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

Sep 6, 2023 – 08:41 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 3VD5 |
| Title | : | E. coli (lacZ) beta-galactosidase (N460S) |
| Authors | : | Wheatley, R.W.; Kappelhoff, J.C.; Hahn, J.N.; Dugdale, M.L.; Dutkoski, M.J.; Tamman, S.D.; Fraser, M.E.; Huber, R.E. |
| Deposited on | : | 2012-01-04 |
| Resolution | : | 2.70 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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The following versions of software and data (see references (i)) were used in the production of this report:

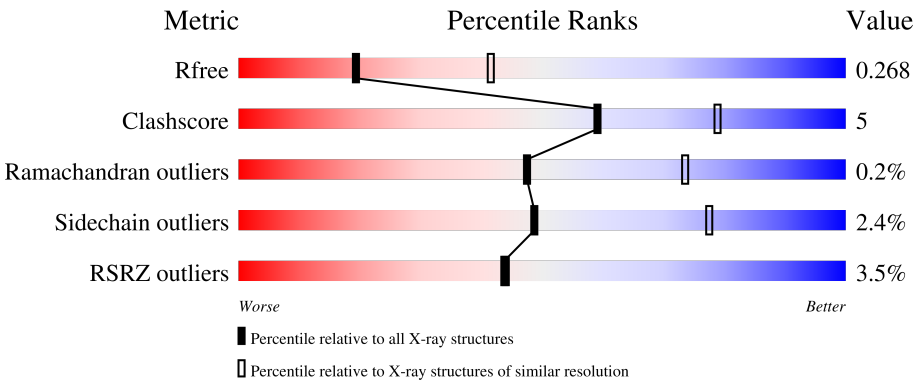
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 2808 (2.70-2.70) |
| Clashscore | 141614 | 3122 (2.70-2.70) |
| Ramachandran outliers | 138981 | 3069 (2.70-2.70) |
| Sidechain outliers | 138945 | 3069 (2.70-2.70) |
| RSRZ outliers | 127900 | 2737 (2.70-2.70) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1052 | 2% 86% 10% • |
| 1 | B | 1052 | 2% 82% 14% • |
| 1 | C | 1052 | 4% 81% 15% • |
| 1 | D | 1052 | 5% 81% 14% • • |

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 33647 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-galactosidase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 1011 | 8124 | 5137 | 1439 | 1510 | 38 | 0 | 0 | 0 |
| 1 | C | 1011 | 8124 | 5137 | 1439 | 1510 | 38 | 0 | 0 | 0 |
| 1 | D | 1011 | 8124 | 5137 | 1439 | 1510 | 38 | 0 | 0 | 0 |
| 1 | B | 1011 | 8124 | 5137 | 1439 | 1510 | 38 | 0 | 0 | 0 |

There are 152 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -28 | MET | - | expression tag | UNP P00722 |
| A | -27 | GLY | - | expression tag | UNP P00722 |
| A | -26 | GLY | - | expression tag | UNP P00722 |
| A | -25 | SER | - | expression tag | UNP P00722 |
| A | -24 | HIS | - | expression tag | UNP P00722 |
| A | -23 | HIS | - | expression tag | UNP P00722 |
| A | -22 | HIS | - | expression tag | UNP P00722 |
| A | -21 | HIS | - | expression tag | UNP P00722 |
| A | -20 | HIS | - | expression tag | UNP P00722 |
| A | -19 | HIS | - | expression tag | UNP P00722 |
| A | -18 | GLY | - | expression tag | UNP P00722 |
| A | -17 | MET | - | expression tag | UNP P00722 |
| A | -16 | ALA | - | expression tag | UNP P00722 |
| A | -15 | SER | - | expression tag | UNP P00722 |
| A | -14 | MET | - | expression tag | UNP P00722 |
| A | -13 | THR | - | expression tag | UNP P00722 |
| A | -12 | GLY | - | expression tag | UNP P00722 |
| A | -11 | GLY | - | expression tag | UNP P00722 |
| A | -10 | GLN | - | expression tag | UNP P00722 |
| A | -9 | GLN | - | expression tag | UNP P00722 |
| A | -8 | MET | - | expression tag | UNP P00722 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -7 | GLY | - | expression tag | UNP P00722 |
| A | -6 | ARG | - | expression tag | UNP P00722 |
| A | -5 | ASP | - | expression tag | UNP P00722 |
| A | -4 | LEU | - | expression tag | UNP P00722 |
| A | -3 | TYR | - | expression tag | UNP P00722 |
| A | -2 | ASP | - | expression tag | UNP P00722 |
| A | -1 | ASP | - | expression tag | UNP P00722 |
| A | 0 | ASP | - | expression tag | UNP P00722 |
| A | 1 | ASP | - | expression tag | UNP P00722 |
| A | 2 | LYS | - | expression tag | UNP P00722 |
| A | 3 | ASP | - | expression tag | UNP P00722 |
| A | 4 | PRO | - | expression tag | UNP P00722 |
| A | 5 | MET | - | expression tag | UNP P00722 |
| A | 6 | ILE | - | expression tag | UNP P00722 |
| A | 7 | ASP | - | expression tag | UNP P00722 |
| A | 8 | PRO | - | expression tag | UNP P00722 |
| A | 460 | SER | ASN | engineered mutation | UNP P00722 |
| C | -28 | MET | - | expression tag | UNP P00722 |
| C | -27 | GLY | - | expression tag | UNP P00722 |
| C | -26 | GLY | - | expression tag | UNP P00722 |
| C | -25 | SER | - | expression tag | UNP P00722 |
| C | -24 | HIS | - | expression tag | UNP P00722 |
| C | -23 | HIS | - | expression tag | UNP P00722 |
| C | -22 | HIS | - | expression tag | UNP P00722 |
| C | -21 | HIS | - | expression tag | UNP P00722 |
| C | -20 | HIS | - | expression tag | UNP P00722 |
| C | -19 | HIS | - | expression tag | UNP P00722 |
| C | -18 | GLY | - | expression tag | UNP P00722 |
| C | -17 | MET | - | expression tag | UNP P00722 |
| C | -16 | ALA | - | expression tag | UNP P00722 |
| C | -15 | SER | - | expression tag | UNP P00722 |
| C | -14 | MET | - | expression tag | UNP P00722 |
| C | -13 | THR | - | expression tag | UNP P00722 |
| C | -12 | GLY | - | expression tag | UNP P00722 |
| C | -11 | GLY | - | expression tag | UNP P00722 |
| C | -10 | GLN | - | expression tag | UNP P00722 |
| C | -9 | GLN | - | expression tag | UNP P00722 |
| C | -8 | MET | - | expression tag | UNP P00722 |
| C | -7 | GLY | - | expression tag | UNP P00722 |
| C | -6 | ARG | - | expression tag | UNP P00722 |
| C | -5 | ASP | - | expression tag | UNP P00722 |
| C | -4 | LEU | - | expression tag | UNP P00722 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | -3 | TYR | - | expression tag | UNP P00722 |
| C | -2 | ASP | - | expression tag | UNP P00722 |
| C | -1 | ASP | - | expression tag | UNP P00722 |
| C | 0 | ASP | - | expression tag | UNP P00722 |
| C | 1 | ASP | - | expression tag | UNP P00722 |
| C | 2 | LYS | - | expression tag | UNP P00722 |
| C | 3 | ASP | - | expression tag | UNP P00722 |
| C | 4 | PRO | - | expression tag | UNP P00722 |
| C | 5 | MET | - | expression tag | UNP P00722 |
| C | 6 | ILE | - | expression tag | UNP P00722 |
| C | 7 | ASP | - | expression tag | UNP P00722 |
| C | 8 | PRO | - | expression tag | UNP P00722 |
| C | 460 | SER | ASN | engineered mutation | UNP P00722 |
| D | -28 | MET | - | expression tag | UNP P00722 |
| D | -27 | GLY | - | expression tag | UNP P00722 |
| D | -26 | GLY | - | expression tag | UNP P00722 |
| D | -25 | SER | - | expression tag | UNP P00722 |
| D | -24 | HIS | - | expression tag | UNP P00722 |
| D | -23 | HIS | - | expression tag | UNP P00722 |
| D | -22 | HIS | - | expression tag | UNP P00722 |
| D | -21 | HIS | - | expression tag | UNP P00722 |
| D | -20 | HIS | - | expression tag | UNP P00722 |
| D | -19 | HIS | - | expression tag | UNP P00722 |
| D | -18 | GLY | - | expression tag | UNP P00722 |
| D | -17 | MET | - | expression tag | UNP P00722 |
| D | -16 | ALA | - | expression tag | UNP P00722 |
| D | -15 | SER | - | expression tag | UNP P00722 |
| D | -14 | MET | - | expression tag | UNP P00722 |
| D | -13 | THR | - | expression tag | UNP P00722 |
| D | -12 | GLY | - | expression tag | UNP P00722 |
| D | -11 | GLY | - | expression tag | UNP P00722 |
| D | -10 | GLN | - | expression tag | UNP P00722 |
| D | -9 | GLN | - | expression tag | UNP P00722 |
| D | -8 | MET | - | expression tag | UNP P00722 |
| D | -7 | GLY | - | expression tag | UNP P00722 |
| D | -6 | ARG | - | expression tag | UNP P00722 |
| D | -5 | ASP | - | expression tag | UNP P00722 |
| D | -4 | LEU | - | expression tag | UNP P00722 |
| D | -3 | TYR | - | expression tag | UNP P00722 |
| D | -2 | ASP | - | expression tag | UNP P00722 |
| D | -1 | ASP | - | expression tag | UNP P00722 |
| D | 0 | ASP | - | expression tag | UNP P00722 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 1 | ASP | - | expression tag | UNP P00722 |
| D | 2 | LYS | - | expression tag | UNP P00722 |
| D | 3 | ASP | - | expression tag | UNP P00722 |
| D | 4 | PRO | - | expression tag | UNP P00722 |
| D | 5 | MET | - | expression tag | UNP P00722 |
| D | 6 | ILE | - | expression tag | UNP P00722 |
| D | 7 | ASP | - | expression tag | UNP P00722 |
| D | 8 | PRO | - | expression tag | UNP P00722 |
| D | 460 | SER | ASN | engineered mutation | UNP P00722 |
| B | -28 | MET | - | expression tag | UNP P00722 |
| B | -27 | GLY | - | expression tag | UNP P00722 |
| B | -26 | GLY | - | expression tag | UNP P00722 |
| B | -25 | SER | - | expression tag | UNP P00722 |
| B | -24 | HIS | - | expression tag | UNP P00722 |
| B | -23 | HIS | - | expression tag | UNP P00722 |
| B | -22 | HIS | - | expression tag | UNP P00722 |
| B | -21 | HIS | - | expression tag | UNP P00722 |
| B | -20 | HIS | - | expression tag | UNP P00722 |
| B | -19 | HIS | - | expression tag | UNP P00722 |
| B | -18 | GLY | - | expression tag | UNP P00722 |
| B | -17 | MET | - | expression tag | UNP P00722 |
| B | -16 | ALA | - | expression tag | UNP P00722 |
| B | -15 | SER | - | expression tag | UNP P00722 |
| B | -14 | MET | - | expression tag | UNP P00722 |
| B | -13 | THR | - | expression tag | UNP P00722 |
| B | -12 | GLY | - | expression tag | UNP P00722 |
| B | -11 | GLY | - | expression tag | UNP P00722 |
| B | -10 | GLN | - | expression tag | UNP P00722 |
| B | -9 | GLN | - | expression tag | UNP P00722 |
| B | -8 | MET | - | expression tag | UNP P00722 |
| B | -7 | GLY | - | expression tag | UNP P00722 |
| B | -6 | ARG | - | expression tag | UNP P00722 |
| B | -5 | ASP | - | expression tag | UNP P00722 |
| B | -4 | LEU | - | expression tag | UNP P00722 |
| B | -3 | TYR | - | expression tag | UNP P00722 |
| B | -2 | ASP | - | expression tag | UNP P00722 |
| B | -1 | ASP | - | expression tag | UNP P00722 |
| B | 0 | ASP | - | expression tag | UNP P00722 |
| B | 1 | ASP | - | expression tag | UNP P00722 |
| B | 2 | LYS | - | expression tag | UNP P00722 |
| B | 3 | ASP | - | expression tag | UNP P00722 |
| B | 4 | PRO | - | expression tag | UNP P00722 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 5 | MET | - | expression tag | UNP P00722 |
| B | 6 | ILE | - | expression tag | UNP P00722 |
| B | 7 | ASP | - | expression tag | UNP P00722 |
| B | 8 | PRO | - | expression tag | UNP P00722 |
| B | 460 | SER | ASN | engineered mutation | UNP P00722 |

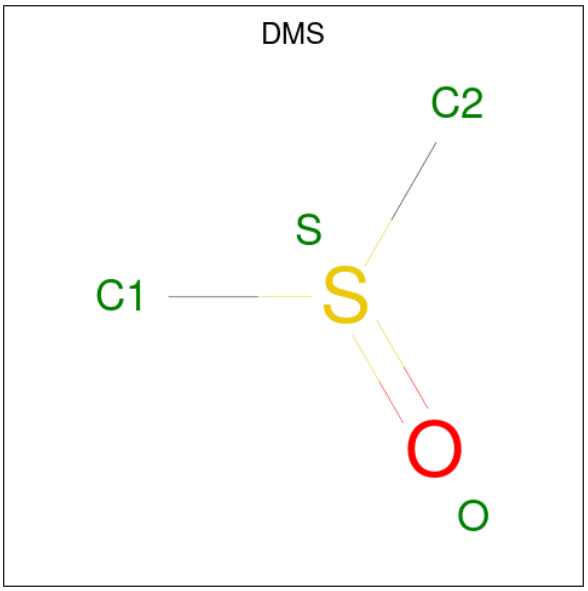
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: $C_2H_6OS$).




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

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

- Molecule 5 is water.

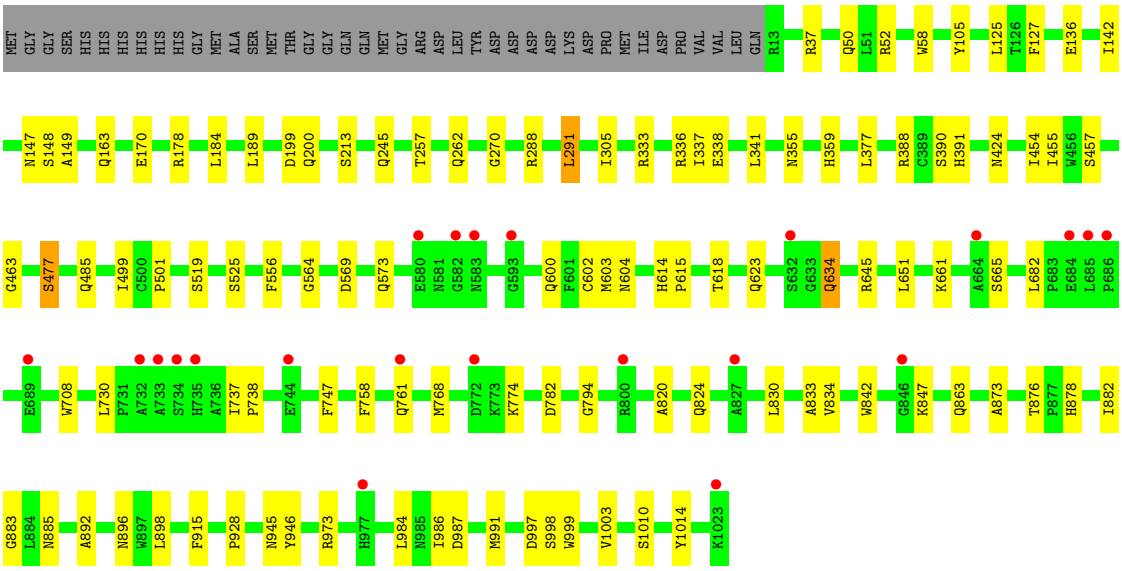
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 5 | A | 314 | 314 | 314 | 0 | 0 |
| | | | Total | O | | |
| 5 | C | 204 | 204 | 204 | 0 | 0 |
| | | | Total | O | | |
| 5 | D | 272 | 272 | 272 | 0 | 0 |
| | | | Total | O | | |
| 5 | B | 246 | 246 | 246 | 0 | 0 |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

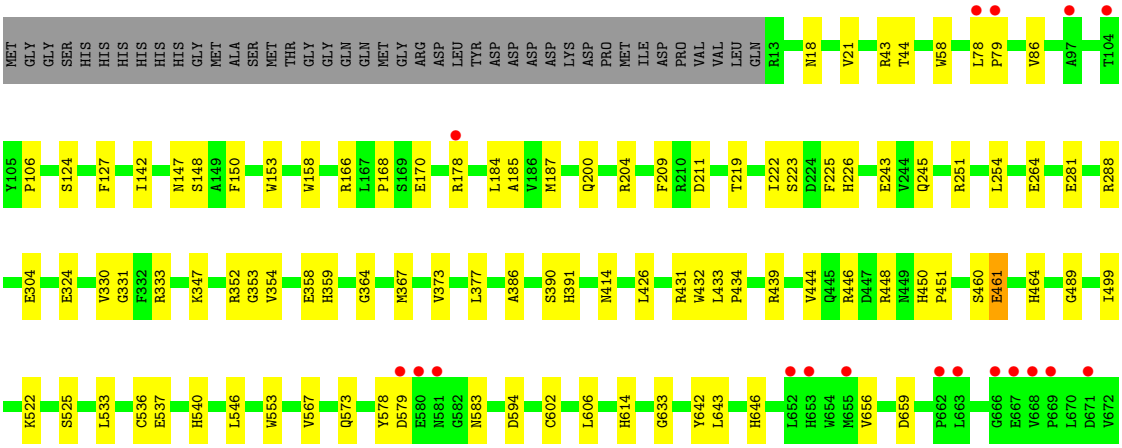
- Molecule 1: Beta-galactosidase

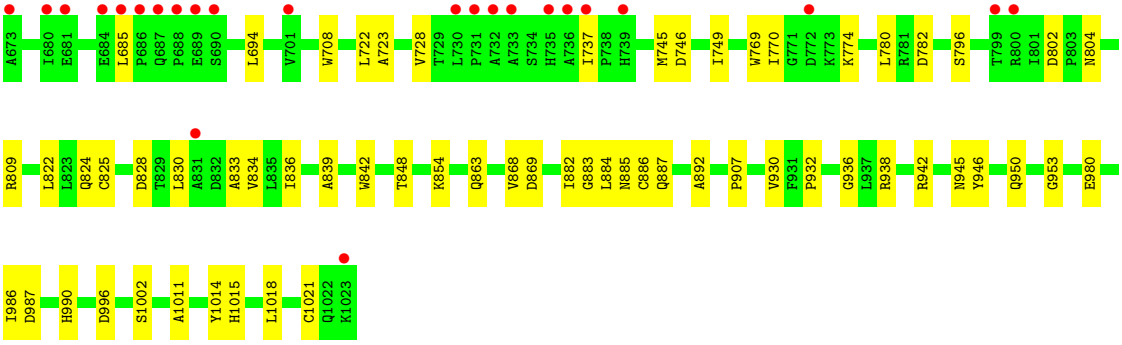
Chain A:




- Molecule 1: Beta-galactosidase

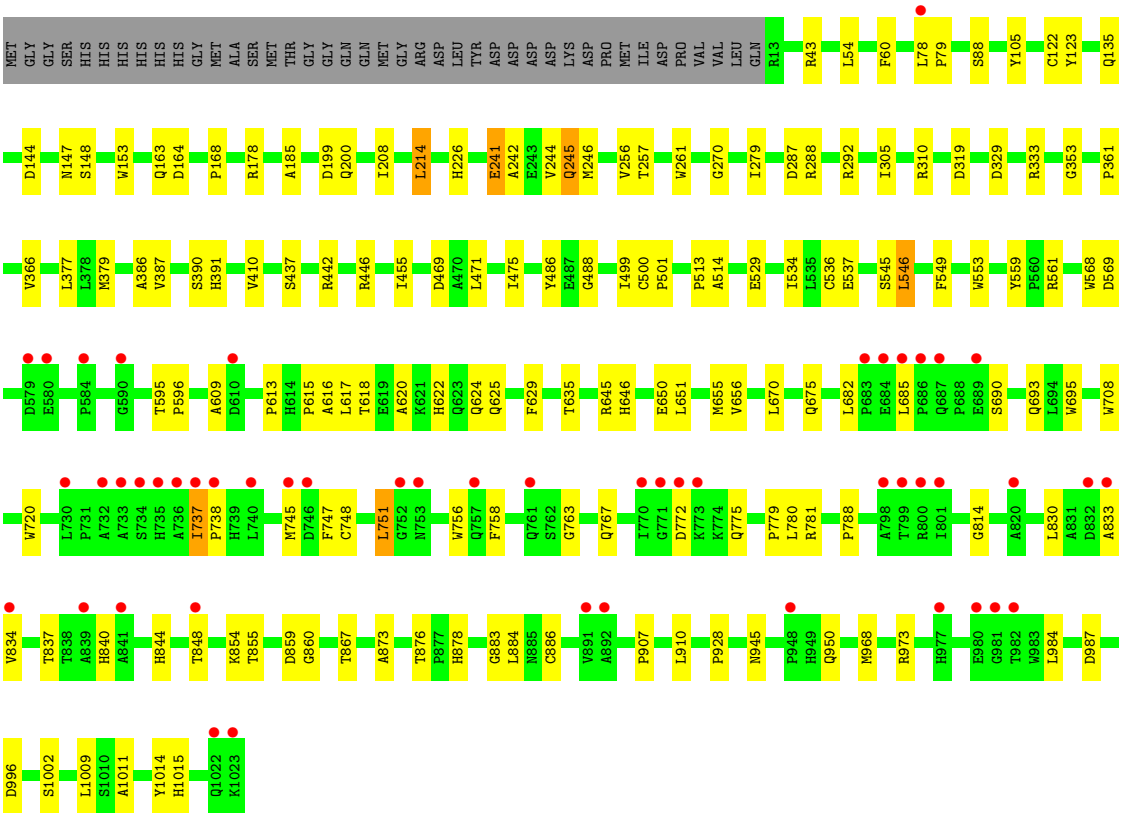
Chain C:





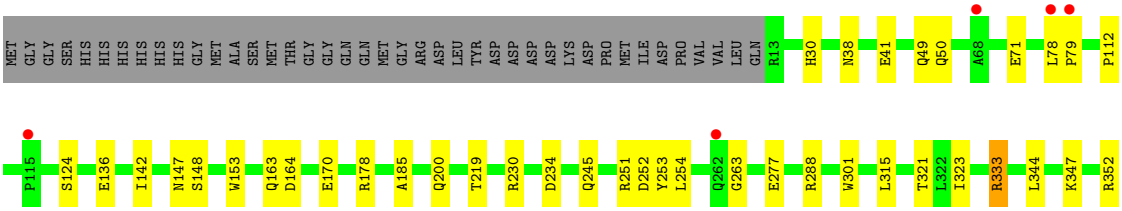

- Molecule 1: Beta-galactosidase

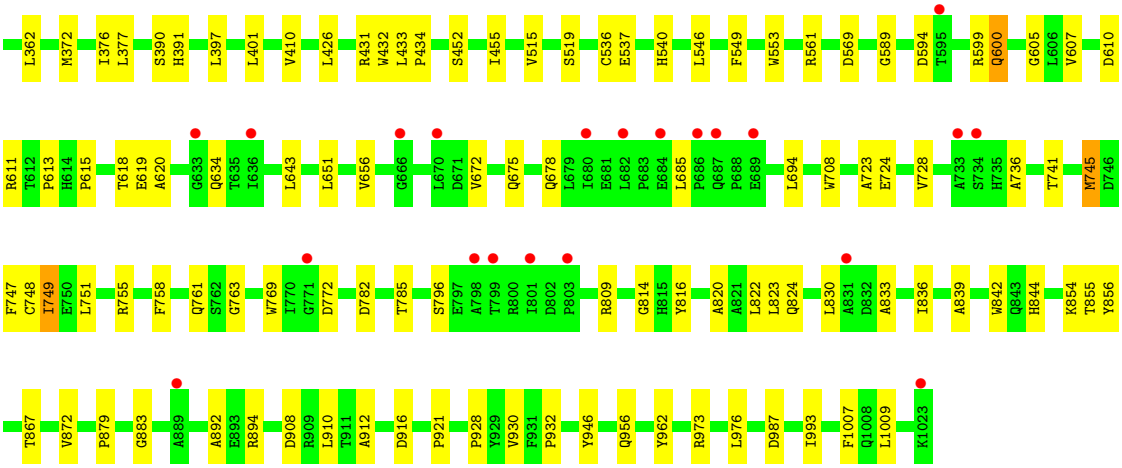
Chain D:




- Molecule 1: Beta-galactosidase

Chain B:




L362
M372
I376
L377
S390
H391
L397
L401
V410
L426
R431
W432
L433
P434
S452
I455
V515
S519
C536
E537
H540
L546
F549
W553
R561
D569
G589
D594
T595
R599
Q600
G605
L606
V607
D610
R611
T612
P613
H614
P615
T618
E619
A620
G633
Q634
T635
I636
L643
L651
V656
G666
L670
D671
V672
Q675
Q678
L679
I680
E681
L682
P683
E684
L685
P686
Q687
P688
E689
L694
W708
A723
E724
V728
A733
S734
H735
A736
T741
M745
D746
F747
C748
I749
E750
L751
R755
F758
Q761
S762
G763
W769
I770
G771
D772
D782
T785
S796
E797
A798
T799
R800
I801
D802
P803
R809
G814
H815
Y816
A820
A821
L822
L823
Q824
L830
A831
D832
A833
I836
A839
W842
Q843
H844
K854
T855
Y856
T867
V872
P879
G883
A889
A892
E893
R894
D908
R909
I910
T911
A912
D916
P921
P928
Y929
V930
F931
P932
Y946
Q956
Y962
R973
L976
D987
I993
F1007
Q1008
L1009
K1023

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 126.30Å 150.75Å 131.09Å<br>90.00° 104.06° 90.00° | Depositor |
| Resolution (Å) | 54.58 – 2.70<br>54.58 – 2.70 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 100.0 (54.58-2.70)<br>91.0 (54.58-2.70) | Depositor<br>EDS |
| $R_{merge}$ | 0.13 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.34 (at 2.69Å) | Xtriage |
| Refinement program | REFMAC 5.5.0109, CNS | Depositor |
| R, $R_{free}$ | 0.203 , 0.276<br>0.194 , 0.268 | Depositor<br>DCC |
| $R_{free}$ test set | 5937 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 36.7 | Xtriage |
| Anisotropy | 0.073 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.33 , 51.1 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.47$, $< L^2 > = 0.30$ | Xtriage |
| Estimated twinning fraction | 0.026 for l,-k,h | Xtriage |
| $F_o$,$F_c$ correlation | 0.92 | EDS |
| Total number of atoms | 33647 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 52.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| >5$ | RMSZ | $\#\|Z\| >5$ |
| 1 | A | 0.40 | 0/8366 | 0.56 | 1/11412 (0.0%) |
| 1 | B | 0.38 | 0/8366 | 0.55 | 0/11412 |
| 1 | C | 0.37 | 0/8366 | 0.53 | 0/11412 |
| 1 | D | 0.39 | 0/8366 | 0.55 | 0/11412 |
| All | All | 0.39 | 0/33464 | 0.55 | 1/45648 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 291 | LEU | CA-CB-CG | 5.33 | 127.57 | 115.30 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 8124 | 0 | 7715 | 55 | 0 |
| 1 | B | 8124 | 0 | 7715 | 75 | 0 |
| 1 | C | 8124 | 0 | 7715 | 90 | 0 |
| 1 | D | 8124 | 0 | 7715 | 85 | 0 |
| 2 | A | 2 | 0 | 0 | 0 | 0 |
| 2 | B | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | C | 2 | 0 | 0 | 0 | 0 |
| 2 | D | 2 | 0 | 0 | 0 | 0 |
| 3 | A | 3 | 0 | 0 | 0 | 0 |
| 3 | B | 3 | 0 | 0 | 0 | 0 |
| 3 | C | 3 | 0 | 0 | 0 | 0 |
| 3 | D | 2 | 0 | 0 | 0 | 0 |
| 4 | A | 32 | 0 | 48 | 2 | 0 |
| 4 | B | 16 | 0 | 24 | 0 | 0 |
| 4 | C | 24 | 0 | 36 | 3 | 0 |
| 4 | D | 24 | 0 | 36 | 0 | 0 |
| 5 | A | 314 | 0 | 0 | 1 | 0 |
| 5 | B | 246 | 0 | 0 | 1 | 0 |
| 5 | C | 204 | 0 | 0 | 3 | 0 |
| 5 | D | 272 | 0 | 0 | 4 | 0 |
| All | All | 33647 | 0 | 31004 | 296 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (296) 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:A:142:ILE:HG12 | 1:A:170:GLU:HG2 | 1.48 | 0.94 |
| 1:C:226:HIS:ND1 | 1:C:448:ARG:HD3 | 1.85 | 0.91 |
| 1:B:656:VAL:HG21 | 1:B:685:LEU:HD22 | 1.56 | 0.88 |
| 1:B:656:VAL:HG21 | 1:B:685:LEU:CD2 | 2.12 | 0.80 |
| 1:D:245:GLN:HG3 | 1:D:288:ARG:HG2 | 1.67 | 0.77 |
| 1:D:615:PRO:O | 1:D:618:THR:HG22 | 1.88 | 0.73 |
| 1:D:305:ILE:HD11 | 1:D:645:ARG:HB3 | 1.72 | 0.70 |
| 1:B:38:ASN:OD1 | 1:B:41:GLU:HG2 | 1.92 | 0.69 |
| 1:C:828:ASP:HB3 | 1:D:830:LEU:HD22 | 1.75 | 0.68 |
| 1:B:153:TRP:HB2 | 1:B:185:ALA:HB3 | 1.76 | 0.68 |
| 1:D:241:GLU:HG3 | 1:D:292:ARG:HG2 | 1.77 | 0.66 |
| 1:A:615:PRO:O | 1:A:618:THR:HG22 | 1.96 | 0.66 |
| 1:C:245:GLN:HG2 | 1:C:288:ARG:HG2 | 1.77 | 0.66 |
| 1:B:928:PRO:HB2 | 1:B:973:ARG:HH11 | 1.60 | 0.65 |
| 1:B:245:GLN:HG2 | 1:B:288:ARG:HG2 | 1.79 | 0.64 |
| 1:C:58:TRP:CD1 | 1:C:86:VAL:HB | 2.33 | 0.64 |
| 1:B:883:GLY:HA3 | 1:B:987:ASP:HA | 1.81 | 0.62 |
| 1:D:135:GLN:HG3 | 5:D:4006:HOH:O | 1.99 | 0.62 |
| 1:B:112:PRO:HG3 | 1:B:431:ARG:HH22 | 1.65 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:127:PHE:HE2 | 1:C:184:LEU:HG | 1.65 | 0.61 |
| 1:C:830:LEU:HD12 | 1:C:833:ALA:HB3 | 1.83 | 0.61 |
| 1:C:331:GLY:H | 4:C:8002:DMS:H22 | 1.66 | 0.60 |
| 1:A:499:ILE:HG22 | 1:A:501:PRO:HD3 | 1.84 | 0.60 |
| 1:B:672:VAL:HG22 | 1:B:678:GLN:HB2 | 1.84 | 0.59 |
| 1:A:896:ASN:HB3 | 1:A:945:ASN:HB2 | 1.85 | 0.59 |
| 1:C:942:ARG:HA | 1:C:953:GLY:O | 2.03 | 0.59 |
| 1:B:836:ILE:HB | 1:B:856:TYR:HB2 | 1.84 | 0.59 |
| 1:D:928:PRO:HB2 | 1:D:973:ARG:HH11 | 1.68 | 0.59 |
| 1:D:779:PRO:O | 1:D:781:ARG:HG3 | 2.03 | 0.58 |
| 1:B:619:GLU:HA | 1:B:912:ALA:HB2 | 1.84 | 0.58 |
| 1:D:200:GLN:HG2 | 1:D:391:HIS:HB2 | 1.86 | 0.58 |
| 1:B:230:ARG:HH11 | 1:B:230:ARG:HG2 | 1.69 | 0.58 |
| 1:C:347:LYS:HE3 | 1:C:643:LEU:HB3 | 1.86 | 0.57 |
| 1:C:142:ILE:HG12 | 1:C:170:GLU:HG2 | 1.86 | 0.57 |
| 1:A:355:ASN:OD1 | 1:A:388:ARG:HD3 | 2.04 | 0.56 |
| 1:B:230:ARG:HH11 | 1:B:230:ARG:CG | 2.17 | 0.56 |
| 1:C:153:TRP:HB2 | 1:C:185:ALA:HB3 | 1.88 | 0.56 |
| 1:C:354:VAL:HG23 | 1:C:567:VAL:HB | 1.88 | 0.56 |
| 1:B:200:GLN:HG2 | 1:B:391:HIS:HB2 | 1.87 | 0.56 |
| 1:D:833:ALA:HB2 | 1:D:859:ASP:HB3 | 1.87 | 0.56 |
| 1:C:304:GLU:HG2 | 1:C:642:TYR:CD2 | 2.40 | 0.55 |
| 1:D:553:TRP:CZ2 | 1:D:624:GLN:HG2 | 2.42 | 0.55 |
| 1:B:251:ARG:H | 1:B:254:LEU:HD12 | 1.71 | 0.55 |
| 1:B:908:ASP:HB3 | 1:B:1007:PHE:CD1 | 2.41 | 0.55 |
| 1:D:656:VAL:HG21 | 1:D:685:LEU:HD22 | 1.87 | 0.55 |
| 1:B:830:LEU:HD12 | 1:B:833:ALA:HB3 | 1.89 | 0.55 |
| 1:D:788:PRO:HD2 | 1:D:968:MET:HB2 | 1.89 | 0.55 |
| 1:A:882:ILE:HD13 | 1:A:1014:TYR:CD1 | 2.41 | 0.54 |
| 1:C:769:TRP:NE1 | 1:C:774:LYS:HG3 | 2.23 | 0.54 |
| 1:B:315:LEU:HG | 1:B:323:ILE:HD12 | 1.89 | 0.54 |
| 1:B:749:ILE:N | 1:B:749:ILE:HD13 | 2.23 | 0.54 |
| 1:B:615:PRO:O | 1:B:618:THR:HG22 | 2.08 | 0.54 |
| 1:D:945:ASN:OD1 | 1:D:950:GLN:HG3 | 2.08 | 0.53 |
| 1:D:595:THR:HA | 1:D:596:PRO:C | 2.29 | 0.53 |
| 1:D:883:GLY:HA3 | 1:D:987:ASP:HA | 1.90 | 0.53 |
| 1:D:873:ALA:O | 1:D:876:THR:HG22 | 2.09 | 0.53 |
| 1:B:372:MET:HE3 | 1:B:397:LEU:HD23 | 1.90 | 0.53 |
| 1:C:304:GLU:HG2 | 1:C:642:TYR:HD2 | 1.73 | 0.53 |
| 1:D:780:LEU:HA | 1:D:886:CYS:HB3 | 1.90 | 0.53 |
| 1:B:536:CYS:O | 1:B:537:GLU:HG3 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:622:HIS:O | 1:D:625:GLN:HG3 | 2.08 | 0.52 |
| 1:D:854:LYS:HA | 1:D:867:THR:O | 2.09 | 0.52 |
| 1:C:106:PRO:HG3 | 1:C:204:ARG:HG3 | 1.90 | 0.52 |
| 1:D:246:MET:HG3 | 1:D:287:ASP:O | 2.09 | 0.52 |
| 1:A:525:SER:O | 1:B:561:ARG:HD3 | 2.10 | 0.52 |
| 1:B:782:ASP:HB2 | 1:B:842:TRP:CZ2 | 2.45 | 0.52 |
| 1:C:127:PHE:CE2 | 1:C:184:LEU:HG | 2.45 | 0.52 |
| 1:D:682:LEU:HD13 | 1:D:685:LEU:HD21 | 1.91 | 0.52 |
| 1:A:730:LEU:HD11 | 1:B:823:LEU:O | 2.10 | 0.51 |
| 1:D:867:THR:HG23 | 1:D:1015:HIS:CE1 | 2.45 | 0.51 |
| 1:B:814:GLY:HA3 | 1:B:844:HIS:CD2 | 2.44 | 0.51 |
| 1:A:52:ARG:O | 1:A:213:SER:HB2 | 2.10 | 0.51 |
| 1:D:353:GLY:HA2 | 1:D:386:ALA:O | 2.11 | 0.51 |
| 1:A:892:ALA:HB3 | 1:A:946:TYR:CE1 | 2.45 | 0.51 |
| 1:A:623:GLN:NE2 | 4:A:8002:DMS:H11 | 2.25 | 0.51 |
| 1:D:500:CYS:HA | 1:D:534:ILE:O | 2.11 | 0.51 |
| 1:B:694:LEU:HB2 | 1:B:723:ALA:O | 2.11 | 0.51 |
| 1:B:333:ARG:HH11 | 1:B:333:ARG:HG2 | 1.76 | 0.51 |
| 1:A:127:PHE:CE2 | 1:A:184:LEU:HG | 2.46 | 0.50 |
| 1:B:377:LEU:HD22 | 1:B:708:TRP:HA | 1.93 | 0.50 |
| 1:D:168:PRO:O | 1:D:442:ARG:NH2 | 2.45 | 0.50 |
| 1:D:54:LEU:HD11 | 1:D:214:LEU:HD13 | 1.92 | 0.50 |
| 1:C:150:PHE:HA | 1:C:187:MET:O | 2.12 | 0.50 |
| 1:C:525:SER:O | 1:D:561:ARG:HD3 | 2.11 | 0.49 |
| 1:D:153:TRP:HB2 | 1:D:185:ALA:HB3 | 1.94 | 0.49 |
| 1:B:892:ALA:HB3 | 1:B:946:TYR:CE1 | 2.47 | 0.49 |
| 1:C:251:ARG:H | 1:C:254:LEU:HD12 | 1.78 | 0.49 |
| 1:C:579:ASP:OD1 | 1:C:583:ASN:HB2 | 2.12 | 0.49 |
| 1:D:379:MET:HE1 | 1:D:387:VAL:HB | 1.93 | 0.49 |
| 1:B:142:ILE:HG12 | 1:B:170:GLU:HG2 | 1.94 | 0.49 |
| 1:C:330:VAL:HG22 | 5:C:4081:HOH:O | 2.12 | 0.49 |
| 1:A:782:ASP:OD1 | 1:A:842:TRP:HH2 | 1.96 | 0.49 |
| 1:C:694:LEU:HD12 | 1:C:723:ALA:HB3 | 1.93 | 0.49 |
| 1:D:549:PHE:CE2 | 1:D:620:ALA:HA | 2.48 | 0.49 |
| 1:D:88:SER:HA | 1:D:366:VAL:HG21 | 1.95 | 0.49 |
| 1:A:377:LEU:HD22 | 1:A:708:TRP:HA | 1.95 | 0.48 |
| 1:C:573:GLN:HB2 | 1:C:602:CYS:O | 2.13 | 0.48 |
| 1:D:1011:ALA:HB3 | 1:D:1014:TYR:CZ | 2.48 | 0.48 |
| 1:D:60:PHE:HA | 1:D:122:CYS:O | 2.14 | 0.48 |
| 1:A:991:MET:HE3 | 1:A:1003:VAL:HG21 | 1.94 | 0.48 |
| 1:D:471:LEU:O | 1:D:475:ILE:HG13 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:878:HIS:HB3 | 1:D:1009:LEU:O | 2.13 | 0.48 |
| 1:B:763:GLY:HA3 | 1:B:822:LEU:HD13 | 1.96 | 0.48 |
| 1:B:908:ASP:OD1 | 1:B:993:ILE:HG12 | 2.13 | 0.48 |
| 1:C:883:GLY:HA3 | 1:C:987:ASP:HA | 1.95 | 0.48 |
| 1:D:147:ASN:HA | 1:D:148:SER:HA | 1.58 | 0.48 |
| 1:A:747:PHE:HB2 | 1:A:758:PHE:HB2 | 1.96 | 0.48 |
| 1:A:991:MET:CE | 1:A:1003:VAL:HG21 | 2.43 | 0.48 |
| 1:C:854:LYS:HG2 | 1:C:868:VAL:HG13 | 1.96 | 0.48 |
| 1:A:457:SER:HA | 1:A:485:GLN:O | 2.13 | 0.47 |
| 1:C:200:GLN:HG2 | 1:C:391:HIS:HB2 | 1.95 | 0.47 |
| 1:C:373:VAL:O | 1:C:377:LEU:HG | 2.14 | 0.47 |
| 1:A:245:GLN:HG3 | 1:A:288:ARG:HG2 | 1.95 | 0.47 |
| 1:B:607:VAL:HG12 | 1:B:613:PRO:HA | 1.95 | 0.47 |
| 1:A:37:ARG:HG2 | 1:A:50:GLN:NE2 | 2.29 | 0.47 |
| 1:D:756:TRP:HB3 | 1:D:758:PHE:HE1 | 1.80 | 0.47 |
| 1:D:546:LEU:HD22 | 1:D:616:ALA:HB1 | 1.95 | 0.47 |
| 1:A:847:LYS:NZ | 1:B:724:GLU:O | 2.48 | 0.47 |
| 1:D:629:PHE:HB3 | 1:D:720:TRP:HH2 | 1.80 | 0.47 |
| 1:D:867:THR:HG23 | 1:D:1015:HIS:HE1 | 1.80 | 0.47 |
| 1:B:656:VAL:HG21 | 1:B:685:LEU:HD21 | 1.95 | 0.47 |
| 1:B:824:GLN:HB3 | 1:B:839:ALA:HB3 | 1.97 | 0.47 |
| 1:D:310:ARG:NH1 | 1:D:329:ASP:OD1 | 2.46 | 0.47 |
| 1:D:377:LEU:HD22 | 1:D:708:TRP:HA | 1.96 | 0.47 |
| 1:C:606:LEU:O | 1:C:614:HIS:HB2 | 2.15 | 0.47 |
| 1:C:377:LEU:HD22 | 1:C:708:TRP:HA | 1.97 | 0.46 |
| 1:C:804:ASN:OD1 | 1:C:809:ARG:NH2 | 2.48 | 0.46 |
| 1:A:873:ALA:O | 1:A:876:THR:HG22 | 2.16 | 0.46 |
| 1:C:168:PRO:HD3 | 1:C:446:ARG:HH11 | 1.80 | 0.46 |
| 1:C:1011:ALA:HB3 | 1:C:1014:TYR:CZ | 2.50 | 0.46 |
| 1:B:749:ILE:N | 1:B:749:ILE:CD1 | 2.79 | 0.46 |
| 1:B:549:PHE:CE2 | 1:B:620:ALA:HA | 2.50 | 0.46 |
| 1:A:830:LEU:HD12 | 1:A:833:ALA:HB3 | 1.98 | 0.46 |
| 1:D:907:PRO:HA | 1:D:910:LEU:HD23 | 1.97 | 0.46 |
| 1:B:277:GLU:CD | 1:B:277:GLU:H | 2.19 | 0.46 |
| 1:C:769:TRP:HE1 | 1:C:774:LYS:HG3 | 1.80 | 0.46 |
| 1:D:410:VAL:HG22 | 1:D:455:ILE:HB | 1.98 | 0.46 |
| 1:B:347:LYS:HB3 | 1:B:643:LEU:HD22 | 1.97 | 0.46 |
| 1:A:424:ASN:OD1 | 1:D:279:ILE:HD11 | 2.16 | 0.46 |
| 1:A:984:LEU:HD21 | 1:A:986:ILE:HD11 | 1.97 | 0.46 |
| 1:C:749:ILE:HD11 | 1:C:836:ILE:HD11 | 1.97 | 0.46 |
| 1:D:814:GLY:HA3 | 1:D:844:HIS:CG | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:863:GLN:HG2 | 1:C:1021:CYS:CB | 2.46 | 0.46 |
| 1:D:257:THR:HA | 1:D:270:GLY:O | 2.16 | 0.46 |
| 1:A:573:GLN:HB2 | 1:A:602:CYS:O | 2.16 | 0.45 |
| 1:B:589:GLY:O | 1:B:599:ARG:HA | 2.16 | 0.45 |
| 1:B:820:ALA:HB2 | 1:B:842:TRP:NE1 | 2.30 | 0.45 |
| 1:C:225:PHE:HA | 1:C:243:GLU:O | 2.16 | 0.45 |
| 1:D:613:PRO:HB3 | 1:D:617:LEU:HD23 | 1.99 | 0.45 |
| 1:D:693:GLN:HG2 | 1:D:695:TRP:NE1 | 2.31 | 0.45 |
| 1:B:741:THR:HB | 1:B:748:CYS:HB3 | 1.96 | 0.45 |
| 1:C:824:GLN:HB3 | 1:C:839:ALA:HB3 | 1.99 | 0.45 |
| 1:A:424:ASN:HB3 | 1:A:463:GLY:HA3 | 1.97 | 0.45 |
| 1:A:898:LEU:HG | 1:A:915:PHE:CZ | 2.51 | 0.45 |
| 1:D:244:VAL:HG21 | 1:D:256:VAL:HG11 | 1.98 | 0.45 |
| 1:B:163:GLN:O | 1:B:164:ASP:HB3 | 2.17 | 0.45 |
| 1:C:166:ARG:HD3 | 1:C:209:PHE:HZ | 1.81 | 0.45 |
| 1:D:163:GLN:O | 1:D:164:ASP:HB3 | 2.15 | 0.45 |
| 1:D:379:MET:CE | 1:D:387:VAL:HB | 2.46 | 0.45 |
| 1:D:996:ASP:HB2 | 1:D:1002:SER:HB2 | 1.98 | 0.45 |
| 1:B:251:ARG:HD2 | 1:B:253:TYR:CE2 | 2.52 | 0.45 |
| 1:C:43:ARG:HH12 | 1:C:264:GLU:CD | 2.20 | 0.45 |
| 4:C:8002:DMS:H21 | 5:C:4081:HOH:O | 2.16 | 0.45 |
| 1:B:301:TRP:CH2 | 1:B:452:SER:HA | 2.51 | 0.45 |
| 1:C:226:HIS:ND1 | 1:C:448:ARG:CD | 2.70 | 0.45 |
| 1:C:431:ARG:NH1 | 5:C:4073:HOH:O | 2.49 | 0.45 |
| 1:C:887:GLN:NE2 | 1:C:980:GLU:O | 2.49 | 0.45 |
| 1:D:390:SER:HA | 1:D:391:HIS:HA | 1.69 | 0.45 |
| 1:B:352:ARG:HG2 | 1:B:553:TRP:CH2 | 2.51 | 0.45 |
| 1:B:410:VAL:HG22 | 1:B:455:ILE:HB | 1.99 | 0.45 |
| 1:B:569:ASP:O | 1:B:605:GLY:HA2 | 2.17 | 0.45 |
| 1:A:147:ASN:HA | 1:A:148:SER:HA | 1.58 | 0.45 |
| 1:C:822:LEU:HD11 | 1:C:825:CYS:HB2 | 1.99 | 0.45 |
| 1:D:615:PRO:O | 1:D:618:THR:CG2 | 2.62 | 0.45 |
| 1:B:376:ILE:HD13 | 1:B:401:LEU:HB3 | 1.99 | 0.45 |
| 1:A:149:ALA:HB2 | 1:A:163:GLN:HG2 | 1.99 | 0.44 |
| 1:C:153:TRP:CD1 | 1:C:158:TRP:HA | 2.52 | 0.44 |
| 1:C:770:ILE:O | 1:C:770:ILE:HG22 | 2.16 | 0.44 |
| 1:C:782:ASP:HA | 1:C:884:LEU:HD23 | 1.98 | 0.44 |
| 1:B:610:ASP:O | 1:B:611:ARG:HB2 | 2.18 | 0.44 |
| 1:C:882:ILE:HG22 | 1:C:882:ILE:O | 2.18 | 0.44 |
| 1:C:945:ASN:OD1 | 1:C:950:GLN:HG3 | 2.17 | 0.44 |
| 1:A:600:GLN:HB2 | 1:A:603:MET:HE2 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:656:VAL:HG21 | 1:C:685:LEU:HD22 | 2.00 | 0.44 |
| 1:B:277:GLU:HG3 | 5:B:4091:HOH:O | 2.17 | 0.44 |
| 1:C:930:VAL:O | 1:C:932:PRO:HD3 | 2.17 | 0.44 |
| 1:A:127:PHE:HE2 | 1:A:184:LEU:HG | 1.83 | 0.44 |
| 1:C:780:LEU:HA | 1:C:886:CYS:HB3 | 1.99 | 0.44 |
| 1:B:49:GLN:HB2 | 1:B:50:GLN:OE1 | 2.18 | 0.44 |
| 1:B:230:ARG:CG | 1:B:230:ARG:NH1 | 2.79 | 0.44 |
| 1:B:333:ARG:HG2 | 1:B:333:ARG:NH1 | 2.33 | 0.44 |
| 1:C:749:ILE:HG12 | 1:C:834:VAL:HG11 | 2.00 | 0.43 |
| 1:D:763:GLY:O | 1:D:840:HIS:CE1 | 2.71 | 0.43 |
| 1:B:930:VAL:O | 1:B:932:PRO:HD3 | 2.17 | 0.43 |
| 1:A:105:TYR:CE2 | 1:A:199:ASP:HB2 | 2.53 | 0.43 |
| 1:A:820:ALA:HB2 | 1:A:842:TRP:NE1 | 2.33 | 0.43 |
| 1:D:43:ARG:HD2 | 1:D:261:TRP:CD2 | 2.53 | 0.43 |
| 1:D:319:ASP:HB2 | 5:D:4088:HOH:O | 2.18 | 0.43 |
| 1:A:200:GLN:HG2 | 1:A:391:HIS:HB2 | 1.99 | 0.43 |
| 1:C:414:ASN:O | 1:C:439:ARG:HD3 | 2.18 | 0.43 |
| 1:D:226:HIS:O | 1:D:242:ALA:HA | 2.18 | 0.43 |
| 1:D:747:PHE:HB2 | 1:D:758:PHE:HB2 | 2.00 | 0.43 |
| 1:B:433:LEU:N | 1:B:434:PRO:CD | 2.80 | 0.43 |
| 1:B:872:VAL:HG11 | 1:B:879:PRO:HD3 | 2.01 | 0.43 |
| 1:C:358:GLU:HG2 | 1:C:367:MET:HG3 | 2.01 | 0.43 |
| 1:A:305:ILE:HD11 | 1:A:645:ARG:HB3 | 2.00 | 0.43 |
| 1:C:444:VAL:O | 1:C:448:ARG:HB3 | 2.18 | 0.43 |
| 1:C:390:SER:HB2 | 1:C:391:HIS:CE1 | 2.52 | 0.43 |
| 1:A:997:ASP:HB2 | 1:A:999:TRP:CE2 | 2.53 | 0.43 |
| 1:C:226:HIS:CE1 | 1:C:448:ARG:HH11 | 2.37 | 0.43 |
| 1:C:863:GLN:HG2 | 1:C:1021:CYS:HB3 | 2.00 | 0.43 |
| 1:B:894:ARG:NH1 | 1:B:921:PRO:HD3 | 2.33 | 0.43 |
| 1:D:105:TYR:CE2 | 1:D:199:ASP:HB2 | 2.54 | 0.43 |
| 1:D:446:ARG:HD2 | 5:D:4142:HOH:O | 2.18 | 0.43 |
| 1:B:745:MET:HE3 | 1:B:745:MET:H | 1.84 | 0.43 |
| 1:B:879:PRO:O | 1:B:1009:LEU:HD12 | 2.18 | 0.43 |
| 1:C:78:LEU:HA | 1:C:79:PRO:HD3 | 1.87 | 0.42 |
| 1:C:124:SER:HA | 1:C:184:LEU:O | 2.19 | 0.42 |
| 1:C:359:HIS:CD2 | 1:C:573:GLN:HA | 2.54 | 0.42 |
| 1:A:634:GLN:HB2 | 1:A:682:LEU:HB2 | 2.01 | 0.42 |
| 1:D:486:TYR:CE2 | 1:D:488:GLY:HA3 | 2.54 | 0.42 |
| 1:B:736:ALA:HB1 | 1:B:751:LEU:HD11 | 2.00 | 0.42 |
| 1:C:147:ASN:HA | 1:C:148:SER:HA | 1.59 | 0.42 |
| 1:C:536:CYS:O | 1:C:537:GLU:HG3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:454:ILE:HG13 | 1:A:455:ILE:HG13 | 2.01 | 0.42 |
| 1:A:359:HIS:CD2 | 1:A:573:GLN:HA | 2.55 | 0.42 |
| 1:C:331:GLY:H | 4:C:8002:DMS:C2 | 2.30 | 0.42 |
| 1:C:986:ILE:HG21 | 1:C:1018:LEU:HD11 | 2.02 | 0.42 |
| 1:B:854:LYS:HA | 1:B:867:THR:O | 2.20 | 0.42 |
| 1:A:794:GLY:HA2 | 1:A:998:SER:O | 2.20 | 0.42 |
| 1:A:878:HIS:HD2 | 5:A:4165:HOH:O | 2.01 | 0.42 |
| 1:C:222:ILE:N | 1:C:324:GLU:OE1 | 2.49 | 0.42 |
| 1:C:996:ASP:HB2 | 1:C:1002:SER:HB2 | 2.02 | 0.42 |
| 1:D:499:ILE:HG22 | 1:D:501:PRO:HD3 | 2.01 | 0.42 |
| 1:A:355:ASN:O | 1:A:569:ASP:HB2 | 2.19 | 0.42 |
| 1:C:907:PRO:HG2 | 1:C:990:HIS:O | 2.20 | 0.42 |
| 1:A:928:PRO:HB2 | 1:A:973:ARG:HH11 | 1.84 | 0.42 |
| 1:C:281:GLU:HG3 | 1:B:515:VAL:HG21 | 2.02 | 0.42 |
| 1:C:353:GLY:HA2 | 1:C:386:ALA:O | 2.20 | 0.42 |
| 1:C:522:LYS:HA | 1:D:559:TYR:CE2 | 2.55 | 0.42 |
| 1:B:747:PHE:HB2 | 1:B:758:PHE:HB2 | 2.00 | 0.42 |
| 1:B:755:ARG:HB3 | 1:B:769:TRP:HB2 | 2.01 | 0.42 |
| 1:C:499:ILE:O | 1:C:533:LEU:HA | 2.20 | 0.42 |
| 1:D:361:PRO:HB3 | 1:D:609:ALA:HB1 | 2.02 | 0.42 |
| 1:D:536:CYS:O | 1:D:537:GLU:HG3 | 2.20 | 0.42 |
| 1:D:737:ILE:HA | 1:D:738:PRO:HD3 | 1.89 | 0.42 |
| 1:B:599:ARG:HB2 | 1:B:600:GLN:NE2 | 2.35 | 0.42 |
| 1:A:291:LEU:HA | 4:A:8004:DMS:O | 2.20 | 0.41 |
| 1:A:336:ARG:HH21 | 1:A:338:GLU:CD | 2.24 | 0.41 |
| 1:A:477:SER:OG | 1:D:469:ASP:OD2 | 2.38 | 0.41 |
| 1:D:738:PRO:HB2 | 1:D:834:VAL:HG23 | 2.02 | 0.41 |
| 1:C:464:HIS:HB2 | 1:C:489:GLY:HA3 | 2.02 | 0.41 |
| 1:D:629:PHE:HB3 | 1:D:720:TRP:CH2 | 2.55 | 0.41 |
| 1:B:390:SER:HA | 1:B:391:HIS:HA | 1.74 | 0.41 |
| 1:D:437:SER:CB | 1:D:471:LEU:HD21 | 2.49 | 0.41 |
| 1:D:844:HIS:HA | 5:D:4126:HOH:O | 2.19 | 0.41 |
| 1:C:18:ASN:ND2 | 1:C:21:VAL:HG23 | 2.35 | 0.41 |
| 1:B:78:LEU:HA | 1:B:79:PRO:HD3 | 1.84 | 0.41 |
| 1:C:892:ALA:HB3 | 1:C:946:TYR:CE1 | 2.56 | 0.41 |
| 1:D:780:LEU:HD11 | 1:D:884:LEU:HD13 | 2.02 | 0.41 |
| 1:C:390:SER:HA | 1:C:391:HIS:HA | 1.75 | 0.41 |
| 1:D:123:TYR:CE1 | 1:D:208:ILE:HG13 | 2.56 | 0.41 |
| 1:C:796:SER:HB2 | 1:C:802:ASP:HB3 | 2.03 | 0.41 |
| 1:C:830:LEU:HD23 | 1:D:830:LEU:HD21 | 2.03 | 0.41 |
| 1:D:78:LEU:HA | 1:D:79:PRO:HD3 | 1.92 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:556:PHE:CD1 | 1:A:564:GLY:HA2 | 2.56 | 0.41 |
| 1:C:460:SER:O | 1:C:461:GLU:C | 2.59 | 0.41 |
| 1:D:144:ASP:OD1 | 1:D:168:PRO:HB3 | 2.21 | 0.41 |
| 1:D:650:GLU:HB3 | 1:D:670:LEU:HD12 | 2.03 | 0.41 |
| 1:A:390:SER:HA | 1:A:391:HIS:HA | 1.71 | 0.41 |
| 1:A:878:HIS:CE1 | 1:A:1010:SER:HB3 | 2.56 | 0.41 |
| 1:C:594:ASP:OD1 | 1:C:594:ASP:N | 2.43 | 0.41 |
| 1:D:499:ILE:HD11 | 1:D:529:GLU:CD | 2.41 | 0.41 |
| 1:D:751:LEU:HD11 | 1:D:860:GLY:HA2 | 2.03 | 0.41 |
| 1:B:426:LEU:HD22 | 1:B:432:TRP:CE2 | 2.56 | 0.41 |
| 1:C:200:GLN:CG | 1:C:391:HIS:HB2 | 2.51 | 0.41 |
| 1:C:426:LEU:HD22 | 1:C:432:TRP:CE2 | 2.56 | 0.41 |
| 1:C:782:ASP:HB2 | 1:C:842:TRP:CZ2 | 2.56 | 0.41 |
| 1:A:257:THR:HA | 1:A:270:GLY:O | 2.21 | 0.40 |
| 1:A:337:ILE:HA | 1:A:341:LEU:O | 2.21 | 0.40 |
| 1:B:147:ASN:HA | 1:B:148:SER:HA | 1.70 | 0.40 |
| 1:A:58:TRP:CD1 | 1:A:125:LEU:HD13 | 2.55 | 0.40 |
| 1:D:568:TRP:HA | 1:D:569:ASP:HA | 1.91 | 0.40 |
| 1:C:433:LEU:HB3 | 1:C:434:PRO:HD3 | 2.03 | 0.40 |
| 1:D:767:GLN:OE1 | 1:D:775:GLN:N | 2.47 | 0.40 |
| 1:B:785:THR:HB | 1:B:816:TYR:CE2 | 2.56 | 0.40 |
| 1:B:962:TYR:CE2 | 1:B:976:LEU:HB3 | 2.57 | 0.40 |
| 1:A:883:GLY:HA3 | 1:A:987:ASP:HA | 2.04 | 0.40 |
| 1:C:352:ARG:HG2 | 1:C:553:TRP:CH2 | 2.57 | 0.40 |
| 1:C:450:HIS:HA | 1:C:451:PRO:HD2 | 1.97 | 0.40 |
| 1:C:936:GLY:O | 1:C:938:ARG:NH1 | 2.51 | 0.40 |
| 1:A:738:PRO:HB2 | 1:A:834:VAL:HG23 | 2.04 | 0.40 |
| 1:C:578:TYR:HA | 1:C:583:ASN:O | 2.22 | 0.40 |
| 1:C:869:ASP:OD2 | 1:C:1015:HIS:ND1 | 2.34 | 0.40 |
| 1:D:513:PRO:O | 1:D:514:ALA:HB3 | 2.22 | 0.40 |
| 1:B:30:HIS:HE2 | 1:B:170:GLU:CD | 2.25 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 1009/1052 (96%) | 972 (96%) | 37 (4%) | 0 | 100 | 100 |
| 1 | B | 1009/1052 (96%) | 965 (96%) | 41 (4%) | 3 (0%) | 41 | 66 |
| 1 | C | 1009/1052 (96%) | 947 (94%) | 56 (6%) | 6 (1%) | 25 | 50 |
| 1 | D | 1009/1052 (96%) | 935 (93%) | 74 (7%) | 0 | 100 | 100 |
| All | All | 4036/4208 (96%) | 3819 (95%) | 208 (5%) | 9 (0%) | 47 | 73 |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 461 | GLU |
| 1 | C | 659 | ASP |
| 1 | C | 722 | LEU |
| 1 | B | 916 | ASP |
| 1 | B | 540 | HIS |
| 1 | C | 633 | GLY |
| 1 | C | 540 | HIS |
| 1 | B | 263 | GLY |
| 1 | C | 364 | GLY |

### 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 | 864/898 (96%) | 844 (98%) | 20 (2%) | 50 | 78 |
| 1 | B | 864/898 (96%) | 836 (97%) | 28 (3%) | 39 | 68 |
| 1 | C | 864/898 (96%) | 850 (98%) | 14 (2%) | 62 | 85 |
| 1 | D | 864/898 (96%) | 842 (98%) | 22 (2%) | 47 | 76 |
| All | All | 3456/3592 (96%) | 3372 (98%) | 84 (2%) | 49 | 77 |

All (84) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 136 | GLU |
| 1 | A | 178 | ARG |
| 1 | A | 189 | LEU |
| 1 | A | 262 | GLN |
| 1 | A | 333 | ARG |
| 1 | A | 477 | SER |
| 1 | A | 519 | SER |
| 1 | A | 604 | ASN |
| 1 | A | 614 | HIS |
| 1 | A | 634 | GLN |
| 1 | A | 651 | LEU |
| 1 | A | 661 | LYS |
| 1 | A | 665 | SER |
| 1 | A | 737 | ILE |
| 1 | A | 761 | GLN |
| 1 | A | 768 | MET |
| 1 | A | 774 | LYS |
| 1 | A | 824 | GLN |
| 1 | A | 863 | GLN |
| 1 | A | 885 | ASN |
| 1 | C | 44 | THR |
| 1 | C | 178 | ARG |
| 1 | C | 211 | ASP |
| 1 | C | 219 | THR |
| 1 | C | 223 | SER |
| 1 | C | 333 | ARG |
| 1 | C | 546 | LEU |
| 1 | C | 646 | HIS |
| 1 | C | 728 | VAL |
| 1 | C | 737 | ILE |
| 1 | C | 745 | MET |
| 1 | C | 746 | ASP |
| 1 | C | 848 | THR |
| 1 | C | 885 | ASN |
| 1 | D | 178 | ARG |
| 1 | D | 214 | LEU |
| 1 | D | 241 | GLU |
| 1 | D | 245 | GLN |
| 1 | D | 333 | ARG |
| 1 | D | 545 | SER |
| 1 | D | 546 | LEU |
| 1 | D | 635 | THR |
| 1 | D | 646 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 651 | LEU |
| 1 | D | 655 | MET |
| 1 | D | 675 | GLN |
| 1 | D | 690 | SER |
| 1 | D | 737 | ILE |
| 1 | D | 745 | MET |
| 1 | D | 748 | CYS |
| 1 | D | 751 | LEU |
| 1 | D | 772 | ASP |
| 1 | D | 837 | THR |
| 1 | D | 848 | THR |
| 1 | D | 855 | THR |
| 1 | D | 984 | LEU |
| 1 | B | 71 | GLU |
| 1 | B | 124 | SER |
| 1 | B | 136 | GLU |
| 1 | B | 178 | ARG |
| 1 | B | 219 | THR |
| 1 | B | 234 | ASP |
| 1 | B | 252 | ASP |
| 1 | B | 321 | THR |
| 1 | B | 333 | ARG |
| 1 | B | 344 | LEU |
| 1 | B | 362 | LEU |
| 1 | B | 519 | SER |
| 1 | B | 546 | LEU |
| 1 | B | 594 | ASP |
| 1 | B | 600 | GLN |
| 1 | B | 634 | GLN |
| 1 | B | 651 | LEU |
| 1 | B | 675 | GLN |
| 1 | B | 728 | VAL |
| 1 | B | 745 | MET |
| 1 | B | 749 | ILE |
| 1 | B | 761 | GLN |
| 1 | B | 772 | ASP |
| 1 | B | 796 | SER |
| 1 | B | 809 | ARG |
| 1 | B | 855 | THR |
| 1 | B | 910 | LEU |
| 1 | B | 956 | GLN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 226 | HIS |
| 1 | A | 307 | ASN |
| 1 | C | 245 | GLN |
| 1 | C | 623 | GLN |
| 1 | C | 878 | HIS |
| 1 | D | 418 | HIS |
| 1 | D | 540 | HIS |
| 1 | B | 93 | HIS |
| 1 | B | 1015 | HIS |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 43 ligands modelled in this entry, 19 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 4 | DMS | B | 8002 | - | 3,3,3 | 2.65 | 1 (33%) | 3,3,3 | 0.51 | 0 |
| 4 | DMS | A | 8002 | - | 3,3,3 | 2.55 | 1 (33%) | 3,3,3 | 0.43 | 0 |
| 4 | DMS | A | 8004 | - | 3,3,3 | 2.61 | 1 (33%) | 3,3,3 | 0.67 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 4 | DMS | B | 8001 | - | 3,3,3 | 2.69 | 1 (33%) | 3,3,3 | 0.63 | 0 |
| 4 | DMS | C | 8003 | - | 3,3,3 | 2.67 | 1 (33%) | 3,3,3 | 0.58 | 0 |
| 4 | DMS | A | 8008 | - | 3,3,3 | 2.67 | 1 (33%) | 3,3,3 | 0.58 | 0 |
| 4 | DMS | D | 8005 | - | 3,3,3 | 2.58 | 1 (33%) | 3,3,3 | 0.59 | 0 |
| 4 | DMS | D | 8003 | - | 3,3,3 | 2.69 | 1 (33%) | 3,3,3 | 0.47 | 0 |
| 4 | DMS | C | 8002 | - | 3,3,3 | 2.67 | 1 (33%) | 3,3,3 | 0.62 | 0 |
| 4 | DMS | D | 8004 | - | 3,3,3 | 2.64 | 1 (33%) | 3,3,3 | 0.55 | 0 |
| 4 | DMS | D | 8006 | - | 3,3,3 | 2.70 | 1 (33%) | 3,3,3 | 0.52 | 0 |
| 4 | DMS | B | 8003 | - | 3,3,3 | 2.66 | 1 (33%) | 3,3,3 | 0.49 | 0 |
| 4 | DMS | D | 8002 | - | 3,3,3 | 2.61 | 1 (33%) | 3,3,3 | 0.38 | 0 |
| 4 | DMS | C | 8004 | - | 3,3,3 | 2.62 | 1 (33%) | 3,3,3 | 0.49 | 0 |
| 4 | DMS | A | 8005 | - | 3,3,3 | 2.70 | 1 (33%) | 3,3,3 | 0.58 | 0 |
| 4 | DMS | A | 8006 | - | 3,3,3 | 2.72 | 1 (33%) | 3,3,3 | 0.64 | 0 |
| 4 | DMS | A | 8001 | - | 3,3,3 | 2.62 | 1 (33%) | 3,3,3 | 0.59 | 0 |
| 4 | DMS | B | 8004 | - | 3,3,3 | 1.66 | 1 (33%) | 3,3,3 | 0.36 | 0 |
| 4 | DMS | A | 8007 | - | 3,3,3 | 2.73 | 1 (33%) | 3,3,3 | 0.70 | 0 |
| 4 | DMS | C | 8005 | - | 3,3,3 | 2.68 | 1 (33%) | 3,3,3 | 0.59 | 0 |
| 4 | DMS | C | 8006 | - | 3,3,3 | 2.74 | 1 (33%) | 3,3,3 | 0.66 | 0 |
| 4 | DMS | A | 8003 | - | 3,3,3 | 2.65 | 1 (33%) | 3,3,3 | 0.70 | 0 |
| 4 | DMS | D | 8001 | - | 3,3,3 | 2.69 | 1 (33%) | 3,3,3 | 0.55 | 0 |
| 4 | DMS | C | 8001 | - | 3,3,3 | 2.66 | 1 (33%) | 3,3,3 | 0.61 | 0 |

All (24) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | A | 8007 | DMS | O-S | 4.57 | 1.81 | 1.50 |
| 4 | C | 8006 | DMS | O-S | 4.57 | 1.81 | 1.50 |
| 4 | A | 8006 | DMS | O-S | 4.56 | 1.81 | 1.50 |
| 4 | A | 8005 | DMS | O-S | 4.54 | 1.80 | 1.50 |
| 4 | D | 8006 | DMS | O-S | 4.53 | 1.80 | 1.50 |
| 4 | D | 8003 | DMS | O-S | 4.51 | 1.80 | 1.50 |
| 4 | C | 8002 | DMS | O-S | 4.50 | 1.80 | 1.50 |
| 4 | D | 8001 | DMS | O-S | 4.50 | 1.80 | 1.50 |
| 4 | B | 8001 | DMS | O-S | 4.49 | 1.80 | 1.50 |
| 4 | C | 8005 | DMS | O-S | 4.48 | 1.80 | 1.50 |
| 4 | A | 8008 | DMS | O-S | 4.47 | 1.80 | 1.50 |
| 4 | C | 8003 | DMS | O-S | 4.46 | 1.80 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | A | 8003 | DMS | O-S | 4.46 | 1.80 | 1.50 |
| 4 | B | 8003 | DMS | O-S | 4.45 | 1.80 | 1.50 |
| 4 | C | 8001 | DMS | O-S | 4.45 | 1.80 | 1.50 |
| 4 | B | 8002 | DMS | O-S | 4.44 | 1.80 | 1.50 |
| 4 | D | 8004 | DMS | O-S | 4.43 | 1.80 | 1.50 |
| 4 | C | 8004 | DMS | O-S | 4.41 | 1.80 | 1.50 |
| 4 | A | 8001 | DMS | O-S | 4.41 | 1.80 | 1.50 |
| 4 | D | 8002 | DMS | O-S | 4.40 | 1.80 | 1.50 |
| 4 | A | 8004 | DMS | O-S | 4.36 | 1.79 | 1.50 |
| 4 | A | 8002 | DMS | O-S | 4.31 | 1.79 | 1.50 |
| 4 | D | 8005 | DMS | O-S | 4.31 | 1.79 | 1.50 |
| 4 | B | 8004 | DMS | O-S | 2.81 | 1.69 | 1.50 |

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | A | 8002 | DMS | 1 | 0 |
| 4 | A | 8004 | DMS | 1 | 0 |
| 4 | C | 8002 | DMS | 3 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

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

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 1011/1052 (96%) | -0.17 | 22 (2%) | 62 | 63 | 24, 43, 79, 114 | 0 |
| 1 | B | 1011/1052 (96%) | -0.04 | 26 (2%) | 56 | 57 | 28, 51, 75, 111 | 0 |
| 1 | C | 1011/1052 (96%) | 0.08 | 42 (4%) | 36 | 35 | 30, 56, 87, 123 | 0 |
| 1 | D | 1011/1052 (96%) | 0.06 | 51 (5%) | 28 | 27 | 27, 48, 94, 127 | 0 |
| All | All | 4044/4208 (96%) | -0.02 | 141 (3%) | 44 | 44 | 24, 50, 84, 127 | 0 |

All (141) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 689 | GLU | 6.5 |
| 1 | D | 732 | ALA | 5.5 |
| 1 | D | 833 | ALA | 5.5 |
| 1 | C | 685 | LEU | 5.4 |
| 1 | D | 771 | GLY | 5.0 |
| 1 | C | 689 | GLU | 4.9 |
| 1 | D | 770 | ILE | 4.8 |
| 1 | D | 745 | MET | 4.8 |
| 1 | D | 737 | ILE | 4.8 |
| 1 | A | 685 | LEU | 4.5 |
| 1 | A | 733 | ALA | 4.5 |
| 1 | D | 733 | ALA | 4.4 |
| 1 | C | 687 | GLN | 4.3 |
| 1 | C | 800 | ARG | 4.3 |
| 1 | B | 686 | PRO | 4.2 |
| 1 | A | 686 | PRO | 4.1 |
| 1 | C | 671 | ASP | 4.1 |
| 1 | C | 731 | PRO | 4.0 |
| 1 | B | 799 | THR | 4.0 |
| 1 | B | 733 | ALA | 4.0 |
| 1 | D | 735 | HIS | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 735 | HIS | 3.9 |
| 1 | C | 732 | ALA | 3.8 |
| 1 | C | 673 | ALA | 3.8 |
| 1 | D | 798 | ALA | 3.8 |
| 1 | A | 583 | ASN | 3.6 |
| 1 | C | 580 | GLU | 3.6 |
| 1 | B | 687 | GLN | 3.5 |
| 1 | C | 739 | HIS | 3.5 |
| 1 | C | 831 | ALA | 3.4 |
| 1 | C | 684 | GLU | 3.3 |
| 1 | D | 948 | PRO | 3.3 |
| 1 | C | 733 | ALA | 3.3 |
| 1 | B | 666 | GLY | 3.2 |
| 1 | C | 737 | ILE | 3.2 |
| 1 | A | 800 | ARG | 3.2 |
| 1 | B | 682 | LEU | 3.2 |
| 1 | D | 761 | GLN | 3.2 |
| 1 | D | 832 | ASP | 3.1 |
| 1 | D | 982 | THR | 3.1 |
| 1 | D | 730 | LEU | 3.1 |
| 1 | A | 977 | HIS | 3.1 |
| 1 | D | 689 | GLU | 3.1 |
| 1 | B | 831 | ALA | 3.0 |
| 1 | C | 666 | GLY | 3.0 |
| 1 | D | 685 | LEU | 2.9 |
| 1 | A | 734 | SER | 2.9 |
| 1 | D | 734 | SER | 2.9 |
| 1 | C | 667 | GLU | 2.9 |
| 1 | D | 738 | PRO | 2.9 |
| 1 | A | 732 | ALA | 2.9 |
| 1 | C | 772 | ASP | 2.9 |
| 1 | D | 981 | GLY | 2.8 |
| 1 | C | 78 | LEU | 2.8 |
| 1 | C | 736 | ALA | 2.8 |
| 1 | D | 740 | LEU | 2.8 |
| 1 | D | 736 | ALA | 2.8 |
| 1 | D | 580 | GLU | 2.8 |
| 1 | B | 684 | GLU | 2.8 |
| 1 | C | 579 | ASP | 2.8 |
| 1 | C | 669 | PRO | 2.7 |
| 1 | D | 892 | ALA | 2.7 |
| 1 | C | 681 | GLU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 761 | GLN | 2.7 |
| 1 | D | 772 | ASP | 2.7 |
| 1 | B | 636 | ILE | 2.7 |
| 1 | C | 655 | MET | 2.7 |
| 1 | D | 977 | HIS | 2.7 |
| 1 | D | 1023 | LYS | 2.7 |
| 1 | B | 79 | PRO | 2.7 |
| 1 | B | 68 | ALA | 2.7 |
| 1 | A | 1023 | LYS | 2.6 |
| 1 | D | 891 | VAL | 2.6 |
| 1 | D | 753 | ASN | 2.6 |
| 1 | B | 1023 | LYS | 2.6 |
| 1 | C | 690 | SER | 2.6 |
| 1 | B | 595 | THR | 2.6 |
| 1 | B | 633 | GLY | 2.6 |
| 1 | B | 78 | LEU | 2.6 |
| 1 | D | 746 | ASP | 2.5 |
| 1 | D | 834 | VAL | 2.5 |
| 1 | B | 689 | GLU | 2.5 |
| 1 | D | 848 | THR | 2.5 |
| 1 | C | 668 | VAL | 2.5 |
| 1 | A | 846 | GLY | 2.5 |
| 1 | C | 1023 | LYS | 2.5 |
| 1 | A | 772 | ASP | 2.5 |
| 1 | C | 686 | PRO | 2.5 |
| 1 | D | 683 | PRO | 2.5 |
| 1 | C | 663 | LEU | 2.5 |
| 1 | D | 839 | ALA | 2.5 |
| 1 | C | 688 | PRO | 2.5 |
| 1 | A | 827 | ALA | 2.5 |
| 1 | C | 104 | THR | 2.4 |
| 1 | D | 820 | ALA | 2.4 |
| 1 | D | 841 | ALA | 2.4 |
| 1 | D | 801 | ILE | 2.4 |
| 1 | B | 680 | ILE | 2.4 |
| 1 | D | 773 | LYS | 2.4 |
| 1 | B | 734 | SER | 2.4 |
| 1 | C | 799 | THR | 2.4 |
| 1 | D | 78 | LEU | 2.4 |
| 1 | B | 262 | GLN | 2.3 |
| 1 | C | 79 | PRO | 2.3 |
| 1 | D | 752 | GLY | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 653 | HIS | 2.3 |
| 1 | A | 582 | GLY | 2.2 |
| 1 | D | 684 | GLU | 2.2 |
| 1 | B | 889 | ALA | 2.2 |
| 1 | B | 771 | GLY | 2.2 |
| 1 | B | 801 | ILE | 2.2 |
| 1 | D | 579 | ASP | 2.2 |
| 1 | B | 670 | LEU | 2.2 |
| 1 | A | 684 | GLU | 2.2 |
| 1 | C | 680 | ILE | 2.2 |
| 1 | C | 581 | ASN | 2.2 |
| 1 | C | 178 | ARG | 2.2 |
| 1 | D | 1022 | GLN | 2.2 |
| 1 | B | 803 | PRO | 2.2 |
| 1 | D | 799 | THR | 2.2 |
| 1 | D | 757 | GLN | 2.2 |
| 1 | C | 97 | ALA | 2.2 |
| 1 | C | 735 | HIS | 2.2 |
| 1 | B | 115 | PRO | 2.2 |
| 1 | A | 632 | SER | 2.1 |
| 1 | D | 590 | GLY | 2.1 |
| 1 | D | 687 | GLN | 2.1 |
| 1 | D | 800 | ARG | 2.1 |
| 1 | A | 593 | GLY | 2.1 |
| 1 | D | 584 | PRO | 2.1 |
| 1 | D | 980 | GLU | 2.1 |
| 1 | C | 652 | LEU | 2.1 |
| 1 | A | 744 | GLU | 2.1 |
| 1 | D | 610 | ASP | 2.1 |
| 1 | C | 701 | VAL | 2.1 |
| 1 | A | 664 | ALA | 2.1 |
| 1 | A | 580 | GLU | 2.1 |
| 1 | C | 662 | PRO | 2.0 |
| 1 | D | 686 | PRO | 2.0 |
| 1 | B | 798 | ALA | 2.0 |
| 1 | C | 730 | LEU | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | NA | D | 3101 | 1/1 | 0.75 | 0.18 | 55,55,55,55 | 0 |
| 3 | NA | C | 3101 | 1/1 | 0.79 | 0.11 | 57,57,57,57 | 0 |
| 3 | NA | C | 3103 | 1/1 | 0.80 | 0.14 | 62,62,62,62 | 0 |
| 3 | NA | B | 3101 | 1/1 | 0.80 | 0.12 | 55,55,55,55 | 0 |
| 2 | MG | B | 3001 | 1/1 | 0.88 | 0.06 | 50,50,50,50 | 0 |
| 4 | DMS | C | 8001 | 4/4 | 0.88 | 0.24 | 75,77,79,80 | 0 |
| 3 | NA | C | 3102 | 1/1 | 0.90 | 0.14 | 41,41,41,41 | 0 |
| 4 | DMS | C | 8003 | 4/4 | 0.91 | 0.30 | 83,84,85,86 | 0 |
| 2 | MG | C | 3002 | 1/1 | 0.93 | 0.10 | 54,54,54,54 | 0 |
| 3 | NA | B | 3102 | 1/1 | 0.93 | 0.15 | 35,35,35,35 | 0 |
| 3 | NA | A | 3103 | 1/1 | 0.93 | 0.12 | 59,59,59,59 | 0 |
| 3 | NA | D | 3102 | 1/1 | 0.93 | 0.15 | 34,34,34,34 | 0 |
| 2 | MG | C | 3001 | 1/1 | 0.94 | 0.09 | 42,42,42,42 | 0 |
| 4 | DMS | A | 8007 | 4/4 | 0.95 | 0.16 | 57,58,59,67 | 0 |
| 4 | DMS | A | 8008 | 4/4 | 0.95 | 0.14 | 81,82,83,86 | 0 |
| 2 | MG | D | 3002 | 1/1 | 0.95 | 0.09 | 42,42,42,42 | 0 |
| 3 | NA | B | 3103 | 1/1 | 0.95 | 0.23 | 58,58,58,58 | 0 |
| 4 | DMS | C | 8005 | 4/4 | 0.95 | 0.21 | 63,64,64,65 | 0 |
| 4 | DMS | C | 8006 | 4/4 | 0.95 | 0.27 | 65,65,66,70 | 0 |
| 4 | DMS | D | 8006 | 4/4 | 0.95 | 0.15 | 58,60,62,65 | 0 |
| 4 | DMS | B | 8003 | 4/4 | 0.95 | 0.15 | 63,65,67,68 | 0 |
| 4 | DMS | B | 8004 | 4/4 | 0.95 | 0.15 | 43,46,46,46 | 0 |
| 2 | MG | B | 3002 | 1/1 | 0.96 | 0.06 | 56,56,56,56 | 0 |
| 2 | MG | D | 3001 | 1/1 | 0.96 | 0.08 | 39,39,39,39 | 0 |
| 4 | DMS | D | 8005 | 4/4 | 0.96 | 0.20 | 53,56,57,61 | 0 |
| 4 | DMS | A | 8001 | 4/4 | 0.96 | 0.22 | 71,71,72,74 | 0 |
| 4 | DMS | C | 8002 | 4/4 | 0.96 | 0.20 | 49,53,53,55 | 0 |
| 4 | DMS | A | 8004 | 4/4 | 0.96 | 0.27 | 60,61,63,64 | 0 |
| 3 | NA | A | 3101 | 1/1 | 0.97 | 0.10 | 51,51,51,51 | 0 |
| 4 | DMS | C | 8004 | 4/4 | 0.97 | 0.18 | 53,54,55,56 | 0 |
| 4 | DMS | B | 8001 | 4/4 | 0.97 | 0.14 | 64,66,67,70 | 0 |
| 4 | DMS | B | 8002 | 4/4 | 0.97 | 0.18 | 58,59,61,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 4 | DMS | D | 8003 | 4/4 | 0.97 | 0.15 | 66,67,68,69 | 0 |
| 4 | DMS | D | 8004 | 4/4 | 0.97 | 0.19 | 74,75,76,76 | 0 |
| 4 | DMS | A | 8006 | 4/4 | 0.98 | 0.14 | 56,58,59,63 | 0 |
| 3 | NA | A | 3102 | 1/1 | 0.98 | 0.10 | 34,34,34,34 | 0 |
| 4 | DMS | A | 8002 | 4/4 | 0.98 | 0.20 | 53,53,53,54 | 0 |
| 2 | MG | A | 3002 | 1/1 | 0.98 | 0.08 | 43,43,43,43 | 0 |
| 4 | DMS | D | 8001 | 4/4 | 0.98 | 0.22 | 56,56,56,58 | 0 |
| 4 | DMS | D | 8002 | 4/4 | 0.98 | 0.30 | 58,62,62,63 | 0 |
| 4 | DMS | A | 8005 | 4/4 | 0.98 | 0.12 | 56,56,57,60 | 0 |
| 4 | DMS | A | 8003 | 4/4 | 0.99 | 0.17 | 44,45,47,47 | 0 |
| 2 | MG | A | 3001 | 1/1 | 0.99 | 0.05 | 51,51,51,51 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.