



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2022 – 12:08 PM JST

PDB ID : 7EAV
Title : The X-ray crystallographic structure of glycogen debranching enzyme from *Sulfolobus solfataricus* STB09
Authors : Li, Z.F.; Ban, X.F.; Tian, Y.X.; Li, C.M.; Cheng, L.; Hong, Y.; Gu, Z.B.
Deposited on : 2021-03-08
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
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)	:	2.27

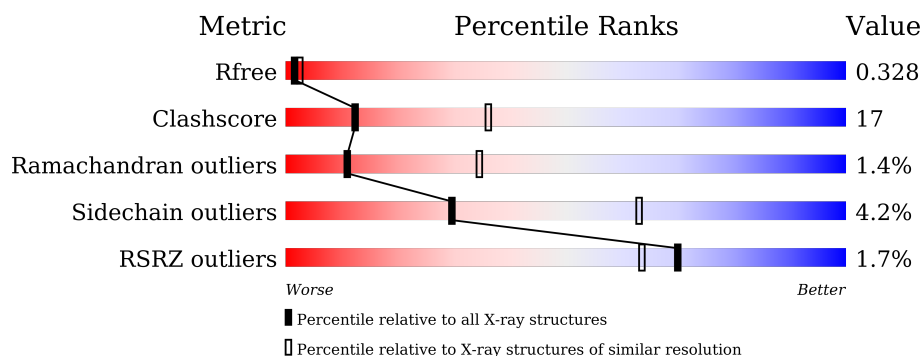
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	718	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>.</div> </div> </div>
1	B	718	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>..</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11872 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 Glycogen debranching enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5848	3753	985	1091	19			
1	B	714	Total	C	N	O	S	0	0	0
			5844	3749	985	1091	19			

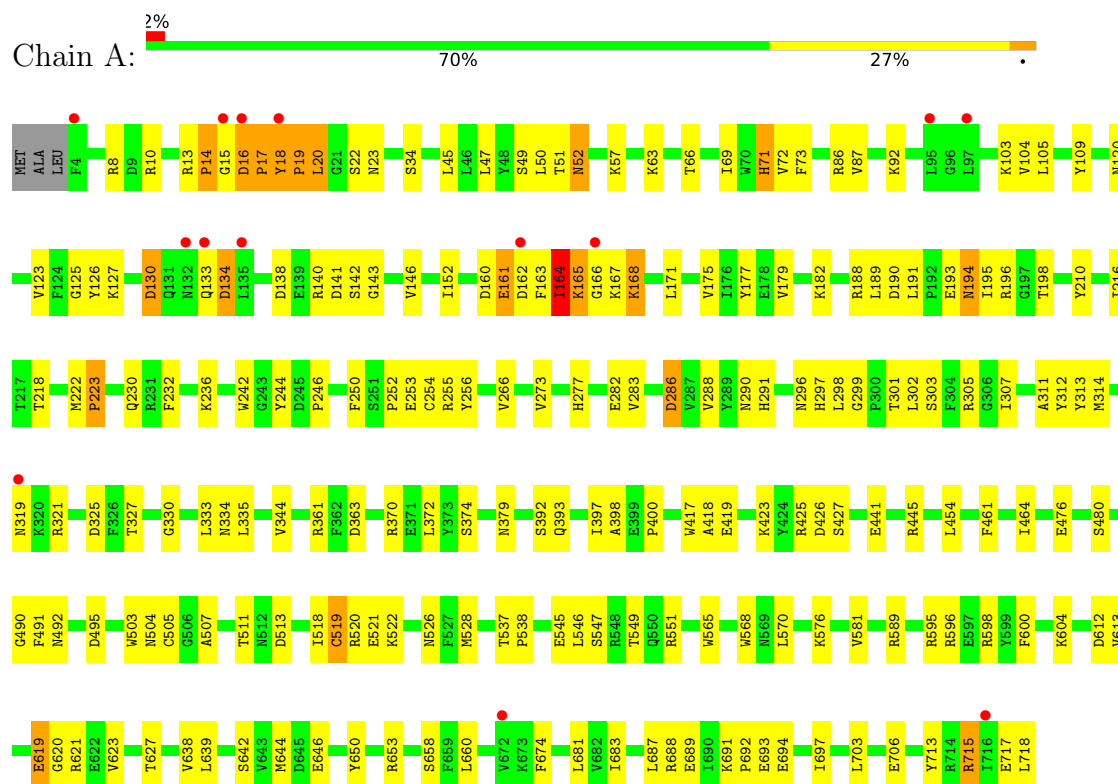
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total	O	0	0
			90	90		
2	B	90	Total	O	0	0
			90	90		

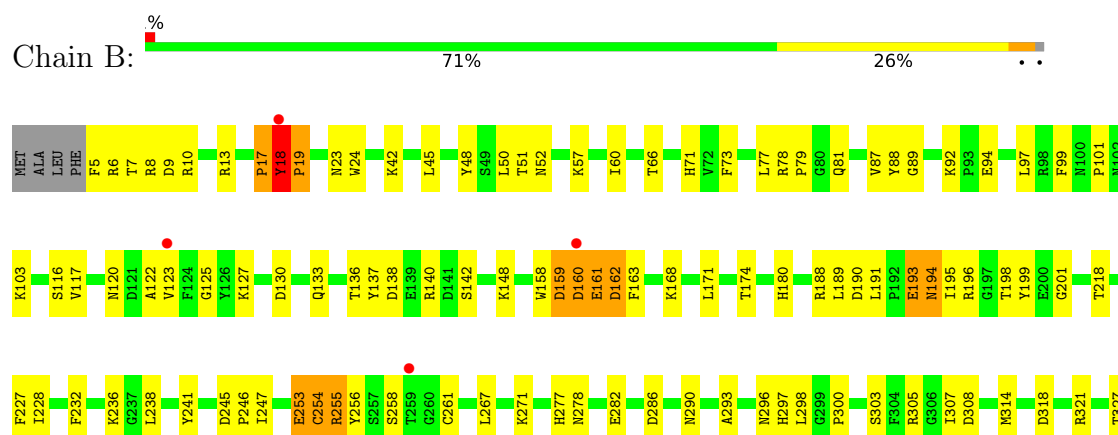
3 Residue-property plots

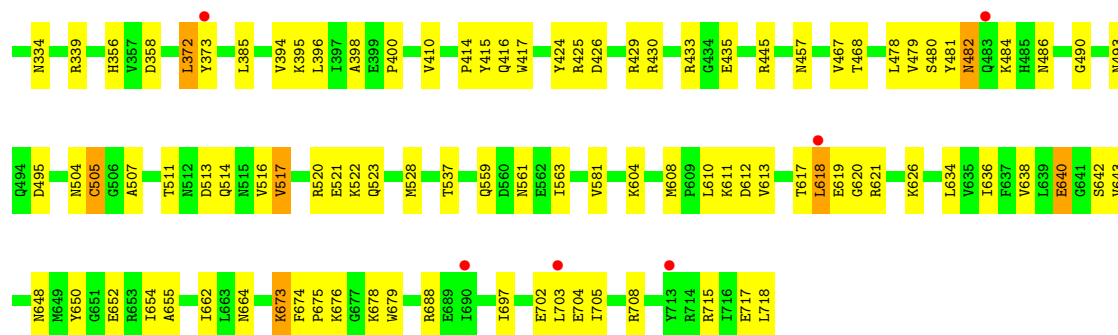
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Glycogen debranching enzyme



• Molecule 1: Glycogen debranching enzyme





4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.54Å 203.54Å 89.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.11 – 2.80 49.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.11-2.80) 99.0 (49.11-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.264 , 0.325 0.271 , 0.328	Depositor DCC
R_{free} test set	2585 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11872	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	0.32	0/6002	0.48	0/8136
1	B	0.30	0/5997	0.47	0/8130
All	All	0.31	0/11999	0.48	0/16266

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5848	0	5662	216	0
1	B	5844	0	5671	181	0
2	A	90	0	0	5	0
2	B	90	0	0	4	0
All	All	11872	0	11333	388	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 17.

All (388) 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:20:LEU:HB3	1:A:109:TYR:CD2	1.37	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:CYS:HB2	1:B:261:CYS:SG	1.59	1.41
1:B:18:TYR:HB3	1:B:19:PRO:CD	1.53	1.38
1:A:20:LEU:HB3	1:A:109:TYR:CE2	1.66	1.28
1:A:20:LEU:HG	1:A:109:TYR:CZ	1.78	1.17
1:A:505:CYS:HB3	1:A:519:CYS:SG	1.85	1.16
1:A:164:ILE:HD13	1:A:277:HIS:HD2	1.10	1.15
1:A:20:LEU:HB3	1:A:109:TYR:CG	1.81	1.15
1:A:20:LEU:CB	1:A:109:TYR:CD2	2.32	1.13
1:A:17:PRO:HG3	1:A:71:HIS:ND1	1.63	1.11
1:A:505:CYS:CB	1:A:519:CYS:SG	2.40	1.10
1:B:254:CYS:CB	1:B:261:CYS:SG	2.40	1.09
1:A:504:ASN:HB2	1:A:507:ALA:O	1.51	1.08
1:A:17:PRO:HG3	1:A:71:HIS:HD1	1.12	1.07
1:B:18:TYR:HB3	1:B:19:PRO:HD3	1.24	1.07
1:A:393:GLN:HG2	1:B:18:TYR:CZ	1.89	1.06
1:A:19:PRO:C	1:A:20:LEU:HD13	1.76	1.05
1:A:393:GLN:HG2	1:B:18:TYR:OH	1.54	1.05
1:B:17:PRO:HG3	1:B:66:THR:OG1	1.56	1.04
1:B:290:ASN:HD22	1:B:327:THR:CG2	1.75	0.99
1:B:18:TYR:CB	1:B:19:PRO:CD	2.42	0.98
1:A:164:ILE:HD13	1:A:277:HIS:CD2	2.00	0.96
1:A:20:LEU:CB	1:A:109:TYR:CG	2.47	0.96
1:B:18:TYR:HB3	1:B:19:PRO:HD2	1.45	0.95
1:A:164:ILE:HG21	1:A:277:HIS:CD2	2.03	0.93
1:A:715:ARG:HH11	1:A:715:ARG:HB3	1.33	0.93
1:A:164:ILE:CD1	1:A:277:HIS:HD2	1.80	0.92
1:A:17:PRO:CG	1:A:71:HIS:CE1	2.53	0.91
1:B:198:THR:HG21	1:B:258:SER:HB3	1.52	0.90
1:A:20:LEU:CB	1:A:109:TYR:CE2	2.51	0.89
1:A:715:ARG:HE	1:A:718:LEU:HD22	1.36	0.89
1:A:17:PRO:HG3	1:A:71:HIS:CE1	2.08	0.89
1:B:198:THR:CG2	1:B:258:SER:HB3	2.02	0.89
1:A:715:ARG:HH21	1:A:718:LEU:CD2	1.85	0.88
1:A:20:LEU:CG	1:A:109:TYR:CZ	2.57	0.87
1:B:504:ASN:HB2	1:B:507:ALA:O	1.75	0.86
1:B:6:ARG:HH21	1:B:8:ARG:HB3	1.41	0.85
1:B:198:THR:HG21	1:B:258:SER:CB	2.06	0.84
1:A:715:ARG:HH21	1:A:718:LEU:HD22	1.40	0.84
1:A:17:PRO:CG	1:A:71:HIS:ND1	2.41	0.82
1:A:8:ARG:HH12	1:A:63:LYS:HZ3	1.22	0.82
1:B:290:ASN:HD22	1:B:327:THR:HG22	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:TYR:HB3	1:A:19:PRO:HD3	1.61	0.81
1:B:290:ASN:HD22	1:B:327:THR:HG21	1.43	0.81
1:B:504:ASN:CB	1:B:507:ALA:O	2.28	0.81
1:A:17:PRO:HD3	1:A:71:HIS:CE1	2.16	0.81
1:A:715:ARG:NE	1:A:718:LEU:HD22	1.95	0.81
1:A:8:ARG:HH12	1:A:63:LYS:NZ	1.79	0.80
1:A:715:ARG:NH2	1:A:718:LEU:HD22	1.96	0.80
1:A:19:PRO:HB3	1:A:23:ASN:ND2	1.98	0.77
1:A:161:GLU:OE1	1:A:277:HIS:CG	2.36	0.77
1:A:193:GLU:O	1:A:194:ASN:ND2	2.18	0.76
1:A:19:PRO:O	1:A:20:LEU:CD1	2.33	0.76
1:B:640:GLU:HB3	1:B:643:VAL:HG22	1.68	0.76
1:A:8:ARG:NH1	1:A:63:LYS:HZ3	1.85	0.75
1:A:17:PRO:CD	1:A:71:HIS:CE1	2.70	0.75
1:A:14:PRO:O	1:A:72:VAL:HA	1.86	0.75
1:A:715:ARG:HH11	1:A:715:ARG:CB	1.99	0.74
1:A:161:GLU:O	1:A:161:GLU:HG3	1.88	0.74
1:A:393:GLN:CG	1:B:18:TYR:OH	2.34	0.74
1:B:619:GLU:OE2	1:B:619:GLU:N	2.17	0.73
1:A:19:PRO:C	1:A:20:LEU:CD1	2.55	0.73
1:A:236:LYS:NZ	1:A:490:GLY:O	2.21	0.73
1:A:290:ASN:ND2	1:A:363:ASP:O	2.22	0.72
1:A:20:LEU:HB3	1:A:109:TYR:CZ	2.23	0.72
1:A:13:ARG:HD3	1:B:650:TYR:HA	1.72	0.72
1:A:17:PRO:HB3	1:A:69:ILE:HG21	1.70	0.72
1:A:504:ASN:CB	1:A:507:ALA:O	2.34	0.72
1:A:198:THR:HB	1:A:256:TYR:O	1.90	0.72
1:B:18:TYR:CB	1:B:19:PRO:HD3	2.14	0.71
1:B:198:THR:CB	1:B:258:SER:HB3	2.20	0.71
1:B:193:GLU:HA	1:B:196:ARG:HG3	1.71	0.71
1:B:522:LYS:NZ	1:B:708:ARG:O	2.24	0.70
1:B:618:LEU:HG	1:B:619:GLU:OE2	1.91	0.70
1:A:19:PRO:HB3	1:A:23:ASN:HD21	1.54	0.70
1:A:193:GLU:HA	1:A:196:ARG:HG3	1.73	0.70
1:B:236:LYS:NZ	1:B:490:GLY:O	2.24	0.70
1:A:105:LEU:HB3	1:A:303:SER:HA	1.74	0.69
1:B:662:ILE:HG21	1:B:705:ILE:HD13	1.75	0.69
1:A:19:PRO:O	1:A:20:LEU:HD13	1.91	0.69
1:A:715:ARG:CZ	1:A:718:LEU:HD22	2.23	0.69
1:A:715:ARG:NH2	1:A:718:LEU:CD2	2.54	0.69
1:A:660:LEU:HB3	1:A:713:TYR:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:THR:HG23	1:A:305:ARG:HB3	1.75	0.68
1:A:109:TYR:CE1	1:A:250:PHE:CZ	2.82	0.68
1:A:8:ARG:HH22	1:A:63:LYS:HZ3	1.42	0.68
1:A:20:LEU:CB	1:A:109:TYR:CD1	2.77	0.67
1:B:429:ARG:HH21	1:B:478:LEU:HD13	1.58	0.67
1:A:164:ILE:CD1	1:A:277:HIS:CD2	2.70	0.67
1:B:504:ASN:O	1:B:505:CYS:HB2	1.95	0.67
1:A:20:LEU:HG	1:A:109:TYR:CE1	2.29	0.67
1:B:482:ASN:HD21	1:B:504:ASN:CG	1.98	0.66
1:B:159:ASP:O	1:B:160:ASP:C	2.33	0.66
1:A:20:LEU:CG	1:A:109:TYR:CE1	2.79	0.66
1:B:103:LYS:HZ2	1:B:125:GLY:H	1.44	0.66
1:A:20:LEU:HD13	1:A:20:LEU:N	2.09	0.66
1:B:520:ARG:O	1:B:523:GLN:N	2.28	0.66
1:B:253:GLU:OE1	1:B:255:ARG:HB3	1.96	0.66
1:B:296:ASN:ND2	1:B:297:HIS:O	2.29	0.65
1:A:20:LEU:HB2	1:A:109:TYR:CG	2.31	0.65
1:B:254:CYS:CB	1:B:261:CYS:HG	2.01	0.65
1:B:199:TYR:CE1	1:B:256:TYR:HB3	2.32	0.65
1:A:164:ILE:CG2	1:A:277:HIS:CD2	2.79	0.64
1:B:504:ASN:ND2	1:B:507:ALA:O	2.30	0.64
1:A:20:LEU:CB	1:A:109:TYR:CZ	2.81	0.64
1:A:134:ASP:OD2	1:A:321:ARG:NH2	2.27	0.64
1:A:188:ARG:HG3	1:A:190:ASP:HB3	1.81	0.63
1:A:20:LEU:HB3	1:A:109:TYR:CD1	2.33	0.63
1:A:123:VAL:HG12	1:A:142:SER:HB2	1.80	0.63
1:B:89:GLY:HA3	1:B:99:PHE:HD2	1.62	0.63
1:B:247:ILE:HG23	1:B:293:ALA:HB3	1.81	0.63
1:B:94:GLU:HA	1:B:321:ARG:HB2	1.80	0.63
1:A:393:GLN:HG2	1:B:18:TYR:CE2	2.33	0.63
1:B:619:GLU:HA	1:B:673:LYS:HD3	1.81	0.62
1:A:522:LYS:O	1:A:526:ASN:ND2	2.32	0.62
1:B:198:THR:HB	1:B:258:SER:HB3	1.81	0.62
1:B:195:ILE:HD12	1:B:201:GLY:HA2	1.80	0.61
1:A:109:TYR:CD1	1:A:250:PHE:CZ	2.88	0.61
1:A:296:ASN:ND2	1:A:297:HIS:O	2.33	0.61
1:A:20:LEU:HG	1:A:109:TYR:CE2	2.34	0.61
1:B:300:PRO:O	1:B:305:ARG:NH1	2.34	0.61
1:A:20:LEU:HD23	1:A:109:TYR:CE1	2.35	0.61
1:A:19:PRO:O	1:A:20:LEU:HD12	1.99	0.60
1:A:549:THR:HG22	1:A:551:ARG:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:TYR:CB	1:B:19:PRO:HD2	2.24	0.60
1:B:480:SER:HA	1:B:520:ARG:NH2	2.17	0.60
1:B:127:LYS:HB3	1:B:130:ASP:HB2	1.84	0.60
1:B:123:VAL:HG12	1:B:142:SER:HB2	1.83	0.59
1:A:218:THR:HG22	1:A:282:GLU:HB2	1.84	0.59
1:B:24:TRP:CD2	1:B:79:PRO:HD3	2.37	0.59
1:A:8:ARG:NH2	1:A:63:LYS:HZ3	1.98	0.59
1:B:161:GLU:OE1	1:B:356:HIS:ND1	2.33	0.59
1:B:168:LYS:NZ	2:B:814:HOH:O	2.36	0.59
1:A:19:PRO:HG3	1:A:23:ASN:ND2	2.18	0.59
1:A:8:ARG:HH22	1:A:63:LYS:NZ	2.00	0.58
1:A:691:LYS:HD2	1:A:693:GLU:HB2	1.83	0.58
1:B:189:LEU:HD12	1:B:189:LEU:H	1.68	0.58
1:A:18:TYR:HB3	1:A:19:PRO:CD	2.31	0.58
1:A:311:ALA:O	1:A:313:TYR:N	2.37	0.58
1:A:193:GLU:HG2	1:A:194:ASN:N	2.19	0.58
1:B:636:ILE:HD12	1:B:662:ILE:HD12	1.86	0.58
1:B:162:ASP:OD1	1:B:162:ASP:N	2.34	0.57
1:B:158:TRP:HB3	1:B:161:GLU:HG2	1.85	0.57
1:B:513:ASP:HB3	1:B:516:VAL:HG23	1.87	0.57
1:B:103:LYS:NZ	1:B:122:ALA:O	2.33	0.57
1:B:290:ASN:ND2	1:B:327:THR:HG21	2.17	0.57
1:B:92:LYS:NZ	2:B:819:HOH:O	2.38	0.56
1:A:161:GLU:OE1	1:A:277:HIS:CB	2.54	0.56
1:B:482:ASN:OD1	1:B:504:ASN:HB3	2.05	0.56
1:A:19:PRO:CB	1:A:23:ASN:ND2	2.67	0.55
1:A:522:LYS:NZ	2:A:814:HOH:O	2.39	0.55
1:A:253:GLU:CG	1:A:255:ARG:HG2	2.36	0.55
1:B:290:ASN:ND2	1:B:327:THR:CG2	2.59	0.55
1:A:688:ARG:NH2	1:A:706:GLU:OE2	2.39	0.55
1:A:16:ASP:O	1:A:18:TYR:N	2.35	0.55
1:A:242:TRP:HB3	1:A:244:TYR:HD1	1.71	0.55
1:B:559:GLN:HG2	1:B:563:ILE:HD12	1.88	0.55
1:A:650:TYR:HA	1:B:13:ARG:HD3	1.88	0.55
1:A:17:PRO:HD3	1:A:71:HIS:ND1	2.22	0.55
1:B:415:TYR:O	1:B:416:GLN:HB3	2.06	0.54
1:A:17:PRO:CD	1:A:71:HIS:ND1	2.70	0.54
1:A:51:THR:OG1	1:A:52:ASN:N	2.40	0.54
1:A:193:GLU:HG2	1:A:194:ASN:H	1.71	0.54
1:A:528:MET:HG2	1:A:581:VAL:HG22	1.89	0.54
1:B:481:TYR:C	1:B:482:ASN:OD1	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLU:C	1:B:195:ILE:H	2.11	0.54
1:A:425:ARG:NH1	1:A:426:ASP:OD1	2.41	0.54
1:B:520:ARG:O	1:B:521:GLU:C	2.40	0.54
1:A:596:ARG:NE	1:A:646:GLU:HG2	2.23	0.53
1:A:8:ARG:CZ	1:A:63:LYS:HZ3	2.21	0.53
1:A:161:GLU:OE1	1:A:277:HIS:ND1	2.40	0.53
1:A:619:GLU:O	1:A:621:ARG:N	2.42	0.53
1:A:105:LEU:HD12	1:A:302:LEU:C	2.29	0.53
1:A:503:TRP:CZ3	1:A:505:CYS:HA	2.42	0.53
1:B:636:ILE:HD12	1:B:662:ILE:CD1	2.39	0.53
1:A:66:THR:HB	1:A:71:HIS:HE1	1.73	0.53
1:A:242:TRP:HB3	1:A:244:TYR:CD1	2.43	0.53
1:A:17:PRO:CB	1:A:69:ILE:HG21	2.37	0.53
1:B:6:ARG:HG2	1:B:7:THR:H	1.72	0.53
1:B:372:LEU:HG	1:B:373:TYR:HD1	1.73	0.53
1:A:400:PRO:HG3	1:A:419:GLU:HB3	1.91	0.53
1:B:198:THR:HG21	1:B:258:SER:HB2	1.89	0.53
1:A:20:LEU:CG	1:A:109:TYR:CE2	2.87	0.52
1:A:596:ARG:HD3	1:A:600:PHE:CE1	2.43	0.52
1:B:171:LEU:HG	1:B:537:THR:HG21	1.90	0.52
1:A:18:TYR:CB	1:A:19:PRO:CD	2.87	0.52
1:A:103:LYS:HE3	1:A:125:GLY:H	1.75	0.52
1:A:20:LEU:CD1	1:A:20:LEU:N	2.73	0.52
1:B:414:PRO:O	1:B:417:TRP:HB2	2.09	0.52
1:A:223:PRO:HD3	1:A:286:ASP:HB3	1.92	0.52
1:B:191:LEU:O	1:B:196:ARG:NH1	2.42	0.52
1:A:16:ASP:C	1:A:18:TYR:H	2.13	0.51
1:B:87:VAL:HG21	1:B:307:ILE:HD13	1.92	0.51
1:A:694:GLU:HG2	1:A:703:LEU:HD21	1.91	0.51
1:B:610:LEU:HB3	1:B:640:GLU:HG2	1.91	0.51
1:A:17:PRO:HG3	1:A:69:ILE:CG2	2.40	0.51
1:A:20:LEU:CB	1:A:109:TYR:CE1	2.94	0.51
1:A:546:LEU:HD22	1:A:570:LEU:HD21	1.93	0.51
1:B:290:ASN:ND2	1:B:327:THR:HG22	2.21	0.51
1:B:640:GLU:HB3	1:B:643:VAL:CG2	2.38	0.51
1:B:218:THR:HG22	1:B:282:GLU:HB2	1.92	0.51
1:A:86:ARG:NH2	1:A:141:ASP:OD2	2.40	0.51
1:A:688:ARG:HG2	1:A:689:GLU:N	2.26	0.51
1:A:50:LEU:HD23	1:A:50:LEU:H	1.76	0.51
1:B:648:ASN:HD21	1:B:652:GLU:HB2	1.76	0.51
1:A:109:TYR:HE1	1:A:250:PHE:CZ	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ARG:HA	1:A:374:SER:O	2.11	0.51
1:A:393:GLN:CG	1:B:18:TYR:CZ	2.81	0.50
1:B:486:ASN:ND2	1:B:495:ASP:O	2.42	0.50
1:A:177:TYR:HB2	1:A:216:ILE:HG21	1.92	0.50
1:A:8:ARG:HH11	1:A:8:ARG:HG3	1.76	0.50
1:A:691:LYS:HD3	1:A:692:PRO:HD2	1.93	0.50
1:B:193:GLU:O	1:B:195:ILE:N	2.40	0.50
1:A:623:VAL:HG13	1:A:627:THR:HG23	1.94	0.50
1:A:681:LEU:HD23	1:A:713:TYR:CZ	2.47	0.50
1:B:48:TYR:CZ	1:B:148:LYS:HE2	2.46	0.50
1:B:679:TRP:CZ3	1:B:715:ARG:HB2	2.46	0.50
1:A:392:SER:HB2	1:B:18:TYR:HE1	1.77	0.50
1:A:521:GLU:HB3	1:A:687:LEU:HD21	1.93	0.50
1:A:312:TYR:O	1:A:333:LEU:HD12	2.12	0.50
1:A:674:PHE:CG	1:A:697:ILE:HG21	2.47	0.50
1:A:120:ASN:O	1:A:123:VAL:HG22	2.12	0.49
1:B:19:PRO:HB2	1:B:23:ASN:OD1	2.12	0.49
1:A:182:LYS:HD3	1:A:565:TRP:CH2	2.46	0.49
1:B:103:LYS:HE3	1:B:125:GLY:HA2	1.94	0.49
1:A:17:PRO:HG3	1:A:69:ILE:HG22	1.95	0.49
1:B:45:LEU:N	1:B:60:ILE:O	2.38	0.49
1:B:398:ALA:HB2	1:B:417:TRP:CE3	2.48	0.49
1:A:20:LEU:CD2	1:A:109:TYR:CE1	2.95	0.49
1:A:398:ALA:HB2	1:A:417:TRP:CZ3	2.48	0.49
1:A:715:ARG:HD3	1:A:717:GLU:O	2.11	0.49
1:B:457:ASN:ND2	2:B:822:HOH:O	2.45	0.49
1:A:127:LYS:HE2	1:A:130:ASP:OD1	2.12	0.49
1:B:480:SER:HA	1:B:520:ARG:HH21	1.77	0.49
1:A:20:LEU:HG	1:A:109:TYR:OH	2.11	0.48
1:B:528:MET:HG2	1:B:581:VAL:HG22	1.95	0.48
1:B:133:GLN:O	1:B:136:THR:OG1	2.28	0.48
1:A:210:TYR:OH	1:A:545:GLU:OE1	2.28	0.48
1:B:77:LEU:HD13	1:B:81:GLN:HG2	1.95	0.48
1:A:393:GLN:CG	1:B:18:TYR:CE2	2.96	0.48
1:B:676:LYS:HE2	1:B:676:LYS:H	1.77	0.48
1:A:152:ILE:O	2:A:801:HOH:O	2.20	0.48
1:B:199:TYR:CZ	1:B:256:TYR:HB2	2.47	0.48
1:B:482:ASN:OD1	1:B:482:ASN:N	2.45	0.48
1:A:17:PRO:CG	1:A:69:ILE:HG21	2.44	0.48
1:A:20:LEU:HB2	1:A:109:TYR:CD1	2.48	0.48
1:A:166:GLY:O	1:A:168:LYS:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HD21	1:A:344:VAL:HG21	1.95	0.48
1:A:18:TYR:CB	1:A:19:PRO:HD3	2.36	0.48
1:B:189:LEU:HA	1:B:196:ARG:NH1	2.29	0.48
1:A:19:PRO:CG	1:A:23:ASN:ND2	2.76	0.47
1:A:191:LEU:HB3	1:A:195:ILE:HD11	1.95	0.47
1:B:17:PRO:HB3	1:B:71:HIS:CD2	2.49	0.47
1:B:282:GLU:CD	1:B:395:LYS:HZ1	2.17	0.47
1:B:673:LYS:HG3	1:B:702:GLU:HG2	1.96	0.47
1:A:87:VAL:HG21	1:A:307:ILE:HA	1.94	0.47
1:B:278:ASN:O	2:B:801:HOH:O	2.20	0.47
1:A:491:PHE:HB2	1:A:495:ASP:OD2	2.15	0.47
1:A:291:HIS:HB3	1:A:327:THR:HG21	1.96	0.47
1:B:159:ASP:O	1:B:161:GLU:N	2.48	0.47
1:B:433:ARG:NH1	1:B:435:GLU:OE1	2.41	0.47
1:A:22:SER:O	1:A:23:ASN:OD1	2.32	0.47
1:A:246:PRO:HG3	1:A:288:VAL:HB	1.97	0.47
1:A:505:CYS:SG	1:A:520:ARG:HG2	2.55	0.47
1:B:715:ARG:HD3	1:B:718:LEU:HB2	1.97	0.47
1:B:120:ASN:O	1:B:123:VAL:HG22	2.14	0.47
1:B:517:VAL:O	1:B:520:ARG:HB2	2.15	0.47
1:A:464:ILE:HD13	1:A:537:THR:HB	1.96	0.46
1:A:715:ARG:CB	1:A:715:ARG:NH1	2.74	0.46
1:B:619:GLU:C	1:B:621:ARG:H	2.17	0.46
1:B:642:SER:HA	1:B:655:ALA:HB1	1.97	0.46
1:A:104:VAL:HG21	1:A:143:GLY:HA2	1.96	0.46
1:B:604:LYS:HA	1:B:611:LYS:HA	1.97	0.46
1:A:164:ILE:O	1:A:164:ILE:HG23	2.15	0.46
1:B:171:LEU:HA	1:B:174:THR:OG1	2.16	0.46
1:A:314:MET:HG3	1:A:334:ASN:HA	1.97	0.46
1:B:429:ARG:O	1:B:433:ARG:HB2	2.16	0.46
1:B:6:ARG:NH2	1:B:8:ARG:HE	2.14	0.46
1:B:619:GLU:O	1:B:621:ARG:N	2.47	0.46
1:B:400:PRO:HG2	1:B:410:VAL:HG22	1.98	0.46
1:A:175:VAL:HG13	1:A:538:PRO:HG2	1.98	0.45
1:A:397:ILE:HG12	1:A:418:ALA:HB3	1.99	0.45
1:A:546:LEU:HD11	1:A:568:TRP:CZ3	2.51	0.45
1:A:596:ARG:HH21	1:A:598:ARG:HB2	1.81	0.45
1:A:619:GLU:HG2	1:A:621:ARG:HG3	1.98	0.45
1:A:639:LEU:O	1:A:658:SER:HA	2.17	0.45
1:B:193:GLU:CD	1:B:194:ASN:H	2.20	0.45
1:B:227:PHE:CE1	1:B:255:ARG:CZ	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLU:OE1	1:A:255:ARG:HG2	2.16	0.45
1:A:20:LEU:HB3	1:A:109:TYR:CE1	2.52	0.45
1:A:612:ASP:OD1	1:A:613:VAL:N	2.49	0.45
1:B:227:PHE:HA	1:B:246:PRO:HA	1.99	0.45
1:A:252:PRO:HD2	1:A:266:VAL:HG12	1.99	0.45
1:B:424:TYR:HA	1:B:445:ARG:HD3	1.97	0.45
1:B:42:LYS:HB3	1:B:88:TYR:HB2	1.99	0.45
1:B:180:HIS:NE2	1:B:241:TYR:O	2.33	0.45
1:A:8:ARG:CZ	1:A:8:ARG:HB2	2.46	0.45
1:A:230:GLN:NE2	1:A:230:GLN:HA	2.31	0.45
1:A:311:ALA:C	1:A:313:TYR:H	2.20	0.45
1:B:51:THR:OG1	1:B:52:ASN:N	2.50	0.45
1:B:648:ASN:ND2	1:B:652:GLU:HB2	2.32	0.45
1:B:648:ASN:HB3	1:B:654:ILE:HD11	1.99	0.44
1:B:78:ARG:HB3	1:B:79:PRO:HD2	2.00	0.44
1:B:314:MET:HG3	1:B:334:ASN:HA	2.00	0.44
1:A:109:TYR:CE1	1:A:250:PHE:HZ	2.34	0.44
1:B:608:MET:HG3	1:B:643:VAL:HG12	1.99	0.44
1:A:372:LEU:HD12	1:A:372:LEU:HA	1.76	0.44
1:B:13:ARG:HB2	1:B:73:PHE:HD2	1.83	0.44
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.74	0.44
1:B:621:ARG:HD2	1:B:621:ARG:HA	1.82	0.44
1:B:358:ASP:O	1:B:394:VAL:HB	2.17	0.44
1:B:174:THR:HG23	1:B:218:THR:HG23	1.99	0.44
1:B:479:VAL:O	1:B:520:ARG:HG2	2.18	0.44
1:B:87:VAL:HG21	1:B:307:ILE:HA	2.00	0.44
1:B:426:ASP:O	1:B:430:ARG:HG3	2.18	0.43
1:B:429:ARG:NH1	1:B:467:VAL:O	2.51	0.43
1:B:612:ASP:N	1:B:612:ASP:OD1	2.50	0.43
1:B:678:LYS:HB3	1:B:717:GLU:HB3	1.99	0.43
1:A:92:LYS:NZ	2:A:824:HOH:O	2.52	0.43
1:A:273:VAL:HG23	1:A:283:VAL:HG21	2.01	0.43
1:A:14:PRO:HB2	1:A:15:GLY:H	1.64	0.43
1:A:163:PHE:C	1:A:165:LYS:H	2.21	0.43
1:A:687:LEU:N	2:A:814:HOH:O	2.46	0.43
1:B:228:ILE:HD11	1:B:247:ILE:HD13	2.01	0.43
1:A:109:TYR:HE1	1:A:250:PHE:HZ	1.66	0.43
1:A:253:GLU:HG3	1:A:255:ARG:HG2	1.99	0.43
1:B:675:PRO:HG2	1:B:679:TRP:CZ2	2.53	0.43
1:A:576:LYS:HD3	1:A:576:LYS:HA	1.67	0.43
1:B:92:LYS:N	1:B:97:LEU:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:VAL:HA	1:B:638:VAL:O	2.19	0.43
1:B:425:ARG:NH1	1:B:426:ASP:OD1	2.46	0.43
1:B:160:ASP:OD1	1:B:163:PHE:HB2	2.19	0.43
1:A:476:GLU:OE1	1:A:547:SER:HB3	2.20	0.42
1:B:13:ARG:HB2	1:B:73:PHE:CD2	2.55	0.42
1:B:116:SER:OG	1:B:117:VAL:N	2.49	0.42
1:A:133:GLN:HB2	1:A:298:LEU:CD2	2.50	0.42
1:B:297:HIS:ND1	1:B:298:LEU:HG	2.33	0.42
1:B:634:LEU:HD12	1:B:664:ASN:HB2	2.01	0.42
1:B:267:LEU:HG	1:B:271:LYS:HE2	2.01	0.42
1:A:325:ASP:OD2	1:A:330:GLY:N	2.53	0.42
1:B:484:LYS:HG3	1:B:493:ASN:HD21	1.84	0.42
1:B:559:GLN:HG3	1:B:561:ASN:HD21	1.83	0.42
1:A:311:ALA:O	1:A:312:TYR:HB2	2.19	0.42
1:B:484:LYS:HG3	1:B:493:ASN:ND2	2.34	0.42
1:B:199:TYR:CE1	1:B:256:TYR:CB	3.01	0.42
1:B:617:THR:OG1	1:B:618:LEU:N	2.52	0.42
1:A:13:ARG:HB2	1:A:73:PHE:HB3	2.02	0.42
1:A:454:LEU:HD12	1:A:454:LEU:HA	1.87	0.42
1:B:127:LYS:HD3	1:B:136:THR:HB	2.02	0.42
1:B:199:TYR:CZ	1:B:256:TYR:CB	3.03	0.42
1:B:467:VAL:HG23	1:B:468:THR:HG23	2.02	0.42
1:B:514:GLN:HA	1:B:517:VAL:HG12	2.02	0.42
1:A:189:LEU:HA	1:A:196:ARG:NE	2.35	0.41
1:B:318:ASP:OD1	1:B:318:ASP:N	2.44	0.41
1:B:516:VAL:O	1:B:520:ARG:HD2	2.19	0.41
1:A:138:ASP:OD1	1:A:140:ARG:HB2	2.20	0.41
1:A:694:GLU:HG2	1:A:703:LEU:HD11	2.02	0.41
1:B:5:PHE:HB3	1:B:9:ASP:HB2	2.02	0.41
1:B:188:ARG:NH1	1:B:190:ASP:OD2	2.52	0.41
1:B:188:ARG:O	1:B:196:ARG:HD3	2.20	0.41
1:B:103:LYS:NZ	1:B:125:GLY:H	2.13	0.41
1:A:126:TYR:HB2	2:A:820:HOH:O	2.20	0.41
1:A:45:LEU:HD21	1:A:47:LEU:HD21	2.02	0.41
1:A:49:SER:HB2	1:A:57:LYS:HD3	2.03	0.41
1:A:104:VAL:CG2	1:A:143:GLY:HA2	2.50	0.41
1:A:232:PHE:O	1:A:236:LYS:HD2	2.20	0.41
1:B:161:GLU:OE2	1:B:277:HIS:ND1	2.52	0.41
1:A:423:LYS:O	1:A:427:SER:OG	2.36	0.41
1:B:253:GLU:OE2	1:B:253:GLU:HA	2.21	0.41
1:B:385:LEU:HD21	1:B:396:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ASN:O	1:B:505:CYS:CB	2.63	0.41
1:B:674:PHE:CZ	1:B:697:ILE:HG13	2.56	0.41
1:A:142:SER:O	1:A:146:VAL:HG23	2.20	0.41
1:A:179:VAL:O	1:A:222:MET:HG3	2.20	0.41
1:B:101:PRO:HD2	1:B:137:TYR:OH	2.21	0.41
1:B:194:ASN:O	1:B:258:SER:HB2	2.21	0.41
1:B:232:PHE:O	1:B:236:LYS:HD2	2.21	0.41
1:A:171:LEU:HD13	1:A:461:PHE:HB3	2.01	0.41
1:A:19:PRO:HB2	1:A:20:LEU:H	1.69	0.40
1:A:441:GLU:O	1:A:445:ARG:HG2	2.21	0.40
1:A:589:ARG:HA	1:A:595:ARG:HE	1.86	0.40
1:A:644:MET:O	1:A:653:ARG:HD2	2.21	0.40
1:B:138:ASP:OD1	1:B:140:ARG:HB2	2.21	0.40
1:A:297:HIS:C	1:A:299:GLY:H	2.24	0.40
1:A:398:ALA:HB2	1:A:417:TRP:CE3	2.57	0.40
1:A:613:VAL:HA	1:A:638:VAL:O	2.21	0.40
1:B:198:THR:HA	1:B:256:TYR:O	2.22	0.40
1:B:513:ASP:HB3	1:B:516:VAL:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	713/718 (99%)	649 (91%)	54 (8%)	10 (1%)	11	34
1	B	712/718 (99%)	651 (91%)	51 (7%)	10 (1%)	11	34
All	All	1425/1436 (99%)	1300 (91%)	105 (7%)	20 (1%)	11	34

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	620	GLY
1	A	683	ILE
1	B	18	TYR
1	B	160	ASP
1	B	193	GLU
1	B	194	ASN
1	A	19	PRO
1	B	303	SER
1	B	372	LEU
1	B	620	GLY
1	A	160	ASP
1	A	168	LYS
1	A	513	ASP
1	B	308	ASP
1	A	164	ILE
1	B	17	PRO
1	A	17	PRO
1	B	19	PRO
1	A	223	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	631/636 (99%)	602 (95%)	29 (5%)	27	60
1	B	633/636 (100%)	609 (96%)	24 (4%)	33	67
All	All	1264/1272 (99%)	1211 (96%)	53 (4%)	30	63

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	16	ASP
1	A	18	TYR
1	A	20	LEU

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Mol	Chain	Res	Type
1	A	34	SER
1	A	52	ASN
1	A	71	HIS
1	A	130	ASP
1	A	134	ASP
1	A	161	GLU
1	A	162	ASP
1	A	164	ILE
1	A	165	LYS
1	A	167	LYS
1	A	194	ASN
1	A	254	CYS
1	A	286	ASP
1	A	319	ASN
1	A	361	ARG
1	A	379	ASN
1	A	480	SER
1	A	492	ASN
1	A	511	THR
1	A	518	ILE
1	A	519	CYS
1	A	604	LYS
1	A	619	GLU
1	A	642	SER
1	A	715	ARG
1	B	10	ARG
1	B	18	TYR
1	B	50	LEU
1	B	57	LYS
1	B	159	ASP
1	B	161	GLU
1	B	162	ASP
1	B	245	ASP
1	B	253	GLU
1	B	254	CYS
1	B	255	ARG
1	B	286	ASP
1	B	339	ARG
1	B	482	ASN
1	B	505	CYS
1	B	511	THR
1	B	517	VAL

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Mol	Chain	Res	Type
1	B	618	LEU
1	B	626	LYS
1	B	640	GLU
1	B	673	LYS
1	B	688	ARG
1	B	703	LEU
1	B	704	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	52	ASN
1	A	277	HIS
1	A	319	ASN
1	A	416	GLN
1	B	274	ASN
1	B	290	ASN
1	B	296	ASN

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](#)

There are no ligands in this entry.

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	715/718 (99%)	0.07	14 (1%) 65 56	30, 62, 81, 101	0
1	B	714/718 (99%)	0.05	10 (1%) 75 70	37, 58, 81, 103	0
All	All	1429/1436 (99%)	0.06	24 (1%) 70 63	30, 60, 81, 103	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	PHE	3.7
1	B	18	TYR	3.5
1	A	18	TYR	3.3
1	A	166	GLY	3.2
1	A	133	GLN	3.1
1	A	135	LEU	2.9
1	A	132	ASN	2.7
1	A	97	LEU	2.6
1	A	672	VAL	2.5
1	A	95	LEU	2.4
1	A	162	ASP	2.4
1	B	160	ASP	2.3
1	B	703	LEU	2.3
1	A	319	ASN	2.2
1	B	259	THR	2.2
1	B	373	TYR	2.2
1	A	15	GLY	2.2
1	B	618	LEU	2.2
1	B	123	VAL	2.2
1	B	713	TYR	2.1
1	B	690	ILE	2.1
1	A	16	ASP	2.1
1	A	716	ILE	2.1
1	B	483	GLN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.