 1:B:777:LEU:HA | 1.90 | 0.41 |
| 1:D:506:VAL:CG1 | 1:D:521:LYS:HE3 | 2.51 | 0.41 |
| 1:D:997:ASP:HB2 | 1:D:999:TRP:CZ2 | 2.56 | 0.41 |
| 1:A:964:GLN:O | 1:A:968:MET:HB2 | 2.21 | 0.41 |
| 1:B:85:VAL:CG1 | 1:B:86:VAL:N | 2.82 | 0.41 |
| 1:B:773:LYS:HA | 1:B:773:LYS:HD2 | 1.68 | 0.41 |
| 1:C:577:LYS:HB3 | 1:C:577:LYS:HE3 | 1.91 | 0.41 |
| 1:C:667:GLU:C | 1:C:668:VAL:HG23 | 2.41 | 0.41 |
| 1:C:753:ASN:N | 1:C:753:ASN:OD1 | 2.52 | 0.41 |
| 1:A:699:ARG:HH11 | 1:A:699:ARG:HD2 | 1.74 | 0.41 |
| 1:A:708:TRP:CZ2 | 4:A:8403:DMS:H12 | 2.56 | 0.41 |
| 1:A:764:PHE:CD1 | 1:A:781:ARG:NH1 | 2.89 | 0.41 |
| 1:B:13:ARG:HD3 | 1:B:13:ARG:HA | 1.78 | 0.41 |
| 1:B:681:GLU:H | 1:B:681:GLU:HG2 | 1.67 | 0.41 |
| 1:C:712:GLY:O | 1:C:713:HIS:C | 2.57 | 0.41 |
| 1:D:225:PHE:HA | 1:D:243:GLU:O | 2.21 | 0.41 |
| 1:C:1022:GLN:HE21 | 1:C:1022:GLN:HB3 | 1.57 | 0.41 |
| 1:A:359:HIS:N | 1:A:367:MET:HE1 | 2.36 | 0.40 |
| 1:A:594:ASP:C | 1:A:595:THR:HG22 | 2.41 | 0.40 |
| 1:B:654:TRP:O | 1:B:665:SER:HB2 | 2.20 | 0.40 |
| 1:B:807:VAL:HG13 | 1:B:808:GLU:N | 2.35 | 0.40 |
| 1:B:1022:GLN:NE2 | 1:B:1023:LYS:O | 2.52 | 0.40 |
| 1:D:843:GLN:HG3 | 1:D:848:THR:HA | 2.02 | 0.40 |
| 1:A:241:GLU:CD | 1:A:292:ARG:NH2 | 2.74 | 0.40 |
| 1:B:37:ARG:HH12 | 4:B:8504:DMS:H23 | 1.86 | 0.40 |
| 1:C:878:HIS:CE1 | 1:C:1010:SER:HB3 | 2.56 | 0.40 |
| 1:D:367:MET:HE2 | 1:D:372:MET:HG3 | 2.03 | 0.40 |
| 1:D:733:ALA:O | 1:D:735:HIS:ND1 | 2.53 | 0.40 |
| 1:A:200:GLN:HG2 | 1:A:391:HIS:HB2 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:615:PRO:O | 1:A:618:THR:HG22 | 2.22 | 0.40 |
| 1:A:634:GLN:NE2 | 1:A:682:LEU:HD12 | 2.36 | 0.40 |
| 1:A:952:ARG:NH2 | 1:A:1021:CYS:SG | 2.94 | 0.40 |
| 1:B:46:ARG:HH11 | 1:B:46:ARG:HD2 | 1.78 | 0.40 |
| 1:C:16:TRP:CD2 | 1:C:189:LEU:CD1 | 3.04 | 0.40 |
| 1:C:296:GLU:HG2 | 4:C:8601:DMS:H12 | 2.03 | 0.40 |
| 1:C:634:GLN:OE1 | 1:C:681:GLU:HG2 | 2.21 | 0.40 |
| 1:C:781:ARG:HG2 | 1:C:781:ARG:HH11 | 1.85 | 0.40 |
| 1:D:687:GLN:HA | 1:D:688:PRO:HD3 | 1.61 | 0.40 |
| 1:A:575:LEU:HD23 | 1:A:575:LEU:HA | 1.69 | 0.40 |
| 1:B:114:VAL:HB | 1:B:115:PRO:CD | 2.51 | 0.40 |
| 1:B:133:TRP:CD1 | 4:B:8504:DMS:C1 | 3.04 | 0.40 |
| 1:C:100:TYR:CE2 | 1:C:602:CYS:HB3 | 2.56 | 0.40 |
| 1:C:584:PRO:O | 4:C:8411:DMS:H22 | 2.21 | 0.40 |
| 1:C:654:TRP:NE1 | 1:C:666:GLY:HA3 | 2.35 | 0.40 |
| 1:A:891:VAL:HG23 | 1:A:981:GLY:HA2 | 2.02 | 0.40 |
| 1:B:16:TRP:CD2 | 1:B:189:LEU:CD1 | 3.04 | 0.40 |
| 1:B:378:LEU:HD23 | 1:B:378:LEU:HA | 1.96 | 0.40 |
| 1:B:379:MET:CE | 1:B:407:LEU:CD1 | 2.99 | 0.40 |
| 1:B:634:GLN:CG | 1:B:682:LEU:HB2 | 2.47 | 0.40 |
| 1:C:670:LEU:HA | 1:C:670:LEU:HD23 | 1.85 | 0.40 |
| 1:C:1011:ALA:HB3 | 1:C:1014:TYR:CZ | 2.57 | 0.40 |
| 1:D:379:MET:HE2 | 1:D:379:MET:HB2 | 1.77 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 1006/1023 (98%) | 972 (97%) | 33 (3%) | 1 (0%) | 51 29 |
| 1 | B | 1005/1023 (98%) | 962 (96%) | 36 (4%) | 7 (1%) | 22 7 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | C | 1003/1023 (98%) | 968 (96%) | 32 (3%) | 3 (0%) | 41 | 21 |
| 1 | D | 1004/1023 (98%) | 961 (96%) | 39 (4%) | 4 (0%) | 34 | 15 |
| All | All | 4018/4092 (98%) | 3863 (96%) | 140 (4%) | 15 (0%) | 34 | 15 |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 690 | SER |
| 1 | B | 731 | PRO |
| 1 | B | 732 | ALA |
| 1 | B | 734 | SER |
| 1 | D | 688 | PRO |
| 1 | C | 734 | SER |
| 1 | D | 734 | SER |
| 1 | A | 688 | PRO |
| 1 | B | 688 | PRO |
| 1 | B | 733 | ALA |
| 1 | D | 164 | ASP |
| 1 | B | 164 | ASP |
| 1 | C | 687 | GLN |
| 1 | C | 732 | ALA |
| 1 | D | 683 | PRO |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 863/875 (99%) | 831 (96%) | 32 (4%) | 34 | 11 |
| 1 | B | 863/875 (99%) | 821 (95%) | 42 (5%) | 25 | 6 |
| 1 | C | 861/875 (98%) | 824 (96%) | 37 (4%) | 29 | 9 |
| 1 | D | 862/875 (98%) | 819 (95%) | 43 (5%) | 24 | 6 |
| All | All | 3449/3500 (98%) | 3295 (96%) | 154 (4%) | 27 | 8 |

All (154) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 71 | GLU |
| 1 | A | 117 | GLU |
| 1 | A | 130 | ASP |
| 1 | A | 250 | LEU |
| 1 | A | 277 | GLU |
| 1 | A | 333 | ARG |
| 1 | A | 362 | LEU |
| 1 | A | 370 | GLN |
| 1 | A | 377 | LEU |
| 1 | A | 394 | ASN |
| 1 | A | 519 | SER |
| 1 | A | 546 | LEU |
| 1 | A | 580 | GLU |
| 1 | A | 595 | THR |
| 1 | A | 600 | GLN |
| 1 | A | 655 | MET |
| 1 | A | 684 | GLU |
| 1 | A | 685 | LEU |
| 1 | A | 735 | HIS |
| 1 | A | 737 | ILE |
| 1 | A | 755 | ARG |
| 1 | A | 773 | LYS |
| 1 | A | 800 | ARG |
| 1 | A | 817 | GLN |
| 1 | A | 829 | THR |
| 1 | A | 843 | GLN |
| 1 | A | 847 | LYS |
| 1 | A | 885 | ASN |
| 1 | A | 956 | GLN |
| 1 | A | 986 | ILE |
| 1 | A | 1017 | GLN |
| 1 | A | 1023 | LYS |
| 1 | B | 13 | ARG |
| 1 | B | 71 | GLU |
| 1 | B | 80 | GLU |
| 1 | B | 230 | ARG |
| 1 | B | 237 | ARG |
| 1 | B | 262 | GLN |
| 1 | B | 277 | GLU |
| 1 | B | 333 | ARG |
| 1 | B | 344 | LEU |
| 1 | B | 370 | GLN |
| 1 | B | 392 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 394 | ASN |
| 1 | B | 546 | LEU |
| 1 | B | 554 | GLN |
| 1 | B | 595 | THR |
| 1 | B | 599 | ARG |
| 1 | B | 600 | GLN |
| 1 | B | 630 | ARG |
| 1 | B | 646 | HIS |
| 1 | B | 651 | LEU |
| 1 | B | 655 | MET |
| 1 | B | 661 | LYS |
| 1 | B | 663 | LEU |
| 1 | B | 672 | VAL |
| 1 | B | 681 | GLU |
| 1 | B | 687 | GLN |
| 1 | B | 689 | GLU |
| 1 | B | 690 | SER |
| 1 | B | 730 | LEU |
| 1 | B | 734 | SER |
| 1 | B | 737 | ILE |
| 1 | B | 745 | MET |
| 1 | B | 766 | SER |
| 1 | B | 768 | MET |
| 1 | B | 773 | LYS |
| 1 | B | 800 | ARG |
| 1 | B | 804 | ASN |
| 1 | B | 847 | LYS |
| 1 | B | 890 | GLN |
| 1 | B | 917 | ARG |
| 1 | B | 1017 | GLN |
| 1 | B | 1023 | LYS |
| 1 | C | 71 | GLU |
| 1 | C | 80 | GLU |
| 1 | C | 117 | GLU |
| 1 | C | 136 | GLU |
| 1 | C | 178 | ARG |
| 1 | C | 262 | GLN |
| 1 | C | 264 | GLU |
| 1 | C | 333 | ARG |
| 1 | C | 344 | LEU |
| 1 | C | 362 | LEU |
| 1 | C | 394 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 437 | SER |
| 1 | C | 519 | SER |
| 1 | C | 535 | LEU |
| 1 | C | 546 | LEU |
| 1 | C | 595 | THR |
| 1 | C | 630 | ARG |
| 1 | C | 634 | GLN |
| 1 | C | 651 | LEU |
| 1 | C | 653 | HIS |
| 1 | C | 655 | MET |
| 1 | C | 663 | LEU |
| 1 | C | 684 | GLU |
| 1 | C | 685 | LEU |
| 1 | C | 687 | GLN |
| 1 | C | 690 | SER |
| 1 | C | 699 | ARG |
| 1 | C | 730 | LEU |
| 1 | C | 737 | ILE |
| 1 | C | 745 | MET |
| 1 | C | 750 | GLU |
| 1 | C | 804 | ASN |
| 1 | C | 819 | GLU |
| 1 | C | 847 | LYS |
| 1 | C | 956 | GLN |
| 1 | C | 1022 | GLN |
| 1 | C | 1023 | LYS |
| 1 | D | 71 | GLU |
| 1 | D | 80 | GLU |
| 1 | D | 128 | ASN |
| 1 | D | 237 | ARG |
| 1 | D | 249 | GLU |
| 1 | D | 277 | GLU |
| 1 | D | 319 | ASP |
| 1 | D | 333 | ARG |
| 1 | D | 362 | LEU |
| 1 | D | 370 | GLN |
| 1 | D | 392 | TYR |
| 1 | D | 394 | ASN |
| 1 | D | 511 | PRO |
| 1 | D | 519 | SER |
| 1 | D | 546 | LEU |
| 1 | D | 580 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 630 | ARG |
| 1 | D | 632 | SER |
| 1 | D | 651 | LEU |
| 1 | D | 655 | MET |
| 1 | D | 661 | LYS |
| 1 | D | 663 | LEU |
| 1 | D | 681 | GLU |
| 1 | D | 684 | GLU |
| 1 | D | 685 | LEU |
| 1 | D | 687 | GLN |
| 1 | D | 689 | GLU |
| 1 | D | 730 | LEU |
| 1 | D | 734 | SER |
| 1 | D | 735 | HIS |
| 1 | D | 737 | ILE |
| 1 | D | 755 | ARG |
| 1 | D | 772 | ASP |
| 1 | D | 817 | GLN |
| 1 | D | 829 | THR |
| 1 | D | 849 | LEU |
| 1 | D | 858 | ILE |
| 1 | D | 859 | ASP |
| 1 | D | 910 | LEU |
| 1 | D | 956 | GLN |
| 1 | D | 986 | ILE |
| 1 | D | 1018 | LEU |
| 1 | D | 1022 | GLN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 135 | GLN |
| 1 | A | 363 | HIS |
| 1 | A | 600 | GLN |
| 1 | A | 634 | GLN |
| 1 | A | 653 | HIS |
| 1 | A | 735 | HIS |
| 1 | A | 739 | HIS |
| 1 | A | 817 | GLN |
| 1 | A | 824 | GLN |
| 1 | A | 844 | HIS |
| 1 | A | 878 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 262 | GLN |
| 1 | B | 363 | HIS |
| 1 | B | 554 | GLN |
| 1 | B | 600 | GLN |
| 1 | B | 624 | GLN |
| 1 | B | 628 | GLN |
| 1 | B | 675 | GLN |
| 1 | B | 687 | GLN |
| 1 | B | 757 | GLN |
| 1 | B | 878 | HIS |
| 1 | B | 977 | HIS |
| 1 | C | 363 | HIS |
| 1 | C | 624 | GLN |
| 1 | C | 646 | HIS |
| 1 | C | 653 | HIS |
| 1 | C | 687 | GLN |
| 1 | C | 824 | GLN |
| 1 | C | 878 | HIS |
| 1 | C | 977 | HIS |
| 1 | C | 1022 | GLN |
| 1 | D | 128 | ASN |
| 1 | D | 135 | GLN |
| 1 | D | 163 | GLN |
| 1 | D | 624 | GLN |
| 1 | D | 628 | GLN |
| 1 | D | 634 | GLN |
| 1 | D | 704 | ASN |
| 1 | D | 761 | GLN |
| 1 | D | 824 | GLN |
| 1 | D | 878 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 113 ligands modelled in this entry, 28 are monoatomic - leaving 85 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 |
| 4 | DMS | A | 8502 | - | 3,3,3 | 2.09 | 1 (33%) | 3,3,3 | 1.00 | 0 |
| 4 | DMS | D | 8404 | - | 3,3,3 | 1.18 | 0 | 3,3,3 | 0.51 | 0 |
| 4 | DMS | B | 8504 | - | 3,3,3 | 0.37 | 0 | 3,3,3 | 0.11 | 0 |
| 4 | DMS | A | 8602 | - | 3,3,3 | 0.72 | 0 | 3,3,3 | 0.22 | 0 |
| 4 | DMS | C | 8601 | - | 3,3,3 | 0.65 | 0 | 3,3,3 | 0.52 | 0 |
| 4 | DMS | C | 8504 | - | 3,3,3 | 1.23 | 0 | 3,3,3 | 1.08 | 0 |
| 4 | DMS | D | 8421 | - | 3,3,3 | 0.32 | 0 | 3,3,3 | 0.49 | 0 |
| 4 | DMS | B | 8601 | - | 3,3,3 | 2.49 | 1 (33%) | 3,3,3 | 0.79 | 0 |
| 4 | DMS | D | 8402 | - | 3,3,3 | 1.36 | 0 | 3,3,3 | 0.23 | 0 |
| 4 | DMS | D | 8401 | - | 3,3,3 | 1.66 | 1 (33%) | 3,3,3 | 0.12 | 0 |
| 4 | DMS | A | 8414 | - | 3,3,3 | 0.40 | 0 | 3,3,3 | 0.20 | 0 |
| 4 | DMS | A | 8504 | - | 3,3,3 | 0.93 | 0 | 3,3,3 | 0.41 | 0 |
| 4 | DMS | C | 8417 | - | 3,3,3 | 0.27 | 0 | 3,3,3 | 0.42 | 0 |
| 4 | DMS | C | 8501 | - | 3,3,3 | 1.53 | 1 (33%) | 3,3,3 | 0.77 | 0 |
| 4 | DMS | C | 8421 | - | 3,3,3 | 1.22 | 0 | 3,3,3 | 0.57 | 0 |
| 4 | DMS | A | 8404 | - | 3,3,3 | 1.48 | 1 (33%) | 3,3,3 | 0.58 | 0 |
| 4 | DMS | C | 8409 | - | 3,3,3 | 2.15 | 1 (33%) | 3,3,3 | 0.32 | 0 |
| 4 | DMS | A | 8501 | - | 3,3,3 | 0.76 | 0 | 3,3,3 | 0.44 | 0 |
| 4 | DMS | C | 8602 | - | 3,3,3 | 0.56 | 0 | 3,3,3 | 0.22 | 0 |
| 4 | DMS | D | 8414 | - | 3,3,3 | 0.40 | 0 | 3,3,3 | 0.55 | 0 |
| 4 | DMS | D | 8703 | - | 3,3,3 | 0.82 | 0 | 3,3,3 | 0.27 | 0 |
| 4 | DMS | C | 8425 | 3 | 3,3,3 | 1.05 | 0 | 3,3,3 | 0.12 | 0 |
| 4 | DMS | A | 8421 | - | 3,3,3 | 0.98 | 0 | 3,3,3 | 0.77 | 0 |
| 4 | DMS | A | 8403 | - | 3,3,3 | 1.77 | 1 (33%) | 3,3,3 | 0.65 | 0 |
| 4 | DMS | A | 8409 | - | 3,3,3 | 2.35 | 2 (66%) | 3,3,3 | 0.51 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | DMS | A | 8401 | - | 3,3,3 | 1.21 | 0 | 3,3,3 | 0.52 | 0 |
| 4 | DMS | A | 8402 | - | 3,3,3 | 1.20 | 0 | 3,3,3 | 0.75 | 0 |
| 4 | DMS | B | 8502 | - | 3,3,3 | 1.49 | 0 | 3,3,3 | 1.22 | 1 (33%) |
| 4 | DMS | D | 8701 | - | 3,3,3 | 1.51 | 1 (33%) | 3,3,3 | 0.46 | 0 |
| 4 | DMS | D | 8410 | - | 3,3,3 | 1.93 | 1 (33%) | 3,3,3 | 0.24 | 0 |
| 4 | DMS | A | 8411 | - | 3,3,3 | 1.50 | 0 | 3,3,3 | 0.49 | 0 |
| 4 | DMS | B | 8402 | - | 3,3,3 | 1.80 | 1 (33%) | 3,3,3 | 1.27 | 1 (33%) |
| 4 | DMS | D | 8413 | - | 3,3,3 | 0.81 | 0 | 3,3,3 | 0.03 | 0 |
| 4 | DMS | A | 8425 | 3 | 3,3,3 | 1.22 | 0 | 3,3,3 | 0.70 | 0 |
| 4 | DMS | B | 8416 | - | 3,3,3 | 1.00 | 0 | 3,3,3 | 0.24 | 0 |
| 4 | DMS | B | 8404 | - | 3,3,3 | 0.99 | 0 | 3,3,3 | 0.51 | 0 |
| 4 | DMS | C | 8403 | - | 3,3,3 | 1.42 | 1 (33%) | 3,3,3 | 0.33 | 0 |
| 4 | DMS | A | 8408 | - | 3,3,3 | 0.55 | 0 | 3,3,3 | 0.34 | 0 |
| 4 | DMS | D | 8705 | - | 3,3,3 | 1.94 | 1 (33%) | 3,3,3 | 0.30 | 0 |
| 4 | DMS | D | 8508 | - | 3,3,3 | 1.39 | 0 | 3,3,3 | 0.90 | 0 |
| 4 | DMS | B | 8508 | - | 3,3,3 | 2.06 | 1 (33%) | 3,3,3 | 0.81 | 0 |
| 4 | DMS | B | 8411 | - | 3,3,3 | 0.54 | 0 | 3,3,3 | 0.82 | 0 |
| 4 | DMS | B | 8412 | - | 3,3,3 | 0.88 | 0 | 3,3,3 | 0.25 | 0 |
| 4 | DMS | D | 8403 | - | 3,3,3 | 1.28 | 0 | 3,3,3 | 0.35 | 0 |
| 4 | DMS | C | 8404 | - | 3,3,3 | 1.29 | 0 | 3,3,3 | 1.11 | 0 |
| 4 | DMS | A | 8405 | - | 3,3,3 | 1.29 | 1 (33%) | 3,3,3 | 0.44 | 0 |
| 4 | DMS | D | 8408 | - | 3,3,3 | 1.31 | 1 (33%) | 3,3,3 | 0.26 | 0 |
| 4 | DMS | C | 8405 | - | 3,3,3 | 2.61 | 2 (66%) | 3,3,3 | 0.27 | 0 |
| 4 | DMS | B | 8417 | - | 3,3,3 | 0.82 | 0 | 3,3,3 | 0.52 | 0 |
| 4 | DMS | C | 8414 | - | 3,3,3 | 1.75 | 1 (33%) | 3,3,3 | 1.19 | 0 |
| 4 | DMS | B | 8421 | - | 3,3,3 | 0.58 | 0 | 3,3,3 | 0.38 | 0 |
| 4 | DMS | A | 8503 | - | 3,3,3 | 1.06 | 0 | 3,3,3 | 0.74 | 0 |
| 4 | DMS | D | 8501 | - | 3,3,3 | 0.84 | 0 | 3,3,3 | 0.37 | 0 |
| 4 | DMS | B | 8401 | - | 3,3,3 | 0.96 | 0 | 3,3,3 | 0.43 | 0 |
| 4 | DMS | C | 8401 | - | 3,3,3 | 1.74 | 1 (33%) | 3,3,3 | 0.38 | 0 |
| 4 | DMS | B | 8409 | - | 3,3,3 | 2.68 | 1 (33%) | 3,3,3 | 0.57 | 0 |
| 4 | DMS | D | 8409 | - | 3,3,3 | 1.96 | 1 (33%) | 3,3,3 | 1.39 | 1 (33%) |
| 4 | DMS | D | 8416 | - | 3,3,3 | 0.26 | 0 | 3,3,3 | 0.54 | 0 |
| 4 | DMS | C | 8408 | - | 3,3,3 | 0.75 | 0 | 3,3,3 | 1.10 | 0 |
| 4 | DMS | A | 8417 | - | 3,3,3 | 1.00 | 0 | 3,3,3 | 0.79 | 0 |
| 4 | DMS | B | 8405 | - | 3,3,3 | 2.22 | 1 (33%) | 3,3,3 | 0.28 | 0 |
| 4 | DMS | C | 8410 | - | 3,3,3 | 0.69 | 0 | 3,3,3 | 0.16 | 0 |
| 4 | DMS | D | 8417 | - | 3,3,3 | 0.46 | 0 | 3,3,3 | 0.21 | 0 |
| 4 | DMS | B | 8414 | - | 3,3,3 | 1.01 | 0 | 3,3,3 | 0.39 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | DMS | D | 8406 | - | 3,3,3 | 0.86 | 0 | 3,3,3 | 0.53 | 0 |
| 4 | DMS | A | 8416 | - | 3,3,3 | 2.03 | 2 (66%) | 3,3,3 | 0.62 | 0 |
| 4 | DMS | D | 8412 | - | 3,3,3 | 1.63 | 1 (33%) | 3,3,3 | 0.54 | 0 |
| 4 | DMS | B | 8408 | - | 3,3,3 | 1.26 | 0 | 3,3,3 | 0.08 | 0 |
| 4 | DMS | D | 8425 | 3 | 3,3,3 | 0.93 | 0 | 3,3,3 | 0.37 | 0 |
| 4 | DMS | D | 8411 | - | 3,3,3 | 1.36 | 0 | 3,3,3 | 0.22 | 0 |
| 4 | DMS | C | 8503 | - | 3,3,3 | 0.85 | 0 | 3,3,3 | 1.43 | 1 (33%) |
| 4 | DMS | B | 8425 | 3 | 3,3,3 | 1.12 | 0 | 3,3,3 | 0.40 | 0 |
| 4 | DMS | A | 8406 | - | 3,3,3 | 1.78 | 1 (33%) | 3,3,3 | 0.42 | 0 |
| 4 | DMS | C | 8413 | - | 3,3,3 | 0.71 | 0 | 3,3,3 | 0.29 | 0 |
| 4 | DMS | A | 8419 | - | 3,3,3 | 1.10 | 0 | 3,3,3 | 0.40 | 0 |
| 4 | DMS | B | 8403 | - | 3,3,3 | 1.10 | 0 | 3,3,3 | 0.13 | 0 |
| 4 | DMS | A | 8412 | - | 3,3,3 | 2.09 | 1 (33%) | 3,3,3 | 0.47 | 0 |
| 4 | DMS | C | 8412 | - | 3,3,3 | 1.20 | 0 | 3,3,3 | 1.37 | 1 (33%) |
| 4 | DMS | C | 8416 | - | 3,3,3 | 0.67 | 0 | 3,3,3 | 0.31 | 0 |
| 4 | DMS | A | 8410 | - | 3,3,3 | 0.58 | 0 | 3,3,3 | 0.55 | 0 |
| 4 | DMS | C | 8402 | - | 3,3,3 | 2.22 | 1 (33%) | 3,3,3 | 0.17 | 0 |
| 4 | DMS | D | 8419 | - | 3,3,3 | 0.59 | 0 | 3,3,3 | 0.49 | 0 |
| 4 | DMS | D | 8405 | - | 3,3,3 | 0.79 | 0 | 3,3,3 | 0.49 | 0 |
| 4 | DMS | C | 8411 | - | 3,3,3 | 1.13 | 0 | 3,3,3 | 0.30 | 0 |
| 4 | DMS | D | 8503 | - | 3,3,3 | 0.68 | 0 | 3,3,3 | 0.79 | 0 |

All (30) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4 | B | 8409 | DMS | O-S | 4.60 | 1.81 | 1.50 |
| 4 | C | 8405 | DMS | O-S | 3.93 | 1.76 | 1.50 |
| 4 | B | 8601 | DMS | C2-S | 3.77 | 2.03 | 1.75 |
| 4 | C | 8409 | DMS | O-S | 3.66 | 1.75 | 1.50 |
| 4 | B | 8405 | DMS | O-S | 3.53 | 1.74 | 1.50 |
| 4 | A | 8409 | DMS | O-S | 3.36 | 1.72 | 1.50 |
| 4 | A | 8502 | DMS | C1-S | 3.32 | 2.00 | 1.75 |
| 4 | C | 8402 | DMS | C2-S | 3.18 | 1.99 | 1.75 |
| 4 | A | 8412 | DMS | C1-S | 3.03 | 1.98 | 1.75 |
| 4 | A | 8406 | DMS | C2-S | -3.00 | 1.53 | 1.75 |
| 4 | B | 8508 | DMS | C1-S | 2.89 | 1.97 | 1.75 |
| 4 | D | 8409 | DMS | O-S | 2.88 | 1.69 | 1.50 |
| 4 | A | 8416 | DMS | O-S | -2.81 | 1.31 | 1.50 |
| 4 | A | 8403 | DMS | C2-S | 2.72 | 1.96 | 1.75 |
| 4 | D | 8705 | DMS | C1-S | -2.69 | 1.55 | 1.75 |
| 4 | B | 8402 | DMS | C2-S | 2.67 | 1.95 | 1.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4 | C | 8401 | DMS | C2-S | 2.36 | 1.93 | 1.75 |
| 4 | D | 8410 | DMS | C2-S | 2.34 | 1.93 | 1.75 |
| 4 | C | 8403 | DMS | O-S | 2.31 | 1.65 | 1.50 |
| 4 | C | 8414 | DMS | O-S | -2.28 | 1.34 | 1.50 |
| 4 | C | 8501 | DMS | C1-S | -2.24 | 1.59 | 1.75 |
| 4 | A | 8405 | DMS | O-S | 2.21 | 1.65 | 1.50 |
| 4 | C | 8405 | DMS | C1-S | 2.20 | 1.92 | 1.75 |
| 4 | D | 8701 | DMS | C1-S | 2.18 | 1.92 | 1.75 |
| 4 | A | 8404 | DMS | O-S | -2.12 | 1.35 | 1.50 |
| 4 | D | 8401 | DMS | O-S | 2.11 | 1.64 | 1.50 |
| 4 | A | 8416 | DMS | C1-S | -2.10 | 1.60 | 1.75 |
| 4 | D | 8412 | DMS | O-S | 2.07 | 1.64 | 1.50 |
| 4 | D | 8408 | DMS | C1-S | 2.01 | 1.90 | 1.75 |
| 4 | A | 8409 | DMS | C1-S | 2.00 | 1.90 | 1.75 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|------|-------------|----------|
| 4 | C | 8503 | DMS | C2-S-C1 | 2.39 | 110.74 | 98.44 |
| 4 | D | 8409 | DMS | C2-S-C1 | 2.36 | 110.58 | 98.44 |
| 4 | C | 8412 | DMS | C2-S-C1 | 2.34 | 110.50 | 98.44 |
| 4 | B | 8402 | DMS | C2-S-C1 | 2.16 | 109.55 | 98.44 |
| 4 | B | 8502 | DMS | C2-S-C1 | 2.11 | 109.32 | 98.44 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 58 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4 | A | 8502 | DMS | 3 | 0 |
| 4 | B | 8504 | DMS | 2 | 0 |
| 4 | A | 8602 | DMS | 1 | 0 |
| 4 | C | 8601 | DMS | 2 | 0 |
| 4 | D | 8421 | DMS | 2 | 0 |
| 4 | B | 8601 | DMS | 1 | 0 |
| 4 | A | 8404 | DMS | 5 | 0 |
| 4 | C | 8602 | DMS | 1 | 0 |
| 4 | D | 8703 | DMS | 5 | 0 |
| 4 | C | 8425 | DMS | 7 | 0 |
| 4 | A | 8403 | DMS | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4 | A | 8425 | DMS | 2 | 0 |
| 4 | D | 8705 | DMS | 1 | 0 |
| 4 | B | 8411 | DMS | 1 | 0 |
| 4 | B | 8412 | DMS | 1 | 0 |
| 4 | D | 8403 | DMS | 1 | 0 |
| 4 | A | 8503 | DMS | 1 | 0 |
| 4 | B | 8409 | DMS | 1 | 0 |
| 4 | C | 8410 | DMS | 1 | 0 |
| 4 | D | 8417 | DMS | 1 | 0 |
| 4 | D | 8406 | DMS | 1 | 0 |
| 4 | A | 8416 | DMS | 2 | 0 |
| 4 | D | 8412 | DMS | 2 | 0 |
| 4 | C | 8503 | DMS | 2 | 0 |
| 4 | C | 8413 | DMS | 1 | 0 |
| 4 | B | 8403 | DMS | 1 | 0 |
| 4 | A | 8412 | DMS | 1 | 0 |
| 4 | C | 8412 | DMS | 1 | 0 |
| 4 | A | 8410 | DMS | 3 | 0 |
| 4 | C | 8402 | DMS | 1 | 0 |
| 4 | D | 8419 | DMS | 1 | 0 |
| 4 | C | 8411 | DMS | 1 | 0 |
| 4 | D | 8503 | DMS | 1 | 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 | 1010/1023 (98%) | -0.37 | 28 (2%) 53 50 | 9, 18, 47, 97 | 0 |
| 1 | B | 1009/1023 (98%) | -0.40 | 19 (1%) 66 65 | 9, 17, 44, 94 | 0 |
| 1 | C | 1007/1023 (98%) | -0.40 | 19 (1%) 66 65 | 8, 17, 45, 99 | 0 |
| 1 | D | 1008/1023 (98%) | -0.40 | 25 (2%) 57 55 | 9, 17, 46, 94 | 0 |
| All | All | 4034/4092 (98%) | -0.39 | 91 (2%) 60 59 | 8, 17, 45, 99 | 0 |

All (91) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 733 | ALA | 7.5 |
| 1 | B | 733 | ALA | 7.4 |
| 1 | A | 730 | LEU | 7.3 |
| 1 | C | 732 | ALA | 7.2 |
| 1 | B | 731 | PRO | 6.9 |
| 1 | A | 735 | HIS | 6.5 |
| 1 | C | 731 | PRO | 6.4 |
| 1 | C | 687 | GLN | 6.1 |
| 1 | B | 730 | LEU | 5.8 |
| 1 | A | 689 | GLU | 5.7 |
| 1 | D | 732 | ALA | 5.7 |
| 1 | D | 733 | ALA | 5.7 |
| 1 | C | 730 | LEU | 5.6 |
| 1 | A | 731 | PRO | 5.4 |
| 1 | A | 686 | PRO | 5.3 |
| 1 | C | 689 | GLU | 5.3 |
| 1 | D | 735 | HIS | 5.1 |
| 1 | B | 732 | ALA | 4.9 |
| 1 | D | 730 | LEU | 4.6 |
| 1 | D | 731 | PRO | 4.6 |
| 1 | C | 686 | PRO | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | C | 735 | HIS | 4.3 |
| 1 | B | 689 | GLU | 4.3 |
| 1 | A | 580 | GLU | 4.3 |
| 1 | D | 689 | GLU | 4.3 |
| 1 | D | 684 | GLU | 4.2 |
| 1 | A | 687 | GLN | 4.1 |
| 1 | A | 798 | ALA | 4.0 |
| 1 | C | 685 | LEU | 4.0 |
| 1 | D | 734 | SER | 3.9 |
| 1 | D | 686 | PRO | 3.9 |
| 1 | D | 687 | GLN | 3.8 |
| 1 | A | 733 | ALA | 3.8 |
| 1 | D | 771 | GLY | 3.7 |
| 1 | B | 735 | HIS | 3.6 |
| 1 | B | 687 | GLN | 3.6 |
| 1 | A | 801 | ILE | 3.6 |
| 1 | B | 686 | PRO | 3.6 |
| 1 | A | 732 | ALA | 3.5 |
| 1 | A | 685 | LEU | 3.4 |
| 1 | A | 795 | VAL | 3.4 |
| 1 | C | 684 | GLU | 3.4 |
| 1 | D | 580 | GLU | 3.3 |
| 1 | D | 76 | CYS | 3.3 |
| 1 | B | 685 | LEU | 3.3 |
| 1 | A | 729 | THR | 3.2 |
| 1 | D | 683 | PRO | 3.2 |
| 1 | C | 580 | GLU | 3.2 |
| 1 | B | 745 | MET | 3.1 |
| 1 | B | 580 | GLU | 3.1 |
| 1 | A | 581 | ASN | 3.0 |
| 1 | A | 1023 | LYS | 3.0 |
| 1 | D | 845 | GLN | 3.0 |
| 1 | C | 634 | GLN | 3.0 |
| 1 | A | 734 | SER | 3.0 |
| 1 | A | 800 | ARG | 2.9 |
| 1 | A | 688 | PRO | 2.9 |
| 1 | B | 684 | GLU | 2.9 |
| 1 | B | 801 | ILE | 2.9 |
| 1 | B | 734 | SER | 2.8 |
| 1 | D | 581 | ASN | 2.8 |
| 1 | D | 736 | ALA | 2.8 |
| 1 | D | 688 | PRO | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 582 | GLY | 2.6 |
| 1 | D | 737 | ILE | 2.6 |
| 1 | D | 685 | LEU | 2.6 |
| 1 | C | 736 | ALA | 2.5 |
| 1 | D | 634 | GLN | 2.5 |
| 1 | B | 583 | ASN | 2.5 |
| 1 | D | 801 | ILE | 2.4 |
| 1 | D | 582 | GLY | 2.4 |
| 1 | B | 581 | ASN | 2.4 |
| 1 | D | 1023 | LYS | 2.3 |
| 1 | A | 736 | ALA | 2.3 |
| 1 | C | 803 | PRO | 2.3 |
| 1 | A | 737 | ILE | 2.3 |
| 1 | A | 71 | GLU | 2.3 |
| 1 | C | 761 | GLN | 2.2 |
| 1 | B | 663 | LEU | 2.2 |
| 1 | D | 772 | ASP | 2.2 |
| 1 | A | 684 | GLU | 2.2 |
| 1 | C | 729 | THR | 2.2 |
| 1 | C | 582 | GLY | 2.2 |
| 1 | C | 830 | LEU | 2.2 |
| 1 | A | 583 | ASN | 2.2 |
| 1 | A | 690 | SER | 2.1 |
| 1 | B | 690 | SER | 2.1 |
| 1 | A | 831 | ALA | 2.1 |
| 1 | B | 582 | GLY | 2.1 |
| 1 | A | 79 | PRO | 2.0 |
| 1 | C | 772 | ASP | 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, 95th 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 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 2 | MG | A | 3005 | 1/1 | 0.74 | 0.12 | 42,42,42,42 | 0 |
| 2 | MG | C | 3004 | 1/1 | 0.78 | 0.10 | 52,52,52,52 | 0 |
| 4 | DMS | C | 8504 | 4/4 | 0.82 | 0.14 | 36,68,72,73 | 0 |
| 4 | DMS | C | 8503 | 4/4 | 0.84 | 0.16 | 30,35,46,59 | 0 |
| 4 | DMS | B | 8425 | 4/4 | 0.86 | 0.12 | 32,33,41,56 | 0 |
| 4 | DMS | C | 8413 | 4/4 | 0.86 | 0.21 | 42,69,100,100 | 0 |
| 4 | DMS | A | 8421 | 4/4 | 0.87 | 0.26 | 35,58,84,100 | 0 |
| 4 | DMS | D | 8419 | 4/4 | 0.87 | 0.20 | 54,72,74,95 | 0 |
| 4 | DMS | D | 8413 | 4/4 | 0.88 | 0.17 | 28,56,73,100 | 0 |
| 4 | DMS | D | 8416 | 4/4 | 0.89 | 0.16 | 25,43,52,77 | 0 |
| 4 | DMS | D | 8417 | 4/4 | 0.90 | 0.13 | 26,32,41,100 | 0 |
| 4 | DMS | C | 8602 | 4/4 | 0.90 | 0.14 | 25,45,68,100 | 0 |
| 4 | DMS | D | 8425 | 4/4 | 0.90 | 0.15 | 16,27,33,36 | 4 |
| 4 | DMS | D | 8503 | 4/4 | 0.90 | 0.19 | 43,44,59,100 | 0 |
| 4 | DMS | D | 8703 | 4/4 | 0.90 | 0.18 | 37,58,59,100 | 0 |
| 4 | DMS | D | 8705 | 4/4 | 0.90 | 0.17 | 18,50,52,67 | 0 |
| 3 | NA | D | 3104 | 1/1 | 0.91 | 0.09 | 35,35,35,35 | 0 |
| 4 | DMS | A | 8419 | 4/4 | 0.91 | 0.20 | 65,67,69,100 | 0 |
| 4 | DMS | B | 8508 | 4/4 | 0.91 | 0.12 | 36,41,50,64 | 0 |
| 4 | DMS | B | 8417 | 4/4 | 0.92 | 0.15 | 31,39,48,62 | 0 |
| 4 | DMS | D | 8501 | 4/4 | 0.92 | 0.08 | 25,33,43,59 | 0 |
| 4 | DMS | D | 8409 | 4/4 | 0.92 | 0.11 | 24,33,33,40 | 0 |
| 4 | DMS | A | 8503 | 4/4 | 0.92 | 0.20 | 41,50,94,100 | 0 |
| 4 | DMS | D | 8421 | 4/4 | 0.92 | 0.19 | 42,61,71,100 | 0 |
| 4 | DMS | C | 8417 | 4/4 | 0.93 | 0.10 | 33,36,45,63 | 0 |
| 4 | DMS | A | 8502 | 4/4 | 0.93 | 0.17 | 23,38,48,83 | 0 |
| 4 | DMS | D | 8508 | 4/4 | 0.93 | 0.10 | 39,47,52,59 | 0 |
| 4 | DMS | A | 8425 | 4/4 | 0.93 | 0.14 | 29,37,46,51 | 0 |
| 4 | DMS | C | 8601 | 4/4 | 0.93 | 0.15 | 49,50,73,100 | 0 |
| 4 | DMS | A | 8404 | 4/4 | 0.94 | 0.10 | 19,26,41,49 | 0 |
| 4 | DMS | B | 8404 | 4/4 | 0.94 | 0.11 | 24,29,41,100 | 0 |
| 4 | DMS | B | 8409 | 4/4 | 0.94 | 0.09 | 21,26,39,44 | 0 |
| 4 | DMS | A | 8417 | 4/4 | 0.94 | 0.12 | 26,26,68,100 | 0 |
| 4 | DMS | B | 8421 | 4/4 | 0.95 | 0.11 | 32,60,64,68 | 0 |
| 3 | NA | D | 3103 | 1/1 | 0.95 | 0.09 | 36,36,36,36 | 0 |
| 4 | DMS | A | 8406 | 4/4 | 0.95 | 0.12 | 12,45,59,77 | 0 |
| 4 | DMS | B | 8601 | 4/4 | 0.95 | 0.14 | 33,36,39,39 | 0 |
| 4 | DMS | A | 8416 | 4/4 | 0.95 | 0.19 | 20,39,63,71 | 0 |
| 4 | DMS | C | 8414 | 4/4 | 0.95 | 0.11 | 23,25,34,42 | 0 |
| 3 | NA | A | 3103 | 1/1 | 0.95 | 0.10 | 38,38,38,38 | 0 |
| 4 | DMS | C | 8501 | 4/4 | 0.95 | 0.10 | 27,31,39,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4 | DMS | B | 8502 | 4/4 | 0.96 | 0.10 | 22,27,37,41 | 0 |
| 4 | DMS | B | 8504 | 4/4 | 0.96 | 0.10 | 30,33,44,82 | 0 |
| 4 | DMS | D | 8406 | 4/4 | 0.96 | 0.09 | 21,25,26,42 | 0 |
| 4 | DMS | A | 8414 | 4/4 | 0.96 | 0.13 | 22,43,69,100 | 0 |
| 4 | DMS | D | 8410 | 4/4 | 0.96 | 0.10 | 40,52,57,60 | 0 |
| 3 | NA | B | 3104 | 1/1 | 0.96 | 0.11 | 33,33,33,33 | 0 |
| 4 | DMS | D | 8414 | 4/4 | 0.96 | 0.15 | 33,50,100,100 | 0 |
| 4 | DMS | C | 8409 | 4/4 | 0.96 | 0.08 | 29,30,33,36 | 0 |
| 3 | NA | C | 3104 | 1/1 | 0.96 | 0.08 | 28,28,28,28 | 0 |
| 2 | MG | D | 3005 | 1/1 | 0.96 | 0.09 | 26,26,26,26 | 0 |
| 4 | DMS | C | 8416 | 4/4 | 0.96 | 0.26 | 44,51,52,100 | 0 |
| 4 | DMS | B | 8416 | 4/4 | 0.96 | 0.12 | 32,33,42,49 | 0 |
| 4 | DMS | C | 8421 | 4/4 | 0.96 | 0.16 | 41,44,60,65 | 0 |
| 4 | DMS | C | 8425 | 4/4 | 0.96 | 0.21 | 44,50,66,88 | 0 |
| 4 | DMS | A | 8409 | 4/4 | 0.96 | 0.09 | 23,25,28,41 | 0 |
| 4 | DMS | A | 8412 | 4/4 | 0.96 | 0.14 | 28,33,41,100 | 0 |
| 4 | DMS | A | 8501 | 4/4 | 0.96 | 0.08 | 20,25,41,42 | 0 |
| 3 | NA | A | 3104 | 1/1 | 0.97 | 0.09 | 29,29,29,29 | 0 |
| 4 | DMS | A | 8410 | 4/4 | 0.97 | 0.11 | 41,49,78,100 | 0 |
| 4 | DMS | D | 8404 | 4/4 | 0.97 | 0.09 | 22,27,43,76 | 0 |
| 4 | DMS | A | 8411 | 4/4 | 0.97 | 0.10 | 25,34,36,44 | 0 |
| 4 | DMS | C | 8404 | 4/4 | 0.97 | 0.07 | 17,23,30,37 | 0 |
| 4 | DMS | C | 8405 | 4/4 | 0.97 | 0.11 | 28,31,31,36 | 0 |
| 4 | DMS | C | 8408 | 4/4 | 0.97 | 0.09 | 26,28,34,40 | 0 |
| 3 | NA | D | 3101 | 1/1 | 0.97 | 0.07 | 24,24,24,24 | 0 |
| 4 | DMS | A | 8408 | 4/4 | 0.97 | 0.10 | 21,34,39,80 | 0 |
| 4 | DMS | C | 8411 | 4/4 | 0.98 | 0.11 | 25,31,31,100 | 0 |
| 4 | DMS | C | 8412 | 4/4 | 0.98 | 0.10 | 30,37,38,41 | 0 |
| 4 | DMS | A | 8504 | 4/4 | 0.98 | 0.07 | 23,40,44,77 | 0 |
| 4 | DMS | D | 8411 | 4/4 | 0.98 | 0.12 | 31,33,34,100 | 0 |
| 4 | DMS | A | 8602 | 4/4 | 0.98 | 0.15 | 35,49,98,100 | 0 |
| 4 | DMS | B | 8401 | 4/4 | 0.98 | 0.09 | 16,19,21,23 | 0 |
| 4 | DMS | B | 8402 | 4/4 | 0.98 | 0.07 | 16,16,21,22 | 0 |
| 2 | MG | C | 3006 | 1/1 | 0.98 | 0.08 | 31,31,31,31 | 0 |
| 4 | DMS | B | 8405 | 4/4 | 0.98 | 0.11 | 31,36,37,40 | 0 |
| 4 | DMS | B | 8408 | 4/4 | 0.98 | 0.11 | 33,34,35,100 | 0 |
| 4 | DMS | A | 8403 | 4/4 | 0.98 | 0.06 | 21,23,28,29 | 0 |
| 4 | DMS | B | 8412 | 4/4 | 0.98 | 0.06 | 26,29,33,36 | 0 |
| 4 | DMS | B | 8414 | 4/4 | 0.98 | 0.13 | 25,36,42,46 | 0 |
| 3 | NA | B | 3101 | 1/1 | 0.98 | 0.07 | 17,17,17,17 | 0 |
| 4 | DMS | D | 8701 | 4/4 | 0.98 | 0.09 | 15,18,24,53 | 0 |
| 4 | DMS | D | 8403 | 4/4 | 0.98 | 0.07 | 21,26,28,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4 | DMS | C | 8410 | 4/4 | 0.98 | 0.11 | 26,40,42,49 | 0 |
| 4 | DMS | C | 8401 | 4/4 | 0.99 | 0.05 | 14,15,19,20 | 0 |
| 4 | DMS | D | 8401 | 4/4 | 0.99 | 0.07 | 14,17,19,20 | 0 |
| 4 | DMS | D | 8402 | 4/4 | 0.99 | 0.05 | 12,20,21,23 | 0 |
| 4 | DMS | C | 8402 | 4/4 | 0.99 | 0.05 | 16,16,23,25 | 0 |
| 4 | DMS | C | 8403 | 4/4 | 0.99 | 0.12 | 16,21,24,30 | 0 |
| 4 | DMS | D | 8405 | 4/4 | 0.99 | 0.06 | 24,25,39,45 | 0 |
| 3 | NA | C | 3102 | 1/1 | 0.99 | 0.06 | 14,14,14,14 | 0 |
| 4 | DMS | D | 8408 | 4/4 | 0.99 | 0.06 | 18,30,35,45 | 0 |
| 4 | DMS | B | 8403 | 4/4 | 0.99 | 0.09 | 22,23,28,30 | 0 |
| 3 | NA | C | 3103 | 1/1 | 0.99 | 0.09 | 27,27,27,27 | 0 |
| 2 | MG | B | 3002 | 1/1 | 0.99 | 0.04 | 15,15,15,15 | 0 |
| 4 | DMS | D | 8412 | 4/4 | 0.99 | 0.06 | 27,27,35,100 | 0 |
| 3 | NA | A | 3101 | 1/1 | 0.99 | 0.07 | 23,23,23,23 | 0 |
| 3 | NA | D | 3102 | 1/1 | 0.99 | 0.04 | 12,12,12,12 | 0 |
| 4 | DMS | B | 8411 | 4/4 | 0.99 | 0.10 | 33,34,34,46 | 0 |
| 3 | NA | A | 3102 | 1/1 | 0.99 | 0.04 | 12,12,12,12 | 0 |
| 2 | MG | A | 3002 | 1/1 | 0.99 | 0.04 | 17,17,17,17 | 0 |
| 4 | DMS | A | 8401 | 4/4 | 0.99 | 0.10 | 12,15,15,17 | 0 |
| 4 | DMS | A | 8402 | 4/4 | 0.99 | 0.05 | 15,17,23,36 | 0 |
| 2 | MG | A | 3001 | 1/1 | 0.99 | 0.04 | 17,17,17,17 | 0 |
| 2 | MG | D | 3001 | 1/1 | 0.99 | 0.03 | 14,14,14,14 | 0 |
| 4 | DMS | A | 8405 | 4/4 | 0.99 | 0.06 | 25,25,26,29 | 0 |
| 3 | NA | B | 3103 | 1/1 | 0.99 | 0.06 | 26,26,26,26 | 0 |
| 2 | MG | D | 3002 | 1/1 | 0.99 | 0.03 | 16,16,16,16 | 0 |
| 3 | NA | C | 3101 | 1/1 | 0.99 | 0.06 | 18,18,18,18 | 0 |
| 3 | NA | B | 3102 | 1/1 | 1.00 | 0.06 | 13,13,13,13 | 0 |
| 2 | MG | C | 3001 | 1/1 | 1.00 | 0.10 | 15,15,15,15 | 0 |
| 2 | MG | C | 3002 | 1/1 | 1.00 | 0.03 | 13,13,13,13 | 0 |
| 2 | MG | B | 3001 | 1/1 | 1.00 | 0.09 | 14,14,14,14 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.