



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2017 – 05:25 PM EDT

PDB ID : 1JZ4
Title : E. COLI (lacZ) BETA-GALACTOSIDASE-TRAPPED 2-DEOXY-GALACTOSYL-ENZYME INTERMEDIATE (Low Bis-Tris)
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : unknown
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

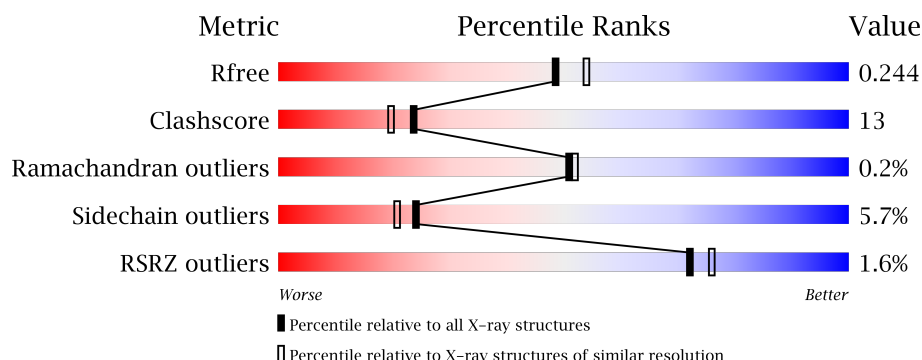
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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} | 100719 | 4243 (2.10-2.10) |
| Clashscore | 112137 | 4788 (2.10-2.10) |
| Ramachandran outliers | 110173 | 4740 (2.10-2.10) |
| Sidechain outliers | 110143 | 4741 (2.10-2.10) |
| RSRZ outliers | 101464 | 4275 (2.10-2.10) |

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 | 2% 64% 29% 5% .. |
| 1 | B | 1023 | % 62% 30% 5% .. |
| 1 | C | 1023 | 2% 63% 28% 7% .. |
| 1 | D | 1023 | 2% 63% 30% 5% .. |

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 crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2 | 2DG | B | 2001 | - | - | - | X |
| 4 | NA | D | 3103 | - | - | - | X |
| 5 | DMS | A | 8406 | - | - | - | X |
| 5 | DMS | A | 8407 | - | - | - | X |
| 5 | DMS | A | 8417 | - | - | - | X |
| 5 | DMS | A | 8420 | - | - | - | X |
| 5 | DMS | A | 8502 | - | - | - | X |
| 5 | DMS | A | 8504 | - | - | - | X |
| 5 | DMS | B | 8404 | - | - | - | X |
| 5 | DMS | B | 8405 | - | - | - | X |
| 5 | DMS | B | 8406 | - | - | - | X |
| 5 | DMS | B | 8407 | - | - | - | X |
| 5 | DMS | B | 8408 | - | - | - | X |
| 5 | DMS | B | 8420 | - | - | - | X |
| 5 | DMS | B | 8423 | - | - | - | X |
| 5 | DMS | B | 8508 | - | X | - | X |
| 5 | DMS | C | 8419 | - | - | - | X |
| 5 | DMS | C | 8420 | - | - | - | X |
| 5 | DMS | C | 8501 | - | - | - | X |
| 5 | DMS | C | 8506 | - | - | X | - |
| 5 | DMS | C | 8602 | - | - | - | X |
| 5 | DMS | D | 8408 | - | - | - | X |
| 5 | DMS | D | 8412 | - | - | X | - |
| 5 | DMS | D | 8703 | - | - | - | X |

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36890 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 | 1011 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8125 | 5138 | 1440 | 1509 | 38 | | | |
| 1 | B | 1011 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8125 | 5138 | 1440 | 1509 | 38 | | | |
| 1 | C | 1011 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8125 | 5138 | 1440 | 1509 | 38 | | | |
| 1 | D | 1011 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8125 | 5138 | 1440 | 1509 | 38 | | | |

There are 32 discrepancies between the modelled and reference sequences:

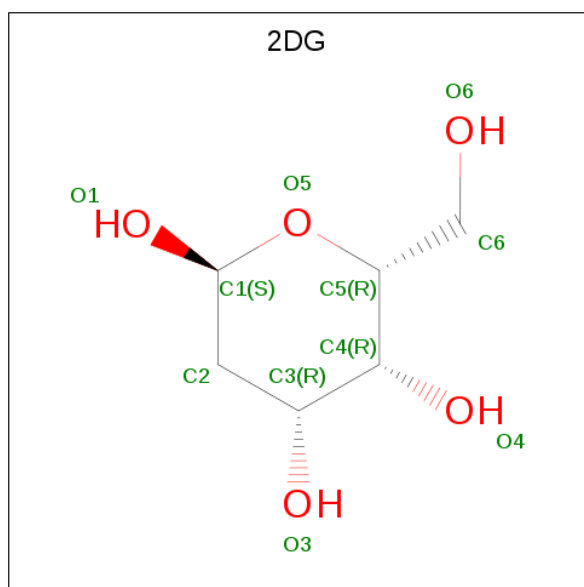
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|-----------|
| A | 1 | GLY | THR | CLONING ARTIFACT | ? P00722 |
| A | 2 | SER | MET | CLONING ARTIFACT | ? P00722 |
| A | 3 | HIS | ILE | CLONING ARTIFACT | ? P00722 |
| A | 4 | MET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

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

- Molecule 2 is 2-DEOXY-BETA-D-GALACTOSE (three-letter code: 2DG) (formula: $C_6H_{12}O_5$).



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

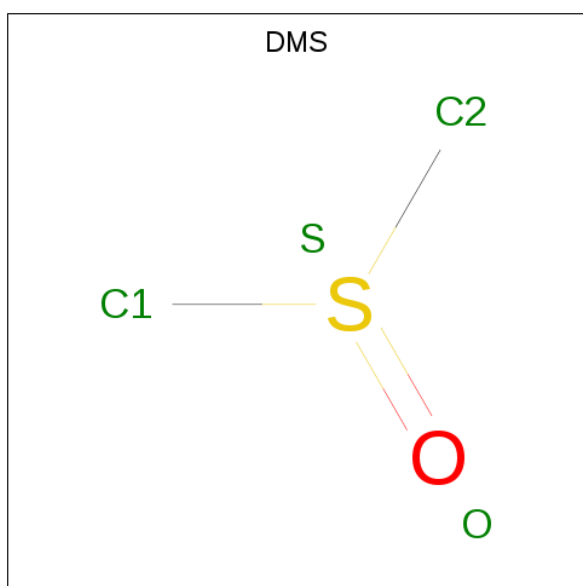
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------------|---------|---------|
| 5 | A | 1 | Total C O S 4 2 1 1 | 0 | 0 |
| 5 | A | 1 | Total C O S 4 2 1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 5 | A | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | A | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | B | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | C | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|--------|---------|---------|
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |
| 5 | D | 1 | Total 4 | C 2 | O 1 | S 1 | 0 | 0 |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 6 | A | 992 | Total 992 | O 992 | 0 | 0 |
| 6 | B | 995 | Total 995 | O 995 | 0 | 0 |

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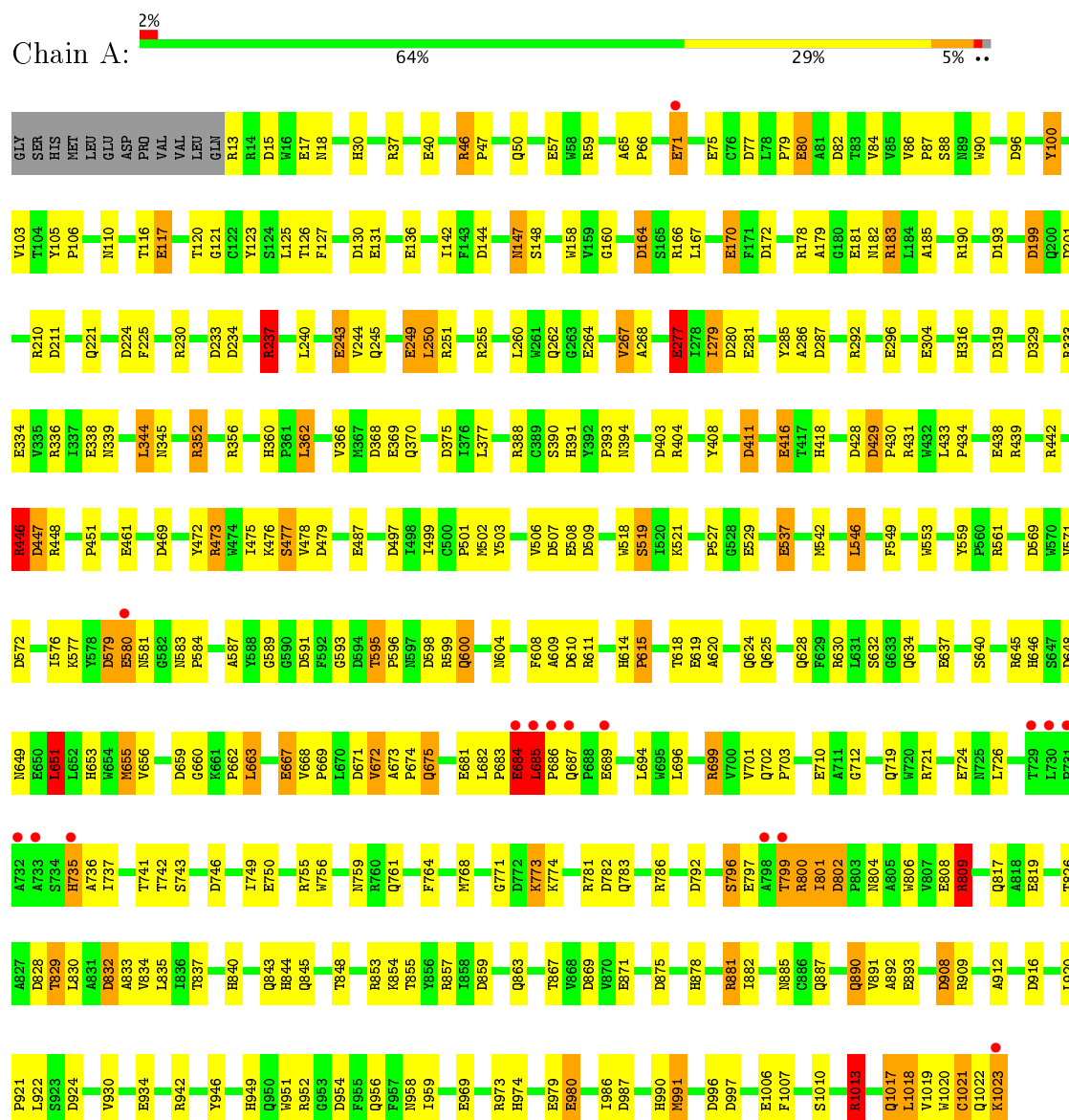
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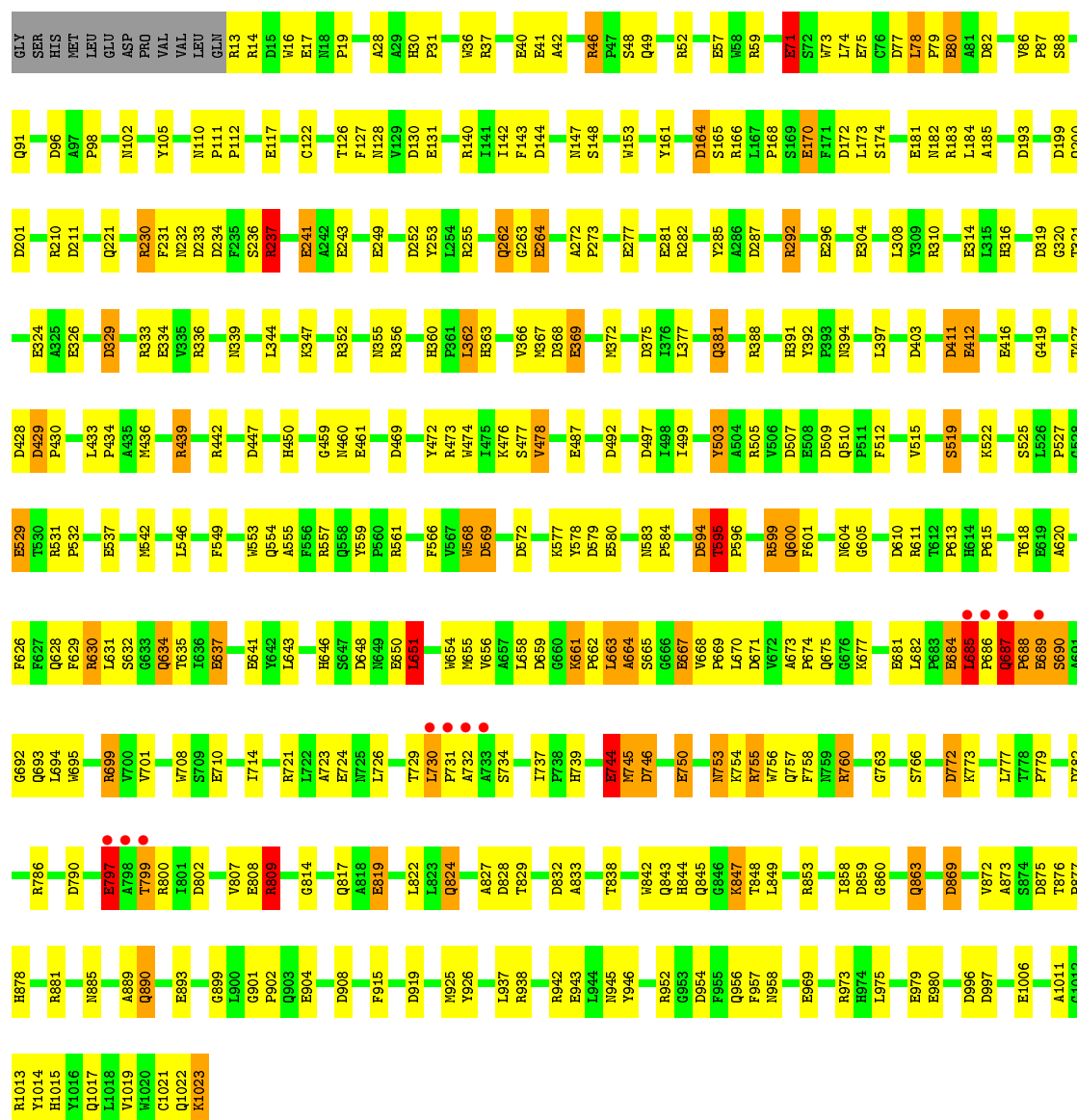
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 6 | C | 946 | Total 946 | O 946 | 0 | 0 |
| 6 | D | 980 | Total 980 | O 980 | 0 | 0 |

3 Residue-property plots

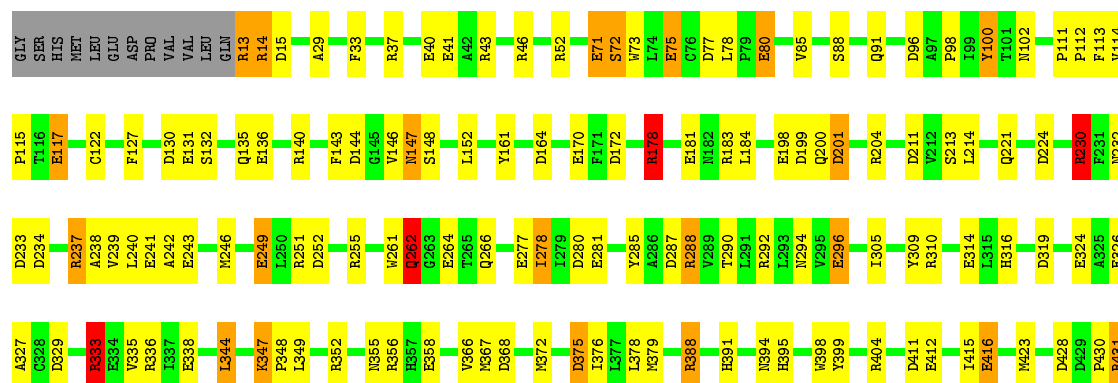
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

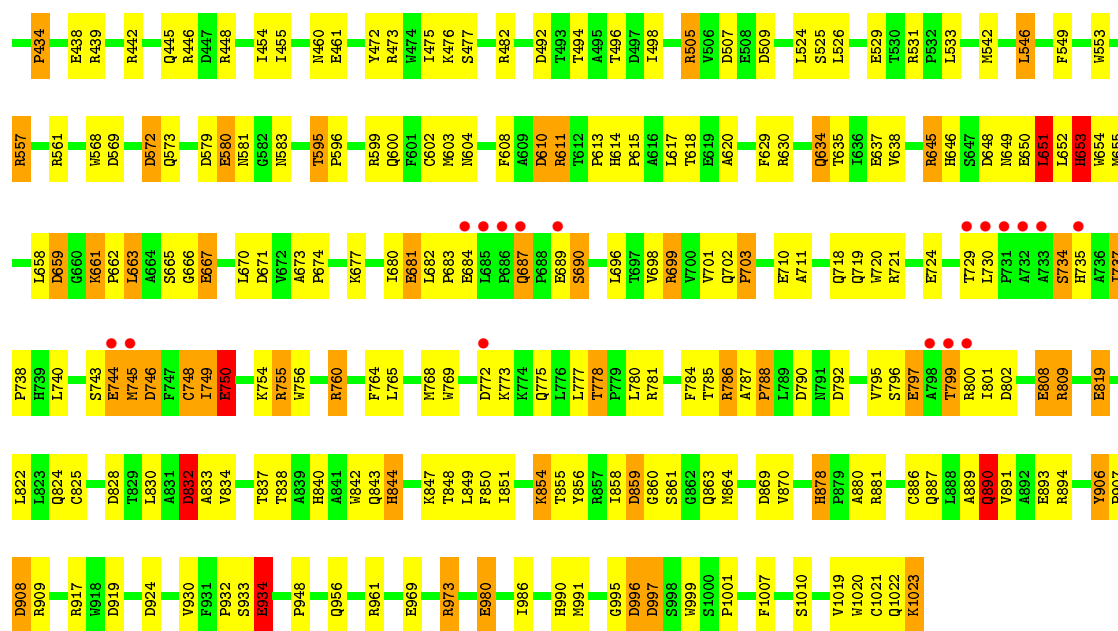
• Molecule 1: Beta-Galactosidase



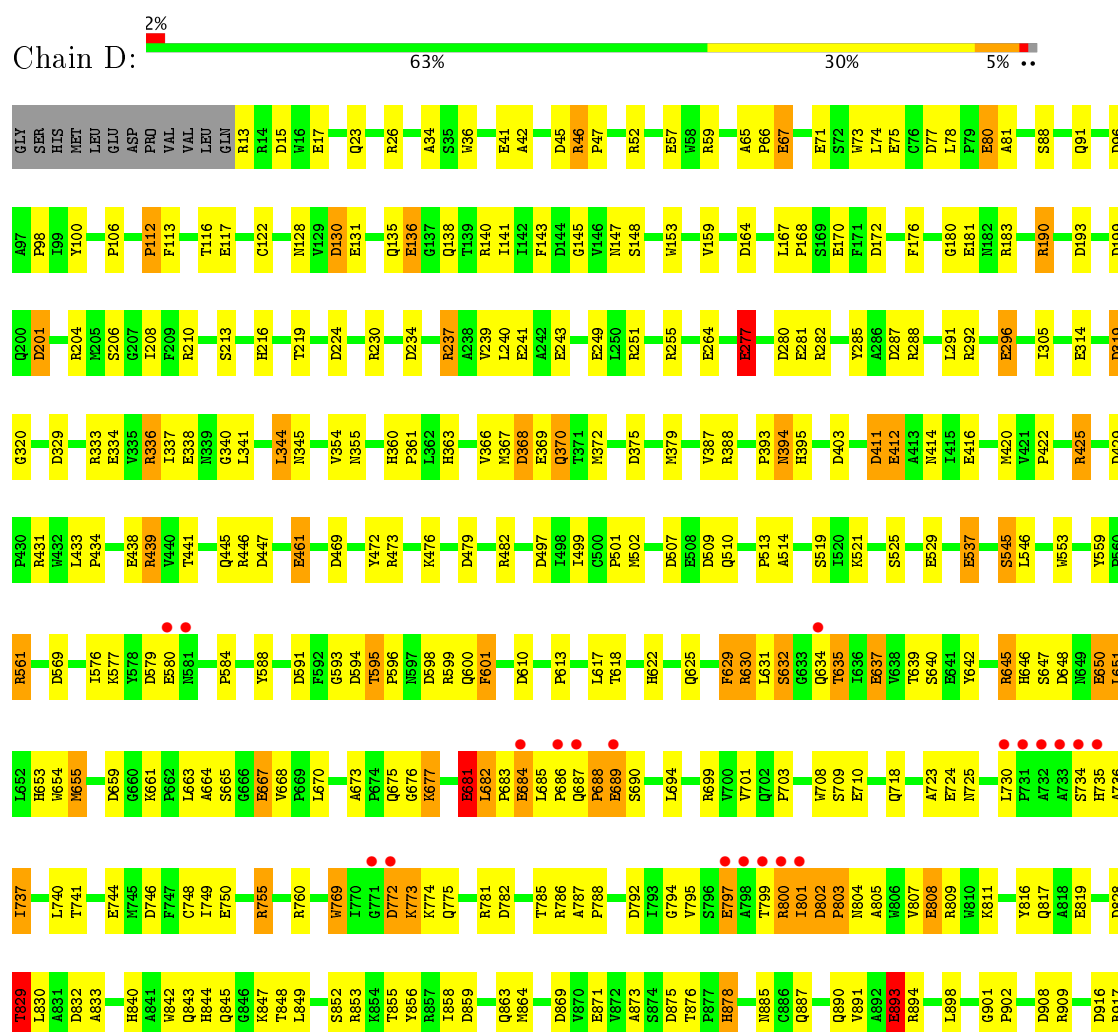


● Molecule 1: Beta-Galactosidase





• Molecule 1: Beta-Galactosidase



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| H918 | D919 | L920 | P921 | E934 | R942 | E943 | L944 | N945 | H949 | Q950 | W951 | R952 | G953 | D954 | F955 | Q956 | I959 | S960 | R961 | Y962 | M968 | E969 | H972 | R973 | H974 | E979 | E980 | G981 | L984 | R985 | I986 | D987 | D996 | D997 | S1004 | S1010 | R1013 | L1018 | V1019 | W1020 | C1021 | Q1022 | K1023 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 149.50 Å 169.00 Å 200.80 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 2.10 19.99 – 2.10 | Depositor EDS |
| % Data completeness (in resolution range) | 90.0 (40.00-2.10) 86.4 (19.99-2.10) | Depositor EDS |
| R_{merge} | 0.08 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.18 (at 2.09 Å) | Xtriage |
| Refinement program | TNT | Depositor |
| R, R_{free} | 0.164 , 0.267 0.152 , 0.244 | Depositor DCC |
| R_{free} test set | 3669 reflections (1.46%) | DCC |
| Wilson B-factor (Å ²) | 11.5 | Xtriage |
| Anisotropy | 0.030 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 95.0 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.96 | EDS |
| Total number of atoms | 36890 | wwPDB-VP |
| Average B, all atoms (Å ²) | 20.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.06 % 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 5.3009e-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, MG, DMS, 2DG

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 | 1.09 | 43/8367 (0.5%) | 1.73 | 174/11415 (1.5%) |
| 1 | B | 1.11 | 48/8367 (0.6%) | 1.69 | 165/11415 (1.4%) |
| 1 | C | 1.11 | 42/8367 (0.5%) | 1.75 | 177/11415 (1.6%) |
| 1 | D | 1.11 | 48/8367 (0.6%) | 1.69 | 151/11415 (1.3%) |
| All | All | 1.10 | 181/33468 (0.5%) | 1.71 | 667/45660 (1.5%) |

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 | B | 0 | 1 |
| 1 | D | 1 | 0 |
| All | All | 1 | 1 |

All (181) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | D | 277 | GLU | CD-OE2 | 10.41 | 1.37 | 1.25 |
| 1 | C | 281 | GLU | CD-OE2 | 10.15 | 1.36 | 1.25 |
| 1 | D | 71 | GLU | CD-OE2 | 10.14 | 1.36 | 1.25 |
| 1 | C | 684 | GLU | CD-OE2 | 9.88 | 1.36 | 1.25 |
| 1 | C | 296 | GLU | CD-OE2 | 9.86 | 1.36 | 1.25 |
| 1 | A | 304 | GLU | CD-OE2 | 9.53 | 1.36 | 1.25 |
| 1 | A | 136 | GLU | CD-OE2 | 9.34 | 1.35 | 1.25 |
| 1 | B | 461 | GLU | CD-OE2 | 8.92 | 1.35 | 1.25 |
| 1 | D | 243 | GLU | CD-OE2 | 8.72 | 1.35 | 1.25 |
| 1 | D | 136 | GLU | CD-OE2 | 8.49 | 1.34 | 1.25 |
| 1 | A | 537 | GLU | CD-OE2 | 8.29 | 1.34 | 1.25 |
| 1 | A | 296 | GLU | CD-OE2 | 8.22 | 1.34 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1 | B | 281 | GLU | CD-OE2 | 8.19 | 1.34 | 1.25 |
| 1 | B | 324 | GLU | CD-OE2 | 7.92 | 1.34 | 1.25 |
| 1 | A | 249 | GLU | CD-OE2 | 7.91 | 1.34 | 1.25 |
| 1 | C | 980 | GLU | CD-OE2 | 7.74 | 1.34 | 1.25 |
| 1 | D | 650 | GLU | CD-OE2 | 7.57 | 1.33 | 1.25 |
| 1 | C | 744 | GLU | CD-OE2 | 7.54 | 1.33 | 1.25 |
| 1 | D | 681 | GLU | CD-OE2 | 7.54 | 1.33 | 1.25 |
| 1 | A | 1006 | GLU | CD-OE2 | 7.54 | 1.33 | 1.25 |
| 1 | D | 980 | GLU | CD-OE2 | 7.47 | 1.33 | 1.25 |
| 1 | A | 281 | GLU | CD-OE2 | 7.42 | 1.33 | 1.25 |
| 1 | C | 819 | GLU | CD-OE2 | 7.40 | 1.33 | 1.25 |
| 1 | D | 979 | GLU | CD-OE2 | 7.33 | 1.33 | 1.25 |
| 1 | B | 296 | GLU | CD-OE2 | 7.29 | 1.33 | 1.25 |
| 1 | A | 243 | GLU | CD-OE2 | 7.26 | 1.33 | 1.25 |
| 1 | B | 980 | GLU | CD-OE2 | 7.26 | 1.33 | 1.25 |
| 1 | A | 684 | GLU | CD-OE2 | 7.24 | 1.33 | 1.25 |
| 1 | D | 41 | GLU | CD-OE2 | 7.20 | 1.33 | 1.25 |
| 1 | A | 689 | GLU | CD-OE2 | 7.18 | 1.33 | 1.25 |
| 1 | B | 529 | GLU | CD-OE2 | 7.18 | 1.33 | 1.25 |
| 1 | D | 580 | GLU | CD-OE2 | 7.12 | 1.33 | 1.25 |
| 1 | B | 71 | GLU | CD-OE2 | 7.10 | 1.33 | 1.25 |
| 1 | D | 893 | GLU | CD-OE2 | 7.07 | 1.33 | 1.25 |
| 1 | B | 650 | GLU | CD-OE2 | 7.03 | 1.33 | 1.25 |
| 1 | B | 819 | GLU | CD-OE2 | 7.00 | 1.33 | 1.25 |
| 1 | C | 750 | GLU | CD-OE2 | 6.98 | 1.33 | 1.25 |
| 1 | D | 969 | GLU | CD-OE2 | 6.98 | 1.33 | 1.25 |
| 1 | B | 904 | GLU | CD-OE1 | -6.97 | 1.18 | 1.25 |
| 1 | C | 198 | GLU | CD-OE2 | 6.95 | 1.33 | 1.25 |
| 1 | A | 57 | GLU | CD-OE2 | 6.92 | 1.33 | 1.25 |
| 1 | C | 893 | GLU | CD-OE2 | 6.89 | 1.33 | 1.25 |
| 1 | B | 314 | GLU | CD-OE1 | -6.88 | 1.18 | 1.25 |
| 1 | A | 71 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | B | 243 | GLU | CD-OE2 | 6.86 | 1.33 | 1.25 |
| 1 | C | 170 | GLU | CD-OE2 | 6.85 | 1.33 | 1.25 |
| 1 | C | 529 | GLU | CD-OE2 | 6.81 | 1.33 | 1.25 |
| 1 | D | 296 | GLU | CD-OE2 | 6.75 | 1.33 | 1.25 |
| 1 | A | 338 | GLU | CD-OE2 | 6.73 | 1.33 | 1.25 |
| 1 | A | 416 | GLU | CD-OE2 | 6.72 | 1.33 | 1.25 |
| 1 | C | 689 | GLU | CD-OE2 | 6.71 | 1.33 | 1.25 |
| 1 | C | 710 | GLU | CD-OE2 | 6.66 | 1.32 | 1.25 |
| 1 | C | 314 | GLU | CD-OE2 | 6.64 | 1.32 | 1.25 |
| 1 | C | 277 | GLU | CD-OE2 | 6.63 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | D | 80 | GLU | CD-OE2 | 6.61 | 1.32 | 1.25 |
| 1 | D | 241 | GLU | CD-OE2 | 6.58 | 1.32 | 1.25 |
| 1 | B | 710 | GLU | CD-OE2 | 6.58 | 1.32 | 1.25 |
| 1 | B | 969 | GLU | CD-OE2 | 6.58 | 1.32 | 1.25 |
| 1 | A | 170 | GLU | CD-OE2 | 6.58 | 1.32 | 1.25 |
| 1 | C | 667 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 1 | D | 170 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 1 | B | 117 | GLU | CD-OE2 | 6.53 | 1.32 | 1.25 |
| 1 | D | 808 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 1 | C | 241 | GLU | CD-OE2 | 6.44 | 1.32 | 1.25 |
| 1 | A | 277 | GLU | CD-OE2 | 6.42 | 1.32 | 1.25 |
| 1 | B | 580 | GLU | CD-OE2 | 6.42 | 1.32 | 1.25 |
| 1 | C | 580 | GLU | CD-OE2 | 6.39 | 1.32 | 1.25 |
| 1 | A | 334 | GLU | CD-OE2 | 6.36 | 1.32 | 1.25 |
| 1 | C | 650 | GLU | CD-OE2 | 6.36 | 1.32 | 1.25 |
| 1 | B | 637 | GLU | CD-OE2 | 6.36 | 1.32 | 1.25 |
| 1 | C | 934 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | B | 689 | GLU | CD-OE2 | 6.34 | 1.32 | 1.25 |
| 1 | D | 819 | GLU | CD-OE2 | 6.34 | 1.32 | 1.25 |
| 1 | A | 637 | GLU | CD-OE2 | 6.32 | 1.32 | 1.25 |
| 1 | B | 943 | GLU | CD-OE2 | 6.31 | 1.32 | 1.25 |
| 1 | A | 969 | GLU | CD-OE2 | 6.29 | 1.32 | 1.25 |
| 1 | B | 40 | GLU | CD-OE2 | 6.26 | 1.32 | 1.25 |
| 1 | B | 684 | GLU | CD-OE2 | 6.26 | 1.32 | 1.25 |
| 1 | C | 969 | GLU | CD-OE2 | 6.26 | 1.32 | 1.25 |
| 1 | B | 181 | GLU | CD-OE2 | 6.24 | 1.32 | 1.25 |
| 1 | D | 117 | GLU | CD-OE2 | 6.24 | 1.32 | 1.25 |
| 1 | B | 264 | GLU | CD-OE2 | 6.22 | 1.32 | 1.25 |
| 1 | C | 181 | GLU | CD-OE2 | 6.22 | 1.32 | 1.25 |
| 1 | B | 41 | GLU | CD-OE2 | 6.19 | 1.32 | 1.25 |
| 1 | C | 338 | GLU | CD-OE2 | 6.18 | 1.32 | 1.25 |
| 1 | D | 934 | GLU | CD-OE2 | 6.17 | 1.32 | 1.25 |
| 1 | C | 136 | GLU | CD-OE2 | 6.14 | 1.32 | 1.25 |
| 1 | C | 249 | GLU | CD-OE2 | 6.14 | 1.32 | 1.25 |
| 1 | C | 71 | GLU | CD-OE2 | 6.13 | 1.32 | 1.25 |
| 1 | A | 117 | GLU | CD-OE2 | 6.13 | 1.32 | 1.25 |
| 1 | B | 744 | GLU | CD-OE2 | 6.12 | 1.32 | 1.25 |
| 1 | D | 416 | GLU | CD-OE2 | 6.12 | 1.32 | 1.25 |
| 1 | D | 281 | GLU | CD-OE2 | 6.10 | 1.32 | 1.25 |
| 1 | A | 893 | GLU | CD-OE2 | 6.10 | 1.32 | 1.25 |
| 1 | C | 442 | ARG | CZ-NH1 | 6.10 | 1.41 | 1.33 |
| 1 | A | 487 | GLU | CD-OE2 | 6.07 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1 | A | 529 | GLU | CD-OE2 | 6.05 | 1.32 | 1.25 |
| 1 | D | 943 | GLU | CD-OE1 | -6.05 | 1.19 | 1.25 |
| 1 | D | 943 | GLU | CD-OE2 | 6.05 | 1.32 | 1.25 |
| 1 | C | 416 | GLU | CD-OE2 | 6.04 | 1.32 | 1.25 |
| 1 | D | 17 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | D | 684 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | A | 80 | GLU | CD-OE2 | 6.02 | 1.32 | 1.25 |
| 1 | D | 797 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | D | 537 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | A | 819 | GLU | CD-OE2 | 5.98 | 1.32 | 1.25 |
| 1 | C | 681 | GLU | CD-OE2 | 5.96 | 1.32 | 1.25 |
| 1 | D | 438 | GLU | CD-OE2 | 5.94 | 1.32 | 1.25 |
| 1 | A | 580 | GLU | CD-OE2 | 5.92 | 1.32 | 1.25 |
| 1 | D | 529 | GLU | CD-OE2 | 5.92 | 1.32 | 1.25 |
| 1 | A | 750 | GLU | CD-OE2 | 5.92 | 1.32 | 1.25 |
| 1 | C | 461 | GLU | CD-OE2 | 5.91 | 1.32 | 1.25 |
| 1 | C | 75 | GLU | CD-OE2 | 5.91 | 1.32 | 1.25 |
| 1 | C | 41 | GLU | CD-OE2 | 5.87 | 1.32 | 1.25 |
| 1 | B | 334 | GLU | CD-OE2 | 5.86 | 1.32 | 1.25 |
| 1 | D | 131 | GLU | CD-OE2 | 5.84 | 1.32 | 1.25 |
| 1 | D | 249 | GLU | CD-OE2 | 5.84 | 1.32 | 1.25 |
| 1 | A | 710 | GLU | CD-OE2 | 5.84 | 1.32 | 1.25 |
| 1 | B | 1006 | GLU | CD-OE2 | 5.84 | 1.32 | 1.25 |
| 1 | B | 893 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | B | 277 | GLU | CD-OE2 | 5.82 | 1.32 | 1.25 |
| 1 | B | 724 | GLU | CD-OE2 | 5.80 | 1.32 | 1.25 |
| 1 | B | 667 | GLU | CD-OE2 | 5.80 | 1.32 | 1.25 |
| 1 | D | 750 | GLU | CD-OE2 | 5.76 | 1.31 | 1.25 |
| 1 | A | 980 | GLU | CD-OE2 | 5.76 | 1.31 | 1.25 |
| 1 | B | 797 | GLU | CD-OE2 | 5.76 | 1.31 | 1.25 |
| 1 | D | 75 | GLU | CD-OE2 | 5.75 | 1.31 | 1.25 |
| 1 | A | 369 | GLU | CD-OE2 | 5.75 | 1.31 | 1.25 |
| 1 | C | 264 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |
| 1 | C | 412 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |
| 1 | D | 264 | GLU | CD-OE2 | 5.71 | 1.31 | 1.25 |
| 1 | A | 724 | GLU | CD-OE2 | 5.68 | 1.31 | 1.25 |
| 1 | A | 131 | GLU | CD-OE2 | 5.67 | 1.31 | 1.25 |
| 1 | B | 241 | GLU | CD-OE2 | 5.65 | 1.31 | 1.25 |
| 1 | B | 75 | GLU | CD-OE2 | 5.64 | 1.31 | 1.25 |
| 1 | B | 170 | GLU | CD-OE2 | 5.63 | 1.31 | 1.25 |
| 1 | B | 487 | GLU | CD-OE2 | 5.61 | 1.31 | 1.25 |
| 1 | B | 326 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | B | 369 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | D | 710 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | C | 358 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | C | 797 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | D | 744 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | A | 979 | GLU | CD-OE2 | 5.56 | 1.31 | 1.25 |
| 1 | A | 264 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | C | 243 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | D | 314 | GLU | CD-OE2 | 5.54 | 1.31 | 1.25 |
| 1 | D | 338 | GLU | CD-OE2 | 5.53 | 1.31 | 1.25 |
| 1 | B | 249 | GLU | CD-OE2 | 5.52 | 1.31 | 1.25 |
| 1 | B | 80 | GLU | CD-OE2 | 5.51 | 1.31 | 1.25 |
| 1 | B | 57 | GLU | CD-OE2 | 5.46 | 1.31 | 1.25 |
| 1 | D | 461 | GLU | CD-OE2 | 5.46 | 1.31 | 1.25 |
| 1 | B | 979 | GLU | CD-OE2 | 5.44 | 1.31 | 1.25 |
| 1 | D | 871 | GLU | CD-OE2 | 5.43 | 1.31 | 1.25 |
| 1 | A | 508 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 |
| 1 | A | 681 | GLU | CD-OE2 | 5.37 | 1.31 | 1.25 |
| 1 | A | 461 | GLU | CD-OE2 | 5.36 | 1.31 | 1.25 |
| 1 | D | 667 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | A | 369 | GLU | CD-OE1 | -5.34 | 1.19 | 1.25 |
| 1 | B | 17 | GLU | CD-OE1 | -5.29 | 1.19 | 1.25 |
| 1 | D | 369 | GLU | CD-OE2 | 5.27 | 1.31 | 1.25 |
| 1 | A | 667 | GLU | CD-OE2 | 5.25 | 1.31 | 1.25 |
| 1 | A | 934 | GLU | CD-OE2 | 5.23 | 1.31 | 1.25 |
| 1 | D | 637 | GLU | CD-OE2 | 5.20 | 1.31 | 1.25 |
| 1 | B | 750 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 1 | B | 304 | GLU | CD-OE1 | -5.15 | 1.20 | 1.25 |
| 1 | A | 40 | GLU | CD-OE2 | 5.14 | 1.31 | 1.25 |
| 1 | C | 438 | GLU | CD-OE2 | 5.14 | 1.31 | 1.25 |
| 1 | D | 689 | GLU | CD-OE1 | -5.14 | 1.20 | 1.25 |
| 1 | D | 57 | GLU | CD-OE2 | 5.13 | 1.31 | 1.25 |
| 1 | C | 808 | GLU | CD-OE2 | 5.13 | 1.31 | 1.25 |
| 1 | C | 80 | GLU | CD-OE2 | 5.12 | 1.31 | 1.25 |
| 1 | A | 181 | GLU | CD-OE2 | 5.11 | 1.31 | 1.25 |
| 1 | A | 334 | GLU | CD-OE1 | -5.11 | 1.20 | 1.25 |
| 1 | D | 181 | GLU | CD-OE2 | 5.08 | 1.31 | 1.25 |
| 1 | C | 324 | GLU | CD-OE2 | 5.08 | 1.31 | 1.25 |
| 1 | B | 131 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |
| 1 | C | 117 | GLU | CD-OE2 | 5.03 | 1.31 | 1.25 |
| 1 | D | 412 | GLU | CD-OE2 | 5.01 | 1.31 | 1.25 |
| 1 | B | 561 | ARG | NE-CZ | 5.01 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | B | 314 | GLU | CD-OE2 | 5.00 | 1.31 | 1.25 |

All (667) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | C | 809 | ARG | NE-CZ-NH1 | 19.72 | 130.16 | 120.30 |
| 1 | C | 442 | ARG | NE-CZ-NH2 | -17.27 | 111.67 | 120.30 |
| 1 | C | 786 | ARG | NE-CZ-NH1 | 15.02 | 127.81 | 120.30 |
| 1 | C | 721 | ARG | NE-CZ-NH1 | 15.00 | 127.80 | 120.30 |
| 1 | A | 46 | ARG | NE-CZ-NH1 | 15.00 | 127.80 | 120.30 |
| 1 | B | 881 | ARG | NE-CZ-NH1 | 14.60 | 127.60 | 120.30 |
| 1 | D | 561 | ARG | NE-CZ-NH1 | 12.89 | 126.74 | 120.30 |
| 1 | C | 43 | ARG | NE-CZ-NH1 | 12.49 | 126.55 | 120.30 |
| 1 | D | 630 | ARG | NE-CZ-NH1 | 12.48 | 126.54 | 120.30 |
| 1 | D | 172 | ASP | CB-CG-OD2 | -12.37 | 107.17 | 118.30 |
| 1 | A | 280 | ASP | CB-CG-OD2 | -12.26 | 107.26 | 118.30 |
| 1 | C | 280 | ASP | CB-CG-OD2 | -12.24 | 107.29 | 118.30 |
| 1 | C | 630 | ARG | NE-CZ-NH1 | 11.98 | 126.29 | 120.30 |
| 1 | D | 224 | ASP | CB-CG-OD1 | 11.97 | 129.07 | 118.30 |
| 1 | C | 611 | ARG | NE-CZ-NH1 | 11.93 | 126.26 | 120.30 |
| 1 | C | 786 | ARG | NE-CZ-NH2 | -11.91 | 114.35 | 120.30 |
| 1 | B | 252 | ASP | CB-CG-OD2 | -11.85 | 107.64 | 118.30 |
| 1 | A | 37 | ARG | NE-CZ-NH1 | 11.76 | 126.18 | 120.30 |
| 1 | C | 204 | ARG | NE-CZ-NH1 | 11.65 | 126.12 | 120.30 |
| 1 | A | 699 | ARG | NE-CZ-NH2 | -11.63 | 114.48 | 120.30 |
| 1 | D | 802 | ASP | C-N-CD | -11.56 | 95.17 | 120.60 |
| 1 | C | 809 | ARG | NE-CZ-NH2 | -11.49 | 114.56 | 120.30 |
| 1 | A | 909 | ARG | NE-CZ-NH1 | 11.43 | 126.01 | 120.30 |
| 1 | A | 699 | ARG | NE-CZ-NH1 | 11.38 | 125.99 | 120.30 |
| 1 | D | 429 | ASP | CB-CG-OD1 | 11.37 | 128.53 | 118.30 |
| 1 | C | 230 | ARG | NE-CZ-NH1 | 11.28 | 125.94 | 120.30 |
| 1 | C | 310 | ARG | NE-CZ-NH1 | 11.21 | 125.91 | 120.30 |
| 1 | A | 497 | ASP | CB-CG-OD1 | 11.20 | 128.38 | 118.30 |
| 1 | B | 772 | ASP | CB-CG-OD2 | -11.13 | 108.28 | 118.30 |
| 1 | D | 172 | ASP | CB-CG-OD1 | 11.09 | 128.28 | 118.30 |
| 1 | D | 255 | ARG | NE-CZ-NH1 | 11.09 | 125.84 | 120.30 |
| 1 | A | 497 | ASP | CB-CG-OD2 | -10.84 | 108.54 | 118.30 |
| 1 | B | 193 | ASP | CB-CG-OD1 | 10.80 | 128.02 | 118.30 |
| 1 | B | 772 | ASP | CB-CG-OD1 | 10.73 | 127.96 | 118.30 |
| 1 | C | 973 | ARG | NE-CZ-NH1 | 10.70 | 125.65 | 120.30 |
| 1 | A | 144 | ASP | CB-CG-OD1 | 10.68 | 127.92 | 118.30 |
| 1 | A | 37 | ARG | NE-CZ-NH2 | -10.52 | 115.04 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | B | 287 | ASP | CB-CG-OD1 | 10.48 | 127.73 | 118.30 |
| 1 | B | 869 | ASP | CB-CG-OD1 | 10.40 | 127.66 | 118.30 |
| 1 | D | 336 | ARG | NE-CZ-NH1 | 10.40 | 125.50 | 120.30 |
| 1 | A | 439 | ARG | NE-CZ-NH1 | 10.36 | 125.48 | 120.30 |
| 1 | D | 786 | ARG | NE-CZ-NH2 | -10.31 | 115.15 | 120.30 |
| 1 | A | 292 | ARG | NE-CZ-NH1 | 10.27 | 125.44 | 120.30 |
| 1 | B | 336 | ARG | NE-CZ-NH1 | 10.23 | 125.41 | 120.30 |
| 1 | B | 572 | ASP | CB-CG-OD2 | -10.19 | 109.13 | 118.30 |
| 1 | C | 439 | ARG | NE-CZ-NH2 | -10.18 | 115.21 | 120.30 |
| 1 | C | 140 | ARG | NE-CZ-NH1 | 10.15 | 125.38 | 120.30 |
| 1 | A | 509 | ASP | CB-CG-OD2 | -10.09 | 109.22 | 118.30 |
| 1 | C | 85 | VAL | CA-CB-CG2 | -10.02 | 95.88 | 110.90 |
| 1 | C | 909 | ARG | NE-CZ-NH2 | -9.94 | 115.33 | 120.30 |
| 1 | A | 166 | ARG | NE-CZ-NH2 | -9.89 | 115.36 | 120.30 |
| 1 | D | 368 | ASP | CB-CG-OD2 | -9.86 | 109.43 | 118.30 |
| 1 | C | 336 | ARG | NE-CZ-NH1 | 9.85 | 125.22 | 120.30 |
| 1 | B | 671 | ASP | CB-CG-OD2 | -9.80 | 109.47 | 118.30 |
| 1 | C | 996 | ASP | CB-CG-OD2 | -9.77 | 109.51 | 118.30 |
| 1 | C | 411 | ASP | CB-CG-OD2 | -9.76 | 109.51 | 118.30 |
| 1 | C | 310 | ARG | NE-CZ-NH2 | -9.74 | 115.43 | 120.30 |
| 1 | A | 997 | ASP | CB-CG-OD2 | -9.72 | 109.55 | 118.30 |
| 1 | D | 193 | ASP | CB-CG-OD1 | 9.71 | 127.03 | 118.30 |
| 1 | D | 594 | ASP | CB-CG-OD2 | -9.67 | 109.59 | 118.30 |
| 1 | D | 782 | ASP | CB-CG-OD2 | -9.67 | 109.60 | 118.30 |
| 1 | D | 429 | ASP | CB-CG-OD2 | -9.66 | 109.61 | 118.30 |
| 1 | A | 201 | ASP | CB-CG-OD2 | -9.66 | 109.61 | 118.30 |
| 1 | D | 853 | ARG | NE-CZ-NH2 | -9.62 | 115.49 | 120.30 |
| 1 | A | 403 | ASP | CB-CG-OD2 | -9.61 | 109.66 | 118.30 |
| 1 | B | 721 | ARG | NE-CZ-NH1 | 9.60 | 125.10 | 120.30 |
| 1 | A | 916 | ASP | CB-CG-OD2 | -9.58 | 109.68 | 118.30 |
| 1 | A | 224 | ASP | CB-CG-OD1 | 9.55 | 126.89 | 118.30 |
| 1 | B | 172 | ASP | CB-CG-OD1 | 9.53 | 126.88 | 118.30 |
| 1 | C | 233 | ASP | CB-CG-OD2 | -9.48 | 109.77 | 118.30 |
| 1 | B | 492 | ASP | CB-CG-OD1 | 9.48 | 126.83 | 118.30 |
| 1 | A | 439 | ARG | NE-CZ-NH2 | -9.43 | 115.59 | 120.30 |
| 1 | B | 329 | ASP | CB-CG-OD2 | -9.42 | 109.82 | 118.30 |
| 1 | A | 987 | ASP | CB-CG-OD2 | -9.37 | 109.87 | 118.30 |
| 1 | A | 916 | ASP | CB-CG-OD1 | 9.37 | 126.73 | 118.30 |
| 1 | D | 507 | ASP | CB-CG-OD2 | -9.36 | 109.88 | 118.30 |
| 1 | C | 973 | ARG | NE-CZ-NH2 | -9.36 | 115.62 | 120.30 |
| 1 | A | 166 | ARG | NE-CZ-NH1 | 9.33 | 124.97 | 120.30 |
| 1 | A | 233 | ASP | CB-CG-OD1 | 9.32 | 126.69 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 403 | ASP | CB-CG-OD1 | 9.32 | 126.69 | 118.30 |
| 1 | A | 610 | ASP | CB-CG-OD1 | 9.31 | 126.68 | 118.30 |
| 1 | D | 45 | ASP | CB-CG-OD1 | 9.26 | 126.63 | 118.30 |
| 1 | A | 755 | ARG | NE-CZ-NH2 | -9.25 | 115.67 | 120.30 |
| 1 | D | 699 | ARG | NE-CZ-NH1 | 9.25 | 124.92 | 120.30 |
| 1 | B | 687 | GLN | C-N-CD | -9.24 | 100.27 | 120.60 |
| 1 | C | 288 | ARG | NE-CZ-NH2 | -9.22 | 115.69 | 120.30 |
| 1 | A | 356 | ARG | NE-CZ-NH1 | 9.22 | 124.91 | 120.30 |
| 1 | D | 561 | ARG | NE-CZ-NH2 | -9.22 | 115.69 | 120.30 |
| 1 | D | 329 | ASP | CB-CG-OD2 | -9.19 | 110.03 | 118.30 |
| 1 | B | 469 | ASP | CB-CG-OD1 | 9.15 | 126.54 | 118.30 |
| 1 | C | 375 | ASP | CB-CG-OD1 | 9.11 | 126.50 | 118.30 |
| 1 | C | 531 | ARG | NE-CZ-NH2 | -9.11 | 115.75 | 120.30 |
| 1 | C | 172 | ASP | CB-CG-OD1 | 9.08 | 126.47 | 118.30 |
| 1 | B | 881 | ARG | NE-CZ-NH2 | -9.06 | 115.77 | 120.30 |
| 1 | B | 755 | ARG | NE-CZ-NH1 | 9.05 | 124.83 | 120.30 |
| 1 | D | 287 | ASP | CB-CG-OD2 | -9.05 | 110.16 | 118.30 |
| 1 | A | 859 | ASP | CB-CG-OD1 | 9.02 | 126.41 | 118.30 |
| 1 | C | 333 | ARG | NE-CZ-NH1 | -9.02 | 115.79 | 120.30 |
| 1 | A | 46 | ARG | NE-CZ-NH2 | -9.01 | 115.80 | 120.30 |
| 1 | C | 13 | ARG | NE-CZ-NH1 | 9.00 | 124.80 | 120.30 |
| 1 | D | 439 | ARG | NE-CZ-NH1 | 9.00 | 124.80 | 120.30 |
| 1 | A | 509 | ASP | CB-CG-OD1 | 8.99 | 126.39 | 118.30 |
| 1 | A | 442 | ARG | NE-CZ-NH2 | -8.98 | 115.81 | 120.30 |
| 1 | B | 319 | ASP | CB-CG-OD2 | -8.97 | 110.22 | 118.30 |
| 1 | C | 448 | ARG | NE-CZ-NH2 | -8.95 | 115.82 | 120.30 |
| 1 | D | 507 | ASP | CB-CG-OD1 | 8.95 | 126.36 | 118.30 |
| 1 | C | 199 | ASP | CB-CG-OD1 | 8.84 | 126.25 | 118.30 |
| 1 | D | 829 | THR | N-CA-CB | 8.83 | 127.08 | 110.30 |
| 1 | C | 579 | ASP | CB-CG-OD2 | -8.81 | 110.37 | 118.30 |
| 1 | D | 781 | ARG | NE-CZ-NH1 | 8.80 | 124.70 | 120.30 |
| 1 | C | 645 | ARG | NE-CZ-NH2 | -8.75 | 115.93 | 120.30 |
| 1 | D | 792 | ASP | CB-CG-OD1 | 8.74 | 126.17 | 118.30 |
| 1 | D | 800 | ARG | NE-CZ-NH1 | 8.71 | 124.65 | 120.30 |
| 1 | C | 748 | CYS | CA-CB-SG | -8.70 | 98.34 | 114.00 |
| 1 | A | 782 | ASP | CB-CG-OD2 | -8.60 | 110.56 | 118.30 |
| 1 | B | 630 | ARG | NE-CZ-NH1 | 8.60 | 124.60 | 120.30 |
| 1 | A | 411 | ASP | CB-CG-OD2 | -8.57 | 110.59 | 118.30 |
| 1 | A | 130 | ASP | CB-CG-OD1 | 8.54 | 125.99 | 118.30 |
| 1 | B | 942 | ARG | NE-CZ-NH1 | 8.53 | 124.57 | 120.30 |
| 1 | C | 553 | TRP | CA-CB-CG | -8.53 | 97.50 | 113.70 |
| 1 | B | 659 | ASP | CB-CG-OD2 | -8.52 | 110.64 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | C | 233 | ASP | CB-CG-OD1 | 8.48 | 125.94 | 118.30 |
| 1 | A | 908 | ASP | CB-CG-OD1 | 8.45 | 125.91 | 118.30 |
| 1 | D | 15 | ASP | CB-CG-OD2 | -8.45 | 110.69 | 118.30 |
| 1 | B | 166 | ARG | NE-CZ-NH2 | -8.44 | 116.08 | 120.30 |
| 1 | A | 172 | ASP | CB-CG-OD1 | 8.44 | 125.90 | 118.30 |
| 1 | D | 224 | ASP | CB-CG-OD2 | -8.44 | 110.70 | 118.30 |
| 1 | A | 319 | ASP | CB-CG-OD2 | -8.44 | 110.70 | 118.30 |
| 1 | A | 987 | ASP | CB-CG-OD1 | 8.42 | 125.88 | 118.30 |
| 1 | D | 193 | ASP | CB-CG-OD2 | -8.42 | 110.72 | 118.30 |
| 1 | D | 875 | ASP | CB-CG-OD2 | -8.41 | 110.73 | 118.30 |
| 1 | D | 786 | ARG | NE-CZ-NH1 | 8.41 | 124.50 | 120.30 |
| 1 | B | 287 | ASP | CB-CG-OD2 | -8.40 | 110.74 | 118.30 |
| 1 | A | 853 | ARG | NE-CZ-NH2 | -8.34 | 116.13 | 120.30 |
| 1 | D | 648 | ASP | CB-CG-OD2 | -8.33 | 110.80 | 118.30 |
| 1 | C | 645 | ARG | NE-CZ-NH1 | 8.27 | 124.44 | 120.30 |
| 1 | A | 721 | ARG | NE-CZ-NH1 | 8.26 | 124.43 | 120.30 |
| 1 | C | 531 | ARG | NE-CZ-NH1 | 8.26 | 124.43 | 120.30 |
| 1 | C | 869 | ASP | CB-CG-OD2 | -8.25 | 110.87 | 118.30 |
| 1 | B | 659 | ASP | CB-CG-OD1 | 8.25 | 125.72 | 118.30 |
| 1 | C | 961 | ARG | NE-CZ-NH1 | 8.24 | 124.42 | 120.30 |
| 1 | B | 648 | ASP | CB-CG-OD1 | 8.20 | 125.68 | 118.30 |
| 1 | D | 439 | ARG | NE-CZ-NH2 | -8.18 | 116.21 | 120.30 |
| 1 | D | 952 | ARG | NE-CZ-NH2 | -8.15 | 116.22 | 120.30 |
| 1 | C | 368 | ASP | CB-CG-OD2 | -8.15 | 110.96 | 118.30 |
| 1 | B | 869 | ASP | CB-CG-OD2 | -8.15 | 110.97 | 118.30 |
| 1 | C | 599 | ARG | NE-CZ-NH1 | 8.14 | 124.37 | 120.30 |
| 1 | A | 996 | ASP | CB-CG-OD2 | -8.13 | 110.99 | 118.30 |
| 1 | C | 855 | THR | N-CA-CB | 8.12 | 125.74 | 110.30 |
| 1 | B | 319 | ASP | CB-CG-OD1 | 8.12 | 125.61 | 118.30 |
| 1 | D | 689 | GLU | N-CA-CB | 8.12 | 125.21 | 110.60 |
| 1 | C | 352 | ARG | NE-CZ-NH2 | -8.09 | 116.26 | 120.30 |
| 1 | C | 428 | ASP | CB-CG-OD2 | -8.09 | 111.02 | 118.30 |
| 1 | C | 505 | ARG | NE-CZ-NH2 | -8.07 | 116.27 | 120.30 |
| 1 | A | 611 | ARG | NE-CZ-NH1 | 8.06 | 124.33 | 120.30 |
| 1 | B | 492 | ASP | CB-CG-OD2 | -8.06 | 111.04 | 118.30 |
| 1 | D | 411 | ASP | CB-CG-OD2 | -8.05 | 111.06 | 118.30 |
| 1 | B | 919 | ASP | CB-CG-OD2 | -8.03 | 111.07 | 118.30 |
| 1 | C | 199 | ASP | CB-CG-OD2 | -8.03 | 111.07 | 118.30 |
| 1 | A | 190 | ARG | NE-CZ-NH2 | -8.03 | 116.29 | 120.30 |
| 1 | D | 204 | ARG | NE-CZ-NH2 | 8.00 | 124.30 | 120.30 |
| 1 | B | 469 | ASP | CB-CG-OD2 | -7.98 | 111.12 | 118.30 |
| 1 | C | 996 | ASP | CB-CG-OD1 | 7.97 | 125.48 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | C | 997 | ASP | CB-CG-OD2 | -7.97 | 111.13 | 118.30 |
| 1 | D | 255 | ARG | NE-CZ-NH2 | -7.96 | 116.32 | 120.30 |
| 1 | B | 233 | ASP | CB-CG-OD2 | -7.96 | 111.14 | 118.30 |
| 1 | C | 572 | ASP | CB-CG-OD2 | -7.96 | 111.14 | 118.30 |
| 1 | A | 287 | ASP | CB-CG-OD1 | 7.95 | 125.45 | 118.30 |
| 1 | A | 292 | ARG | NE-CZ-NH2 | -7.95 | 116.33 | 120.30 |
| 1 | D | 287 | ASP | CB-CG-OD1 | 7.94 | 125.44 | 118.30 |
| 1 | B | 429 | ASP | CB-CG-OD2 | -7.93 | 111.16 | 118.30 |
| 1 | B | 648 | ASP | CB-CG-OD2 | -7.93 | 111.16 | 118.30 |
| 1 | B | 77 | ASP | CB-CG-OD2 | -7.91 | 111.18 | 118.30 |
| 1 | C | 442 | ARG | NE-CZ-NH1 | 7.90 | 124.25 | 120.30 |
| 1 | A | 908 | ASP | CB-CG-OD2 | -7.89 | 111.20 | 118.30 |
| 1 | A | 721 | ARG | NE-CZ-NH2 | -7.83 | 116.38 | 120.30 |
| 1 | C | 204 | ARG | NE-CZ-NH2 | -7.79 | 116.41 | 120.30 |
| 1 | D | 997 | ASP | N-CA-CB | 7.78 | 124.59 | 110.60 |
| 1 | C | 448 | ARG | NE-CZ-NH1 | 7.76 | 124.18 | 120.30 |
| 1 | A | 507 | ASP | CB-CG-OD1 | 7.76 | 125.28 | 118.30 |
| 1 | C | 699 | ARG | NE-CZ-NH2 | -7.75 | 116.42 | 120.30 |
| 1 | C | 630 | ARG | NE-CZ-NH2 | -7.75 | 116.43 | 120.30 |
| 1 | B | 632 | SER | N-CA-CB | 7.74 | 122.12 | 110.50 |
| 1 | A | 280 | ASP | CB-CG-OD1 | 7.73 | 125.25 | 118.30 |
| 1 | B | 199 | ASP | CB-CG-OD2 | -7.73 | 111.34 | 118.30 |
| 1 | C | 230 | ARG | NE-CZ-NH2 | -7.73 | 116.44 | 120.30 |
| 1 | A | 234 | ASP | CB-CG-OD2 | -7.72 | 111.35 | 118.30 |
| 1 | A | 201 | ASP | CB-CG-OD1 | 7.71 | 125.24 | 118.30 |
| 1 | A | 553 | TRP | CA-CB-CG | -7.70 | 99.07 | 113.70 |
| 1 | D | 875 | ASP | CB-CG-OD1 | 7.70 | 125.23 | 118.30 |
| 1 | B | 786 | ARG | NE-CZ-NH1 | 7.70 | 124.15 | 120.30 |
| 1 | A | 469 | ASP | CB-CG-OD1 | 7.69 | 125.22 | 118.30 |
| 1 | A | 572 | ASP | CB-CG-OD2 | -7.68 | 111.38 | 118.30 |
| 1 | B | 832 | ASP | CB-CG-OD1 | 7.68 | 125.22 | 118.30 |
| 1 | A | 267 | VAL | CG1-CB-CG2 | -7.67 | 98.63 | 110.90 |
| 1 | A | 130 | ASP | CB-CG-OD2 | -7.66 | 111.40 | 118.30 |
| 1 | C | 388 | ARG | NE-CZ-NH1 | 7.64 | 124.12 | 120.30 |
| 1 | B | 497 | ASP | CB-CG-OD1 | 7.64 | 125.17 | 118.30 |
| 1 | C | 280 | ASP | CB-CG-OD1 | 7.63 | 125.17 | 118.30 |
| 1 | B | 199 | ASP | CB-CG-OD1 | 7.63 | 125.17 | 118.30 |
| 1 | A | 809 | ARG | NE-CZ-NH1 | 7.61 | 124.10 | 120.30 |
| 1 | B | 908 | ASP | CB-CG-OD2 | -7.59 | 111.47 | 118.30 |
| 1 | D | 594 | ASP | CB-CG-OD1 | 7.59 | 125.13 | 118.30 |
| 1 | D | 952 | ARG | NE-CZ-NH1 | 7.58 | 124.09 | 120.30 |
| 1 | C | 234 | ASP | CB-CG-OD2 | -7.58 | 111.48 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | B | 997 | ASP | CB-CG-OD2 | -7.57 | 111.49 | 118.30 |
| 1 | A | 741 | THR | CA-CB-CG2 | -7.56 | 101.81 | 112.40 |
| 1 | B | 375 | ASP | CB-CG-OD2 | -7.56 | 111.50 | 118.30 |
| 1 | A | 287 | ASP | CB-CG-OD2 | -7.56 | 111.50 | 118.30 |
| 1 | B | 28 | ALA | CB-CA-C | -7.56 | 98.77 | 110.10 |
| 1 | A | 469 | ASP | CB-CG-OD2 | -7.55 | 111.50 | 118.30 |
| 1 | B | 292 | ARG | NE-CZ-NH2 | -7.55 | 116.52 | 120.30 |
| 1 | D | 632 | SER | N-CA-CB | 7.55 | 121.83 | 110.50 |
| 1 | A | 234 | ASP | CB-CG-OD1 | 7.54 | 125.08 | 118.30 |
| 1 | C | 234 | ASP | CB-CG-OD1 | 7.54 | 125.08 | 118.30 |
| 1 | C | 659 | ASP | CB-CG-OD2 | -7.53 | 111.52 | 118.30 |
| 1 | C | 859 | ASP | CB-CG-OD2 | -7.53 | 111.52 | 118.30 |
| 1 | D | 859 | ASP | CB-CG-OD2 | -7.53 | 111.53 | 118.30 |
| 1 | D | 832 | ASP | CB-CG-OD1 | 7.52 | 125.07 | 118.30 |
| 1 | C | 224 | ASP | CB-CG-OD1 | 7.50 | 125.05 | 118.30 |
| 1 | A | 172 | ASP | CB-CG-OD2 | -7.49 | 111.56 | 118.30 |
| 1 | C | 492 | ASP | CB-CG-OD2 | -7.49 | 111.56 | 118.30 |
| 1 | D | 802 | ASP | CB-CG-OD2 | -7.48 | 111.56 | 118.30 |
| 1 | A | 123 | TYR | CB-CG-CD2 | -7.48 | 116.51 | 121.00 |
| 1 | C | 172 | ASP | CB-CG-OD2 | -7.47 | 111.57 | 118.30 |
| 1 | C | 832 | ASP | CB-CG-OD1 | 7.47 | 125.02 | 118.30 |
| 1 | B | 802 | ASP | CB-CG-OD1 | 7.46 | 125.02 | 118.30 |
| 1 | A | 786 | ARG | NE-CZ-NH2 | -7.45 | 116.58 | 120.30 |
| 1 | D | 659 | ASP | CB-CG-OD2 | -7.42 | 111.62 | 118.30 |
| 1 | B | 429 | ASP | CB-CG-OD1 | 7.42 | 124.98 | 118.30 |
| 1 | B | 611 | ARG | NE-CZ-NH1 | 7.37 | 123.99 | 120.30 |
| 1 | B | 569 | ASP | CB-CG-OD1 | 7.37 | 124.93 | 118.30 |
| 1 | A | 404 | ARG | NE-CZ-NH1 | 7.37 | 123.98 | 120.30 |
| 1 | B | 164 | ASP | CB-CG-OD2 | -7.36 | 111.68 | 118.30 |
| 1 | A | 755 | ARG | NE-CZ-NH1 | 7.35 | 123.97 | 120.30 |
| 1 | B | 356 | ARG | NE-CZ-NH1 | 7.34 | 123.97 | 120.30 |
| 1 | C | 917 | ARG | NE-CZ-NH1 | -7.33 | 116.64 | 120.30 |
| 1 | B | 610 | ASP | CB-CG-OD1 | 7.30 | 124.87 | 118.30 |
| 1 | D | 96 | ASP | CB-CG-OD2 | -7.30 | 111.73 | 118.30 |
| 1 | B | 82 | ASP | CB-CG-OD2 | -7.29 | 111.74 | 118.30 |
| 1 | A | 991 | MET | CG-SD-CE | 7.29 | 111.86 | 100.20 |
| 1 | C | 721 | ARG | NE-CZ-NH2 | -7.24 | 116.68 | 120.30 |
| 1 | D | 1018 | LEU | CB-CA-C | -7.24 | 96.45 | 110.20 |
| 1 | C | 144 | ASP | CB-CG-OD1 | 7.24 | 124.81 | 118.30 |
| 1 | B | 1013 | ARG | NE-CZ-NH1 | 7.23 | 123.92 | 120.30 |
| 1 | D | 403 | ASP | CB-CG-OD1 | 7.23 | 124.80 | 118.30 |
| 1 | A | 802 | ASP | CB-CG-OD2 | -7.22 | 111.80 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | B | 594 | ASP | CB-CG-OD1 | 7.22 | 124.80 | 118.30 |
| 1 | B | 368 | ASP | CB-CG-OD1 | 7.21 | 124.79 | 118.30 |
| 1 | D | 859 | ASP | CB-CG-OD1 | 7.20 | 124.78 | 118.30 |
| 1 | C | 178 | ARG | NE-CZ-NH1 | 7.20 | 123.90 | 120.30 |
| 1 | B | 599 | ARG | NE-CZ-NH1 | 7.20 | 123.90 | 120.30 |
| 1 | C | 43 | ARG | NE-CZ-NH2 | -7.19 | 116.70 | 120.30 |
| 1 | D | 997 | ASP | CB-CG-OD2 | -7.18 | 111.84 | 118.30 |
| 1 | B | 832 | ASP | N-CA-CB | -7.16 | 97.71 | 110.60 |
| 1 | A | 164 | ASP | CB-CG-OD2 | -7.16 | 111.86 | 118.30 |
| 1 | C | 579 | ASP | CB-CG-OD1 | 7.16 | 124.74 | 118.30 |
| 1 | A | 15 | ASP | CB-CG-OD2 | -7.15 | 111.87 | 118.30 |
| 1 | D | 46 | ARG | NE-CZ-NH1 | 7.13 | 123.87 | 120.30 |
| 1 | C | 505 | ARG | NE-CZ-NH1 | 7.12 | 123.86 | 120.30 |
| 1 | C | 961 | ARG | NE-CZ-NH2 | -7.12 | 116.74 | 120.30 |
| 1 | D | 645 | ARG | NE-CZ-NH1 | -7.11 | 116.74 | 120.30 |
| 1 | B | 439 | ARG | NE-CZ-NH1 | 7.11 | 123.86 | 120.30 |
| 1 | A | 1013 | ARG | NE-CZ-NH2 | 7.11 | 123.85 | 120.30 |
| 1 | A | 997 | ASP | CB-CG-OD1 | 7.11 | 124.70 | 118.30 |
| 1 | C | 140 | ARG | NE-CZ-NH2 | -7.10 | 116.75 | 120.30 |
| 1 | B | 832 | ASP | CB-CG-OD2 | -7.10 | 111.91 | 118.30 |
| 1 | B | 144 | ASP | CB-CG-OD1 | 7.09 | 124.68 | 118.30 |
| 1 | A | 479 | ASP | CB-CG-OD2 | -7.08 | 111.93 | 118.30 |
| 1 | B | 140 | ARG | NE-CZ-NH2 | -7.08 | 116.76 | 120.30 |
| 1 | D | 746 | ASP | CB-CG-OD2 | -7.07 | 111.94 | 118.30 |
| 1 | A | 648 | ASP | CB-CG-OD2 | -7.06 | 111.94 | 118.30 |
| 1 | B | 411 | ASP | CB-CG-OD2 | -7.04 | 111.96 | 118.30 |
| 1 | D | 553 | TRP | CA-CB-CG | -7.03 | 100.34 | 113.70 |
| 1 | A | 448 | ARG | NE-CZ-NH1 | 7.01 | 123.81 | 120.30 |
| 1 | D | 869 | ASP | CB-CG-OD2 | -7.00 | 112.00 | 118.30 |
| 1 | B | 746 | ASP | CB-CG-OD2 | -6.98 | 112.02 | 118.30 |
| 1 | D | 828 | ASP | CB-CG-OD2 | -6.98 | 112.02 | 118.30 |
| 1 | B | 561 | ARG | NE-CZ-NH1 | 6.96 | 123.78 | 120.30 |
| 1 | B | 368 | ASP | CB-CG-OD2 | -6.96 | 112.04 | 118.30 |
| 1 | A | 859 | ASP | CB-CG-OD2 | -6.95 | 112.04 | 118.30 |
| 1 | C | 428 | ASP | CB-CG-OD1 | 6.95 | 124.56 | 118.30 |
| 1 | A | 786 | ARG | NE-CZ-NH1 | 6.94 | 123.77 | 120.30 |
| 1 | A | 659 | ASP | CB-CG-OD2 | -6.94 | 112.06 | 118.30 |
| 1 | B | 375 | ASP | CB-CG-OD1 | 6.93 | 124.54 | 118.30 |
| 1 | D | 853 | ARG | NE-CZ-NH1 | 6.93 | 123.77 | 120.30 |
| 1 | A | 368 | ASP | CB-CG-OD2 | -6.93 | 112.06 | 118.30 |
| 1 | C | 659 | ASP | CB-CG-OD1 | 6.92 | 124.53 | 118.30 |
| 1 | B | 610 | ASP | CB-CG-OD2 | -6.92 | 112.07 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | D | 916 | ASP | CB-CG-OD2 | -6.92 | 112.07 | 118.30 |
| 1 | C | 997 | ASP | N-CA-CB | 6.92 | 123.05 | 110.60 |
| 1 | A | 447 | ASP | CB-CG-OD2 | -6.90 | 112.09 | 118.30 |
| 1 | A | 828 | ASP | CB-CG-OD2 | -6.89 | 112.09 | 118.30 |
| 1 | A | 632 | SER | N-CA-CB | 6.88 | 120.83 | 110.50 |
| 1 | D | 782 | ASP | CB-CG-OD1 | 6.88 | 124.50 | 118.30 |
| 1 | B | 356 | ARG | NE-CZ-NH2 | -6.88 | 116.86 | 120.30 |
| 1 | C | 164 | ASP | CB-CG-OD2 | -6.88 | 112.11 | 118.30 |
| 1 | A | 210 | ARG | NE-CZ-NH1 | 6.88 | 123.74 | 120.30 |
| 1 | B | 555 | ALA | CB-CA-C | -6.86 | 99.81 | 110.10 |
| 1 | D | 190 | ARG | NE-CZ-NH2 | -6.85 | 116.88 | 120.30 |
| 1 | C | 997 | ASP | CB-CG-OD1 | 6.84 | 124.46 | 118.30 |
| 1 | D | 282 | ARG | NE-CZ-NH1 | 6.84 | 123.72 | 120.30 |
| 1 | B | 553 | TRP | CA-CB-CG | -6.83 | 100.73 | 113.70 |
| 1 | C | 52 | ARG | NE-CZ-NH2 | 6.83 | 123.71 | 120.30 |
| 1 | B | 185 | ALA | N-CA-CB | 6.82 | 119.64 | 110.10 |
| 1 | C | 492 | ASP | CB-CG-OD1 | 6.82 | 124.43 | 118.30 |
| 1 | A | 579 | ASP | CB-CG-OD1 | 6.81 | 124.43 | 118.30 |
| 1 | D | 832 | ASP | CB-CG-OD2 | -6.78 | 112.20 | 118.30 |
| 1 | C | 161 | TYR | CB-CG-CD2 | -6.77 | 116.94 | 121.00 |
| 1 | A | 164 | ASP | CB-CG-OD1 | 6.76 | 124.38 | 118.30 |
| 1 | B | 926 | TYR | CB-CG-CD1 | 6.76 | 125.05 | 121.00 |
| 1 | B | 572 | ASP | CB-CG-OD1 | 6.75 | 124.38 | 118.30 |
| 1 | A | 569 | ASP | CB-CG-OD1 | 6.75 | 124.37 | 118.30 |
| 1 | B | 519 | SER | N-CA-CB | -6.73 | 100.40 | 110.50 |
| 1 | C | 144 | ASP | CB-CG-OD2 | -6.71 | 112.26 | 118.30 |
| 1 | D | 319 | ASP | CB-CG-OD2 | -6.71 | 112.26 | 118.30 |
| 1 | B | 958 | ASN | N-CA-CB | 6.71 | 122.68 | 110.60 |
| 1 | A | 952 | ARG | NE-CZ-NH1 | 6.71 | 123.65 | 120.30 |
| 1 | A | 579 | ASP | CB-CG-OD2 | -6.70 | 112.27 | 118.30 |
| 1 | B | 336 | ARG | NE-CZ-NH2 | -6.69 | 116.96 | 120.30 |
| 1 | B | 505 | ARG | NE-CZ-NH1 | 6.66 | 123.63 | 120.30 |
| 1 | C | 809 | ARG | CD-NE-CZ | 6.65 | 132.91 | 123.60 |
| 1 | A | 237 | ARG | NE-CZ-NH1 | 6.65 | 123.62 | 120.30 |
| 1 | C | 352 | ARG | NE-CZ-NH1 | 6.64 | 123.62 | 120.30 |
| 1 | A | 746 | ASP | CB-CG-OD2 | -6.63 | 112.34 | 118.30 |
| 1 | D | 368 | ASP | CB-CG-OD1 | 6.61 | 124.25 | 118.30 |
| 1 | C | 368 | ASP | CB-CG-OD1 | 6.61 | 124.25 | 118.30 |
| 1 | D | 642 | TYR | CB-CG-CD2 | -6.61 | 117.04 | 121.00 |
| 1 | B | 594 | ASP | CB-CG-OD2 | -6.60 | 112.36 | 118.30 |
| 1 | B | 828 | ASP | CB-CG-OD2 | -6.60 | 112.36 | 118.30 |
| 1 | D | 431 | ARG | NE-CZ-NH1 | 6.60 | 123.60 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 82 | ASP | CB-CG-OD1 | 6.59 | 124.23 | 118.30 |
| 1 | D | 569 | ASP | CB-CG-OD2 | -6.58 | 112.37 | 118.30 |
| 1 | D | 201 | ASP | CB-CG-OD2 | -6.58 | 112.37 | 118.30 |
| 1 | B | 595 | THR | CA-CB-CG2 | -6.58 | 103.19 | 112.40 |
| 1 | D | 579 | ASP | CB-CG-OD2 | -6.57 | 112.39 | 118.30 |
| 1 | B | 671 | ASP | CB-CG-OD1 | 6.55 | 124.19 | 118.30 |
| 1 | A | 210 | ARG | NE-CZ-NH2 | -6.55 | 117.03 | 120.30 |
| 1 | B | 352 | ARG | NE-CZ-NH1 | 6.55 | 123.57 | 120.30 |
| 1 | D | 610 | ASP | CB-CG-OD2 | -6.55 | 112.41 | 118.30 |
| 1 | C | 77 | ASP | CB-CG-OD1 | 6.52 | 124.17 | 118.30 |
| 1 | B | 859 | ASP | CB-CG-OD2 | -6.51 | 112.44 | 118.30 |
| 1 | B | 172 | ASP | CB-CG-OD2 | -6.50 | 112.45 | 118.30 |
| 1 | C | 411 | ASP | CB-CG-OD1 | 6.50 | 124.15 | 118.30 |
| 1 | D | 699 | ARG | NE-CZ-NH2 | -6.49 | 117.05 | 120.30 |
| 1 | D | 987 | ASP | CB-CG-OD1 | 6.48 | 124.13 | 118.30 |
| 1 | A | 473 | ARG | NE-CZ-NH2 | 6.46 | 123.53 | 120.30 |
| 1 | C | 399 | TYR | CB-CG-CD2 | -6.45 | 117.13 | 121.00 |
| 1 | B | 144 | ASP | CB-CG-OD2 | -6.43 | 112.51 | 118.30 |
| 1 | A | 446 | ARG | NE-CZ-NH1 | 6.43 | 123.51 | 120.30 |
| 1 | C | 671 | ASP | CB-CG-OD2 | -6.41 | 112.53 | 118.30 |
| 1 | B | 699 | ARG | NE-CZ-NH2 | 6.41 | 123.50 | 120.30 |
| 1 | B | 46 | ARG | CD-NE-CZ | -6.41 | 114.63 | 123.60 |
| 1 | B | 233 | ASP | CB-CG-OD1 | 6.40 | 124.06 | 118.30 |
| 1 | D | 792 | ASP | CB-CG-OD2 | -6.40 | 112.54 | 118.30 |
| 1 | A | 356 | ARG | NE-CZ-NH2 | -6.40 | 117.10 | 120.30 |
| 1 | A | 285 | TYR | CB-CG-CD1 | -6.39 | 117.17 | 121.00 |
| 1 | A | 771 | GLY | N-CA-C | -6.38 | 97.14 | 113.10 |
| 1 | C | 832 | ASP | CB-CG-OD2 | -6.37 | 112.57 | 118.30 |
| 1 | B | 996 | ASP | CB-CG-OD1 | 6.36 | 124.02 | 118.30 |
| 1 | C | 130 | ASP | CB-CG-OD2 | -6.34 | 112.59 | 118.30 |
| 1 | D | 15 | ASP | CB-CG-OD1 | 6.34 | 124.00 | 118.30 |
| 1 | B | 285 | TYR | CB-CG-CD2 | -6.33 | 117.20 | 121.00 |
| 1 | D | 411 | ASP | CB-CG-OD1 | 6.33 | 124.00 | 118.30 |
| 1 | D | 869 | ASP | CB-CG-OD1 | 6.33 | 124.00 | 118.30 |
| 1 | C | 924 | ASP | CB-CG-OD2 | -6.32 | 112.61 | 118.30 |
| 1 | D | 77 | ASP | CB-CG-OD2 | -6.31 | 112.62 | 118.30 |
| 1 | B | 557 | ARG | NE-CZ-NH2 | -6.31 | 117.14 | 120.30 |
| 1 | C | 333 | ARG | NE-CZ-NH2 | 6.30 | 123.45 | 120.30 |
| 1 | B | 442 | ARG | NE-CZ-NH1 | 6.30 | 123.45 | 120.30 |
| 1 | B | 411 | ASP | CB-CG-OD1 | 6.29 | 123.97 | 118.30 |
| 1 | C | 1019 | VAL | CA-CB-CG1 | -6.29 | 101.47 | 110.90 |
| 1 | C | 183 | ARG | NE-CZ-NH2 | -6.28 | 117.16 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 924 | ASP | CB-CG-OD2 | -6.27 | 112.66 | 118.30 |
| 1 | A | 997 | ASP | N-CA-CB | 6.27 | 121.88 | 110.60 |
| 1 | A | 285 | TYR | CD1-CE1-CZ | -6.27 | 114.16 | 119.80 |
| 1 | A | 233 | ASP | CB-CG-OD2 | -6.26 | 112.66 | 118.30 |
| 1 | C | 375 | ASP | CB-CG-OD2 | -6.26 | 112.67 | 118.30 |
| 1 | A | 211 | ASP | CB-CG-OD1 | 6.26 | 123.93 | 118.30 |
| 1 | D | 916 | ASP | CB-CG-OD1 | 6.25 | 123.92 | 118.30 |
| 1 | B | 130 | ASP | CB-CG-OD2 | -6.24 | 112.68 | 118.30 |
| 1 | A | 123 | TYR | CB-CG-CD1 | 6.22 | 124.73 | 121.00 |
| 1 | D | 319 | ASP | CB-CG-OD1 | 6.22 | 123.90 | 118.30 |
| 1 | A | 782 | ASP | CB-CG-OD1 | 6.22 | 123.90 | 118.30 |
| 1 | C | 648 | ASP | CB-CG-OD2 | -6.21 | 112.71 | 118.30 |
| 1 | C | 288 | ARG | NE-CZ-NH1 | 6.21 | 123.41 | 120.30 |
| 1 | C | 890 | GLN | N-CA-CB | -6.20 | 99.44 | 110.60 |
| 1 | B | 908 | ASP | CB-CG-OD1 | 6.19 | 123.87 | 118.30 |
| 1 | A | 375 | ASP | CB-CG-OD2 | -6.19 | 112.73 | 118.30 |
| 1 | D | 469 | ASP | CB-CG-OD2 | -6.19 | 112.73 | 118.30 |
| 1 | B | 59 | ARG | NE-CZ-NH1 | -6.17 | 117.21 | 120.30 |
| 1 | C | 859 | ASP | CB-CG-OD1 | 6.17 | 123.86 | 118.30 |
| 1 | B | 237 | ARG | NE-CZ-NH2 | -6.17 | 117.22 | 120.30 |
| 1 | A | 429 | ASP | CB-CG-OD1 | 6.16 | 123.85 | 118.30 |
| 1 | C | 77 | ASP | CB-CG-OD2 | -6.16 | 112.75 | 118.30 |
| 1 | B | 875 | ASP | CB-CG-OD2 | -6.16 | 112.76 | 118.30 |
| 1 | B | 497 | ASP | CB-CG-OD2 | -6.15 | 112.76 | 118.30 |
| 1 | C | 183 | ARG | NE-CZ-NH1 | 6.15 | 123.37 | 120.30 |
| 1 | A | 507 | ASP | CB-CG-OD2 | -6.14 | 112.77 | 118.30 |
| 1 | D | 183 | ARG | NE-CZ-NH1 | -6.14 | 117.23 | 120.30 |
| 1 | C | 557 | ARG | NE-CZ-NH1 | 6.13 | 123.36 | 120.30 |
| 1 | A | 225 | PHE | N-CA-CB | 6.13 | 121.63 | 110.60 |
| 1 | C | 399 | TYR | CB-CG-CD1 | 6.12 | 124.67 | 121.00 |
| 1 | B | 926 | TYR | CB-CG-CD2 | -6.12 | 117.33 | 121.00 |
| 1 | C | 703 | PRO | N-CA-CB | 6.11 | 110.64 | 103.30 |
| 1 | A | 954 | ASP | CB-CG-OD2 | -6.11 | 112.80 | 118.30 |
| 1 | B | 166 | ARG | NE-CZ-NH1 | 6.10 | 123.35 | 120.30 |
| 1 | D | 986 | ILE | CG1-CB-CG2 | -6.10 | 97.98 | 111.40 |
| 1 | D | 908 | ASP | CB-CG-OD2 | -6.09 | 112.81 | 118.30 |
| 1 | B | 210 | ARG | N-CA-CB | 6.09 | 121.56 | 110.60 |
| 1 | B | 52 | ARG | CB-CA-C | -6.09 | 98.22 | 110.40 |
| 1 | C | 610 | ASP | CB-CG-OD1 | 6.09 | 123.78 | 118.30 |
| 1 | B | 412 | GLU | OE1-CD-OE2 | -6.08 | 116.00 | 123.30 |
| 1 | D | 772 | ASP | CB-CG-OD2 | -6.08 | 112.83 | 118.30 |
| 1 | D | 479 | ASP | CB-CG-OD2 | -6.08 | 112.83 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | D | 746 | ASP | CB-CG-OD1 | 6.08 | 123.77 | 118.30 |
| 1 | A | 183 | ARG | NE-CZ-NH1 | -6.07 | 117.26 | 120.30 |
| 1 | A | 958 | ASN | N-CA-CB | 6.07 | 121.53 | 110.60 |
| 1 | C | 699 | ARG | CB-CA-C | -6.07 | 98.26 | 110.40 |
| 1 | A | 630 | ARG | NE-CZ-NH1 | 6.07 | 123.33 | 120.30 |
| 1 | B | 352 | ARG | NE-CZ-NH2 | -6.07 | 117.27 | 120.30 |
| 1 | D | 96 | ASP | CB-CG-OD1 | 6.06 | 123.75 | 118.30 |
| 1 | A | 477 | SER | N-CA-CB | 6.05 | 119.58 | 110.50 |
| 1 | D | 394 | ASN | N-CA-CB | -6.05 | 99.71 | 110.60 |
| 1 | D | 100 | TYR | N-CA-CB | 6.05 | 121.49 | 110.60 |
| 1 | C | 648 | ASP | CB-CG-OD1 | 6.03 | 123.72 | 118.30 |
| 1 | C | 482 | ARG | NE-CZ-NH1 | 6.02 | 123.31 | 120.30 |
| 1 | C | 894 | ARG | NE-CZ-NH2 | 6.02 | 123.31 | 120.30 |
| 1 | D | 190 | ARG | NE-CZ-NH1 | 6.01 | 123.31 | 120.30 |
| 1 | D | 855 | THR | N-CA-CB | 6.00 | 121.70 | 110.30 |
| 1 | A | 615 | PRO | N-CA-CB | 6.00 | 110.50 | 103.30 |
| 1 | B | 809 | ARG | NE-CZ-NH1 | 6.00 | 123.30 | 120.30 |
| 1 | B | 853 | ARG | NE-CZ-NH1 | 5.99 | 123.29 | 120.30 |
| 1 | D | 787 | ALA | N-CA-CB | -5.97 | 101.74 | 110.10 |
| 1 | A | 411 | ASP | CB-CG-OD1 | 5.96 | 123.67 | 118.30 |
| 1 | C | 772 | ASP | CB-CG-OD1 | 5.96 | 123.67 | 118.30 |
| 1 | D | 52 | ARG | NE-CZ-NH1 | 5.96 | 123.28 | 120.30 |
| 1 | C | 40 | GLU | CG-CD-OE1 | 5.96 | 130.22 | 118.30 |
| 1 | D | 497 | ASP | CB-CG-OD2 | -5.96 | 112.94 | 118.30 |
| 1 | A | 809 | ARG | N-CA-CB | -5.95 | 99.89 | 110.60 |
| 1 | A | 572 | ASP | CB-CG-OD1 | 5.95 | 123.65 | 118.30 |
| 1 | D | 431 | ARG | NE-CZ-NH2 | -5.95 | 117.33 | 120.30 |
| 1 | A | 100 | TYR | CB-CG-CD2 | 5.94 | 124.56 | 121.00 |
| 1 | A | 875 | ASP | CB-CG-OD2 | -5.94 | 112.96 | 118.30 |
| 1 | A | 802 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 1 | C | 147 | ASN | N-CA-CB | -5.92 | 99.94 | 110.60 |
| 1 | D | 479 | ASP | CB-CG-OD1 | 5.92 | 123.63 | 118.30 |
| 1 | D | 140 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 1 | A | 144 | ASP | CB-CG-OD2 | -5.91 | 112.98 | 118.30 |
| 1 | B | 77 | ASP | CB-CG-OD1 | 5.91 | 123.62 | 118.30 |
| 1 | D | 329 | ASP | CB-CG-OD1 | 5.91 | 123.62 | 118.30 |
| 1 | D | 917 | ARG | NE-CZ-NH2 | -5.91 | 117.35 | 120.30 |
| 1 | D | 601 | PHE | CA-CB-CG | -5.90 | 99.73 | 113.90 |
| 1 | B | 321 | THR | CA-CB-CG2 | -5.90 | 104.14 | 112.40 |
| 1 | B | 507 | ASP | CB-CG-OD2 | -5.89 | 113.00 | 118.30 |
| 1 | C | 329 | ASP | CB-CG-OD2 | -5.89 | 113.00 | 118.30 |
| 1 | C | 651 | LEU | N-CA-CB | 5.88 | 122.15 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | B | 828 | ASP | CB-CG-OD1 | 5.87 | 123.58 | 118.30 |
| 1 | B | 611 | ARG | NE-CZ-NH2 | -5.85 | 117.37 | 120.30 |
| 1 | B | 782 | ASP | CB-CG-OD1 | 5.85 | 123.56 | 118.30 |
| 1 | B | 82 | ASP | CB-CG-OD1 | 5.84 | 123.56 | 118.30 |
| 1 | D | 234 | ASP | CB-CG-OD1 | 5.84 | 123.56 | 118.30 |
| 1 | A | 255 | ARG | NE-CZ-NH1 | 5.84 | 123.22 | 120.30 |
| 1 | A | 663 | LEU | CB-CA-C | -5.82 | 99.15 | 110.20 |
| 1 | D | 996 | ASP | CB-CG-OD2 | -5.81 | 113.07 | 118.30 |
| 1 | B | 252 | ASP | CB-CG-OD1 | 5.79 | 123.52 | 118.30 |
| 1 | C | 294 | ASN | CA-CB-CG | -5.79 | 100.66 | 113.40 |
| 1 | C | 772 | ASP | CB-CG-OD2 | -5.79 | 113.09 | 118.30 |
| 1 | D | 856 | TYR | CB-CG-CD2 | -5.78 | 117.53 | 121.00 |
| 1 | C | 919 | ASP | CB-CG-OD1 | 5.77 | 123.50 | 118.30 |
| 1 | A | 869 | ASP | CB-CG-OD1 | 5.77 | 123.49 | 118.30 |
| 1 | B | 579 | ASP | CB-CG-OD1 | 5.77 | 123.49 | 118.30 |
| 1 | C | 546 | LEU | N-CA-CB | 5.75 | 121.91 | 110.40 |
| 1 | D | 509 | ASP | CB-CG-OD1 | 5.75 | 123.47 | 118.30 |
| 1 | D | 199 | ASP | CB-CG-OD2 | -5.74 | 113.13 | 118.30 |
| 1 | A | 1019 | VAL | CA-CB-CG2 | -5.74 | 102.29 | 110.90 |
| 1 | B | 699 | ARG | NE-CZ-NH1 | 5.74 | 123.17 | 120.30 |
| 1 | B | 859 | ASP | CB-CG-OD1 | 5.73 | 123.46 | 118.30 |
| 1 | C | 494 | THR | CA-CB-CG2 | -5.73 | 104.37 | 112.40 |
| 1 | C | 909 | ARG | NE-CZ-NH1 | 5.73 | 123.16 | 120.30 |
| 1 | B | 611 | ARG | N-CA-CB | 5.73 | 120.91 | 110.60 |
| 1 | D | 694 | LEU | CB-CG-CD1 | -5.72 | 101.28 | 111.00 |
| 1 | A | 13 | ARG | NE-CZ-NH2 | -5.72 | 117.44 | 120.30 |
| 1 | D | 878 | HIS | CA-CB-CG | -5.71 | 103.89 | 113.60 |
| 1 | C | 792 | ASP | CB-CG-OD2 | -5.71 | 113.17 | 118.30 |
| 1 | D | 420 | MET | CG-SD-CE | -5.71 | 91.07 | 100.20 |
| 1 | A | 185 | ALA | N-CA-CB | 5.69 | 118.07 | 110.10 |
| 1 | A | 221 | GLN | N-CA-CB | -5.69 | 100.36 | 110.60 |
| 1 | C | 13 | ARG | NE-CZ-NH2 | -5.67 | 117.46 | 120.30 |
| 1 | A | 610 | ASP | CB-CG-OD2 | -5.67 | 113.20 | 118.30 |
| 1 | D | 71 | GLU | CB-CA-C | 5.67 | 121.73 | 110.40 |
| 1 | C | 509 | ASP | CB-CG-OD2 | -5.66 | 113.20 | 118.30 |
| 1 | C | 431 | ARG | NE-CZ-NH2 | -5.66 | 117.47 | 120.30 |
| 1 | B | 193 | ASP | CB-CG-OD2 | -5.66 | 113.21 | 118.30 |
| 1 | D | 648 | ASP | CB-CG-OD1 | 5.64 | 123.38 | 118.30 |
| 1 | C | 894 | ARG | NE-CZ-NH1 | -5.64 | 117.48 | 120.30 |
| 1 | C | 690 | SER | N-CA-CB | -5.64 | 102.05 | 110.50 |
| 1 | C | 869 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |
| 1 | C | 790 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 428 | ASP | CB-CG-OD1 | 5.62 | 123.36 | 118.30 |
| 1 | A | 672 | VAL | CB-CA-C | -5.60 | 100.76 | 111.40 |
| 1 | B | 308 | LEU | CB-CA-C | -5.60 | 99.56 | 110.20 |
| 1 | D | 319 | ASP | N-CA-CB | 5.59 | 120.66 | 110.60 |
| 1 | A | 211 | ASP | CB-CG-OD2 | -5.58 | 113.28 | 118.30 |
| 1 | A | 319 | ASP | CB-CG-OD1 | 5.58 | 123.32 | 118.30 |
| 1 | B | 568 | TRP | CA-CB-CG | -5.57 | 103.11 | 113.70 |
| 1 | B | 952 | ARG | NE-CZ-NH1 | 5.57 | 123.08 | 120.30 |
| 1 | C | 507 | ASP | CB-CG-OD1 | 5.57 | 123.31 | 118.30 |
| 1 | A | 881 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 1 | B | 699 | ARG | NH1-CZ-NH2 | -5.54 | 113.30 | 119.40 |
| 1 | C | 844 | HIS | CA-CB-CG | -5.54 | 104.18 | 113.60 |
| 1 | D | 77 | ASP | CB-CG-OD1 | 5.54 | 123.29 | 118.30 |
| 1 | D | 34 | ALA | N-CA-CB | 5.54 | 117.85 | 110.10 |
| 1 | B | 211 | ASP | CB-CG-OD1 | 5.54 | 123.28 | 118.30 |
| 1 | A | 15 | ASP | CB-CG-OD1 | 5.53 | 123.28 | 118.30 |
| 1 | A | 147 | ASN | N-CA-CB | -5.53 | 100.65 | 110.60 |
| 1 | A | 408 | TYR | CB-CG-CD1 | 5.53 | 124.32 | 121.00 |
| 1 | C | 52 | ARG | CB-CA-C | -5.53 | 99.35 | 110.40 |
| 1 | C | 908 | ASP | CB-CG-OD1 | 5.53 | 123.27 | 118.30 |
| 1 | D | 469 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |
| 1 | A | 651 | LEU | N-CA-CB | 5.49 | 121.39 | 110.40 |
| 1 | B | 721 | ARG | NE-CZ-NH2 | -5.49 | 117.55 | 120.30 |
| 1 | D | 802 | ASP | CB-CG-OD1 | 5.49 | 123.24 | 118.30 |
| 1 | B | 161 | TYR | CB-CG-CD1 | -5.49 | 117.71 | 121.00 |
| 1 | B | 509 | ASP | CB-CG-OD2 | -5.48 | 113.37 | 118.30 |
| 1 | A | 329 | ASP | CB-CG-OD1 | 5.47 | 123.23 | 118.30 |
| 1 | A | 292 | ARG | CD-NE-CZ | 5.47 | 131.26 | 123.60 |
| 1 | C | 15 | ASP | CB-CG-OD1 | 5.47 | 123.22 | 118.30 |
| 1 | B | 439 | ARG | NE-CZ-NH2 | -5.47 | 117.57 | 120.30 |
| 1 | D | 130 | ASP | CB-CG-OD1 | 5.47 | 123.22 | 118.30 |
| 1 | C | 917 | ARG | NE-CZ-NH2 | 5.46 | 123.03 | 120.30 |
| 1 | D | 760 | ARG | NE-CZ-NH1 | -5.46 | 117.57 | 120.30 |
| 1 | A | 506 | VAL | CA-CB-CG1 | -5.45 | 102.72 | 110.90 |
| 1 | A | 1018 | LEU | CB-CA-C | -5.44 | 99.86 | 110.20 |
| 1 | C | 659 | ASP | N-CA-CB | 5.44 | 120.39 | 110.60 |
| 1 | C | 446 | ARG | NE-CZ-NH2 | -5.43 | 117.58 | 120.30 |
| 1 | A | 882 | ILE | CA-CB-CG1 | -5.42 | 100.70 | 111.00 |
| 1 | B | 938 | ARG | N-CA-CB | 5.42 | 120.36 | 110.60 |
| 1 | B | 842 | TRP | CB-CA-C | -5.42 | 99.56 | 110.40 |
| 1 | A | 685 | LEU | CB-CA-C | 5.42 | 120.50 | 110.20 |
| 1 | B | 833 | ALA | N-CA-CB | -5.42 | 102.52 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 103 | VAL | CA-CB-CG1 | -5.42 | 102.78 | 110.90 |
| 1 | A | 832 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 1 | C | 828 | ASP | CB-CG-OD2 | -5.41 | 113.43 | 118.30 |
| 1 | C | 878 | HIS | CA-CB-CG | -5.41 | 104.41 | 113.60 |
| 1 | D | 772 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 1 | A | 1021 | CYS | CA-CB-SG | -5.40 | 104.28 | 114.00 |
| 1 | B | 78 | LEU | C-N-CD | -5.40 | 108.72 | 120.60 |
| 1 | B | 629 | PHE | CB-CA-C | -5.40 | 99.61 | 110.40 |
| 1 | C | 434 | PRO | N-CA-CB | 5.39 | 109.77 | 103.30 |
| 1 | B | 428 | ASP | CB-CG-OD1 | 5.37 | 123.14 | 118.30 |
| 1 | C | 745 | MET | CB-CA-C | 5.37 | 121.15 | 110.40 |
| 1 | C | 14 | ARG | NE-CZ-NH1 | 5.37 | 122.98 | 120.30 |
| 1 | C | 287 | ASP | CB-CG-OD1 | 5.37 | 123.13 | 118.30 |
| 1 | C | 113 | PHE | CB-CG-CD2 | -5.36 | 117.05 | 120.80 |
| 1 | B | 946 | TYR | CB-CG-CD1 | 5.36 | 124.22 | 121.00 |
| 1 | D | 840 | HIS | CB-CA-C | -5.36 | 99.69 | 110.40 |
| 1 | D | 987 | ASP | CB-CG-OD2 | -5.35 | 113.49 | 118.30 |
| 1 | B | 221 | GLN | N-CA-CB | -5.35 | 100.98 | 110.60 |
| 1 | A | 996 | ASP | CB-CG-OD1 | 5.34 | 123.11 | 118.30 |
| 1 | D | 908 | ASP | CB-CG-OD1 | 5.34 | 123.11 | 118.30 |
| 1 | B | 164 | ASP | CB-CG-OD1 | 5.34 | 123.10 | 118.30 |
| 1 | B | 234 | ASP | CB-CG-OD1 | 5.33 | 123.10 | 118.30 |
| 1 | D | 769 | TRP | N-CA-CB | 5.33 | 120.19 | 110.60 |
| 1 | D | 800 | ARG | NE-CZ-NH2 | -5.33 | 117.64 | 120.30 |
| 1 | A | 675 | GLN | N-CA-CB | 5.33 | 120.19 | 110.60 |
| 1 | B | 161 | TYR | N-CA-CB | -5.32 | 101.03 | 110.60 |
| 1 | C | 319 | ASP | CB-CG-OD2 | -5.31 | 113.52 | 118.30 |
| 1 | D | 659 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 1 | A | 438 | GLU | CG-CD-OE2 | -5.31 | 107.68 | 118.30 |
| 1 | C | 854 | LYS | CB-CA-C | -5.30 | 99.79 | 110.40 |
| 1 | D | 425 | ARG | NE-CZ-NH2 | 5.30 | 122.95 | 120.30 |
| 1 | A | 447 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |
| 1 | A | 244 | VAL | CA-CB-CG1 | 5.29 | 118.84 | 110.90 |
| 1 | C | 201 | ASP | CB-CG-OD2 | -5.29 | 113.54 | 118.30 |
| 1 | A | 17 | GLU | CG-CD-OE2 | -5.29 | 107.72 | 118.30 |
| 1 | B | 128 | ASN | CB-CA-C | -5.28 | 99.84 | 110.40 |
| 1 | B | 760 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 1 | D | 80 | GLU | CG-CD-OE2 | -5.27 | 107.75 | 118.30 |
| 1 | C | 33 | PHE | CB-CA-C | -5.27 | 99.86 | 110.40 |
| 1 | D | 919 | ASP | CB-CG-OD1 | 5.26 | 123.04 | 118.30 |
| 1 | C | 131 | GLU | CG-CD-OE1 | 5.26 | 128.83 | 118.30 |
| 1 | D | 446 | ARG | NE-CZ-NH1 | 5.26 | 122.93 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | D | 864 | MET | CG-SD-CE | 5.26 | 108.61 | 100.20 |
| 1 | C | 438 | GLU | CB-CA-C | -5.26 | 99.89 | 110.40 |
| 1 | A | 796 | SER | N-CA-CB | 5.26 | 118.39 | 110.50 |
| 1 | C | 653 | HIS | N-CA-CB | 5.25 | 120.06 | 110.60 |
| 1 | A | 645 | ARG | NE-CZ-NH2 | -5.25 | 117.67 | 120.30 |
| 1 | D | 723 | ALA | N-CA-CB | 5.25 | 117.45 | 110.10 |
| 1 | C | 164 | ASP | CB-CG-OD1 | 5.25 | 123.02 | 118.30 |
| 1 | A | 100 | TYR | CB-CG-CD1 | -5.24 | 117.85 | 121.00 |
| 1 | B | 403 | ASP | CB-CA-C | -5.24 | 99.91 | 110.40 |
| 1 | D | 800 | ARG | CD-NE-CZ | 5.24 | 130.94 | 123.60 |
| 1 | A | 840 | HIS | CB-CA-C | -5.24 | 99.92 | 110.40 |
| 1 | C | 262 | GLN | N-CA-C | -5.24 | 96.86 | 111.00 |
| 1 | D | 320 | GLY | C-N-CA | -5.24 | 108.61 | 121.70 |
| 1 | B | 753 | ASN | CA-CB-CG | -5.23 | 101.89 | 113.40 |
| 1 | B | 973 | ARG | NE-CZ-NH1 | -5.23 | 117.68 | 120.30 |
| 1 | C | 786 | ARG | CD-NE-CZ | 5.22 | 130.91 | 123.60 |
| 1 | A | 853 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 1 | C | 113 | PHE | CA-CB-CG | -5.22 | 101.37 | 113.90 |
| 1 | A | 179 | ALA | N-CA-CB | 5.22 | 117.41 | 110.10 |
| 1 | B | 559 | TYR | CB-CG-CD1 | 5.22 | 124.13 | 121.00 |
| 1 | C | 507 | ASP | CB-CG-OD2 | -5.22 | 113.61 | 118.30 |
| 1 | D | 52 | ARG | CB-CA-C | -5.22 | 99.97 | 110.40 |
| 1 | D | 199 | ASP | CB-CG-OD1 | 5.22 | 123.00 | 118.30 |
| 1 | B | 569 | ASP | CB-CG-OD2 | -5.21 | 113.61 | 118.30 |
| 1 | C | 347 | LYS | CB-CA-C | -5.21 | 99.98 | 110.40 |
| 1 | A | 96 | ASP | CB-CG-OD1 | 5.21 | 122.99 | 118.30 |
| 1 | C | 572 | ASP | CB-CG-OD1 | 5.21 | 122.99 | 118.30 |
| 1 | D | 234 | ASP | CB-CG-OD2 | -5.21 | 113.61 | 118.30 |
| 1 | C | 524 | LEU | CB-CG-CD1 | -5.20 | 102.16 | 111.00 |
| 1 | A | 952 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |
| 1 | B | 253 | TYR | CB-CG-CD2 | -5.20 | 117.88 | 121.00 |
| 1 | C | 721 | ARG | CD-NE-CZ | 5.20 | 130.88 | 123.60 |
| 1 | C | 919 | ASP | CB-CG-OD2 | -5.20 | 113.62 | 118.30 |
| 1 | D | 510 | GLN | N-CA-C | -5.19 | 96.98 | 111.00 |
| 1 | A | 828 | ASP | CB-CG-OD1 | 5.18 | 122.96 | 118.30 |
| 1 | C | 211 | ASP | CB-CG-OD1 | 5.17 | 122.95 | 118.30 |
| 1 | A | 792 | ASP | CB-CG-OD2 | -5.17 | 113.65 | 118.30 |
| 1 | C | 760 | ARG | N-CA-CB | 5.17 | 119.90 | 110.60 |
| 1 | A | 82 | ASP | CB-CG-OD2 | -5.16 | 113.65 | 118.30 |
| 1 | D | 482 | ARG | NE-CZ-NH2 | -5.16 | 117.72 | 120.30 |
| 1 | C | 261 | TRP | CB-CA-C | -5.15 | 100.09 | 110.40 |
| 1 | D | 755 | ARG | NE-CZ-NH1 | 5.15 | 122.88 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 559 | TYR | CB-CG-CD2 | -5.15 | 117.91 | 121.00 |
| 1 | C | 100 | TYR | CB-CG-CD1 | 5.14 | 124.09 | 121.00 |
| 1 | D | 559 | TYR | CB-CG-CD2 | -5.14 | 117.91 | 121.00 |
| 1 | B | 164 | ASP | N-CA-CB | 5.14 | 119.86 | 110.60 |
| 1 | C | 856 | TYR | CG-CD2-CE2 | -5.14 | 117.19 | 121.30 |
| 1 | B | 381 | GLN | CA-CB-CG | -5.14 | 102.09 | 113.40 |
| 1 | B | 954 | ASP | CB-CG-OD2 | -5.13 | 113.68 | 118.30 |
| 1 | A | 598 | ASP | CB-CG-OD1 | 5.12 | 122.91 | 118.30 |
| 1 | D | 769 | TRP | CB-CA-C | -5.12 | 100.16 | 110.40 |
| 1 | A | 368 | ASP | CB-CG-OD1 | 5.12 | 122.90 | 118.30 |
| 1 | B | 875 | ASP | CB-CG-OD1 | 5.11 | 122.90 | 118.30 |
| 1 | D | 67 | GLU | CG-CD-OE2 | -5.11 | 108.08 | 118.30 |
| 1 | A | 375 | ASP | CB-CG-OD1 | 5.10 | 122.89 | 118.30 |
| 1 | B | 363 | HIS | CA-CB-CG | -5.09 | 104.94 | 113.60 |
| 1 | B | 546 | LEU | N-CA-CB | 5.09 | 120.59 | 110.40 |
| 1 | A | 352 | ARG | CG-CD-NE | 5.09 | 122.49 | 111.80 |
| 1 | D | 629 | PHE | CB-CA-C | -5.09 | 100.22 | 110.40 |
| 1 | C | 473 | ARG | NE-CZ-NH1 | -5.08 | 117.76 | 120.30 |
| 1 | C | 788 | PRO | N-CA-CB | 5.08 | 109.40 | 103.30 |
| 1 | B | 503 | TYR | CB-CG-CD2 | -5.08 | 117.95 | 121.00 |
| 1 | C | 113 | PHE | CB-CA-C | -5.07 | 100.27 | 110.40 |
| 1 | A | 199 | ASP | CB-CG-OD2 | -5.06 | 113.74 | 118.30 |
| 1 | B | 827 | ALA | N-CA-CB | 5.06 | 117.18 | 110.10 |
| 1 | B | 310 | ARG | NE-CZ-NH1 | 5.05 | 122.83 | 120.30 |
| 1 | B | 782 | ASP | CB-CG-OD2 | -5.04 | 113.76 | 118.30 |
| 1 | B | 130 | ASP | CB-CG-OD1 | 5.04 | 122.83 | 118.30 |
| 1 | C | 252 | ASP | CB-CG-OD2 | -5.04 | 113.77 | 118.30 |
| 1 | B | 790 | ASP | CB-CG-OD1 | 5.03 | 122.83 | 118.30 |
| 1 | C | 404 | ARG | NE-CZ-NH2 | -5.03 | 117.78 | 120.30 |
| 1 | C | 130 | ASP | CB-CG-OD1 | 5.03 | 122.83 | 118.30 |
| 1 | C | 239 | VAL | CG1-CB-CG2 | -5.03 | 102.85 | 110.90 |
| 1 | C | 906 | TYR | CA-CB-CG | -5.03 | 103.85 | 113.40 |
| 1 | D | 280 | ASP | CB-CG-OD2 | -5.03 | 113.78 | 118.30 |
| 1 | B | 664 | ALA | N-CA-CB | -5.03 | 103.06 | 110.10 |
| 1 | D | 954 | ASP | CB-CG-OD2 | -5.02 | 113.78 | 118.30 |
| 1 | A | 120 | THR | CA-CB-CG2 | -5.02 | 105.37 | 112.40 |
| 1 | B | 651 | LEU | CB-CA-C | 5.02 | 119.74 | 110.20 |
| 1 | A | 503 | TYR | CD1-CE1-CZ | -5.02 | 115.28 | 119.80 |
| 1 | D | 610 | ASP | CB-CG-OD1 | 5.02 | 122.82 | 118.30 |
| 1 | A | 942 | ARG | NE-CZ-NH2 | -5.01 | 117.79 | 120.30 |
| 1 | B | 685 | LEU | CB-CA-C | 5.01 | 119.72 | 110.20 |
| 1 | D | 686 | PRO | N-CA-CB | 5.01 | 109.31 | 103.30 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | D | 689 | GLU | CA |

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | B | 329 | ASP | Sidechain |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 8125 | 0 | 7716 | 188 | 1 |
| 1 | B | 8125 | 0 | 7716 | 201 | 0 |
| 1 | C | 8125 | 0 | 7716 | 219 | 0 |
| 1 | D | 8125 | 0 | 7716 | 208 | 0 |
| 2 | A | 10 | 0 | 9 | 0 | 0 |
| 2 | B | 10 | 0 | 9 | 1 | 0 |
| 2 | C | 10 | 0 | 9 | 0 | 0 |
| 2 | D | 10 | 0 | 9 | 2 | 0 |
| 3 | A | 3 | 0 | 0 | 0 | 0 |
| 3 | B | 2 | 0 | 0 | 0 | 0 |
| 3 | C | 2 | 0 | 0 | 0 | 0 |
| 3 | D | 3 | 0 | 0 | 0 | 0 |
| 4 | A | 4 | 0 | 0 | 0 | 0 |
| 4 | B | 4 | 0 | 0 | 0 | 0 |
| 4 | C | 4 | 0 | 0 | 0 | 0 |
| 4 | D | 3 | 0 | 0 | 0 | 0 |
| 5 | A | 100 | 0 | 150 | 9 | 0 |
| 5 | B | 108 | 0 | 162 | 10 | 0 |
| 5 | C | 112 | 0 | 168 | 15 | 0 |
| 5 | D | 92 | 0 | 138 | 13 | 0 |
| 6 | A | 992 | 0 | 0 | 21 | 0 |
| 6 | B | 995 | 0 | 0 | 14 | 0 |
| 6 | C | 946 | 0 | 0 | 14 | 1 |
| 6 | D | 980 | 0 | 0 | 18 | 0 |
| All | All | 36890 | 0 | 31518 | 810 | 1 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (810) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:634:GLN:NE2 | 1:C:634:GLN:H | 1.47 | 1.13 |
| 1:C:746:ASP:HA | 1:C:760:ARG:HG3 | 1.33 | 1.10 |
| 1:D:804:ASN:HD22 | 1:D:809:ARG:NH2 | 1.54 | 1.05 |
| 1:B:142:ILE:HG12 | 1:B:170:GLU:HG2 | 1.37 | 1.02 |
| 1:B:797:GLU:HG2 | 1:B:799:THR:HG23 | 1.35 | 1.02 |
| 1:B:600:GLN:H | 1:B:600:GLN:HE21 | 1.09 | 0.98 |
| 1:C:230:ARG:HG3 | 1:C:230:ARG:HH11 | 1.30 | 0.94 |
| 1:D:653:HIS:CD2 | 1:D:667:GLU:HB3 | 2.03 | 0.93 |
| 1:C:755:ARG:HG2 | 1:C:769:TRP:CE3 | 2.02 | 0.93 |
| 1:D:804:ASN:HA | 1:D:809:ARG:HE | 1.30 | 0.93 |
| 1:D:653:HIS:HD2 | 1:D:667:GLU:HB3 | 1.36 | 0.91 |
| 1:A:600:GLN:H | 1:A:600:GLN:HE21 | 1.17 | 0.91 |
| 1:B:809:ARG:HH11 | 1:B:809:ARG:HG2 | 1.34 | 0.91 |
| 1:D:651:LEU:CD2 | 1:D:701:VAL:HB | 2.01 | 0.91 |
| 1:D:804:ASN:HD22 | 1:D:809:ARG:CZ | 1.85 | 0.90 |
| 1:B:232:ASN:ND2 | 1:B:237:ARG:HG3 | 1.88 | 0.89 |
| 1:B:655:MET:HE2 | 1:B:665:SER:HB3 | 1.54 | 0.89 |
| 1:D:237:ARG:HH11 | 1:D:237:ARG:HB3 | 1.38 | 0.88 |
| 1:D:804:ASN:HA | 1:D:809:ARG:NE | 1.89 | 0.85 |
| 1:A:735:HIS:N | 1:A:735:HIS:ND1 | 2.24 | 0.85 |
| 1:B:668:VAL:HG12 | 1:B:669:PRO:HD2 | 1.57 | 0.83 |
| 1:C:634:GLN:N | 1:C:634:GLN:NE2 | 2.26 | 0.83 |
| 1:A:797:GLU:O | 1:A:801:ILE:HD13 | 1.79 | 0.82 |
| 1:D:843:GLN:HG2 | 1:D:848:THR:HA | 1.61 | 0.82 |
| 1:B:730:LEU:HD12 | 1:B:730:LEU:H | 1.44 | 0.82 |
| 1:D:804:ASN:ND2 | 1:D:809:ARG:NH2 | 2.29 | 0.81 |
| 1:B:634:GLN:HG2 | 1:B:682:LEU:O | 1.80 | 0.81 |
| 1:C:356:ARG:HD2 | 1:C:379:MET:HE1 | 1.62 | 0.81 |
| 1:C:824:GLN:HG2 | 1:C:825:CYS:N | 1.96 | 0.81 |
| 1:A:863:GLN:HG2 | 1:A:1021:CYS:HB3 | 1.62 | 0.80 |
| 1:D:804:ASN:CB | 1:D:809:ARG:HH21 | 1.93 | 0.80 |
| 1:B:360:HIS:CE1 | 1:B:362:LEU:HB2 | 2.17 | 0.79 |
| 1:D:807:VAL:O | 1:D:811:LYS:HG3 | 1.83 | 0.79 |
| 1:D:802:ASP:OD1 | 1:D:803:PRO:HD2 | 1.83 | 0.79 |
| 1:C:634:GLN:HE21 | 1:C:634:GLN:H | 1.30 | 0.79 |
| 1:D:651:LEU:HD23 | 1:D:701:VAL:HB | 1.63 | 0.78 |
| 1:A:797:GLU:HB3 | 1:A:799:THR:HG23 | 1.63 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:72:SER:HB3 | 6:C:9337:HOH:O | 1.84 | 0.77 |
| 1:C:102:ASN:HD22 | 5:C:8506:DMS:H13 | 1.50 | 0.77 |
| 1:C:778:THR:HG23 | 1:C:887:GLN:HB3 | 1.67 | 0.77 |
| 1:D:230:ARG:HD3 | 6:D:9630:HOH:O | 1.84 | 0.76 |
| 1:A:646:HIS:ND1 | 6:A:9408:HOH:O | 2.17 | 0.76 |
| 1:C:777:LEU:HG | 1:C:889:ALA:HA | 1.68 | 0.76 |
| 1:D:797:GLU:O | 1:D:801:ILE:HD13 | 1.85 | 0.76 |
| 1:A:809:ARG:HH11 | 1:A:809:ARG:HG2 | 1.50 | 0.76 |
| 1:B:655:MET:HG3 | 6:B:8989:HOH:O | 1.85 | 0.75 |
| 1:B:142:ILE:CG1 | 1:B:170:GLU:HG2 | 2.14 | 0.75 |
| 1:A:65:ALA:HB1 | 1:A:66:PRO:HD2 | 1.67 | 0.75 |
| 1:C:785:THR:O | 1:C:881:ARG:HD2 | 1.88 | 0.74 |
| 1:B:797:GLU:HG2 | 1:B:799:THR:CG2 | 2.17 | 0.74 |
| 1:A:668:VAL:HG13 | 1:A:669:PRO:HD2 | 1.69 | 0.74 |
| 1:A:887:GLN:NE2 | 1:A:980:GLU:O | 2.20 | 0.74 |
| 1:D:237:ARG:NH1 | 6:D:9257:HOH:O | 2.20 | 0.74 |
| 1:B:142:ILE:HG12 | 1:B:170:GLU:CG | 2.18 | 0.74 |
| 1:B:531:ARG:HB3 | 1:B:532:PRO:HD2 | 1.70 | 0.73 |
| 1:C:749:ILE:N | 1:C:749:ILE:HD12 | 2.03 | 0.73 |
| 1:A:473:ARG:NH1 | 1:A:476:LYS:HB2 | 2.04 | 0.73 |
| 1:C:878:HIS:HD2 | 6:C:8694:HOH:O | 1.71 | 0.73 |
| 1:C:687:GLN:N | 1:C:687:GLN:HE21 | 1.86 | 0.73 |
| 1:D:634:GLN:NE2 | 1:D:682:LEU:O | 2.22 | 0.73 |
| 1:D:651:LEU:HD21 | 1:D:653:HIS:CE1 | 2.23 | 0.72 |
| 1:A:46:ARG:HB3 | 1:A:47:PRO:HD2 | 1.69 | 0.72 |
| 1:C:102:ASN:HD22 | 5:C:8506:DMS:C1 | 2.03 | 0.72 |
| 1:D:237:ARG:HH11 | 1:D:237:ARG:CB | 2.01 | 0.72 |
| 1:D:292:ARG:HH12 | 5:D:8412:DMS:C2 | 2.03 | 0.72 |
| 1:B:863:GLN:HG3 | 1:B:1021:CYS:HB3 | 1.69 | 0.72 |
| 1:B:360:HIS:HE1 | 1:B:362:LEU:HB2 | 1.55 | 0.71 |
| 1:D:749:ILE:N | 1:D:749:ILE:HD12 | 2.04 | 0.71 |
| 1:C:797:GLU:O | 1:C:801:ILE:HD13 | 1.90 | 0.71 |
| 1:B:651:LEU:O | 1:B:651:LEU:HD23 | 1.91 | 0.71 |
| 1:C:652:LEU:HD11 | 1:C:698:VAL:HB | 1.72 | 0.70 |
| 1:C:356:ARG:HD2 | 1:C:379:MET:CE | 2.22 | 0.70 |
| 1:B:772:ASP:OD1 | 1:B:773:LYS:HD3 | 1.92 | 0.70 |
| 1:B:434:PRO:HB3 | 1:C:434:PRO:HB3 | 1.74 | 0.70 |
| 1:C:748:CYS:C | 1:C:749:ILE:HD12 | 2.12 | 0.70 |
| 1:D:112:PRO:HD2 | 1:D:113:PHE:CE1 | 2.26 | 0.69 |
| 1:A:473:ARG:NH1 | 6:A:9273:HOH:O | 2.24 | 0.69 |
| 1:A:84:VAL:HA | 5:A:8414:DMS:O | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:730:LEU:H | 1:B:730:LEU:CD1 | 2.00 | 0.69 |
| 1:B:878:HIS:HD2 | 6:B:8690:HOH:O | 1.74 | 0.69 |
| 1:D:622:HIS:O | 1:D:625:GLN:HG3 | 1.92 | 0.68 |
| 1:A:800:ARG:HG2 | 1:A:800:ARG:O | 1.92 | 0.68 |
| 1:A:749:ILE:N | 1:A:749:ILE:HD12 | 2.08 | 0.68 |
| 1:B:634:GLN:HE22 | 1:B:684:GLU:HA | 1.57 | 0.68 |
| 1:A:243:GLU:OE2 | 1:A:245:GLN:NE2 | 2.22 | 0.68 |
| 1:A:249:GLU:OE2 | 1:A:251:ARG:NE | 2.23 | 0.68 |
| 1:A:804:ASN:OD1 | 1:A:809:ARG:NH2 | 2.27 | 0.68 |
| 1:C:651:LEU:HD21 | 1:C:653:HIS:HE1 | 1.57 | 0.68 |
| 1:A:433:LEU:HB3 | 1:A:434:PRO:HD3 | 1.76 | 0.68 |
| 1:C:765:LEU:HD21 | 1:C:768:MET:CE | 2.24 | 0.68 |
| 1:D:237:ARG:NH1 | 1:D:296:GLU:OE2 | 2.27 | 0.67 |
| 1:D:804:ASN:HD22 | 1:D:809:ARG:HH21 | 1.39 | 0.67 |
| 1:A:829:THR:HG23 | 1:A:834:VAL:HG22 | 1.77 | 0.67 |
| 1:A:277:GLU:CD | 1:A:277:GLU:H | 1.98 | 0.67 |
| 1:B:634:GLN:CG | 1:B:682:LEU:HB2 | 2.24 | 0.67 |
| 1:C:651:LEU:CD1 | 1:C:701:VAL:HB | 2.24 | 0.67 |
| 1:B:1022:GLN:HG2 | 1:B:1023:LYS:N | 2.09 | 0.67 |
| 1:D:725:ASN:HB2 | 6:D:9521:HOH:O | 1.94 | 0.67 |
| 1:D:88:SER:HA | 1:D:366:VAL:HG21 | 1.76 | 0.67 |
| 1:D:887:GLN:NE2 | 1:D:980:GLU:O | 2.28 | 0.66 |
| 1:B:651:LEU:C | 1:B:651:LEU:HD23 | 2.15 | 0.66 |
| 1:A:599:ARG:HG3 | 1:A:600:GLN:NE2 | 2.10 | 0.66 |
| 1:A:595:THR:HA | 1:A:596:PRO:C | 2.16 | 0.66 |
| 1:D:844:HIS:ND1 | 1:D:845:GLN:HG2 | 2.11 | 0.66 |
| 1:B:637:GLU:OE2 | 1:B:677:LYS:HD3 | 1.95 | 0.66 |
| 1:C:858:ILE:CD1 | 1:C:864:MET:HB2 | 2.26 | 0.66 |
| 1:C:718:GLN:HG2 | 5:C:8503:DMS:C1 | 2.26 | 0.65 |
| 1:D:635:THR:HG23 | 1:D:681:GLU:OE1 | 1.95 | 0.65 |
| 1:B:634:GLN:HG3 | 1:B:682:LEU:HB2 | 1.78 | 0.65 |
| 1:B:102:ASN:HD22 | 5:B:8506:DMS:C1 | 2.10 | 0.65 |
| 1:B:684:GLU:O | 1:B:686:PRO:HD3 | 1.97 | 0.65 |
| 1:B:634:GLN:NE2 | 1:B:684:GLU:HA | 2.12 | 0.65 |
| 1:C:232:ASN:ND2 | 1:C:237:ARG:HG3 | 2.12 | 0.65 |
| 1:D:804:ASN:HA | 1:D:809:ARG:CZ | 2.26 | 0.65 |
| 1:A:857:ARG:HG2 | 6:A:9068:HOH:O | 1.97 | 0.64 |
| 1:A:46:ARG:HB3 | 1:A:47:PRO:CD | 2.28 | 0.64 |
| 1:B:809:ARG:NH1 | 1:B:809:ARG:HG2 | 2.08 | 0.64 |
| 1:D:804:ASN:CA | 1:D:809:ARG:HH21 | 2.09 | 0.64 |
| 1:D:237:ARG:HH11 | 1:D:237:ARG:CG | 2.10 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:658:LEU:O | 1:C:661:LYS:HB2 | 1.98 | 0.64 |
| 1:C:743:SER:O | 1:C:760:ARG:NH1 | 2.28 | 0.64 |
| 1:D:135:GLN:C | 1:D:136:GLU:HG2 | 2.18 | 0.64 |
| 1:D:804:ASN:HA | 1:D:809:ARG:NH2 | 2.13 | 0.64 |
| 1:C:749:ILE:HG13 | 1:C:834:VAL:HG11 | 1.81 | 0.63 |
| 1:A:86:VAL:HG13 | 1:A:87:PRO:HA | 1.79 | 0.63 |
| 1:B:668:VAL:CG1 | 1:B:669:PRO:HD2 | 2.29 | 0.63 |
| 1:C:765:LEU:HD21 | 1:C:768:MET:HE3 | 1.81 | 0.63 |
| 1:A:930:VAL:HA | 1:A:973:ARG:HD3 | 1.79 | 0.63 |
| 1:B:945:ASN:HB3 | 1:B:1023:LYS:HE2 | 1.78 | 0.63 |
| 1:C:230:ARG:HG3 | 1:C:230:ARG:NH1 | 2.04 | 0.63 |
| 1:D:804:ASN:ND2 | 1:D:809:ARG:HH21 | 1.95 | 0.63 |
| 1:A:1017:GLN:O | 1:A:1017:GLN:HG3 | 1.99 | 0.63 |
| 1:B:367:MET:CE | 1:B:372:MET:HG3 | 2.29 | 0.63 |
| 1:C:754:LYS:NZ | 1:C:1022:GLN:OE1 | 2.30 | 0.63 |
| 1:B:241:GLU:HG3 | 1:B:292:ARG:HG3 | 1.79 | 0.62 |
| 1:C:596:PRO:HB3 | 6:C:9379:HOH:O | 1.98 | 0.62 |
| 1:D:1022:GLN:HG3 | 1:D:1023:LYS:N | 2.14 | 0.62 |
| 1:D:748:CYS:C | 1:D:749:ILE:HD12 | 2.19 | 0.62 |
| 1:B:615:PRO:O | 1:B:618:THR:HG22 | 1.99 | 0.62 |
| 1:C:822:LEU:HD13 | 1:C:840:HIS:NE2 | 2.14 | 0.62 |
| 1:D:46:ARG:HB3 | 1:D:47:PRO:HD2 | 1.81 | 0.62 |
| 1:A:237:ARG:HH11 | 1:A:237:ARG:HB3 | 1.64 | 0.62 |
| 1:C:292:ARG:HH12 | 5:C:8412:DMS:C2 | 2.12 | 0.62 |
| 1:D:334:GLU:OE1 | 1:D:336:ARG:NH1 | 2.29 | 0.62 |
| 1:B:236:SER:C | 1:B:237:ARG:HG2 | 2.17 | 0.62 |
| 1:A:878:HIS:HD2 | 6:A:8674:HOH:O | 1.83 | 0.62 |
| 1:D:805:ALA:O | 1:D:809:ARG:HG3 | 2.00 | 0.61 |
| 1:C:858:ILE:HD11 | 1:C:864:MET:HB2 | 1.81 | 0.61 |
| 1:A:599:ARG:HG3 | 1:A:600:GLN:HE21 | 1.65 | 0.61 |
| 1:A:892:ALA:HB3 | 1:A:946:TYR:CE1 | 2.35 | 0.61 |
| 1:C:613:PRO:HB3 | 1:C:617:LEU:HD23 | 1.82 | 0.61 |
| 1:D:804:ASN:HA | 1:D:809:ARG:HH21 | 1.65 | 0.61 |
| 1:A:844:HIS:HD2 | 6:A:9406:HOH:O | 1.83 | 0.61 |
| 1:A:431:ARG:HG3 | 6:A:9338:HOH:O | 1.99 | 0.61 |
| 1:C:887:GLN:NE2 | 1:C:980:GLU:O | 2.32 | 0.61 |
| 1:C:454:ILE:HG13 | 1:C:455:ILE:HG13 | 1.83 | 0.61 |
| 1:D:795:VAL:HG23 | 6:D:9473:HOH:O | 1.99 | 0.61 |
| 1:D:844:HIS:CE1 | 1:D:845:GLN:HG2 | 2.36 | 0.60 |
| 1:D:230:ARG:HH12 | 1:D:239:VAL:HG11 | 1.65 | 0.60 |
| 1:D:634:GLN:HB3 | 1:D:682:LEU:HB2 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:804:ASN:CA | 1:D:809:ARG:HE | 2.07 | 0.60 |
| 1:C:1020:TRP:HD1 | 1:C:1021:CYS:N | 1.99 | 0.60 |
| 1:D:804:ASN:HB2 | 1:D:809:ARG:HH21 | 1.66 | 0.60 |
| 1:D:472:TYR:O | 1:D:476:LYS:HG2 | 2.02 | 0.60 |
| 1:A:110:ASN:OD1 | 6:A:9307:HOH:O | 2.15 | 0.60 |
| 1:C:745:MET:CE | 1:C:745:MET:HA | 2.32 | 0.60 |
| 1:B:367:MET:HE2 | 1:B:372:MET:HG3 | 1.83 | 0.59 |
| 1:C:88:SER:HA | 1:C:366:VAL:HG21 | 1.83 | 0.59 |
| 1:C:278:ILE:N | 1:C:278:ILE:HD13 | 2.16 | 0.59 |
| 1:D:794:GLY:HA3 | 6:D:8986:HOH:O | 2.01 | 0.59 |
| 1:D:91:GLN:HB3 | 1:D:98:PRO:HD3 | 1.84 | 0.59 |
| 1:A:640:SER:O | 1:A:675:GLN:HA | 2.03 | 0.59 |
| 1:D:128:ASN:HB3 | 1:D:180:GLY:O | 2.03 | 0.59 |
| 1:A:599:ARG:HD2 | 1:A:600:GLN:HE22 | 1.68 | 0.59 |
| 5:A:8420:DMS:H21 | 6:D:9470:HOH:O | 2.02 | 0.59 |
| 1:A:890:GLN:HG3 | 1:A:891:VAL:N | 2.17 | 0.59 |
| 1:D:473:ARG:NH1 | 1:D:476:LYS:HB2 | 2.17 | 0.58 |
| 1:C:237:ARG:HB2 | 1:C:237:ARG:HH11 | 1.68 | 0.58 |
| 1:D:795:VAL:HG12 | 6:D:9678:HOH:O | 2.03 | 0.58 |
| 1:B:200:GLN:HG2 | 1:B:391:HIS:HB2 | 1.84 | 0.58 |
| 1:A:587:ALA:HB1 | 1:A:591:ASP:HB2 | 1.85 | 0.58 |
| 1:C:690:SER:HB2 | 6:C:9334:HOH:O | 2.03 | 0.58 |
| 1:C:744:GLU:O | 1:C:760:ARG:HD3 | 2.03 | 0.58 |
| 1:D:595:THR:HA | 1:D:596:PRO:C | 2.23 | 0.58 |
| 1:A:832:ASP:OD1 | 1:A:832:ASP:N | 2.33 | 0.58 |
| 1:B:630:ARG:NE | 1:B:637:GLU:OE1 | 2.36 | 0.58 |
| 1:C:796:SER:OG | 1:C:802:ASP:N | 2.28 | 0.58 |
| 1:A:878:HIS:CE1 | 1:A:1010:SER:HB3 | 2.39 | 0.58 |
| 1:B:1022:GLN:HG2 | 1:B:1023:LYS:O | 2.04 | 0.58 |
| 1:B:600:GLN:N | 1:B:600:GLN:HE21 | 1.91 | 0.58 |
| 1:D:593:GLY:O | 1:D:595:THR:HG22 | 2.03 | 0.58 |
| 1:D:393:PRO:HD3 | 1:D:412:GLU:O | 2.03 | 0.58 |
| 1:B:631:LEU:HD12 | 1:B:635:THR:O | 2.04 | 0.58 |
| 1:A:687:GLN:HG3 | 6:A:9416:HOH:O | 2.02 | 0.57 |
| 1:C:768:MET:O | 1:C:775:GLN:N | 2.37 | 0.57 |
| 1:C:778:THR:HG23 | 1:C:887:GLN:CB | 2.34 | 0.57 |
| 1:A:599:ARG:HG3 | 1:A:600:GLN:H | 1.68 | 0.57 |
| 1:D:375:ASP:O | 1:D:379:MET:HG3 | 2.05 | 0.57 |
| 1:C:249:GLU:OE2 | 1:C:251:ARG:HD3 | 2.04 | 0.57 |
| 1:C:305:ILE:HD11 | 1:C:645:ARG:HB3 | 1.85 | 0.57 |
| 1:A:1022:GLN:HG2 | 1:A:1023:LYS:H | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:873:ALA:O | 1:D:876:THR:HG22 | 2.05 | 0.57 |
| 1:D:878:HIS:HD2 | 6:D:8814:HOH:O | 1.88 | 0.57 |
| 1:A:683:PRO:O | 1:A:685:LEU:HG | 2.04 | 0.56 |
| 1:C:906:TYR:HB3 | 1:C:907:PRO:HD2 | 1.87 | 0.56 |
| 1:A:279:ILE:HD11 | 1:D:422:PRO:HG2 | 1.86 | 0.56 |
| 1:C:781:ARG:NH1 | 6:C:9326:HOH:O | 2.38 | 0.56 |
| 1:C:802:ASP:O | 1:C:808:GLU:HG3 | 2.05 | 0.56 |
| 1:B:577:LYS:O | 1:B:584:PRO:HA | 2.04 | 0.56 |
| 1:D:240:LEU:C | 1:D:240:LEU:HD23 | 2.25 | 0.56 |
| 1:B:429:ASP:OD1 | 1:B:430:PRO:HD2 | 2.04 | 0.56 |
| 1:D:682:LEU:HD22 | 1:D:683:PRO:HD2 | 1.85 | 0.56 |
| 1:C:651:LEU:HD11 | 1:C:701:VAL:HB | 1.88 | 0.56 |
| 1:C:734:SER:HB3 | 1:C:860:GLY:C | 2.26 | 0.56 |
| 1:C:843:GLN:NE2 | 1:C:848:THR:OG1 | 2.37 | 0.56 |
| 1:A:949:HIS:O | 1:A:1023:LYS:NZ | 2.38 | 0.56 |
| 1:A:768:MET:HE1 | 1:A:1020:TRP:CZ2 | 2.40 | 0.55 |
| 1:A:668:VAL:CG1 | 1:A:669:PRO:HD2 | 2.36 | 0.55 |
| 1:B:646:HIS:CE1 | 1:B:673:ALA:HB2 | 2.42 | 0.55 |
| 1:D:277:GLU:OE1 | 5:D:8412:DMS:O | 2.25 | 0.55 |
| 1:A:649:ASN:OD1 | 1:A:703:PRO:HD2 | 2.06 | 0.55 |
| 1:A:625:GLN:NE2 | 6:A:8804:HOH:O | 2.39 | 0.55 |
| 1:C:651:LEU:CD2 | 1:C:653:HIS:HE1 | 2.19 | 0.55 |
| 1:C:568:TRP:CD2 | 1:C:569:ASP:HB3 | 2.42 | 0.55 |
| 1:A:653:HIS:CD2 | 1:A:667:GLU:HG2 | 2.42 | 0.55 |
| 1:D:629:PHE:O | 1:D:630:ARG:NH1 | 2.35 | 0.55 |
| 1:D:891:VAL:HG23 | 1:D:981:GLY:HA2 | 1.89 | 0.55 |
| 1:C:786:ARG:HG2 | 1:C:880:ALA:HB1 | 1.89 | 0.55 |
| 1:A:673:ALA:HB1 | 1:A:674:PRO:HD2 | 1.89 | 0.55 |
| 1:B:634:GLN:HG2 | 1:B:682:LEU:HB2 | 1.89 | 0.55 |
| 1:B:655:MET:SD | 1:B:656:VAL:N | 2.80 | 0.54 |
| 1:C:655:MET:HE2 | 1:C:665:SER:HB3 | 1.89 | 0.54 |
| 1:C:654:TRP:O | 1:C:665:SER:HB2 | 2.07 | 0.54 |
| 1:D:128:ASN:HB2 | 6:D:9631:HOH:O | 2.06 | 0.54 |
| 1:B:499:ILE:HD11 | 1:B:529:GLU:CG | 2.36 | 0.54 |
| 1:B:878:HIS:CD2 | 6:B:8690:HOH:O | 2.54 | 0.54 |
| 1:D:920:LEU:HB3 | 1:D:921:PRO:HD2 | 1.89 | 0.54 |
| 1:A:843:GLN:HG2 | 1:A:848:THR:HA | 1.89 | 0.54 |
| 1:B:73:TRP:CE2 | 1:B:122:CYS:HB3 | 2.42 | 0.54 |
| 1:B:863:GLN:HG3 | 1:B:1021:CYS:CB | 2.37 | 0.54 |
| 1:A:416:GLU:OE2 | 1:A:418:HIS:HB2 | 2.07 | 0.54 |
| 1:D:521:LYS:HE2 | 6:D:9163:HOH:O | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:759:ASN:OD1 | 1:A:761:GLN:N | 2.38 | 0.54 |
| 1:A:830:LEU:HD12 | 1:A:833:ALA:HB3 | 1.90 | 0.54 |
| 1:B:30:HIS:HB2 | 1:B:31:PRO:HD2 | 1.89 | 0.54 |
| 1:D:340:GLY:O | 1:D:561:ARG:HG2 | 2.08 | 0.54 |
| 1:D:718:GLN:NE2 | 5:D:8503:DMS:H13 | 2.23 | 0.54 |
| 1:D:847:LYS:HG3 | 1:D:848:THR:N | 2.18 | 0.54 |
| 1:D:843:GLN:CG | 1:D:848:THR:HA | 2.35 | 0.54 |
| 1:C:824:GLN:OE1 | 1:C:837:THR:HG22 | 2.08 | 0.54 |
| 1:A:764:PHE:CD1 | 1:A:781:ARG:NH1 | 2.76 | 0.54 |
| 1:C:890:GLN:HG3 | 1:C:891:VAL:N | 2.22 | 0.54 |
| 1:B:377:LEU:CD2 | 1:B:708:TRP:HA | 2.38 | 0.53 |
| 1:C:764:PHE:CE1 | 1:C:781:ARG:NH1 | 2.76 | 0.53 |
| 1:D:801:ILE:CG2 | 1:D:802:ASP:H | 2.21 | 0.53 |
| 1:C:652:LEU:HD23 | 1:C:680:ILE:HD13 | 1.90 | 0.53 |
| 1:C:832:ASP:N | 1:C:832:ASP:OD1 | 2.41 | 0.53 |
| 1:C:843:GLN:HA | 1:C:847:LYS:O | 2.07 | 0.53 |
| 1:D:292:ARG:HH12 | 5:D:8412:DMS:H22 | 1.71 | 0.53 |
| 1:D:577:LYS:O | 1:D:584:PRO:HA | 2.08 | 0.53 |
| 1:D:804:ASN:C | 1:D:809:ARG:HE | 2.12 | 0.53 |
| 1:B:685:LEU:O | 1:B:686:PRO:C | 2.47 | 0.53 |
| 1:C:878:HIS:CE1 | 1:C:1010:SER:HB3 | 2.43 | 0.53 |
| 5:B:8601:DMS:H13 | 6:B:9437:HOH:O | 2.07 | 0.53 |
| 1:C:948:PRO:O | 1:C:1023:LYS:N | 2.34 | 0.53 |
| 1:B:599:ARG:HH11 | 1:B:600:GLN:NE2 | 2.05 | 0.53 |
| 1:C:367:MET:CE | 1:C:367:MET:HA | 2.39 | 0.53 |
| 1:C:549:PHE:CE2 | 1:C:620:ALA:HA | 2.43 | 0.53 |
| 1:D:36:TRP:CD2 | 1:D:42:ALA:HA | 2.43 | 0.53 |
| 1:C:333:ARG:O | 1:C:333:ARG:HD3 | 2.08 | 0.53 |
| 1:C:367:MET:HA | 1:C:367:MET:HE3 | 1.91 | 0.53 |
| 1:C:46:ARG:HG2 | 6:C:9473:HOH:O | 2.07 | 0.53 |
| 1:D:863:GLN:HG2 | 1:D:1021:CYS:CB | 2.39 | 0.53 |
| 1:D:802:ASP:O | 1:D:804:ASN:N | 2.42 | 0.53 |
| 1:D:843:GLN:HG2 | 1:D:848:THR:CA | 2.36 | 0.53 |
| 1:A:577:LYS:O | 1:A:584:PRO:HA | 2.09 | 0.53 |
| 1:C:809:ARG:NH2 | 1:C:1001:PRO:CG | 2.72 | 0.53 |
| 1:A:77:ASP:O | 1:A:79:PRO:HD3 | 2.10 | 0.52 |
| 1:B:272:ALA:HB1 | 1:B:273:PRO:HD2 | 1.90 | 0.52 |
| 1:C:292:ARG:HH12 | 5:C:8412:DMS:H22 | 1.74 | 0.52 |
| 1:D:237:ARG:HB3 | 1:D:237:ARG:NH1 | 2.17 | 0.52 |
| 1:C:796:SER:HB2 | 1:C:802:ASP:HB3 | 1.92 | 0.52 |
| 1:D:986:ILE:HG22 | 1:D:986:ILE:O | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:797:GLU:HB3 | 1:B:800:ARG:H | 1.73 | 0.52 |
| 1:C:755:ARG:HG2 | 1:C:769:TRP:HE3 | 1.70 | 0.52 |
| 1:B:699:ARG:NH2 | 5:B:8415:DMS:C1 | 2.72 | 0.52 |
| 1:C:572:ASP:HB3 | 1:C:603:MET:HG2 | 1.91 | 0.52 |
| 1:A:279:ILE:HD11 | 1:D:422:PRO:CG | 2.39 | 0.52 |
| 1:A:527:PRO:HB3 | 1:B:339:ASN:O | 2.09 | 0.52 |
| 1:C:687:GLN:H | 1:C:687:GLN:HE21 | 1.56 | 0.52 |
| 1:B:890:GLN:HB3 | 6:B:9524:HOH:O | 2.09 | 0.52 |
| 1:C:430:PRO:HD3 | 5:C:8420:DMS:H22 | 1.92 | 0.52 |
| 1:D:801:ILE:HG22 | 1:D:802:ASP:N | 2.25 | 0.52 |
| 1:A:1022:GLN:CG | 1:A:1023:LYS:H | 2.22 | 0.52 |
| 1:A:446:ARG:HG2 | 1:A:447:ASP:OD1 | 2.09 | 0.52 |
| 1:B:744:GLU:HB2 | 1:B:745:MET:HE3 | 1.91 | 0.52 |
| 1:C:78:LEU:HB3 | 1:C:80:GLU:HG3 | 1.92 | 0.52 |
| 1:A:268:ALA:HA | 5:A:8602:DMS:H22 | 1.92 | 0.52 |
| 1:C:861:SER:OG | 1:C:863:GLN:HG3 | 2.10 | 0.52 |
| 1:C:750:GLU:OE2 | 1:C:755:ARG:HB2 | 2.10 | 0.52 |
| 1:B:863:GLN:CG | 1:B:1021:CYS:HB3 | 2.38 | 0.51 |
| 1:C:600:GLN:HB2 | 1:C:603:MET:HE2 | 1.92 | 0.51 |
| 1:D:285:TYR:HB3 | 1:D:288:ARG:HG3 | 1.92 | 0.51 |
| 1:D:167:LEU:HB3 | 1:D:168:PRO:HD2 | 1.92 | 0.51 |
| 1:A:433:LEU:N | 1:A:434:PRO:CD | 2.73 | 0.51 |
| 1:B:646:HIS:CE1 | 1:B:673:ALA:HA | 2.45 | 0.51 |
| 1:C:824:GLN:HG2 | 1:C:825:CYS:H | 1.74 | 0.51 |
| 1:D:800:ARG:O | 1:D:801:ILE:O | 2.29 | 0.51 |
| 1:C:746:ASP:CA | 1:C:760:ARG:HG3 | 2.24 | 0.51 |
| 1:D:433:LEU:HB3 | 1:D:434:PRO:HD3 | 1.93 | 0.51 |
| 1:D:972:HIS:HB3 | 1:D:974:HIS:ND1 | 2.25 | 0.51 |
| 1:B:847:LYS:HG2 | 1:B:849:LEU:HD23 | 1.93 | 0.51 |
| 1:C:749:ILE:CG1 | 1:C:834:VAL:HG11 | 2.40 | 0.51 |
| 1:A:949:HIS:HB2 | 1:A:951:TRP:CH2 | 2.46 | 0.51 |
| 1:B:105:TYR:CE1 | 1:B:419:GLY:HA3 | 2.46 | 0.51 |
| 1:B:873:ALA:O | 1:B:876:THR:HG22 | 2.11 | 0.51 |
| 1:D:372:MET:HE1 | 1:D:395:HIS:HB3 | 1.93 | 0.51 |
| 1:D:640:SER:O | 1:D:675:GLN:HA | 2.10 | 0.51 |
| 1:A:250:LEU:HD11 | 1:A:286:ALA:O | 2.11 | 0.51 |
| 1:C:615:PRO:O | 1:C:618:THR:HG22 | 2.11 | 0.51 |
| 1:A:433:LEU:N | 1:A:434:PRO:HD2 | 2.26 | 0.51 |
| 1:D:65:ALA:HB1 | 1:D:66:PRO:HD2 | 1.93 | 0.51 |
| 1:A:735:HIS:O | 1:A:736:ALA:HB2 | 2.09 | 0.51 |
| 1:C:796:SER:CB | 1:C:802:ASP:H | 2.24 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:595:THR:HA | 1:B:596:PRO:C | 2.32 | 0.50 |
| 1:C:114:VAL:HB | 1:C:115:PRO:HD2 | 1.92 | 0.50 |
| 1:C:655:MET:HE3 | 1:C:662:PRO:HB3 | 1.93 | 0.50 |
| 1:B:730:LEU:HD12 | 1:B:730:LEU:N | 2.21 | 0.50 |
| 1:B:739:HIS:ND1 | 1:B:750:GLU:OE1 | 2.36 | 0.50 |
| 1:C:784:PHE:CD1 | 1:C:850:PHE:CD1 | 2.99 | 0.50 |
| 1:C:906:TYR:HB3 | 1:C:907:PRO:CD | 2.42 | 0.50 |
| 1:A:352:ARG:HD3 | 1:A:624:GLN:HB3 | 1.93 | 0.50 |
| 1:A:844:HIS:CE1 | 1:A:845:GLN:HG3 | 2.47 | 0.50 |
| 1:B:230:ARG:NH1 | 1:B:241:GLU:OE1 | 2.44 | 0.50 |
| 1:B:531:ARG:HB3 | 1:B:532:PRO:CD | 2.41 | 0.50 |
| 1:B:753:ASN:OD1 | 1:B:753:ASN:N | 2.45 | 0.50 |
| 1:C:680:ILE:O | 1:C:680:ILE:HG22 | 2.07 | 0.50 |
| 1:D:355:ASN:OD1 | 1:D:388:ARG:HD3 | 2.10 | 0.50 |
| 1:D:891:VAL:CG2 | 1:D:981:GLY:HA2 | 2.42 | 0.50 |
| 1:A:237:ARG:HH11 | 1:A:237:ARG:CB | 2.23 | 0.50 |
| 1:C:673:ALA:HB1 | 1:C:674:PRO:HD2 | 1.93 | 0.50 |
| 1:C:833:ALA:HB1 | 1:C:858:ILE:O | 2.11 | 0.50 |
| 1:D:599:ARG:HG3 | 1:D:600:GLN:H | 1.76 | 0.50 |
| 1:A:768:MET:CE | 1:A:1020:TRP:CZ2 | 2.94 | 0.50 |
| 1:A:473:ARG:NH1 | 1:A:476:LYS:CB | 2.74 | 0.50 |
| 1:B:763:GLY:HA3 | 1:B:822:LEU:HD13 | 1.93 | 0.50 |
| 1:C:132:SER:HB2 | 5:C:8504:DMS:H11 | 1.94 | 0.50 |
| 1:C:653:HIS:CE1 | 1:C:667:GLU:HG2 | 2.46 | 0.50 |
| 1:C:847:LYS:NZ | 1:D:724:GLU:O | 2.45 | 0.50 |
| 1:D:688:PRO:C | 1:D:690:SER:H | 2.14 | 0.50 |
| 1:A:127:PHE:N | 1:A:127:PHE:CD2 | 2.79 | 0.50 |
| 1:A:167:LEU:HD21 | 1:A:393:PRO:HG2 | 1.94 | 0.50 |
| 1:C:355:ASN:OD1 | 1:C:388:ARG:HD3 | 2.12 | 0.50 |
| 1:D:78:LEU:HD23 | 6:D:9218:HOH:O | 2.11 | 0.50 |
| 1:D:801:ILE:CG2 | 1:D:802:ASP:N | 2.75 | 0.50 |
| 1:B:1017:GLN:HB2 | 6:B:9517:HOH:O | 2.12 | 0.50 |
| 1:B:499:ILE:HD11 | 1:B:529:GLU:CD | 2.32 | 0.50 |
| 1:C:266:GLN:NE2 | 5:C:8602:DMS:S | 2.85 | 0.50 |
| 1:D:513:PRO:O | 1:D:514:ALA:HB3 | 2.12 | 0.50 |
| 1:B:320:GLY:O | 5:B:8406:DMS:O | 2.29 | 0.49 |
| 1:C:37:ARG:HH11 | 1:C:37:ARG:HG3 | 1.77 | 0.49 |
| 1:B:684:GLU:HG2 | 1:B:685:LEU:N | 2.27 | 0.49 |
| 1:C:724:GLU:O | 1:D:847:LYS:NZ | 2.44 | 0.49 |
| 1:A:599:ARG:HH11 | 1:A:600:GLN:NE2 | 2.09 | 0.49 |
| 1:A:809:ARG:CG | 1:A:809:ARG:HH11 | 2.20 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:450:HIS:HE1 | 6:B:9574:HOH:O | 1.95 | 0.49 |
| 1:B:797:GLU:CG | 1:B:799:THR:HG23 | 2.25 | 0.49 |
| 5:C:8503:DMS:H13 | 6:C:9034:HOH:O | 2.11 | 0.49 |
| 1:D:219:THR:HG21 | 6:D:9649:HOH:O | 2.12 | 0.49 |
| 1:A:663:LEU:HD12 | 1:A:686:PRO:HG2 | 1.95 | 0.49 |
| 1:A:920:LEU:HB3 | 1:A:921:PRO:HD2 | 1.94 | 0.49 |
| 1:B:869:ASP:OD1 | 1:B:1015:HIS:ND1 | 2.45 | 0.49 |
| 1:B:142:ILE:HG22 | 6:B:8857:HOH:O | 2.12 | 0.49 |
| 1:C:608:PHE:CE1 | 1:C:614:HIS:CD2 | 3.00 | 0.49 |
| 1:C:824:GLN:O | 1:C:838:THR:HA | 2.13 | 0.49 |
| 6:B:9363:HOH:O | 5:C:8420:DMS:H21 | 2.12 | 0.49 |
| 1:D:441:THR:O | 1:D:445:GLN:HG3 | 2.12 | 0.49 |
| 1:D:829:THR:HG22 | 1:D:830:LEU:N | 2.28 | 0.49 |
| 1:D:945:ASN:OD1 | 1:D:950:GLN:HG3 | 2.12 | 0.49 |
| 1:A:624:GLN:NE2 | 6:A:8624:HOH:O | 2.45 | 0.49 |
| 1:D:251:ARG:HD2 | 5:D:8416:DMS:C1 | 2.42 | 0.49 |
| 1:B:699:ARG:NH2 | 5:B:8415:DMS:H11 | 2.28 | 0.49 |
| 1:C:595:THR:HA | 1:C:596:PRO:C | 2.32 | 0.49 |
| 1:D:654:TRP:CZ3 | 1:D:665:SER:HA | 2.48 | 0.49 |
| 1:A:518:TRP:O | 1:A:519:SER:C | 2.51 | 0.49 |
| 1:B:729:THR:HG23 | 6:B:9217:HOH:O | 2.12 | 0.49 |
| 1:B:843:GLN:HA | 1:B:847:LYS:O | 2.13 | 0.49 |
| 1:C:696:LEU:O | 1:C:719:GLN:HA | 2.12 | 0.49 |
| 1:D:847:LYS:HG2 | 1:D:849:LEU:HD23 | 1.95 | 0.49 |
| 1:B:601:PHE:HB3 | 6:B:9551:HOH:O | 2.13 | 0.48 |
| 1:B:694:LEU:HD12 | 1:B:723:ALA:HB3 | 1.94 | 0.48 |
| 1:C:796:SER:OG | 1:C:801:ILE:HA | 2.13 | 0.48 |
| 1:D:502:MET:HA | 1:D:537:GLU:O | 2.13 | 0.48 |
| 1:A:702:GLN:O | 1:A:712:GLY:N | 2.43 | 0.48 |
| 1:A:619:GLU:HA | 1:A:912:ALA:HB2 | 1.95 | 0.48 |
| 1:C:237:ARG:CB | 1:C:237:ARG:NH1 | 2.76 | 0.48 |
| 1:C:285:TYR:HB3 | 1:C:288:ARG:HG3 | 1.95 | 0.48 |
| 1:D:863:GLN:HG2 | 1:D:1021:CYS:HB3 | 1.95 | 0.48 |
| 1:A:237:ARG:HH11 | 1:A:237:ARG:CG | 2.26 | 0.48 |
| 1:A:240:LEU:HD23 | 1:A:240:LEU:C | 2.32 | 0.48 |
| 1:B:843:GLN:HG2 | 1:B:848:THR:HA | 1.95 | 0.48 |
| 1:C:781:ARG:HG2 | 1:C:781:ARG:HH11 | 1.77 | 0.48 |
| 1:C:844:HIS:HD2 | 6:C:9418:HOH:O | 1.95 | 0.48 |
| 1:D:143:PHE:O | 1:D:168:PRO:HA | 2.13 | 0.48 |
| 1:D:305:ILE:HD11 | 1:D:645:ARG:HB3 | 1.95 | 0.48 |
| 1:C:546:LEU:HA | 6:C:8749:HOH:O | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:893:GLU:HG3 | 1:D:894:ARG:CD | 2.44 | 0.48 |
| 1:A:587:ALA:HB1 | 1:A:591:ASP:CB | 2.42 | 0.48 |
| 1:A:764:PHE:CE1 | 1:A:781:ARG:NH1 | 2.81 | 0.48 |
| 1:B:262:GLN:NE2 | 1:B:263:GLY:N | 2.61 | 0.48 |
| 1:C:651:LEU:HD11 | 1:C:653:HIS:CE1 | 2.49 | 0.48 |
| 1:D:598:ASP:O | 1:D:601:PHE:HB2 | 2.14 | 0.48 |
| 1:B:102:ASN:OD1 | 1:B:201:ASP:HB2 | 2.12 | 0.48 |
| 1:C:703:PRO:O | 1:C:711:ALA:HB1 | 2.13 | 0.48 |
| 1:C:740:LEU:HA | 1:C:748:CYS:O | 2.14 | 0.48 |
| 1:C:242:ALA:O | 1:C:290:THR:HA | 2.14 | 0.48 |
| 1:D:159:VAL:HG22 | 1:D:176:PHE:CE2 | 2.48 | 0.48 |
| 1:A:434:PRO:HB3 | 1:D:434:PRO:HB3 | 1.95 | 0.48 |
| 1:D:736:ALA:C | 1:D:737:ILE:HG22 | 2.34 | 0.48 |
| 1:B:91:GLN:HG3 | 1:B:96:ASP:OD1 | 2.13 | 0.48 |
| 1:C:746:ASP:HA | 1:C:760:ARG:CG | 2.23 | 0.48 |
| 1:D:201:ASP:OD2 | 2:D:2001:2DG:O4 | 2.25 | 0.48 |
| 1:D:808:GLU:OE1 | 1:D:811:LYS:HE3 | 2.13 | 0.48 |
| 1:B:355:ASN:OD1 | 1:B:388:ARG:HD3 | 2.14 | 0.48 |
| 1:B:568:TRP:CH2 | 2:B:2001:2DG:H3 | 2.49 | 0.48 |
| 1:B:701:VAL:HG22 | 1:B:714:ILE:HG12 | 1.96 | 0.48 |
| 1:A:279:ILE:HD13 | 1:A:279:ILE:HG23 | 1.62 | 0.47 |
| 1:A:974:HIS:HB3 | 6:A:9019:HOH:O | 2.14 | 0.47 |
| 1:B:14:ARG:HA | 1:B:16:TRP:CZ3 | 2.48 | 0.47 |
| 1:B:36:TRP:CD1 | 1:B:48:SER:HB2 | 2.48 | 0.47 |
| 1:D:1020:TRP:HD1 | 1:D:1021:CYS:N | 2.11 | 0.47 |
| 1:D:145:GLY:N | 1:D:210:ARG:HB2 | 2.28 | 0.47 |
| 1:D:773:LYS:HG3 | 1:D:775:GLN:NE2 | 2.28 | 0.47 |
| 1:D:354:VAL:O | 1:D:387:VAL:HA | 2.14 | 0.47 |
| 1:A:249:GLU:HG2 | 1:A:251:ARG:NE | 2.29 | 0.47 |
| 1:B:537:GLU:HA | 1:B:566:PHE:O | 2.14 | 0.47 |
| 1:D:718:GLN:HG2 | 5:D:8503:DMS:C1 | 2.44 | 0.47 |
| 1:A:646:HIS:NE2 | 1:A:671:ASP:OD1 | 2.40 | 0.47 |
| 1:C:542:MET:HA | 1:C:604:ASN:HA | 1.95 | 0.47 |
| 1:A:360:HIS:CE1 | 1:A:362:LEU:HB2 | 2.49 | 0.47 |
| 1:B:646:HIS:CE1 | 1:B:673:ALA:CB | 2.97 | 0.47 |
| 1:C:178:ARG:O | 1:C:178:ARG:HG2 | 2.14 | 0.47 |
| 1:C:200:GLN:HG2 | 1:C:391:HIS:HB2 | 1.96 | 0.47 |
| 1:C:651:LEU:CD1 | 1:C:653:HIS:CE1 | 2.97 | 0.47 |
| 1:A:655:MET:HE2 | 1:A:656:VAL:O | 2.14 | 0.47 |
| 1:B:863:GLN:HG2 | 1:B:1019:VAL:CG1 | 2.45 | 0.47 |
| 1:B:126:THR:HA | 1:B:182:ASN:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:859:ASP:OD1 | 1:C:861:SER:OG | 2.27 | 0.47 |
| 1:D:654:TRP:CZ2 | 1:D:683:PRO:HG2 | 2.50 | 0.47 |
| 1:A:411:ASP:OD2 | 1:A:447:ASP:OD2 | 2.31 | 0.47 |
| 1:B:377:LEU:O | 1:B:381:GLN:HG3 | 2.15 | 0.47 |
| 1:B:807:VAL:CG1 | 1:B:808:GLU:N | 2.76 | 0.47 |
| 1:C:780:LEU:HA | 1:C:886:CYS:HB3 | 1.97 | 0.47 |
| 1:C:670:LEU:HD23 | 1:C:670:LEU:HA | 1.68 | 0.47 |
| 1:D:230:ARG:HH12 | 1:D:239:VAL:CG1 | 2.25 | 0.47 |
| 1:D:545:SER:O | 1:D:909:ARG:HD3 | 2.15 | 0.47 |
| 1:D:292:ARG:NH1 | 5:D:8412:DMS:C2 | 2.76 | 0.47 |
| 1:D:893:GLU:HG3 | 1:D:894:ARG:HD2 | 1.96 | 0.47 |
| 1:B:655:MET:SD | 1:B:656:VAL:O | 2.72 | 0.47 |
| 1:C:91:GLN:HG2 | 1:C:98:PRO:HA | 1.96 | 0.47 |
| 1:A:871:GLU:OE1 | 1:B:726:LEU:HD22 | 2.15 | 0.47 |
| 1:A:1013:ARG:HD3 | 1:A:1013:ARG:HH11 | 1.58 | 0.47 |
| 1:A:628:GLN:HG3 | 6:A:9028:HOH:O | 2.15 | 0.47 |
| 1:A:959:ILE:O | 1:A:959:ILE:HG23 | 2.14 | 0.47 |
| 1:B:628:GLN:HE22 | 5:B:8402:DMS:C2 | 2.28 | 0.47 |
| 1:C:525:SER:HB3 | 1:D:525:SER:HB3 | 1.97 | 0.47 |
| 1:B:807:VAL:HG13 | 1:B:808:GLU:N | 2.31 | 0.46 |
| 1:D:785:THR:HB | 1:D:816:TYR:CE2 | 2.50 | 0.46 |
| 1:A:260:LEU:O | 1:A:267:VAL:HG22 | 2.15 | 0.46 |
| 1:C:749:ILE:O | 1:C:755:ARG:HA | 2.15 | 0.46 |
| 5:C:8506:DMS:H11 | 6:C:9396:HOH:O | 2.16 | 0.46 |
| 1:D:473:ARG:HH11 | 1:D:476:LYS:HB2 | 1.79 | 0.46 |
| 1:A:125:LEU:O | 1:A:183:ARG:HA | 2.15 | 0.46 |
| 1:B:578:TYR:HA | 1:B:583:ASN:O | 2.15 | 0.46 |
| 1:B:661:LYS:O | 1:B:663:LEU:HD23 | 2.15 | 0.46 |
| 1:C:651:LEU:HD22 | 1:C:667:GLU:HG2 | 1.97 | 0.46 |
| 1:D:363:HIS:HD2 | 6:D:9298:HOH:O | 1.97 | 0.46 |
| 1:A:80:GLU:O | 1:A:80:GLU:HG2 | 2.15 | 0.46 |
| 1:B:105:TYR:CD1 | 1:B:419:GLY:HA3 | 2.51 | 0.46 |
| 1:D:112:PRO:HD2 | 1:D:113:PHE:CD1 | 2.51 | 0.46 |
| 1:D:291:LEU:HD22 | 1:D:291:LEU:N | 2.30 | 0.46 |
| 1:D:499:ILE:HG22 | 1:D:501:PRO:HD3 | 1.98 | 0.46 |
| 1:D:654:TRP:CZ2 | 1:D:683:PRO:CG | 2.98 | 0.46 |
| 1:A:117:GLU:HG3 | 6:A:9004:HOH:O | 2.16 | 0.46 |
| 1:A:599:ARG:CG | 1:A:600:GLN:NE2 | 2.79 | 0.46 |
| 1:A:806:TRP:CE2 | 1:A:991:MET:HE3 | 2.50 | 0.46 |
| 1:A:863:GLN:HG2 | 1:A:1021:CYS:CB | 2.39 | 0.46 |
| 1:B:411:ASP:OD2 | 1:B:447:ASP:OD2 | 2.34 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:519:SER:HB3 | 1:B:522:LYS:HB3 | 1.96 | 0.46 |
| 1:B:282:ARG:HB2 | 1:C:423:MET:N | 2.31 | 0.46 |
| 1:C:749:ILE:N | 1:C:749:ILE:CD1 | 2.75 | 0.46 |
| 1:C:765:LEU:HD21 | 1:C:768:MET:HE2 | 1.97 | 0.46 |
| 1:A:65:ALA:CB | 1:A:66:PRO:HD2 | 2.39 | 0.46 |
| 1:C:1020:TRP:CD1 | 1:C:1021:CYS:N | 2.82 | 0.46 |
| 1:C:292:ARG:HG3 | 1:C:292:ARG:HH11 | 1.80 | 0.46 |
| 1:B:433:LEU:N | 1:B:434:PRO:CD | 2.79 | 0.46 |
| 1:B:744:GLU:HB3 | 1:B:745:MET:HE2 | 1.98 | 0.46 |
| 1:B:746:ASP:OD1 | 1:B:757:GLN:NE2 | 2.49 | 0.46 |
| 1:D:65:ALA:HB1 | 1:D:67:GLU:OE1 | 2.15 | 0.46 |
| 1:D:972:HIS:HB3 | 1:D:974:HIS:HD1 | 1.79 | 0.46 |
| 1:A:106:PRO:O | 5:A:8410:DMS:H22 | 2.16 | 0.46 |
| 1:B:173:LEU:O | 1:B:174:SER:C | 2.52 | 0.46 |
| 1:B:673:ALA:HB1 | 1:B:674:PRO:HD2 | 1.98 | 0.46 |
| 1:D:618:THR:HG21 | 6:D:9054:HOH:O | 2.15 | 0.46 |
| 1:B:183:ARG:NH1 | 6:B:8921:HOH:O | 2.39 | 0.46 |
| 1:B:88:SER:HA | 1:B:366:VAL:HG21 | 1.98 | 0.46 |
| 1:C:629:PHE:HA | 1:C:637:GLU:O | 2.16 | 0.46 |
| 1:C:858:ILE:HD13 | 1:C:864:MET:HB2 | 1.97 | 0.46 |
| 1:C:96:ASP:HB2 | 6:C:8977:HOH:O | 2.15 | 0.46 |
| 1:A:158:TRP:CZ2 | 1:A:160:GLY:HA2 | 2.50 | 0.45 |
| 1:A:59:ARG:HG2 | 5:A:8502:DMS:C1 | 2.47 | 0.45 |
| 1:C:178:ARG:HB3 | 1:C:178:ARG:HE | 1.28 | 0.45 |
| 1:D:344:LEU:O | 1:D:345:ASN:C | 2.52 | 0.45 |
| 5:A:8502:DMS:H12 | 6:A:9319:HOH:O | 2.15 | 0.45 |
| 1:B:658:LEU:O | 1:B:661:LYS:HG3 | 2.16 | 0.45 |
| 1:B:661:LYS:HA | 1:B:662:PRO:HD3 | 1.48 | 0.45 |
| 1:B:744:GLU:CB | 1:B:745:MET:CE | 2.95 | 0.45 |
| 1:C:372:MET:HE1 | 1:C:395:HIS:HB3 | 1.99 | 0.45 |
| 1:C:475:ILE:HD13 | 1:C:475:ILE:HG21 | 1.52 | 0.45 |
| 1:D:664:ALA:O | 1:D:665:SER:HB3 | 2.15 | 0.45 |
| 1:A:783:GLN:HG2 | 1:A:881:ARG:HD2 | 1.98 | 0.45 |
| 1:B:91:GLN:HG2 | 1:B:98:PRO:HA | 1.98 | 0.45 |
| 1:C:230:ARG:O | 1:C:238:ALA:HA | 2.17 | 0.45 |
| 1:C:651:LEU:CD2 | 1:C:653:HIS:CE1 | 2.99 | 0.45 |
| 1:A:593:GLY:O | 1:A:595:THR:HG22 | 2.15 | 0.45 |
| 1:A:88:SER:HA | 1:A:366:VAL:HG21 | 1.98 | 0.45 |
| 1:B:925:MET:HB3 | 6:B:8644:HOH:O | 2.16 | 0.45 |
| 1:C:581:ASN:HB2 | 1:C:583:ASN:ND2 | 2.32 | 0.45 |
| 1:D:73:TRP:CE2 | 1:D:122:CYS:HB3 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:804:ASN:HD22 | 1:D:809:ARG:NE | 2.12 | 0.45 |
| 1:A:802:ASP:O | 1:A:808:GLU:HG3 | 2.17 | 0.45 |
| 1:D:749:ILE:N | 1:D:749:ILE:CD1 | 2.72 | 0.45 |
| 1:A:685:LEU:CB | 1:A:686:PRO:CD | 2.95 | 0.45 |
| 1:A:921:PRO:O | 1:A:922:LEU:C | 2.55 | 0.45 |
| 1:B:474:TRP:O | 1:B:478:VAL:HG13 | 2.16 | 0.45 |
| 1:B:756:TRP:CD2 | 1:B:858:ILE:HD13 | 2.51 | 0.45 |
| 1:B:734:SER:CB | 1:B:860:GLY:HA3 | 2.47 | 0.45 |
| 1:D:367:MET:HB3 | 1:D:372:MET:HE2 | 1.97 | 0.45 |
| 1:D:942:ARG:HA | 1:D:953:GLY:O | 2.17 | 0.45 |
| 1:B:46:ARG:HD2 | 1:B:46:ARG:HH11 | 1.44 | 0.45 |
| 1:B:549:PHE:CE2 | 1:B:620:ALA:HA | 2.52 | 0.45 |
| 1:B:663:LEU:O | 1:B:664:ALA:HB2 | 2.16 | 0.45 |
| 1:C:838:THR:OG1 | 1:C:854:LYS:HB2 | 2.17 | 0.45 |
| 1:D:237:ARG:CG | 1:D:237:ARG:NH1 | 2.77 | 0.45 |
| 1:D:473:ARG:HD2 | 1:D:473:ARG:HA | 1.80 | 0.45 |
| 1:D:654:TRP:CE3 | 1:D:655:MET:HA | 2.51 | 0.45 |
| 1:D:667:GLU:C | 1:D:668:VAL:HG23 | 2.36 | 0.45 |
| 1:B:73:TRP:CZ2 | 1:B:122:CYS:HB3 | 2.52 | 0.45 |
| 1:B:822:LEU:HD11 | 1:B:824:GLN:O | 2.17 | 0.45 |
| 1:B:937:LEU:HA | 1:B:957:PHE:O | 2.16 | 0.45 |
| 1:C:737:ILE:HA | 1:C:738:PRO:HD3 | 1.90 | 0.45 |
| 1:A:768:MET:HE1 | 1:A:1020:TRP:CH2 | 2.52 | 0.45 |
| 1:B:102:ASN:ND2 | 5:B:8506:DMS:C1 | 2.77 | 0.45 |
| 1:B:734:SER:HB2 | 1:B:860:GLY:HA3 | 1.99 | 0.45 |
| 1:B:872:VAL:O | 1:B:873:ALA:C | 2.55 | 0.45 |
| 1:C:809:ARG:HH21 | 1:C:1001:PRO:HG3 | 1.81 | 0.45 |
| 1:A:701:VAL:O | 1:A:703:PRO:HD3 | 2.17 | 0.45 |
| 1:A:990:HIS:HD2 | 1:A:991:MET:O | 2.00 | 0.45 |
| 1:B:646:HIS:CE1 | 1:B:673:ALA:CA | 3.00 | 0.45 |
| 1:D:370:GLN:HB2 | 6:D:9235:HOH:O | 2.16 | 0.45 |
| 1:D:639:THR:OG1 | 1:D:677:LYS:HG3 | 2.16 | 0.45 |
| 1:D:708:TRP:CE3 | 1:D:709:SER:HB3 | 2.52 | 0.45 |
| 1:B:945:ASN:HB3 | 1:B:1023:LYS:CE | 2.46 | 0.44 |
| 1:C:249:GLU:CD | 1:C:251:ARG:HD3 | 2.38 | 0.44 |
| 1:C:777:LEU:HA | 1:C:777:LEU:HD23 | 1.69 | 0.44 |
| 1:C:756:TRP:CE2 | 1:C:858:ILE:HD12 | 2.52 | 0.44 |
| 1:A:262:GLN:HG3 | 6:A:9568:HOH:O | 2.17 | 0.44 |
| 1:A:429:ASP:HA | 1:A:430:PRO:HD2 | 1.86 | 0.44 |
| 1:A:472:TYR:O | 1:A:476:LYS:HG2 | 2.18 | 0.44 |
| 1:C:557:ARG:HD2 | 6:C:8638:HOH:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:147:ASN:HA | 1:D:148:SER:HA | 1.60 | 0.44 |
| 1:B:262:GLN:C | 1:B:262:GLN:HE21 | 2.21 | 0.44 |
| 1:B:814:GLY:HA3 | 1:B:844:HIS:CG | 2.52 | 0.44 |
| 1:D:650:GLU:HB3 | 1:D:670:LEU:HD12 | 1.99 | 0.44 |
| 1:A:126:THR:HA | 1:A:182:ASN:O | 2.18 | 0.44 |
| 1:A:577:LYS:HD3 | 1:A:587:ALA:HB2 | 1.98 | 0.44 |
| 1:B:347:LYS:HB2 | 1:B:643:LEU:HD13 | 1.99 | 0.44 |
| 1:B:674:PRO:O | 1:B:675:GLN:HB2 | 2.18 | 0.44 |
| 1:B:817:GLN:HA | 1:B:817:GLN:NE2 | 2.32 | 0.44 |
| 1:B:670:LEU:HD23 | 1:B:670:LEU:HA | 1.68 | 0.44 |
| 1:B:687:GLN:HA | 1:B:688:PRO:HD3 | 1.69 | 0.44 |
| 1:D:878:HIS:CE1 | 1:D:1010:SER:HB3 | 2.52 | 0.44 |
| 1:A:90:TRP:CZ3 | 1:A:121:GLY:HA3 | 2.53 | 0.44 |
| 1:A:339:ASN:O | 1:B:527:PRO:HB3 | 2.17 | 0.44 |
| 1:A:59:ARG:HG2 | 5:A:8502:DMS:H11 | 1.99 | 0.44 |
| 1:A:549:PHE:CE2 | 1:A:620:ALA:HA | 2.52 | 0.44 |
| 1:A:668:VAL:HA | 1:A:669:PRO:HD3 | 1.81 | 0.44 |
| 1:B:876:THR:OG1 | 1:B:877:PRO:HD2 | 2.18 | 0.44 |
| 1:C:682:LEU:HB3 | 1:C:683:PRO:HD2 | 1.99 | 0.44 |
| 1:C:152:LEU:HD11 | 1:C:184:LEU:HD22 | 2.00 | 0.44 |
| 1:C:326:GLU:O | 1:C:327:ALA:HB2 | 2.17 | 0.44 |
| 1:C:781:ARG:HG2 | 1:C:781:ARG:NH1 | 2.33 | 0.44 |
| 1:B:416:GLU:HA | 1:B:460:ASN:O | 2.17 | 0.44 |
| 1:C:100:TYR:OH | 1:C:201:ASP:OD1 | 2.26 | 0.44 |
| 1:C:240:LEU:HD23 | 1:C:240:LEU:C | 2.37 | 0.44 |
| 1:D:411:ASP:OD2 | 1:D:447:ASP:OD2 | 2.36 | 0.44 |
| 1:D:588:TYR:O | 1:D:591:ASP:HB2 | 2.17 | 0.44 |
| 1:D:599:ARG:HG3 | 1:D:600:GLN:N | 2.33 | 0.44 |
| 1:A:600:GLN:N | 1:A:600:GLN:HE21 | 1.99 | 0.44 |
| 1:D:190:ARG:HG3 | 1:D:206:SER:HB3 | 2.00 | 0.44 |
| 1:D:368:ASP:O | 1:D:372:MET:HG3 | 2.18 | 0.44 |
| 1:C:561:ARG:HD3 | 1:D:525:SER:O | 2.18 | 0.44 |
| 1:A:178:ARG:HD2 | 6:A:9436:HOH:O | 2.16 | 0.43 |
| 1:A:344:LEU:O | 1:A:345:ASN:C | 2.56 | 0.43 |
| 1:A:561:ARG:HD3 | 1:B:525:SER:O | 2.18 | 0.43 |
| 1:A:651:LEU:HD12 | 1:A:651:LEU:C | 2.39 | 0.43 |
| 1:A:696:LEU:O | 1:A:719:GLN:HA | 2.18 | 0.43 |
| 1:B:824:GLN:O | 1:B:838:THR:HA | 2.18 | 0.43 |
| 1:C:255:ARG:HB2 | 1:C:316:HIS:CE1 | 2.53 | 0.43 |
| 1:C:472:TYR:O | 1:C:476:LYS:HG2 | 2.18 | 0.43 |
| 1:D:138:GLN:O | 1:D:216:HIS:HA | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:630:ARG:NH1 | 6:D:9277:HOH:O | 2.50 | 0.43 |
| 1:B:255:ARG:HB2 | 1:B:316:HIS:CE1 | 2.53 | 0.43 |
| 1:B:847:LYS:HG3 | 1:B:848:THR:N | 2.33 | 0.43 |
| 1:C:638:VAL:O | 1:C:677:LYS:HA | 2.18 | 0.43 |
| 1:C:842:TRP:O | 1:C:849:LEU:N | 2.44 | 0.43 |
| 1:C:990:HIS:HD2 | 1:C:991:MET:O | 2.01 | 0.43 |
| 1:C:505:ARG:HG2 | 1:C:996:ASP:OD2 | 2.18 | 0.43 |
| 1:B:262:GLN:HE21 | 1:B:263:GLY:N | 2.14 | 0.43 |
| 1:B:613:PRO:HG2 | 6:B:9240:HOH:O | 2.17 | 0.43 |
| 1:B:693:GLN:HG2 | 1:B:695:TRP:NE1 | 2.34 | 0.43 |
| 1:C:111:PRO:HA | 1:C:112:PRO:HA | 1.67 | 0.43 |
| 1:A:742:THR:HG22 | 1:A:743:SER:N | 2.32 | 0.43 |
| 1:B:110:ASN:N | 1:B:111:PRO:CD | 2.82 | 0.43 |
| 1:C:262:GLN:HB2 | 1:C:309:TYR:CE2 | 2.53 | 0.43 |
| 1:D:701:VAL:O | 1:D:703:PRO:HD3 | 2.19 | 0.43 |
| 1:A:608:PHE:CD1 | 1:A:614:HIS:HD2 | 2.36 | 0.43 |
| 1:C:378:LEU:HD23 | 1:C:378:LEU:HA | 1.85 | 0.43 |
| 1:C:799:THR:O | 1:C:800:ARG:HG2 | 2.18 | 0.43 |
| 1:D:23:GLN:HB2 | 1:D:26:ARG:HB2 | 2.00 | 0.43 |
| 1:D:46:ARG:HB3 | 1:D:47:PRO:CD | 2.48 | 0.43 |
| 1:A:142:ILE:HG23 | 1:A:170:GLU:HG2 | 2.00 | 0.43 |
| 1:A:774:LYS:NZ | 6:A:9275:HOH:O | 2.51 | 0.43 |
| 1:B:369:GLU:HB2 | 1:B:397:LEU:CD2 | 2.49 | 0.43 |
| 1:B:427:THR:HG22 | 1:B:436:MET:SD | 2.59 | 0.43 |
| 1:B:599:ARG:HH11 | 1:B:599:ARG:HG3 | 1.84 | 0.43 |
| 1:C:375:ASP:O | 1:C:379:MET:HG3 | 2.18 | 0.43 |
| 1:D:901:GLY:HA3 | 1:D:902:PRO:HA | 1.77 | 0.43 |
| 1:A:105:TYR:CE2 | 1:A:199:ASP:HB2 | 2.54 | 0.43 |
| 1:B:74:LEU:HD22 | 1:B:153:TRP:CG | 2.54 | 0.43 |
| 1:C:344:LEU:CB | 1:C:349:LEU:HD21 | 2.49 | 0.43 |
| 1:C:610:ASP:O | 1:C:611:ARG:HB2 | 2.18 | 0.43 |
| 1:C:608:PHE:CZ | 1:C:614:HIS:CD2 | 3.06 | 0.43 |
| 1:C:663:LEU:HD22 | 1:C:663:LEU:HA | 1.82 | 0.43 |
| 1:C:743:SER:O | 1:C:744:GLU:C | 2.56 | 0.43 |
| 1:D:833:ALA:HB1 | 1:D:858:ILE:O | 2.18 | 0.43 |
| 1:D:986:ILE:HD13 | 1:D:986:ILE:HG21 | 1.51 | 0.43 |
| 1:A:1017:GLN:HE21 | 1:A:1017:GLN:HB2 | 1.74 | 0.43 |
| 1:A:583:ASN:HB3 | 1:A:584:PRO:HD2 | 2.00 | 0.43 |
| 1:B:1011:ALA:HB3 | 1:B:1014:TYR:CZ | 2.54 | 0.43 |
| 1:B:626:PHE:O | 1:B:641:GLU:N | 2.36 | 0.43 |
| 1:D:433:LEU:N | 1:D:434:PRO:CD | 2.81 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:842:TRP:HZ3 | 1:D:852:SER:HB3 | 1.84 | 0.43 |
| 1:A:749:ILE:H | 1:A:749:ILE:HD12 | 1.83 | 0.43 |
| 1:B:651:LEU:CD2 | 1:B:701:VAL:HB | 2.49 | 0.43 |
| 1:B:377:LEU:HD22 | 1:B:708:TRP:HA | 2.01 | 0.43 |
| 1:B:899:GLY:HA2 | 1:B:915:PHE:CE1 | 2.54 | 0.43 |
| 1:A:499:ILE:HG22 | 1:A:501:PRO:HD3 | 2.01 | 0.43 |
| 1:B:143:PHE:O | 1:B:168:PRO:HA | 2.19 | 0.43 |
| 1:B:360:HIS:CE1 | 1:B:362:LEU:H | 2.36 | 0.43 |
| 1:B:37:ARG:NH1 | 5:B:8504:DMS:C2 | 2.82 | 0.43 |
| 1:B:901:GLY:HA3 | 1:B:902:PRO:HA | 1.80 | 0.43 |
| 1:C:431:ARG:NH2 | 6:C:9033:HOH:O | 2.29 | 0.43 |
| 1:C:526:LEU:HA | 1:C:526:LEU:HD23 | 1.78 | 0.43 |
| 1:A:835:LEU:HD11 | 1:A:855:THR:HB | 2.02 | 0.42 |
| 1:B:654:TRP:O | 1:B:665:SER:HB2 | 2.19 | 0.42 |
| 1:D:629:PHE:HA | 1:D:637:GLU:O | 2.19 | 0.42 |
| 1:A:655:MET:HE2 | 1:A:656:VAL:H | 1.84 | 0.42 |
| 1:C:533:LEU:C | 1:C:533:LEU:HD23 | 2.39 | 0.42 |
| 1:B:869:ASP:HA | 1:B:1014:TYR:O | 2.18 | 0.42 |
| 1:B:797:GLU:O | 1:B:800:ARG:N | 2.51 | 0.42 |
| 1:C:655:MET:CE | 1:C:662:PRO:HB3 | 2.49 | 0.42 |
| 1:C:73:TRP:CE2 | 1:C:122:CYS:HB3 | 2.55 | 0.42 |
| 1:D:1022:GLN:O | 1:D:1023:LYS:HB2 | 2.20 | 0.42 |
| 1:A:100:TYR:HB3 | 1:A:589:GLY:HA2 | 2.01 | 0.42 |
| 1:A:75:GLU:HA | 1:A:75:GLU:OE1 | 2.18 | 0.42 |
| 1:B:36:TRP:CD2 | 1:B:42:ALA:HA | 2.54 | 0.42 |
| 1:C:237:ARG:NH2 | 1:C:296:GLU:OE2 | 2.52 | 0.42 |
| 1:C:653:HIS:ND1 | 1:C:667:GLU:HG2 | 2.34 | 0.42 |
| 1:C:795:VAL:HG12 | 5:C:8506:DMS:H22 | 2.01 | 0.42 |
| 1:C:908:ASP:HB3 | 1:C:1007:PHE:CG | 2.55 | 0.42 |
| 1:C:930:VAL:HA | 1:C:973:ARG:HD3 | 2.01 | 0.42 |
| 1:D:36:TRP:NE1 | 1:D:46:ARG:O | 2.43 | 0.42 |
| 1:D:673:ALA:O | 1:D:676:GLY:N | 2.40 | 0.42 |
| 1:D:59:ARG:NH2 | 1:D:81:ALA:HB3 | 2.34 | 0.42 |
| 1:A:360:HIS:HE1 | 1:A:362:LEU:HB2 | 1.84 | 0.42 |
| 1:B:71:GLU:H | 1:B:71:GLU:CD | 2.22 | 0.42 |
| 1:C:127:PHE:CD2 | 1:C:127:PHE:N | 2.87 | 0.42 |
| 1:C:335:VAL:HG22 | 1:C:344:LEU:HD12 | 2.01 | 0.42 |
| 1:C:649:ASN:O | 1:C:702:GLN:HG2 | 2.20 | 0.42 |
| 1:D:962:TYR:CE1 | 5:D:8508:DMS:H21 | 2.55 | 0.42 |
| 1:D:959:ILE:O | 1:D:960:SER:HB3 | 2.19 | 0.42 |
| 1:D:984:LEU:HD11 | 1:D:986:ILE:HG13 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:127:PHE:CE2 | 1:B:184:LEU:HG | 2.54 | 0.42 |
| 1:B:975:LEU:HD23 | 1:B:975:LEU:HA | 1.82 | 0.42 |
| 5:C:8601:DMS:H22 | 6:C:9543:HOH:O | 2.19 | 0.42 |
| 1:D:208:ILE:HD13 | 1:D:208:ILE:HG21 | 1.75 | 0.42 |
| 1:A:599:ARG:HG3 | 1:A:600:GLN:N | 2.32 | 0.42 |
| 1:C:720:TRP:HA | 5:C:8427:DMS:C1 | 2.50 | 0.42 |
| 1:C:930:VAL:O | 1:C:932:PRO:HD3 | 2.20 | 0.42 |
| 1:D:830:LEU:N | 1:D:833:ALA:O | 2.45 | 0.42 |
| 1:A:521:LYS:HE2 | 6:A:9023:HOH:O | 2.19 | 0.42 |
| 1:B:473:ARG:O | 1:B:474:TRP:C | 2.56 | 0.42 |
| 1:C:237:ARG:HH11 | 1:C:237:ARG:CB | 2.31 | 0.42 |
| 1:C:416:GLU:HA | 1:C:460:ASN:O | 2.19 | 0.42 |
| 1:D:141:ILE:HD13 | 1:D:143:PHE:CE1 | 2.54 | 0.42 |
| 1:D:360:HIS:ND1 | 1:D:361:PRO:HD2 | 2.35 | 0.42 |
| 1:A:655:MET:HG3 | 1:A:656:VAL:N | 2.25 | 0.42 |
| 1:A:726:LEU:HD12 | 1:B:848:THR:HG22 | 2.01 | 0.42 |
| 1:B:13:ARG:O | 1:B:14:ARG:C | 2.58 | 0.42 |
| 1:B:658:LEU:HD11 | 1:B:692:GLY:HA3 | 2.02 | 0.42 |
| 1:B:777:LEU:HG | 1:B:889:ALA:HA | 2.01 | 0.42 |
| 1:C:91:GLN:HG3 | 1:C:96:ASP:OD1 | 2.19 | 0.42 |
| 1:D:613:PRO:HB3 | 1:D:617:LEU:HD23 | 2.02 | 0.42 |
| 1:D:898:LEU:HD12 | 1:D:898:LEU:HA | 1.81 | 0.42 |
| 1:A:660:GLY:O | 1:A:662:PRO:HD3 | 2.20 | 0.42 |
| 1:B:86:VAL:HG13 | 1:B:87:PRO:HA | 2.02 | 0.42 |
| 1:C:376:ILE:HG13 | 1:C:398:TRP:CH2 | 2.55 | 0.42 |
| 1:D:277:GLU:H | 1:D:277:GLU:CD | 2.19 | 0.42 |
| 1:D:588:TYR:N | 1:D:591:ASP:OD2 | 2.37 | 0.42 |
| 1:D:788:PRO:HD2 | 1:D:968:MET:HG3 | 2.02 | 0.42 |
| 1:A:646:HIS:ND1 | 1:A:673:ALA:HA | 2.34 | 0.41 |
| 5:A:8420:DMS:C2 | 6:D:9470:HOH:O | 2.64 | 0.41 |
| 1:B:757:GLN:HG2 | 1:B:758:PHE:N | 2.27 | 0.41 |
| 1:C:415:ILE:HG21 | 1:C:415:ILE:HD13 | 1.87 | 0.41 |
| 1:C:608:PHE:CE1 | 1:C:614:HIS:HD2 | 2.37 | 0.41 |
| 1:D:251:ARG:HD2 | 5:D:8416:DMS:H11 | 2.02 | 0.41 |
| 1:B:292:ARG:NH1 | 5:B:8412:DMS:H22 | 2.35 | 0.41 |
| 1:B:472:TYR:O | 1:B:476:LYS:HG2 | 2.19 | 0.41 |
| 1:C:787:ALA:HA | 1:C:788:PRO:HD3 | 1.95 | 0.41 |
| 1:C:147:ASN:HA | 1:C:148:SER:HA | 1.59 | 0.41 |
| 1:C:13:ARG:O | 1:C:14:ARG:C | 2.58 | 0.41 |
| 1:C:661:LYS:HE3 | 1:C:661:LYS:HB2 | 1.39 | 0.41 |
| 1:C:995:GLY:O | 1:C:996:ASP:C | 2.57 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:997:ASP:HB2 | 1:C:999:TRP:CZ2 | 2.55 | 0.41 |
| 1:A:475:ILE:HD13 | 1:A:475:ILE:HG21 | 1.80 | 0.41 |
| 1:B:569:ASP:O | 1:B:605:GLY:HA2 | 2.20 | 0.41 |
| 1:C:347:LYS:HB3 | 1:C:348:PRO:HD2 | 2.01 | 0.41 |
| 1:A:542:MET:HA | 1:A:604:ASN:HA | 2.02 | 0.41 |
| 1:C:654:TRP:NE1 | 1:C:666:GLY:HA3 | 2.34 | 0.41 |
| 1:C:851:ILE:O | 1:C:870:VAL:HA | 2.20 | 0.41 |
| 1:A:279:ILE:CD1 | 1:D:422:PRO:CG | 2.98 | 0.41 |
| 1:A:390:SER:HA | 1:A:391:HIS:HA | 1.88 | 0.41 |
| 1:A:615:PRO:O | 1:A:618:THR:HG22 | 2.20 | 0.41 |
| 1:A:845:GLN:HB3 | 1:A:845:GLN:HE21 | 1.62 | 0.41 |
| 1:B:147:ASN:HA | 1:B:148:SER:HA | 1.61 | 0.41 |
| 1:D:106:PRO:C | 5:D:8419:DMS:H22 | 2.41 | 0.41 |
| 1:D:646:HIS:CD2 | 1:D:647:SER:N | 2.88 | 0.41 |
| 1:D:801:ILE:HG22 | 1:D:802:ASP:H | 1.85 | 0.41 |
| 1:A:30:HIS:NE2 | 1:A:170:GLU:OE1 | 2.53 | 0.41 |
| 1:A:854:LYS:HA | 1:A:867:THR:O | 2.21 | 0.41 |
| 1:B:542:MET:HA | 1:B:604:ASN:HA | 2.02 | 0.41 |
| 1:C:658:LEU:O | 1:C:659:ASP:C | 2.57 | 0.41 |
| 1:C:769:TRP:HA | 1:C:773:LYS:O | 2.21 | 0.41 |
| 1:D:461:GLU:OE1 | 2:D:2001:2DG:H21 | 2.21 | 0.41 |
| 1:D:74:LEU:HD22 | 1:D:153:TRP:CG | 2.55 | 0.41 |
| 1:A:316:HIS:HB2 | 5:A:8406:DMS:H23 | 2.02 | 0.41 |
| 1:A:781:ARG:NH1 | 6:A:9309:HOH:O | 2.53 | 0.41 |
| 1:B:19:PRO:HD3 | 1:B:112:PRO:HB3 | 2.02 | 0.41 |
| 1:C:143:PHE:HB3 | 1:C:146:VAL:HG23 | 2.00 | 0.41 |
| 1:D:414:ASN:ND2 | 1:D:439:ARG:NH1 | 2.69 | 0.41 |
| 1:A:577:LYS:HE3 | 1:A:577:LYS:HB3 | 1.91 | 0.41 |
| 1:B:231:PHE:N | 1:B:231:PHE:CD1 | 2.89 | 0.41 |
| 1:B:412:GLU:CG | 1:B:459:GLY:HA2 | 2.50 | 0.41 |
| 1:B:744:GLU:CB | 1:B:745:MET:HE3 | 2.51 | 0.41 |
| 1:C:344:LEU:HB3 | 1:C:349:LEU:HD21 | 2.03 | 0.41 |
| 1:C:29:ALA:HB3 | 1:C:445:GLN:OE1 | 2.21 | 0.41 |
| 1:A:147:ASN:HA | 1:A:148:SER:HA | 1.54 | 0.41 |
| 1:A:50:GLN:N | 1:A:50:GLN:CD | 2.73 | 0.41 |
| 1:A:571:VAL:CG2 | 1:A:609:ALA:HA | 2.51 | 0.41 |
| 1:A:655:MET:HE2 | 1:A:656:VAL:N | 2.35 | 0.41 |
| 1:A:694:LEU:HA | 1:A:694:LEU:HD23 | 1.89 | 0.41 |
| 1:C:498:ILE:HD13 | 1:C:498:ILE:HG21 | 1.89 | 0.41 |
| 1:C:718:GLN:CG | 5:C:8503:DMS:C1 | 2.97 | 0.41 |
| 1:D:337:ILE:HA | 1:D:341:LEU:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:232:ASN:C | 5:B:8417:DMS:H22 | 2.40 | 0.41 |
| 1:B:78:LEU:HA | 1:B:79:PRO:HD3 | 1.75 | 0.41 |
| 1:D:251:ARG:HD2 | 5:D:8416:DMS:H12 | 2.03 | 0.41 |
| 1:D:654:TRP:CE3 | 1:D:665:SER:HA | 2.56 | 0.41 |
| 1:D:890:GLN:HG3 | 1:D:891:VAL:N | 2.36 | 0.41 |
| 1:D:949:HIS:HB3 | 1:D:951:TRP:CH2 | 2.56 | 0.41 |
| 1:A:370:GLN:HB2 | 6:A:9098:HOH:O | 2.21 | 0.40 |
| 1:A:502:MET:HB2 | 1:A:537:GLU:HB2 | 2.02 | 0.40 |
| 1:B:367:MET:HE1 | 1:B:372:MET:HG3 | 2.00 | 0.40 |
| 1:B:510:GLN:O | 1:B:512:PHE:N | 2.49 | 0.40 |
| 1:B:689:GLU:O | 1:B:690:SER:CB | 2.69 | 0.40 |
| 1:A:908:ASP:HB3 | 1:A:1007:PHE:CD1 | 2.56 | 0.40 |
| 1:A:352:ARG:HG3 | 1:A:352:ARG:HH11 | 1.86 | 0.40 |
| 1:B:766:SER:HA | 1:B:779:PRO:HB3 | 2.04 | 0.40 |
| 1:C:221:GLN:O | 1:C:246:MET:HA | 2.22 | 0.40 |
| 1:C:496:THR:O | 1:C:496:THR:HG23 | 2.21 | 0.40 |
| 1:C:765:LEU:CD2 | 1:C:768:MET:HE3 | 2.49 | 0.40 |
| 1:D:130:ASP:OD2 | 5:D:8703:DMS:H22 | 2.21 | 0.40 |
| 5:D:8413:DMS:H21 | 6:D:9300:HOH:O | 2.20 | 0.40 |
| 1:A:663:LEU:CD1 | 1:A:686:PRO:HG2 | 2.51 | 0.40 |
| 1:A:826:THR:OG1 | 1:A:837:THR:HB | 2.21 | 0.40 |
| 1:B:744:GLU:HB3 | 1:B:745:MET:CE | 2.51 | 0.40 |
| 1:D:740:LEU:HD12 | 1:D:741:THR:N | 2.36 | 0.40 |
| 1:A:240:LEU:HD13 | 1:A:260:LEU:HD13 | 2.04 | 0.40 |
| 1:A:388:ARG:HD3 | 1:A:388:ARG:HH11 | 1.63 | 0.40 |
| 1:A:579:ASP:OD1 | 1:A:581:ASN:HB2 | 2.22 | 0.40 |
| 1:B:746:ASP:HA | 1:B:760:ARG:HG3 | 2.04 | 0.40 |
| 1:C:573:GLN:HB2 | 1:C:602:CYS:O | 2.22 | 0.40 |
| 1:C:933:SER:O | 1:C:934:GLU:C | 2.58 | 0.40 |
| 1:D:576:ILE:HA | 1:D:576:ILE:HD13 | 1.82 | 0.40 |
| 1:A:18:ASN:N | 1:A:193:ASP:OD2 | 2.53 | 0.40 |
| 1:A:546:LEU:HA | 6:A:8730:HOH:O | 2.20 | 0.40 |
| 1:A:576:ILE:HA | 1:A:576:ILE:HD13 | 1.84 | 0.40 |
| 1:A:684:GLU:HG2 | 1:A:685:LEU:N | 2.34 | 0.40 |
| 1:A:756:TRP:CD1 | 1:A:768:MET:HG2 | 2.57 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:A:773:LYS:NZ | 6:C:9410:HOH:O[3_544] | 2.18 | 0.02 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 1009/1023 (99%) | 964 (96%) | 44 (4%) | 1 (0%) | 55 | 57 |
| 1 | B | 1009/1023 (99%) | 956 (95%) | 48 (5%) | 5 (0%) | 32 | 28 |
| 1 | C | 1009/1023 (99%) | 963 (95%) | 46 (5%) | 0 | 100 | 100 |
| 1 | D | 1009/1023 (99%) | 962 (95%) | 43 (4%) | 4 (0%) | 38 | 35 |
| All | All | 4036/4092 (99%) | 3845 (95%) | 181 (4%) | 10 (0%) | 51 | 52 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 690 | SER |
| 1 | B | 731 | PRO |
| 1 | D | 688 | PRO |
| 1 | D | 801 | ILE |
| 1 | B | 688 | PRO |
| 1 | D | 803 | PRO |
| 1 | B | 732 | ALA |
| 1 | D | 164 | ASP |
| 1 | B | 164 | ASP |
| 1 | A | 164 | ASP |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | A | 864/875 (99%) | 816 (94%) | 48 (6%) | 25 | 21 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | B | 864/875 (99%) | 815 (94%) | 49 (6%) | 24 | 21 |
| 1 | C | 864/875 (99%) | 817 (95%) | 47 (5%) | 26 | 23 |
| 1 | D | 864/875 (99%) | 812 (94%) | 52 (6%) | 22 | 19 |
| All | All | 3456/3500 (99%) | 3260 (94%) | 196 (6%) | 24 | 21 |

All (196) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 71 | GLU |
| 1 | A | 116 | THR |
| 1 | A | 230 | ARG |
| 1 | A | 237 | ARG |
| 1 | A | 250 | LEU |
| 1 | A | 277 | GLU |
| 1 | A | 279 | ILE |
| 1 | A | 333 | ARG |
| 1 | A | 336 | ARG |
| 1 | A | 344 | LEU |
| 1 | A | 362 | LEU |
| 1 | A | 377 | LEU |
| 1 | A | 394 | ASN |
| 1 | A | 446 | ARG |
| 1 | A | 451 | PRO |
| 1 | A | 477 | SER |
| 1 | A | 478 | VAL |
| 1 | A | 519 | SER |
| 1 | A | 546 | LEU |
| 1 | A | 580 | GLU |
| 1 | A | 595 | THR |
| 1 | A | 600 | GLN |
| 1 | A | 634 | GLN |
| 1 | A | 651 | LEU |
| 1 | A | 655 | MET |
| 1 | A | 672 | VAL |
| 1 | A | 682 | LEU |
| 1 | A | 684 | GLU |
| 1 | A | 685 | LEU |
| 1 | A | 699 | ARG |
| 1 | A | 735 | HIS |
| 1 | A | 737 | ILE |
| 1 | A | 773 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 796 | SER |
| 1 | A | 799 | THR |
| 1 | A | 800 | ARG |
| 1 | A | 801 | ILE |
| 1 | A | 809 | ARG |
| 1 | A | 817 | GLN |
| 1 | A | 829 | THR |
| 1 | A | 885 | ASN |
| 1 | A | 890 | GLN |
| 1 | A | 956 | GLN |
| 1 | A | 986 | ILE |
| 1 | A | 1013 | ARG |
| 1 | A | 1017 | GLN |
| 1 | A | 1018 | LEU |
| 1 | A | 1023 | LYS |
| 1 | B | 49 | GLN |
| 1 | B | 71 | GLU |
| 1 | B | 80 | GLU |
| 1 | B | 165 | SER |
| 1 | B | 230 | ARG |
| 1 | B | 237 | ARG |
| 1 | B | 262 | GLN |
| 1 | B | 264 | GLU |
| 1 | B | 333 | ARG |
| 1 | B | 344 | LEU |
| 1 | B | 362 | LEU |
| 1 | B | 392 | TYR |
| 1 | B | 394 | ASN |
| 1 | B | 439 | ARG |
| 1 | B | 477 | SER |
| 1 | B | 478 | VAL |
| 1 | B | 503 | TYR |
| 1 | B | 515 | VAL |
| 1 | B | 554 | GLN |
| 1 | B | 594 | ASP |
| 1 | B | 595 | THR |
| 1 | B | 600 | GLN |
| 1 | B | 634 | GLN |
| 1 | B | 651 | LEU |
| 1 | B | 661 | LYS |
| 1 | B | 663 | LEU |
| 1 | B | 667 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 681 | GLU |
| 1 | B | 685 | LEU |
| 1 | B | 687 | GLN |
| 1 | B | 730 | LEU |
| 1 | B | 737 | ILE |
| 1 | B | 744 | GLU |
| 1 | B | 745 | MET |
| 1 | B | 754 | LYS |
| 1 | B | 755 | ARG |
| 1 | B | 797 | GLU |
| 1 | B | 799 | THR |
| 1 | B | 809 | ARG |
| 1 | B | 819 | GLU |
| 1 | B | 824 | GLN |
| 1 | B | 829 | THR |
| 1 | B | 845 | GLN |
| 1 | B | 847 | LYS |
| 1 | B | 863 | GLN |
| 1 | B | 885 | ASN |
| 1 | B | 890 | GLN |
| 1 | B | 956 | GLN |
| 1 | B | 1023 | LYS |
| 1 | C | 71 | GLU |
| 1 | C | 72 | SER |
| 1 | C | 75 | GLU |
| 1 | C | 117 | GLU |
| 1 | C | 135 | GLN |
| 1 | C | 178 | ARG |
| 1 | C | 213 | SER |
| 1 | C | 214 | LEU |
| 1 | C | 230 | ARG |
| 1 | C | 237 | ARG |
| 1 | C | 262 | GLN |
| 1 | C | 278 | ILE |
| 1 | C | 333 | ARG |
| 1 | C | 344 | LEU |
| 1 | C | 394 | ASN |
| 1 | C | 477 | SER |
| 1 | C | 580 | GLU |
| 1 | C | 595 | THR |
| 1 | C | 634 | GLN |
| 1 | C | 635 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 646 | HIS |
| 1 | C | 651 | LEU |
| 1 | C | 653 | HIS |
| 1 | C | 661 | LYS |
| 1 | C | 663 | LEU |
| 1 | C | 681 | GLU |
| 1 | C | 687 | GLN |
| 1 | C | 699 | ARG |
| 1 | C | 729 | THR |
| 1 | C | 730 | LEU |
| 1 | C | 734 | SER |
| 1 | C | 735 | HIS |
| 1 | C | 737 | ILE |
| 1 | C | 746 | ASP |
| 1 | C | 749 | ILE |
| 1 | C | 750 | GLU |
| 1 | C | 755 | ARG |
| 1 | C | 778 | THR |
| 1 | C | 799 | THR |
| 1 | C | 819 | GLU |
| 1 | C | 830 | LEU |
| 1 | C | 832 | ASP |
| 1 | C | 890 | GLN |
| 1 | C | 934 | GLU |
| 1 | C | 956 | GLN |
| 1 | C | 986 | ILE |
| 1 | C | 1023 | LYS |
| 1 | D | 13 | ARG |
| 1 | D | 80 | GLU |
| 1 | D | 112 | PRO |
| 1 | D | 116 | THR |
| 1 | D | 213 | SER |
| 1 | D | 237 | ARG |
| 1 | D | 277 | GLU |
| 1 | D | 319 | ASP |
| 1 | D | 333 | ARG |
| 1 | D | 344 | LEU |
| 1 | D | 370 | GLN |
| 1 | D | 394 | ASN |
| 1 | D | 425 | ARG |
| 1 | D | 519 | SER |
| 1 | D | 545 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 546 | LEU |
| 1 | D | 595 | THR |
| 1 | D | 631 | LEU |
| 1 | D | 632 | SER |
| 1 | D | 635 | THR |
| 1 | D | 651 | LEU |
| 1 | D | 655 | MET |
| 1 | D | 661 | LYS |
| 1 | D | 663 | LEU |
| 1 | D | 677 | LYS |
| 1 | D | 681 | GLU |
| 1 | D | 682 | LEU |
| 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 | 769 | TRP |
| 1 | D | 772 | ASP |
| 1 | D | 773 | LYS |
| 1 | D | 774 | LYS |
| 1 | D | 799 | THR |
| 1 | D | 817 | GLN |
| 1 | D | 829 | THR |
| 1 | D | 885 | ASN |
| 1 | D | 893 | GLU |
| 1 | D | 956 | GLN |
| 1 | D | 980 | GLU |
| 1 | D | 986 | ILE |
| 1 | D | 1004 | SER |
| 1 | D | 1013 | ARG |
| 1 | D | 1022 | GLN |
| 1 | D | 1023 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 558 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 600 | GLN |
| 1 | A | 624 | GLN |
| 1 | A | 653 | HIS |
| 1 | A | 675 | GLN |
| 1 | A | 757 | GLN |
| 1 | A | 761 | GLN |
| 1 | A | 817 | GLN |
| 1 | A | 824 | GLN |
| 1 | A | 844 | HIS |
| 1 | A | 845 | GLN |
| 1 | A | 878 | HIS |
| 1 | A | 977 | HIS |
| 1 | A | 1017 | GLN |
| 1 | B | 102 | ASN |
| 1 | B | 262 | GLN |
| 1 | B | 266 | GLN |
| 1 | B | 363 | HIS |
| 1 | B | 485 | GLN |
| 1 | B | 600 | GLN |
| 1 | B | 624 | GLN |
| 1 | B | 628 | GLN |
| 1 | B | 646 | HIS |
| 1 | B | 757 | GLN |
| 1 | B | 817 | GLN |
| 1 | B | 824 | GLN |
| 1 | B | 878 | HIS |
| 1 | C | 102 | ASN |
| 1 | C | 163 | GLN |
| 1 | C | 262 | GLN |
| 1 | C | 266 | GLN |
| 1 | C | 583 | ASN |
| 1 | C | 634 | GLN |
| 1 | C | 653 | HIS |
| 1 | C | 687 | GLN |
| 1 | C | 843 | GLN |
| 1 | C | 844 | HIS |
| 1 | C | 878 | HIS |
| 1 | D | 135 | GLN |
| 1 | D | 163 | GLN |
| 1 | D | 363 | HIS |
| 1 | D | 583 | ASN |
| 1 | D | 624 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 628 | GLN |
| 1 | D | 653 | HIS |
| 1 | D | 804 | ASN |
| 1 | D | 878 | HIS |
| 1 | D | 977 | HIS |
| 1 | D | 1017 | GLN |
| 1 | D | 1022 | GLN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 132 ligands modelled in this entry, 25 are monoatomic - leaving 107 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 | $\# Z > 2$ |
| 2 | 2DG | A | 2001 | 1,4 | 10,10,11 | 1.02 | 1 (10%) | 10,13,15 | 1.82 | 2 (20%) |
| 5 | DMS | A | 8401 | - | 3,3,3 | 1.93 | 1 (33%) | 3,3,3 | 0.12 | 0 |
| 5 | DMS | A | 8402 | - | 3,3,3 | 1.55 | 1 (33%) | 3,3,3 | 0.14 | 0 |
| 5 | DMS | A | 8403 | - | 3,3,3 | 0.96 | 0 | 3,3,3 | 0.73 | 0 |
| 5 | DMS | A | 8404 | - | 3,3,3 | 1.80 | 1 (33%) | 3,3,3 | 0.30 | 0 |
| 5 | DMS | A | 8405 | - | 3,3,3 | 1.49 | 1 (33%) | 3,3,3 | 0.23 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 5 | DMS | A | 8406 | - | 3,3,3 | 1.85 | 1 (33%) | 3,3,3 | 0.45 | 0 |
| 5 | DMS | A | 8407 | - | 3,3,3 | 1.73 | 2 (66%) | 3,3,3 | 0.53 | 0 |
| 5 | DMS | A | 8408 | - | 3,3,3 | 1.04 | 0 | 3,3,3 | 0.23 | 0 |
| 5 | DMS | A | 8409 | - | 3,3,3 | 2.32 | 2 (66%) | 3,3,3 | 0.35 | 0 |
| 5 | DMS | A | 8410 | - | 3,3,3 | 0.71 | 0 | 3,3,3 | 0.09 | 0 |
| 5 | DMS | A | 8411 | - | 3,3,3 | 1.54 | 1 (33%) | 3,3,3 | 0.15 | 0 |
| 5 | DMS | A | 8412 | - | 3,3,3 | 0.75 | 0 | 3,3,3 | 0.20 | 0 |
| 5 | DMS | A | 8413 | - | 3,3,3 | 2.01 | 2 (66%) | 3,3,3 | 0.16 | 0 |
| 5 | DMS | A | 8414 | - | 3,3,3 | 0.75 | 0 | 3,3,3 | 0.44 | 0 |
| 5 | DMS | A | 8415 | - | 3,3,3 | 1.91 | 1 (33%) | 3,3,3 | 0.15 | 0 |
| 5 | DMS | A | 8417 | - | 3,3,3 | 1.11 | 0 | 3,3,3 | 0.50 | 0 |
| 5 | DMS | A | 8419 | - | 3,3,3 | 0.65 | 0 | 3,3,3 | 0.39 | 0 |
| 5 | DMS | A | 8420 | - | 3,3,3 | 1.55 | 1 (33%) | 3,3,3 | 1.01 | 0 |
| 5 | DMS | A | 8421 | - | 3,3,3 | 0.88 | 0 | 3,3,3 | 0.97 | 0 |
| 5 | DMS | A | 8425 | 4 | 3,3,3 | 1.40 | 1 (33%) | 3,3,3 | 0.55 | 0 |
| 5 | DMS | A | 8501 | - | 3,3,3 | 1.43 | 1 (33%) | 3,3,3 | 0.31 | 0 |
| 5 | DMS | A | 8502 | - | 3,3,3 | 1.15 | 0 | 3,3,3 | 1.35 | 1 (33%) |
| 5 | DMS | A | 8503 | - | 3,3,3 | 0.65 | 0 | 3,3,3 | 0.17 | 0 |
| 5 | DMS | A | 8504 | - | 3,3,3 | 0.34 | 0 | 3,3,3 | 0.42 | 0 |
| 5 | DMS | A | 8602 | - | 3,3,3 | 0.86 | 0 | 3,3,3 | 0.82 | 0 |
| 2 | 2DG | B | 2001 | 1,4 | 10,10,11 | 1.41 | 1 (10%) | 10,13,15 | 1.37 | 1 (10%) |
| 5 | DMS | B | 8401 | - | 3,3,3 | 0.65 | 0 | 3,3,3 | 0.42 | 0 |
| 5 | DMS | B | 8402 | - | 3,3,3 | 1.87 | 2 (66%) | 3,3,3 | 0.18 | 0 |
| 5 | DMS | B | 8403 | - | 3,3,3 | 1.44 | 0 | 3,3,3 | 1.24 | 1 (33%) |
| 5 | DMS | B | 8404 | - | 3,3,3 | 0.80 | 0 | 3,3,3 | 0.35 | 0 |
| 5 | DMS | B | 8405 | - | 3,3,3 | 0.88 | 0 | 3,3,3 | 0.38 | 0 |
| 5 | DMS | B | 8406 | - | 3,3,3 | 1.24 | 1 (33%) | 3,3,3 | 0.25 | 0 |
| 5 | DMS | B | 8407 | - | 3,3,3 | 1.50 | 0 | 3,3,3 | 0.25 | 0 |
| 5 | DMS | B | 8408 | - | 3,3,3 | 1.40 | 0 | 3,3,3 | 0.40 | 0 |
| 5 | DMS | B | 8409 | - | 3,3,3 | 0.71 | 0 | 3,3,3 | 1.27 | 1 (33%) |
| 5 | DMS | B | 8410 | - | 3,3,3 | 1.29 | 0 | 3,3,3 | 0.48 | 0 |
| 5 | DMS | B | 8411 | - | 3,3,3 | 0.36 | 0 | 3,3,3 | 0.75 | 0 |
| 5 | DMS | B | 8412 | - | 3,3,3 | 1.89 | 1 (33%) | 3,3,3 | 0.17 | 0 |
| 5 | DMS | B | 8413 | - | 3,3,3 | 2.20 | 2 (66%) | 3,3,3 | 0.82 | 0 |
| 5 | DMS | B | 8414 | - | 3,3,3 | 0.55 | 0 | 3,3,3 | 0.75 | 0 |
| 5 | DMS | B | 8415 | - | 3,3,3 | 1.09 | 0 | 3,3,3 | 1.32 | 1 (33%) |
| 5 | DMS | B | 8416 | - | 3,3,3 | 1.29 | 0 | 3,3,3 | 0.06 | 0 |
| 5 | DMS | B | 8417 | - | 3,3,3 | 1.17 | 0 | 3,3,3 | 0.47 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 5 | DMS | B | 8420 | - | 3,3,3 | 1.28 | 1 (33%) | 3,3,3 | 0.39 | 0 |
| 5 | DMS | B | 8421 | - | 3,3,3 | 0.83 | 0 | 3,3,3 | 0.14 | 0 |
| 5 | DMS | B | 8423 | - | 3,3,3 | 0.57 | 0 | 3,3,3 | 0.15 | 0 |
| 5 | DMS | B | 8425 | 4 | 3,3,3 | 1.91 | 1 (33%) | 3,3,3 | 0.37 | 0 |
| 5 | DMS | B | 8427 | - | 3,3,3 | 0.87 | 0 | 3,3,3 | 0.61 | 0 |
| 5 | DMS | B | 8502 | - | 3,3,3 | 0.73 | 0 | 3,3,3 | 1.25 | 1 (33%) |
| 5 | DMS | B | 8504 | - | 3,3,3 | 0.11 | 0 | 3,3,3 | 0.08 | 0 |
| 5 | DMS | B | 8506 | - | 3,3,3 | 1.38 | 0 | 3,3,3 | 0.78 | 0 |
| 5 | DMS | B | 8508 | - | 3,3,3 | 2.47 | 3 (100%) | 3,3,3 | 0.38 | 0 |
| 5 | DMS | B | 8601 | - | 3,3,3 | 0.42 | 0 | 3,3,3 | 0.28 | 0 |
| 2 | 2DG | C | 2001 | 1,4 | 10,10,11 | 1.27 | 1 (10%) | 10,13,15 | 1.99 | 1 (10%) |
| 5 | DMS | C | 8401 | - | 3,3,3 | 0.87 | 0 | 3,3,3 | 0.75 | 0 |
| 5 | DMS | C | 8402 | - | 3,3,3 | 2.05 | 1 (33%) | 3,3,3 | 0.72 | 0 |
| 5 | DMS | C | 8403 | - | 3,3,3 | 0.83 | 0 | 3,3,3 | 0.42 | 0 |
| 5 | DMS | C | 8404 | - | 3,3,3 | 1.29 | 0 | 3,3,3 | 0.67 | 0 |
| 5 | DMS | C | 8405 | - | 3,3,3 | 1.82 | 1 (33%) | 3,3,3 | 0.25 | 0 |
| 5 | DMS | C | 8407 | - | 3,3,3 | 1.15 | 0 | 3,3,3 | 0.10 | 0 |
| 5 | DMS | C | 8408 | - | 3,3,3 | 0.67 | 0 | 3,3,3 | 0.25 | 0 |
| 5 | DMS | C | 8409 | - | 3,3,3 | 1.57 | 1 (33%) | 3,3,3 | 0.37 | 0 |
| 5 | DMS | C | 8410 | - | 3,3,3 | 1.09 | 0 | 3,3,3 | 0.36 | 0 |
| 5 | DMS | C | 8411 | - | 3,3,3 | 1.66 | 1 (33%) | 3,3,3 | 0.33 | 0 |
| 5 | DMS | C | 8412 | - | 3,3,3 | 0.86 | 0 | 3,3,3 | 0.55 | 0 |
| 5 | DMS | C | 8413 | - | 3,3,3 | 2.93 | 2 (66%) | 3,3,3 | 0.43 | 0 |
| 5 | DMS | C | 8414 | - | 3,3,3 | 1.56 | 1 (33%) | 3,3,3 | 0.35 | 0 |
| 5 | DMS | C | 8415 | - | 3,3,3 | 1.55 | 1 (33%) | 3,3,3 | 0.96 | 0 |
| 5 | DMS | C | 8416 | - | 3,3,3 | 1.10 | 0 | 3,3,3 | 0.71 | 0 |
| 5 | DMS | C | 8417 | - | 3,3,3 | 0.85 | 0 | 3,3,3 | 0.51 | 0 |
| 5 | DMS | C | 8419 | - | 3,3,3 | 1.38 | 0 | 3,3,3 | 0.18 | 0 |
| 5 | DMS | C | 8420 | - | 3,3,3 | 1.28 | 0 | 3,3,3 | 0.65 | 0 |
| 5 | DMS | C | 8421 | - | 3,3,3 | 0.60 | 0 | 3,3,3 | 0.23 | 0 |
| 5 | DMS | C | 8423 | - | 3,3,3 | 1.29 | 0 | 3,3,3 | 0.31 | 0 |
| 5 | DMS | C | 8425 | 4 | 3,3,3 | 1.47 | 1 (33%) | 3,3,3 | 1.63 | 1 (33%) |
| 5 | DMS | C | 8427 | - | 3,3,3 | 0.89 | 0 | 3,3,3 | 0.09 | 0 |
| 5 | DMS | C | 8501 | - | 3,3,3 | 1.50 | 0 | 3,3,3 | 1.18 | 1 (33%) |
| 5 | DMS | C | 8503 | - | 3,3,3 | 0.79 | 0 | 3,3,3 | 0.41 | 0 |
| 5 | DMS | C | 8504 | - | 3,3,3 | 1.09 | 0 | 3,3,3 | 0.22 | 0 |
| 5 | DMS | C | 8506 | - | 3,3,3 | 1.56 | 1 (33%) | 3,3,3 | 1.24 | 1 (33%) |
| 5 | DMS | C | 8601 | - | 3,3,3 | 1.08 | 0 | 3,3,3 | 0.61 | 0 |
| 5 | DMS | C | 8602 | - | 3,3,3 | 1.04 | 0 | 3,3,3 | 0.15 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | 2DG | D | 2001 | 1,4 | 10,10,11 | 1.38 | 2 (20%) | 10,13,15 | 2.50 | 3 (30%) |
| 5 | DMS | D | 8401 | - | 3,3,3 | 1.77 | 1 (33%) | 3,3,3 | 0.32 | 0 |
| 5 | DMS | D | 8402 | - | 3,3,3 | 1.14 | 0 | 3,3,3 | 0.63 | 0 |
| 5 | DMS | D | 8403 | - | 3,3,3 | 0.51 | 0 | 3,3,3 | 0.31 | 0 |
| 5 | DMS | D | 8404 | - | 3,3,3 | 1.56 | 1 (33%) | 3,3,3 | 0.51 | 0 |
| 5 | DMS | D | 8405 | - | 3,3,3 | 0.82 | 0 | 3,3,3 | 0.24 | 0 |
| 5 | DMS | D | 8406 | - | 3,3,3 | 1.01 | 0 | 3,3,3 | 0.37 | 0 |
| 5 | DMS | D | 8408 | - | 3,3,3 | 1.12 | 0 | 3,3,3 | 0.31 | 0 |
| 5 | DMS | D | 8409 | - | 3,3,3 | 2.21 | 1 (33%) | 3,3,3 | 0.58 | 0 |
| 5 | DMS | D | 8410 | - | 3,3,3 | 1.28 | 0 | 3,3,3 | 0.48 | 0 |
| 5 | DMS | D | 8411 | - | 3,3,3 | 0.92 | 0 | 3,3,3 | 0.49 | 0 |
| 5 | DMS | D | 8412 | - | 3,3,3 | 1.48 | 1 (33%) | 3,3,3 | 0.59 | 0 |
| 5 | DMS | D | 8413 | - | 3,3,3 | 0.89 | 0 | 3,3,3 | 0.65 | 0 |
| 5 | DMS | D | 8414 | - | 3,3,3 | 1.20 | 0 | 3,3,3 | 0.08 | 0 |
| 5 | DMS | D | 8416 | - | 3,3,3 | 0.75 | 0 | 3,3,3 | 0.23 | 0 |
| 5 | DMS | D | 8417 | - | 3,3,3 | 1.25 | 0 | 3,3,3 | 0.72 | 0 |
| 5 | DMS | D | 8419 | - | 3,3,3 | 0.87 | 0 | 3,3,3 | 0.36 | 0 |
| 5 | DMS | D | 8421 | - | 3,3,3 | 1.02 | 0 | 3,3,3 | 0.08 | 0 |
| 5 | DMS | D | 8501 | - | 3,3,3 | 0.83 | 0 | 3,3,3 | 0.89 | 0 |
| 5 | DMS | D | 8503 | - | 3,3,3 | 1.33 | 1 (33%) | 3,3,3 | 0.77 | 0 |
| 5 | DMS | D | 8508 | - | 3,3,3 | 0.56 | 0 | 3,3,3 | 0.59 | 0 |
| 5 | DMS | D | 8701 | - | 3,3,3 | 2.87 | 2 (66%) | 3,3,3 | 0.74 | 0 |
| 5 | DMS | D | 8703 | - | 3,3,3 | 0.83 | 0 | 3,3,3 | 0.32 | 0 |
| 5 | DMS | D | 8705 | - | 3,3,3 | 1.22 | 0 | 3,3,3 | 0.21 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 2 | 2DG | A | 2001 | 1,4 | - | 0/2/16/18 | 0/1/1/1 |
| 5 | DMS | A | 8401 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8402 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8403 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8404 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8405 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8406 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8407 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8408 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8409 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 5 | DMS | A | 8410 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8411 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8412 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8413 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8414 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8415 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8417 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8419 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8420 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8421 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8425 | 4 | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8502 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8503 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8504 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | A | 8602 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | 2DG | B | 2001 | 1,4 | - | 0/2/16/18 | 0/1/1/1 |
| 5 | DMS | B | 8401 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8402 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8403 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8404 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8405 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8406 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8407 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8408 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8409 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8410 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8411 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8412 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8413 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8414 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8415 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8416 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8417 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8420 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8421 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8423 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8425 | 4 | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8427 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8502 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8504 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8506 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 5 | DMS | B | 8508 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | B | 8601 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | 2DG | C | 2001 | 1,4 | - | 0/2/16/18 | 0/1/1/1 |
| 5 | DMS | C | 8401 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8402 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8403 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8404 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8405 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8407 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8408 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8409 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8410 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8411 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8412 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8413 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8414 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8415 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8416 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8417 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8419 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8420 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8421 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8423 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8425 | 4 | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8427 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8503 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8504 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8506 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8601 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | C | 8602 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | 2DG | D | 2001 | 1,4 | - | 0/2/16/18 | 0/1/1/1 |
| 5 | DMS | D | 8401 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8402 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8403 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8404 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8405 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8406 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8408 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8409 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8410 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8411 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 5 | DMS | D | 8412 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8413 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8414 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8416 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8417 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8419 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8421 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8503 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8508 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8701 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8703 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | DMS | D | 8705 | - | - | 0/0/0/0 | 0/0/0/0 |

All (49) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 5 | A | 8406 | DMS | C2-S | -3.20 | 1.51 | 1.75 |
| 5 | C | 8414 | DMS | C1-S | -2.54 | 1.56 | 1.75 |
| 5 | A | 8407 | DMS | O-S | 2.00 | 1.63 | 1.50 |
| 5 | C | 8411 | DMS | C1-S | 2.02 | 1.91 | 1.75 |
| 5 | D | 8412 | DMS | O-S | 2.03 | 1.64 | 1.50 |
| 5 | B | 8402 | DMS | O-S | 2.04 | 1.64 | 1.50 |
| 5 | D | 8503 | DMS | C1-S | 2.05 | 1.91 | 1.75 |
| 5 | A | 8407 | DMS | C2-S | 2.07 | 1.91 | 1.75 |
| 5 | A | 8425 | DMS | C2-S | 2.09 | 1.91 | 1.75 |
| 2 | D | 2001 | 2DG | C4-C5 | 2.10 | 1.57 | 1.53 |
| 5 | C | 8413 | DMS | C2-S | 2.11 | 1.91 | 1.75 |
| 5 | B | 8406 | DMS | C1-S | 2.12 | 1.91 | 1.75 |
| 5 | B | 8508 | DMS | C2-S | 2.12 | 1.91 | 1.75 |
| 5 | C | 8506 | DMS | C2-S | 2.13 | 1.91 | 1.75 |
| 5 | B | 8508 | DMS | O-S | 2.13 | 1.64 | 1.50 |
| 5 | B | 8420 | DMS | C2-S | 2.14 | 1.92 | 1.75 |
| 5 | A | 8501 | DMS | C2-S | 2.16 | 1.92 | 1.75 |
| 2 | A | 2001 | 2DG | C2-C3 | 2.17 | 1.55 | 1.52 |
| 5 | C | 8425 | DMS | C2-S | 2.24 | 1.92 | 1.75 |
| 5 | A | 8413 | DMS | O-S | 2.27 | 1.65 | 1.50 |
| 5 | A | 8405 | DMS | O-S | 2.30 | 1.65 | 1.50 |
| 5 | A | 8402 | DMS | C2-S | 2.32 | 1.93 | 1.75 |
| 5 | A | 8409 | DMS | C1-S | 2.33 | 1.93 | 1.75 |
| 5 | B | 8413 | DMS | O-S | 2.35 | 1.66 | 1.50 |
| 5 | D | 8404 | DMS | C2-S | 2.40 | 1.93 | 1.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 5 | D | 8401 | DMS | C2-S | 2.44 | 1.94 | 1.75 |
| 2 | C | 2001 | 2DG | C4-C5 | 2.48 | 1.58 | 1.53 |
| 5 | B | 8402 | DMS | C2-S | 2.50 | 1.94 | 1.75 |
| 5 | A | 8411 | DMS | C1-S | 2.52 | 1.94 | 1.75 |
| 5 | C | 8415 | DMS | C2-S | 2.57 | 1.95 | 1.75 |
| 5 | A | 8413 | DMS | C2-S | 2.59 | 1.95 | 1.75 |
| 5 | C | 8409 | DMS | O-S | 2.60 | 1.67 | 1.50 |
| 5 | C | 8405 | DMS | O-S | 2.62 | 1.68 | 1.50 |
| 5 | A | 8420 | DMS | C2-S | 2.64 | 1.95 | 1.75 |
| 5 | B | 8413 | DMS | C1-S | 2.71 | 1.96 | 1.75 |
| 5 | D | 8701 | DMS | C2-S | 2.76 | 1.96 | 1.75 |
| 5 | B | 8425 | DMS | O-S | 2.81 | 1.69 | 1.50 |
| 5 | A | 8404 | DMS | C2-S | 2.84 | 1.97 | 1.75 |
| 5 | B | 8412 | DMS | C2-S | 2.90 | 1.97 | 1.75 |
| 5 | A | 8415 | DMS | C2-S | 2.96 | 1.98 | 1.75 |
| 2 | B | 2001 | 2DG | C4-C5 | 2.99 | 1.59 | 1.53 |
| 5 | B | 8508 | DMS | C1-S | 3.04 | 1.98 | 1.75 |
| 5 | C | 8402 | DMS | C2-S | 3.08 | 1.99 | 1.75 |
| 5 | A | 8401 | DMS | O-S | 3.12 | 1.71 | 1.50 |
| 2 | D | 2001 | 2DG | C2-C3 | 3.23 | 1.57 | 1.52 |
| 5 | A | 8409 | DMS | O-S | 3.28 | 1.72 | 1.50 |
| 5 | D | 8409 | DMS | O-S | 3.72 | 1.75 | 1.50 |
| 5 | D | 8701 | DMS | O-S | 3.74 | 1.75 | 1.50 |
| 5 | C | 8413 | DMS | O-S | 4.48 | 1.80 | 1.50 |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2 | C | 2001 | 2DG | C3-C4-C5 | -5.69 | 104.22 | 109.91 |
| 2 | A | 2001 | 2DG | C3-C4-C5 | -4.66 | 105.25 | 109.91 |
| 2 | D | 2001 | 2DG | C3-C4-C5 | -4.14 | 105.77 | 109.91 |
| 2 | A | 2001 | 2DG | O4-C4-C3 | -2.41 | 105.64 | 110.02 |
| 2 | B | 2001 | 2DG | O3-C3-C2 | -2.06 | 104.93 | 110.02 |
| 5 | C | 8501 | DMS | C2-S-C1 | -2.02 | 88.00 | 98.44 |
| 5 | B | 8403 | DMS | C2-S-C1 | 2.07 | 109.16 | 98.44 |
| 5 | C | 8506 | DMS | C2-S-C1 | 2.14 | 109.54 | 98.44 |
| 5 | B | 8502 | DMS | C2-S-C1 | 2.16 | 109.65 | 98.44 |
| 5 | B | 8409 | DMS | C2-S-C1 | 2.18 | 109.74 | 98.44 |
| 5 | B | 8415 | DMS | C2-S-C1 | 2.26 | 110.17 | 98.44 |
| 5 | A | 8502 | DMS | C2-S-C1 | 2.34 | 110.59 | 98.44 |
| 5 | C | 8425 | DMS | C2-S-C1 | 2.82 | 113.06 | 98.44 |
| 2 | D | 2001 | 2DG | C1-O5-C5 | 4.17 | 119.43 | 112.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 2 | D | 2001 | 2DG | C2-C3-C4 | 4.27 | 116.04 | 111.23 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

31 monomers are involved in 50 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5 | A | 8406 | DMS | 1 | 0 |
| 5 | A | 8410 | DMS | 1 | 0 |
| 5 | A | 8414 | DMS | 1 | 0 |
| 5 | A | 8420 | DMS | 2 | 0 |
| 5 | A | 8502 | DMS | 3 | 0 |
| 5 | A | 8602 | DMS | 1 | 0 |
| 2 | B | 2001 | 2DG | 1 | 0 |
| 5 | B | 8402 | DMS | 1 | 0 |
| 5 | B | 8406 | DMS | 1 | 0 |
| 5 | B | 8412 | DMS | 1 | 0 |
| 5 | B | 8415 | DMS | 2 | 0 |
| 5 | B | 8417 | DMS | 1 | 0 |
| 5 | B | 8504 | DMS | 1 | 0 |
| 5 | B | 8506 | DMS | 2 | 0 |
| 5 | B | 8601 | DMS | 1 | 0 |
| 5 | C | 8412 | DMS | 2 | 0 |
| 5 | C | 8420 | DMS | 2 | 0 |
| 5 | C | 8427 | DMS | 1 | 0 |
| 5 | C | 8503 | DMS | 3 | 0 |
| 5 | C | 8504 | DMS | 1 | 0 |
| 5 | C | 8506 | DMS | 4 | 0 |
| 5 | C | 8601 | DMS | 1 | 0 |
| 5 | C | 8602 | DMS | 1 | 0 |
| 2 | D | 2001 | 2DG | 2 | 0 |
| 5 | D | 8412 | DMS | 4 | 0 |
| 5 | D | 8413 | DMS | 1 | 0 |
| 5 | D | 8416 | DMS | 3 | 0 |
| 5 | D | 8419 | DMS | 1 | 0 |
| 5 | D | 8503 | DMS | 2 | 0 |
| 5 | D | 8508 | DMS | 1 | 0 |
| 5 | D | 8703 | DMS | 1 | 0 |

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 | 1011/1023 (98%) | -0.76 | 16 (1%) 72 76 | 5, 15, 44, 98 | 0 |
| 1 | B | 1011/1023 (98%) | -0.73 | 11 (1%) 80 84 | 5, 15, 45, 100 | 0 |
| 1 | C | 1011/1023 (98%) | -0.70 | 17 (1%) 70 75 | 6, 15, 46, 100 | 0 |
| 1 | D | 1011/1023 (98%) | -0.70 | 20 (1%) 65 70 | 4, 16, 46, 99 | 0 |
| All | All | 4044/4092 (98%) | -0.72 | 64 (1%) 72 76 | 4, 15, 45, 100 | 0 |

All (64) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 731 | PRO | 8.1 |
| 1 | A | 735 | HIS | 8.1 |
| 1 | A | 686 | PRO | 7.9 |
| 1 | B | 731 | PRO | 7.2 |
| 1 | D | 732 | ALA | 6.7 |
| 1 | D | 735 | HIS | 5.8 |
| 1 | C | 732 | ALA | 5.8 |
| 1 | B | 730 | LEU | 5.4 |
| 1 | B | 689 | GLU | 5.3 |
| 1 | D | 799 | THR | 5.1 |
| 1 | B | 733 | ALA | 4.9 |
| 1 | D | 686 | PRO | 4.9 |
| 1 | C | 689 | GLU | 4.6 |
| 1 | D | 730 | LEU | 4.5 |
| 1 | A | 732 | ALA | 4.5 |
| 1 | B | 732 | ALA | 4.5 |
| 1 | A | 730 | LEU | 4.4 |
| 1 | D | 800 | ARG | 4.2 |
| 1 | C | 730 | LEU | 4.0 |
| 1 | D | 731 | PRO | 3.9 |
| 1 | D | 797 | GLU | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 731 | PRO | 3.7 |
| 1 | D | 734 | SER | 3.7 |
| 1 | A | 689 | GLU | 3.7 |
| 1 | C | 733 | ALA | 3.7 |
| 1 | C | 735 | HIS | 3.6 |
| 1 | A | 687 | GLN | 3.5 |
| 1 | B | 687 | GLN | 3.4 |
| 1 | A | 799 | THR | 3.4 |
| 1 | B | 799 | THR | 3.4 |
| 1 | D | 689 | GLU | 3.3 |
| 1 | B | 685 | LEU | 3.3 |
| 1 | C | 798 | ALA | 3.3 |
| 1 | A | 733 | ALA | 3.2 |
| 1 | D | 581 | ASN | 3.1 |
| 1 | A | 685 | LEU | 3.1 |
| 1 | D | 687 | GLN | 3.0 |
| 1 | D | 684 | GLU | 2.9 |
| 1 | C | 800 | ARG | 2.8 |
| 1 | B | 798 | ALA | 2.8 |
| 1 | B | 686 | PRO | 2.8 |
| 1 | C | 729 | THR | 2.7 |
| 1 | D | 771 | GLY | 2.7 |
| 1 | A | 71 | GLU | 2.6 |
| 1 | A | 729 | THR | 2.5 |
| 1 | C | 744 | GLU | 2.5 |
| 1 | C | 687 | GLN | 2.5 |
| 1 | C | 685 | LEU | 2.4 |
| 1 | A | 684 | GLU | 2.4 |
| 1 | B | 797 | GLU | 2.4 |
| 1 | C | 799 | THR | 2.4 |
| 1 | C | 686 | PRO | 2.3 |
| 1 | D | 772 | ASP | 2.3 |
| 1 | D | 733 | ALA | 2.3 |
| 1 | A | 580 | GLU | 2.3 |
| 1 | D | 801 | ILE | 2.2 |
| 1 | A | 798 | ALA | 2.2 |
| 1 | A | 1023 | LYS | 2.2 |
| 1 | C | 745 | MET | 2.1 |
| 1 | D | 634 | GLN | 2.1 |
| 1 | C | 684 | GLU | 2.1 |
| 1 | C | 772 | ASP | 2.1 |
| 1 | D | 798 | ALA | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 580 | GLU | 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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 | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 5 | DMS | D | 8703 | 4/4 | 0.89 | 0.20 | 12.90 | 24,53,80,80 | 0 |
| 5 | DMS | A | 8417 | 4/4 | 0.93 | 0.17 | 9.23 | 25,26,61,100 | 0 |
| 5 | DMS | A | 8406 | 4/4 | 0.96 | 0.13 | 9.02 | 7,53,55,100 | 0 |
| 5 | DMS | C | 8420 | 4/4 | 0.98 | 0.12 | 9.01 | 34,36,53,100 | 0 |
| 5 | DMS | A | 8407 | 4/4 | 0.95 | 0.13 | 7.94 | 28,40,42,43 | 0 |
| 5 | DMS | B | 8407 | 4/4 | 0.95 | 0.17 | 7.22 | 34,34,63,66 | 0 |
| 5 | DMS | B | 8420 | 4/4 | 0.96 | 0.13 | 6.63 | 36,45,63,100 | 0 |
| 5 | DMS | B | 8508 | 4/4 | 0.90 | 0.11 | 5.84 | 27,31,46,64 | 0 |
| 5 | DMS | A | 8504 | 4/4 | 0.98 | 0.10 | 5.55 | 23,35,38,100 | 0 |
| 5 | DMS | B | 8406 | 4/4 | 0.92 | 0.19 | 5.50 | 34,40,61,78 | 0 |
| 5 | DMS | B | 8423 | 4/4 | 0.96 | 0.10 | 5.16 | 28,44,71,87 | 0 |
| 5 | DMS | C | 8501 | 4/4 | 0.98 | 0.12 | 4.88 | 23,23,34,38 | 0 |
| 5 | DMS | B | 8408 | 4/4 | 0.94 | 0.17 | 4.33 | 15,25,43,60 | 0 |
| 5 | DMS | C | 8602 | 4/4 | 0.95 | 0.11 | 4.25 | 27,32,53,77 | 0 |
| 5 | DMS | C | 8419 | 4/4 | 0.94 | 0.14 | 4.05 | 33,44,54,61 | 0 |
| 2 | 2DG | B | 2001 | 10/11 | 0.97 | 0.11 | 2.99 | 13,15,19,24 | 0 |
| 5 | DMS | B | 8405 | 4/4 | 0.99 | 0.11 | 2.60 | 23,28,62,71 | 0 |
| 5 | DMS | A | 8420 | 4/4 | 0.98 | 0.09 | 2.49 | 33,35,39,46 | 0 |
| 5 | DMS | A | 8502 | 4/4 | 0.93 | 0.12 | 2.48 | 14,21,75,84 | 0 |
| 5 | DMS | B | 8404 | 4/4 | 0.99 | 0.07 | 2.29 | 16,20,30,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 5 | DMS | D | 8408 | 4/4 | 0.99 | 0.10 | 2.10 | 14,27,28,36 | 0 |
| 4 | NA | D | 3103 | 1/1 | 0.91 | 0.11 | 2.10 | 38,38,38,38 | 0 |
| 5 | DMS | D | 8417 | 4/4 | 0.94 | 0.14 | 1.87 | 18,26,39,73 | 0 |
| 5 | DMS | A | 8419 | 4/4 | 0.98 | 0.12 | 1.77 | 24,26,55,100 | 0 |
| 5 | DMS | B | 8425 | 4/4 | 0.95 | 0.13 | 1.71 | 22,30,32,54 | 0 |
| 5 | DMS | C | 8407 | 4/4 | 0.98 | 0.11 | 1.71 | 35,39,51,52 | 0 |
| 5 | DMS | A | 8401 | 4/4 | 0.99 | 0.09 | 1.68 | 6,13,16,19 | 0 |
| 5 | DMS | B | 8506 | 4/4 | 0.98 | 0.10 | 1.63 | 31,39,63,100 | 0 |
| 5 | DMS | C | 8423 | 4/4 | 0.95 | 0.10 | 1.58 | 26,27,32,61 | 0 |
| 5 | DMS | C | 8405 | 4/4 | 0.99 | 0.09 | 1.53 | 16,23,25,38 | 0 |
| 5 | DMS | B | 8403 | 4/4 | 0.99 | 0.12 | 1.47 | 12,12,18,21 | 0 |
| 5 | DMS | D | 8403 | 4/4 | 0.99 | 0.09 | 1.46 | 21,26,27,45 | 0 |
| 5 | DMS | C | 8403 | 4/4 | 0.99 | 0.10 | 1.44 | 10,12,16,19 | 0 |
| 5 | DMS | D | 8701 | 4/4 | 0.98 | 0.09 | 1.38 | 15,17,22,37 | 0 |
| 5 | DMS | C | 8425 | 4/4 | 0.96 | 0.11 | 1.29 | 33,37,39,48 | 0 |
| 5 | DMS | A | 8412 | 4/4 | 0.98 | 0.10 | 1.25 | 24,33,37,37 | 0 |
| 5 | DMS | A | 8403 | 4/4 | 0.99 | 0.09 | 1.12 | 15,20,21,23 | 0 |
| 5 | DMS | B | 8502 | 4/4 | 0.96 | 0.09 | 1.09 | 13,30,45,50 | 0 |
| 5 | DMS | B | 8412 | 4/4 | 0.96 | 0.11 | 1.05 | 21,33,34,38 | 0 |
| 4 | NA | A | 3103 | 1/1 | 0.98 | 0.10 | 0.98 | 25,25,25,25 | 0 |
| 2 | 2DG | C | 2001 | 10/11 | 0.97 | 0.08 | 0.97 | 7,15,26,27 | 0 |
| 5 | DMS | C | 8417 | 4/4 | 0.95 | 0.10 | 0.95 | 24,51,57,58 | 0 |
| 5 | DMS | A | 8425 | 4/4 | 0.95 | 0.16 | 0.82 | 34,40,45,45 | 0 |
| 5 | DMS | C | 8401 | 4/4 | 0.99 | 0.08 | 0.80 | 10,11,21,30 | 0 |
| 5 | DMS | B | 8504 | 4/4 | 0.98 | 0.10 | 0.74 | 31,37,51,52 | 0 |
| 5 | DMS | D | 8404 | 4/4 | 0.99 | 0.07 | 0.70 | 14,19,26,80 | 0 |
| 2 | 2DG | A | 2001 | 10/11 | 0.97 | 0.07 | 0.65 | 10,15,18,25 | 0 |
| 5 | DMS | D | 8705 | 4/4 | 0.96 | 0.12 | 0.62 | 24,32,51,51 | 0 |
| 5 | DMS | A | 8408 | 4/4 | 0.99 | 0.08 | 0.55 | 14,23,31,82 | 0 |
| 5 | DMS | D | 8405 | 4/4 | 0.99 | 0.08 | 0.55 | 18,23,42,100 | 0 |
| 5 | DMS | B | 8401 | 4/4 | 0.99 | 0.07 | 0.54 | 13,13,21,22 | 0 |
| 5 | DMS | D | 8406 | 4/4 | 0.96 | 0.08 | 0.52 | 18,19,20,34 | 0 |
| 5 | DMS | C | 8408 | 4/4 | 0.97 | 0.09 | 0.51 | 13,35,46,83 | 0 |
| 2 | 2DG | D | 2001 | 10/11 | 0.96 | 0.08 | 0.47 | 9,15,24,24 | 0 |
| 5 | DMS | B | 8417 | 4/4 | 0.96 | 0.10 | 0.46 | 26,31,34,63 | 0 |
| 5 | DMS | D | 8410 | 4/4 | 0.98 | 0.10 | 0.44 | 22,35,39,100 | 0 |
| 5 | DMS | D | 8501 | 4/4 | 0.97 | 0.09 | 0.37 | 16,34,36,46 | 0 |
| 5 | DMS | A | 8411 | 4/4 | 0.98 | 0.08 | 0.33 | 24,26,28,100 | 0 |
| 5 | DMS | C | 8404 | 4/4 | 0.99 | 0.06 | 0.21 | 11,13,21,21 | 0 |
| 5 | DMS | D | 8508 | 4/4 | 0.98 | 0.08 | 0.20 | 19,46,50,80 | 0 |
| 3 | MG | B | 3001 | 1/1 | 0.98 | 0.06 | 0.15 | 11,11,11,11 | 0 |
| 5 | DMS | D | 8412 | 4/4 | 0.98 | 0.10 | 0.10 | 15,25,32,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 5 | DMS | C | 8411 | 4/4 | 0.99 | 0.08 | 0.03 | 18,20,34,50 | 0 |
| 4 | NA | C | 3104 | 1/1 | 0.97 | 0.09 | -0.06 | 26,26,26,26 | 0 |
| 5 | DMS | B | 8402 | 4/4 | 0.98 | 0.07 | -0.13 | 8,21,25,29 | 0 |
| 5 | DMS | D | 8401 | 4/4 | 0.99 | 0.06 | -0.21 | 10,11,20,27 | 0 |
| 5 | DMS | A | 8501 | 4/4 | 0.97 | 0.08 | -0.21 | 12,13,29,33 | 0 |
| 5 | DMS | A | 8410 | 4/4 | 0.99 | 0.09 | -0.26 | 28,39,55,58 | 0 |
| 5 | DMS | D | 8402 | 4/4 | 0.98 | 0.07 | -0.27 | 9,23,27,32 | 0 |
| 4 | NA | B | 3104 | 1/1 | 0.96 | 0.09 | -0.32 | 37,37,37,37 | 0 |
| 5 | DMS | A | 8402 | 4/4 | 0.98 | 0.07 | -0.32 | 11,26,30,47 | 0 |
| 5 | DMS | C | 8412 | 4/4 | 0.99 | 0.07 | -0.41 | 18,31,67,100 | 0 |
| 5 | DMS | C | 8402 | 4/4 | 0.99 | 0.07 | -0.43 | 6,31,38,40 | 0 |
| 5 | DMS | D | 8419 | 4/4 | 0.98 | 0.07 | -0.53 | 18,32,40,44 | 0 |
| 3 | MG | D | 3002 | 1/1 | 0.98 | 0.07 | -0.55 | 19,19,19,19 | 0 |
| 4 | NA | B | 3101 | 1/1 | 0.98 | 0.06 | -0.55 | 13,13,13,13 | 0 |
| 4 | NA | A | 3101 | 1/1 | 0.98 | 0.05 | -0.65 | 13,13,13,13 | 0 |
| 5 | DMS | A | 8404 | 4/4 | 0.99 | 0.06 | -0.80 | 9,22,22,30 | 0 |
| 4 | NA | D | 3101 | 1/1 | 0.99 | 0.04 | -0.82 | 16,16,16,16 | 0 |
| 4 | NA | B | 3102 | 1/1 | 0.99 | 0.06 | -0.84 | 13,13,13,13 | 0 |
| 4 | NA | C | 3103 | 1/1 | 0.97 | 0.06 | -0.86 | 22,22,22,22 | 0 |
| 3 | MG | C | 3002 | 1/1 | 0.99 | 0.05 | -0.88 | 12,12,12,12 | 0 |
| 4 | NA | A | 3104 | 1/1 | 0.99 | 0.06 | -0.96 | 21,21,21,21 | 0 |
| 5 | DMS | A | 8405 | 4/4 | 0.99 | 0.05 | -1.13 | 11,22,25,27 | 0 |
| 4 | NA | C | 3101 | 1/1 | 0.98 | 0.05 | -1.22 | 11,11,11,11 | 0 |
| 5 | DMS | D | 8411 | 4/4 | 0.99 | 0.05 | -1.27 | 11,27,27,100 | 0 |
| 4 | NA | D | 3102 | 1/1 | 0.99 | 0.06 | -1.30 | 18,18,18,18 | 0 |
| 5 | DMS | B | 8411 | 4/4 | 0.99 | 0.05 | -1.38 | 15,17,32,100 | 0 |
| 4 | NA | A | 3102 | 1/1 | 0.99 | 0.04 | -1.53 | 15,15,15,15 | 0 |
| 3 | MG | A | 3002 | 1/1 | 0.98 | 0.05 | -1.68 | 14,14,14,14 | 0 |
| 4 | NA | B | 3103 | 1/1 | 0.99 | 0.03 | -1.83 | 19,19,19,19 | 0 |
| 4 | NA | C | 3102 | 1/1 | 0.99 | 0.04 | -2.03 | 16,16,16,16 | 0 |
| 3 | MG | B | 3002 | 1/1 | 0.99 | 0.04 | -3.01 | 14,14,14,14 | 0 |
| 3 | MG | C | 3001 | 1/1 | 0.99 | 0.03 | -4.34 | 12,12,12,12 | 0 |
| 3 | MG | A | 3001 | 1/1 | 0.99 | 0.02 | -7.96 | 13,13,13,13 | 0 |
| 3 | MG | D | 3001 | 1/1 | 0.99 | 0.02 | -8.37 | 15,15,15,15 | 0 |
| 5 | DMS | C | 8416 | 4/4 | 0.96 | 0.26 | - | 31,33,49,64 | 0 |
| 3 | MG | A | 3005 | 1/1 | 0.89 | 0.05 | - | 36,36,36,36 | 0 |
| 5 | DMS | B | 8409 | 4/4 | 0.97 | 0.09 | - | 18,32,33,38 | 0 |
| 5 | DMS | D | 8413 | 4/4 | 0.98 | 0.13 | - | 21,24,34,35 | 0 |
| 5 | DMS | B | 8410 | 4/4 | 0.98 | 0.09 | - | 18,27,41,54 | 0 |
| 5 | DMS | D | 8414 | 4/4 | 0.97 | 0.14 | - | 17,32,44,92 | 0 |
| 5 | DMS | C | 8414 | 4/4 | 0.98 | 0.08 | - | 17,18,23,39 | 0 |
| 5 | DMS | C | 8409 | 4/4 | 0.97 | 0.09 | - | 23,35,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 5 | DMS | C | 8504 | 4/4 | 0.98 | 0.08 | - | 32,34,42,64 | 0 |
| 5 | DMS | A | 8414 | 4/4 | 0.98 | 0.10 | - | 16,37,47,100 | 0 |
| 5 | DMS | D | 8503 | 4/4 | 0.97 | 0.17 | - | 33,53,64,100 | 0 |
| 5 | DMS | C | 8410 | 4/4 | 0.99 | 0.07 | - | 21,35,37,43 | 0 |
| 5 | DMS | C | 8413 | 4/4 | 0.95 | 0.15 | - | 31,32,34,38 | 0 |
| 5 | DMS | C | 8601 | 4/4 | 0.96 | 0.14 | - | 31,53,55,100 | 0 |
| 5 | DMS | A | 8602 | 4/4 | 0.98 | 0.18 | - | 42,45,100,100 | 0 |
| 5 | DMS | A | 8415 | 4/4 | 0.94 | 0.10 | - | 24,27,28,70 | 0 |
| 5 | DMS | C | 8503 | 4/4 | 0.96 | 0.19 | - | 20,31,54,100 | 0 |
| 5 | DMS | C | 8506 | 4/4 | 0.96 | 0.10 | - | 15,24,47,89 | 0 |
| 5 | DMS | C | 8415 | 4/4 | 0.95 | 0.11 | - | 20,26,33,52 | 0 |
| 5 | DMS | B | 8421 | 4/4 | 0.97 | 0.10 | - | 14,46,60,85 | 0 |
| 5 | DMS | D | 8421 | 4/4 | 0.97 | 0.12 | - | 36,45,48,52 | 0 |
| 5 | DMS | B | 8415 | 4/4 | 0.94 | 0.12 | - | 22,26,33,67 | 0 |
| 5 | DMS | B | 8601 | 4/4 | 0.97 | 0.12 | - | 36,60,100,100 | 0 |
| 5 | DMS | A | 8413 | 4/4 | 0.97 | 0.12 | - | 34,34,53,100 | 0 |
| 5 | DMS | C | 8427 | 4/4 | 0.98 | 0.15 | - | 37,43,81,82 | 0 |
| 5 | DMS | B | 8414 | 4/4 | 0.97 | 0.14 | - | 24,43,49,100 | 0 |
| 5 | DMS | D | 8416 | 4/4 | 0.97 | 0.21 | - | 16,34,42,89 | 0 |
| 5 | DMS | D | 8409 | 4/4 | 0.96 | 0.08 | - | 25,30,39,53 | 0 |
| 5 | DMS | B | 8416 | 4/4 | 0.97 | 0.12 | - | 35,42,52,88 | 0 |
| 3 | MG | D | 3005 | 1/1 | 0.97 | 0.05 | - | 43,43,43,43 | 0 |
| 5 | DMS | B | 8427 | 4/4 | 0.93 | 0.10 | - | 28,31,42,65 | 0 |
| 5 | DMS | A | 8503 | 4/4 | 0.97 | 0.20 | - | 42,47,48,100 | 0 |
| 5 | DMS | A | 8421 | 4/4 | 0.95 | 0.19 | - | 42,43,67,100 | 0 |
| 5 | DMS | B | 8413 | 4/4 | 0.93 | 0.15 | - | 22,32,35,42 | 0 |
| 5 | DMS | C | 8421 | 4/4 | 0.98 | 0.11 | - | 26,26,41,64 | 0 |
| 5 | DMS | A | 8409 | 4/4 | 0.96 | 0.11 | - | 24,27,39,42 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.