



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 12:34 PM EDT

PDB ID : 2EC5
Title : Crystal structures reveal a thiol-protease like catalytic triad in the C-terminal region of Pasteurella multocida toxin
Authors : Kitadokoro, K.; Horiguchi, Y.; Kamitani, S.
Deposited on : 2007-02-09
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

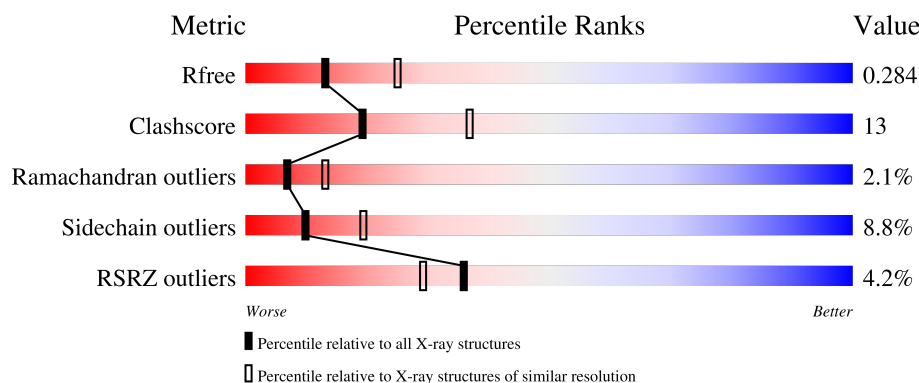
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	746	 4% 69% 22% • 5%
1	B	746	 4% 68% 23% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11528 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 Dermonecrotic toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	711	Total	C	N	O	S	0	0	0
			5643	3603	939	1075	26			
1	B	711	Total	C	N	O	S	0	0	0
			5643	3603	939	1075	26			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	540	MET	-	cloning artifact	UNP P17452
A	541	GLY	-	cloning artifact	UNP P17452
A	542	HIS	-	expression tag	UNP P17452
A	543	HIS	-	expression tag	UNP P17452
A	544	HIS	-	expression tag	UNP P17452
A	545	HIS	-	expression tag	UNP P17452
A	546	HIS	-	expression tag	UNP P17452
A	547	HIS	-	expression tag	UNP P17452
A	548	ASP	-	cloning artifact	UNP P17452
A	549	TYR	-	cloning artifact	UNP P17452
A	550	ASP	-	cloning artifact	UNP P17452
A	551	ILE	-	cloning artifact	UNP P17452
A	552	PRO	-	cloning artifact	UNP P17452
A	553	THR	-	cloning artifact	UNP P17452
A	554	THR	-	cloning artifact	UNP P17452
A	555	GLU	-	cloning artifact	UNP P17452
A	556	ASN	-	cloning artifact	UNP P17452
A	557	LEU	-	cloning artifact	UNP P17452
A	558	TYR	-	cloning artifact	UNP P17452
A	559	PHE	-	cloning artifact	UNP P17452
A	560	GLN	-	cloning artifact	UNP P17452
A	561	GLY	-	cloning artifact	UNP P17452
A	562	ALA	-	cloning artifact	UNP P17452
A	563	HIS	-	cloning artifact	UNP P17452
A	564	MET	-	cloning artifact	UNP P17452

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Chain	Residue	Modelled	Actual	Comment	Reference
A	565	GLY	-	cloning artifact	UNP P17452
A	566	ILE	-	cloning artifact	UNP P17452
A	567	GLN	-	cloning artifact	UNP P17452
A	568	ARG	-	cloning artifact	UNP P17452
A	1159	SER	CYS	engineered mutation	UNP P17452
B	540	MET	-	cloning artifact	UNP P17452
B	541	GLY	-	cloning artifact	UNP P17452
B	542	HIS	-	expression tag	UNP P17452
B	543	HIS	-	expression tag	UNP P17452
B	544	HIS	-	expression tag	UNP P17452
B	545	HIS	-	expression tag	UNP P17452
B	546	HIS	-	expression tag	UNP P17452
B	547	HIS	-	expression tag	UNP P17452
B	548	ASP	-	cloning artifact	UNP P17452
B	549	TYR	-	cloning artifact	UNP P17452
B	550	ASP	-	cloning artifact	UNP P17452
B	551	ILE	-	cloning artifact	UNP P17452
B	552	PRO	-	cloning artifact	UNP P17452
B	553	THR	-	cloning artifact	UNP P17452
B	554	THR	-	cloning artifact	UNP P17452
B	555	GLU	-	cloning artifact	UNP P17452
B	556	ASN	-	cloning artifact	UNP P17452
B	557	LEU	-	cloning artifact	UNP P17452
B	558	TYR	-	cloning artifact	UNP P17452
B	559	PHE	-	cloning artifact	UNP P17452
B	560	GLN	-	cloning artifact	UNP P17452
B	561	GLY	-	cloning artifact	UNP P17452
B	562	ALA	-	cloning artifact	UNP P17452
B	563	HIS	-	cloning artifact	UNP P17452
B	564	MET	-	cloning artifact	UNP P17452
B	565	GLY	-	cloning artifact	UNP P17452
B	566	ILE	-	cloning artifact	UNP P17452
B	567	GLN	-	cloning artifact	UNP P17452
B	568	ARG	-	cloning artifact	UNP P17452
B	1159	SER	CYS	engineered mutation	UNP P17452

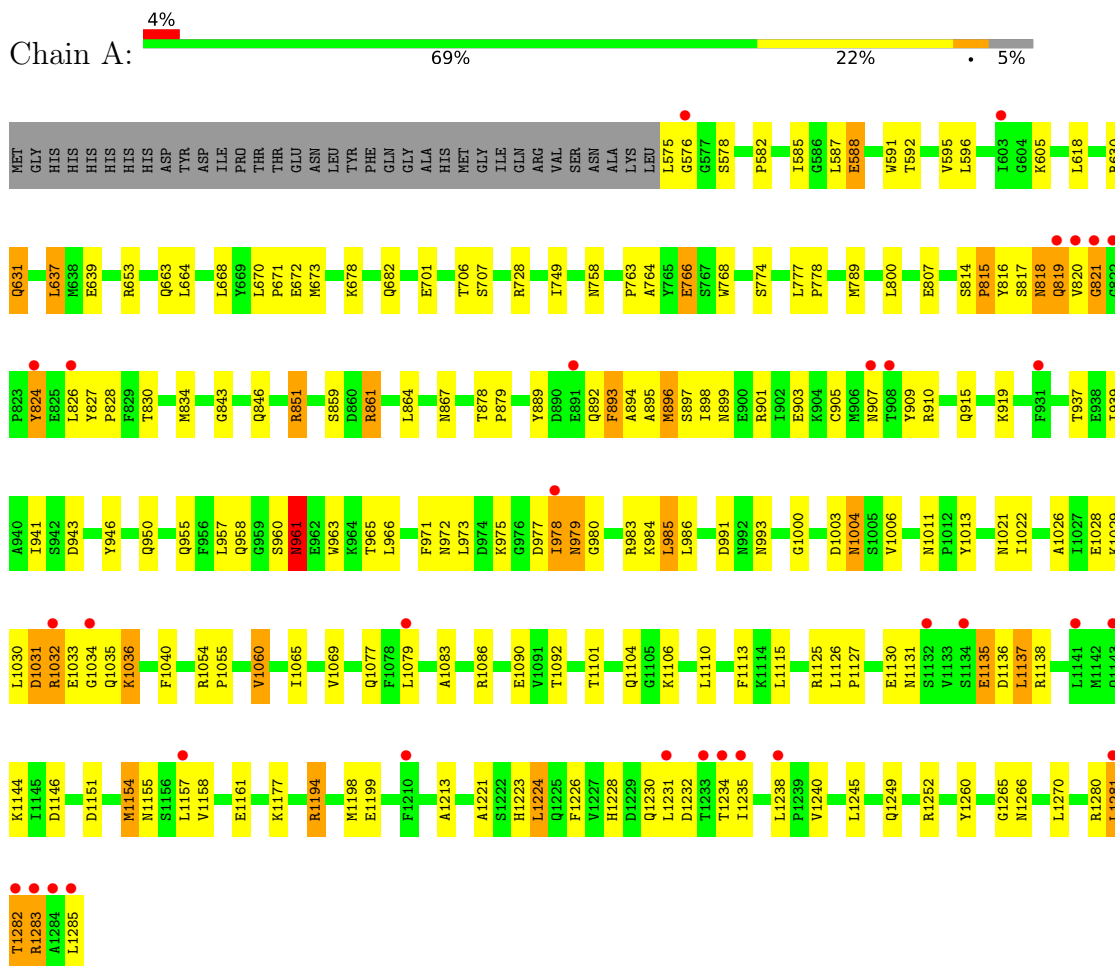
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	119	Total O 119 119	0	0
2	B	123	Total O 123 123	0	0

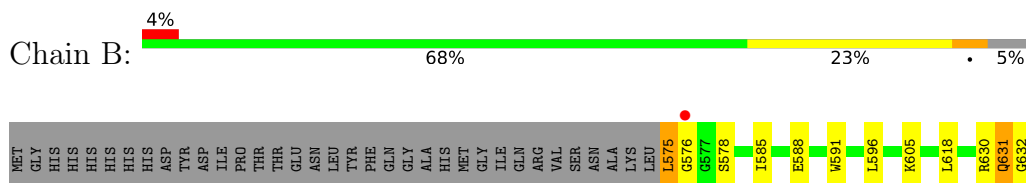
3 Residue-property plots [i](#)

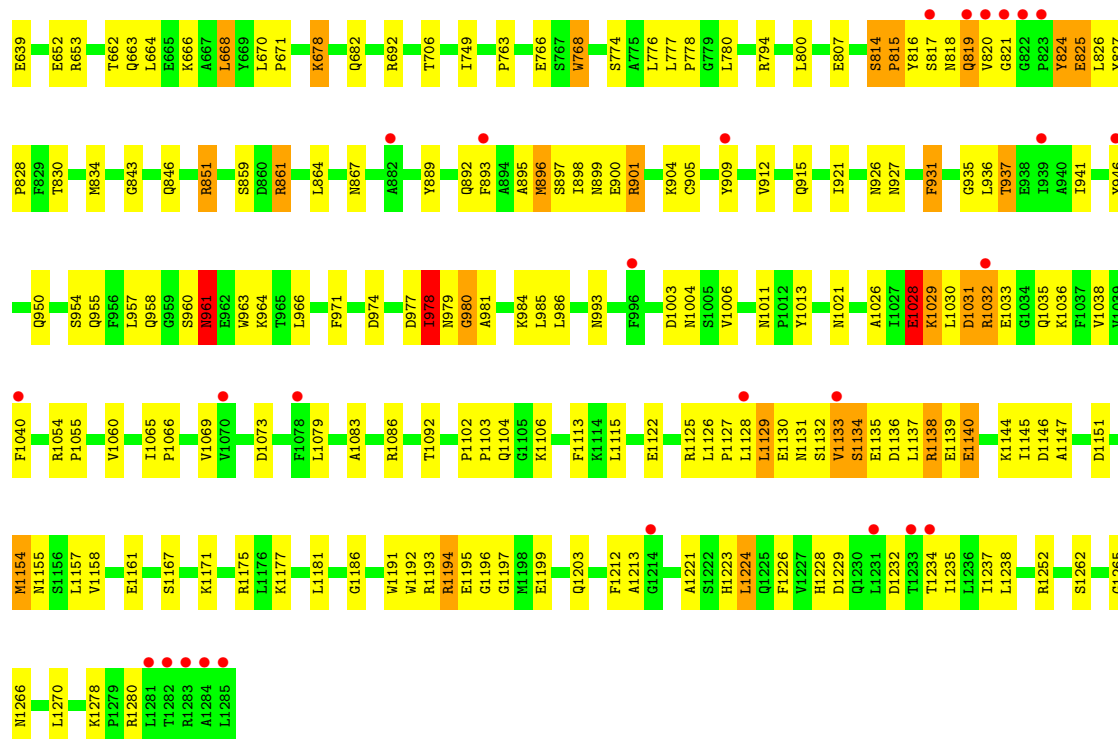
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Dermonecrotic toxin





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.36Å 132.82Å 82.55Å 90.00° 114.74° 90.00°	Depositor
Resolution (Å)	44.81 – 2.60 44.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (44.81-2.60) 96.9 (44.81-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.286 0.230 , 0.284	Depositor DCC
R_{free} test set	2921 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.478 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11528	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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	0.41	0/5769	0.59	0/7811
1	B	0.46	2/5769 (0.0%)	0.60	2/7811 (0.0%)
All	All	0.44	2/11538 (0.0%)	0.60	2/15622 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	926	ASN	CG-ND2	7.94	1.52	1.32
1	B	926	ASN	CG-OD1	6.53	1.38	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1073	ASP	CB-CG-OD2	-9.03	110.17	118.30
1	B	1073	ASP	CB-CG-OD1	8.22	125.69	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	824	TYR	Peptide
1	B	824	TYR	Peptide

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	5643	0	5575	137	0
1	B	5643	0	5575	153	0
2	A	119	0	0	6	0
2	B	123	0	0	4	0
All	All	11528	0	11150	289	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 13.

All (289) 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:B:1129:LEU:CB	1:B:1130:GLU:HA	1.66	1.22
1:B:1129:LEU:HB3	1:B:1130:GLU:CA	1.69	1.21
1:B:817:SER:CB	1:B:818:ASN:HA	1.72	1.18
1:B:817:SER:HB3	1:B:818:ASN:HA	1.27	1.15
1:A:893:PHE:HA	1:A:894:ALA:HB2	1.30	1.10
1:B:814:SER:HB3	1:B:815:PRO:HD3	1.37	1.07
1:A:575:LEU:HB3	1:A:576:GLY:HA2	1.37	1.06
1:A:1032:ARG:HA	1:A:1033:GLU:HB2	1.39	1.04
1:A:1136:ASP:HA	1:A:1138:ARG:H	1.20	1.01
1:A:1030:LEU:HB3	1:A:1031:ASP:HA	1.43	1.00
1:A:1136:ASP:HA	1:A:1138:ARG:N	1.76	1.00
1:B:977:ASP:HB2	1:B:979:ASN:H	1.27	0.99
1:B:1032:ARG:HA	1:B:1033:GLU:HB2	1.41	0.99
1:B:1133:VAL:N	1:B:1134:SER:HA	1.80	0.95
1:B:974:ASP:HB3	1:B:977:ASP:HB3	1.50	0.94
1:B:817:SER:HB2	1:B:971:PHE:HE2	1.31	0.93
1:A:653:ARG:NH2	2:A:219:HOH:O	2.01	0.93
1:B:817:SER:HB3	1:B:818:ASN:CA	2.00	0.91
1:A:1282:THR:O	1:A:1283:ARG:HB2	1.71	0.91
1:A:977:ASP:HA	1:A:978:ILE:O	1.75	0.87
1:B:977:ASP:HB2	1:B:979:ASN:N	1.90	0.87
1:A:1194:ARG:HG3	1:A:1194:ARG:HH11	1.41	0.86
1:B:653:ARG:HD3	2:B:8:HOH:O	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:GLY:H	1:A:846:GLN:HE21	1.25	0.83
1:B:941:ILE:HG22	1:B:1040:PHE:HB2	1.61	0.83
1:B:1032:ARG:HA	1:B:1033:GLU:CB	2.09	0.82
1:A:1030:LEU:HB3	1:A:1031:ASP:CA	2.08	0.82
1:B:1030:LEU:HB3	1:B:1031:ASP:HA	1.61	0.82
1:B:977:ASP:CB	1:B:979:ASN:H	1.93	0.81
1:B:1030:LEU:HB3	1:B:1031:ASP:CA	2.12	0.79
1:B:1130:GLU:N	1:B:1131:ASN:HA	1.97	0.79
1:B:575:LEU:HB3	1:B:576:GLY:HA2	1.63	0.79
1:B:974:ASP:CB	1:B:977:ASP:HB3	2.14	0.78
1:B:817:SER:HB2	1:B:818:ASN:HA	1.61	0.77
1:B:1135:GLU:HG2	1:B:1136:ASP:N	2.00	0.77
1:A:1032:ARG:HA	1:A:1033:GLU:CB	2.15	0.77
1:B:1125:ARG:HD3	1:B:1238:LEU:HD11	1.66	0.77
1:B:1028:GLU:HG3	1:B:1029:LYS:HG2	1.66	0.76
1:A:818:ASN:HB3	1:A:971:PHE:CE2	2.22	0.75
1:B:843:GLY:H	1:B:846:GLN:HE21	1.36	0.74
1:B:814:SER:CB	1:B:815:PRO:HD3	2.16	0.74
1:A:955:GLN:HG3	1:A:960:SER:OG	1.88	0.74
1:B:1028:GLU:HG3	1:B:1029:LYS:N	2.02	0.73
1:B:817:SER:HB3	1:B:819:GLN:H	1.53	0.73
1:A:894:ALA:HB1	1:A:896:MET:HG2	1.71	0.72
1:B:889:TYR:HA	1:B:892:GLN:HB3	1.70	0.72
1:A:815:PRO:HG2	1:A:972:ASN:HB3	1.70	0.72
1:B:639:GLU:OE2	1:B:851:ARG:NH2	2.21	0.72
1:A:578:SER:HB3	2:A:20:HOH:O	1.88	0.71
1:A:1194:ARG:HH11	1:A:1194:ARG:CG	2.02	0.71
1:B:1132:SER:C	1:B:1134:SER:HA	2.11	0.71
1:A:979:ASN:CG	1:A:980:GLY:HA3	2.10	0.71
1:B:1194:ARG:HG3	1:B:1194:ARG:HH11	1.56	0.71
1:A:893:PHE:HA	1:A:894:ALA:CB	2.06	0.70
1:A:1130:GLU:HA	1:A:1131:ASN:C	2.11	0.70
1:A:575:LEU:HB3	1:A:576:GLY:CA	2.19	0.70
1:A:814:SER:HA	1:A:817:SER:O	1.91	0.70
1:B:768:TRP:HD1	1:B:768:TRP:H	1.38	0.70
1:A:977:ASP:HA	1:A:978:ILE:C	2.12	0.69
1:A:1125:ARG:HD3	1:A:1238:LEU:HD11	1.75	0.69
1:A:591:TRP:H	1:A:663:GLN:HE22	1.40	0.69
1:A:893:PHE:CA	1:A:894:ALA:HB2	2.18	0.69
1:A:895:ALA:HB3	1:A:896:MET:HA	1.75	0.69
1:B:977:ASP:HA	1:B:978:ILE:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:817:SER:HB3	1:B:819:GLN:N	2.07	0.68
1:B:817:SER:HB2	1:B:971:PHE:CE2	2.23	0.68
1:B:591:TRP:H	1:B:663:GLN:HE22	1.41	0.68
1:A:1151:ASP:HB3	1:A:1154:MET:HB2	1.76	0.68
1:B:1194:ARG:HH11	1:B:1194:ARG:CG	2.07	0.68
1:A:941:ILE:HG22	1:A:1040:PHE:HB2	1.75	0.66
1:A:639:GLU:OE2	1:A:851:ARG:NH2	2.26	0.66
1:A:749:ILE:HD11	1:A:800:LEU:HB2	1.76	0.66
1:A:1199:GLU:HG3	2:A:224:HOH:O	1.96	0.66
1:A:901:ARG:O	1:A:903:GLU:N	2.28	0.66
1:A:728:ARG:NH2	1:B:1193:ARG:HD3	2.11	0.65
1:A:896:MET:N	1:A:897:SER:HA	2.11	0.65
1:A:1135:GLU:O	1:A:1137:LEU:HB2	1.95	0.65
1:A:1136:ASP:HB3	1:A:1138:ARG:HB3	1.80	0.64
1:B:1028:GLU:HG3	1:B:1029:LYS:CG	2.28	0.64
1:A:1032:ARG:CA	1:A:1033:GLU:HB2	2.23	0.64
1:B:899:ASN:C	1:B:901:ARG:H	2.02	0.64
1:B:1030:LEU:HB3	1:B:1031:ASP:CB	2.27	0.64
1:A:701:GLU:O	1:A:1101:THR:HG22	1.98	0.63
1:B:1060:VAL:HG13	1:B:1065:ILE:O	1.98	0.63
1:B:1136:ASP:HA	1:B:1137:LEU:C	2.19	0.63
1:B:1126:LEU:HB3	1:B:1127:PRO:HD3	1.81	0.62
1:A:961:ASN:C	1:A:961:ASN:HD22	2.02	0.62
1:A:653:ARG:HD3	2:A:4:HOH:O	1.99	0.61
1:A:1032:ARG:HB2	1:A:1035:GLN:CG	2.30	0.61
1:B:1147:ALA:O	1:B:1151:ASP:HB2	1.99	0.61
1:B:1083:ALA:HA	1:B:1086:ARG:HD2	1.82	0.61
1:A:1125:ARG:HH12	1:A:1232:ASP:HB2	1.67	0.60
1:B:1226:PHE:O	1:B:1228:HIS:HD2	1.85	0.60
1:B:678:LYS:O	1:B:682:GLN:HB2	2.02	0.60
1:A:895:ALA:HB3	1:A:896:MET:CA	2.31	0.59
1:A:1032:ARG:HB2	1:A:1035:GLN:HG2	1.84	0.59
1:B:1167:SER:O	1:B:1171:LYS:HD3	2.02	0.59
1:A:843:GLY:H	1:A:846:GLN:NE2	1.97	0.59
1:A:943:ASP:HB3	1:A:973:LEU:HD21	1.83	0.59
1:A:961:ASN:HA	1:A:963:TRP:NE1	2.18	0.59
1:B:671:PRO:HD2	1:B:1280:ARG:HH21	1.68	0.59
1:A:898:ILE:HG13	1:A:901:ARG:NH2	2.18	0.58
1:B:768:TRP:N	1:B:768:TRP:CD1	2.69	0.58
1:B:632:GLY:HA2	1:B:692:ARG:HG3	1.87	0.57
1:B:1133:VAL:HG12	1:B:1133:VAL:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:TYR:HA	1:A:892:GLN:HB2	1.86	0.57
1:B:1032:ARG:CA	1:B:1033:GLU:HB2	2.26	0.57
1:B:630:ARG:NH1	2:B:234:HOH:O	2.36	0.57
1:A:946:TYR:HD1	1:A:950:GLN:NE2	2.03	0.57
1:B:898:ILE:HG22	1:B:898:ILE:O	2.04	0.57
1:A:585:ILE:HG22	1:A:585:ILE:O	2.05	0.56
1:A:815:PRO:N	1:A:816:TYR:HA	2.20	0.56
1:A:768:TRP:N	1:A:768:TRP:CD1	2.71	0.56
1:B:662:THR:HG22	1:B:666:LYS:HE2	1.86	0.56
1:A:980:GLY:H	1:A:983:ARG:HB3	1.71	0.55
1:A:591:TRP:H	1:A:663:GLN:NE2	2.04	0.55
1:A:637:LEU:HD13	1:A:664:LEU:HD11	1.89	0.55
1:A:1234:THR:HG23	1:A:1235:ILE:HG13	1.88	0.55
1:B:814:SER:HB3	1:B:815:PRO:CD	2.24	0.55
1:B:1125:ARG:HH12	1:B:1232:ASP:HB2	1.71	0.55
1:B:1135:GLU:HG2	1:B:1136:ASP:H	1.69	0.55
1:A:878:THR:HB	1:A:879:PRO:HD3	1.88	0.54
1:B:585:ILE:O	1:B:585:ILE:HG22	2.07	0.54
1:A:895:ALA:HB3	1:A:896:MET:HB3	1.90	0.54
1:B:1011:ASN:ND2	1:B:1013:TYR:H	2.05	0.54
1:A:1011:ASN:ND2	1:A:1013:TYR:H	2.05	0.54
1:A:1194:ARG:CG	1:A:1194:ARG:NH1	2.69	0.54
1:B:1129:LEU:HB3	1:B:1130:GLU:HA	0.73	0.54
1:A:895:ALA:H	1:A:896:MET:HB3	1.73	0.54
1:A:1032:ARG:HB3	1:A:1033:GLU:C	2.29	0.53
1:A:1060:VAL:HG13	1:A:1065:ILE:O	2.09	0.53
1:B:905:CYS:HA	1:B:909:TYR:HB2	1.91	0.53
1:A:861:ARG:HD3	1:A:1003:ASP:OD1	2.09	0.53
1:B:1234:THR:HG23	1:B:1235:ILE:HG13	1.90	0.53
1:A:895:ALA:HB3	1:A:896:MET:CB	2.39	0.53
1:B:637:LEU:HD13	1:B:664:LEU:HD11	1.91	0.52
1:A:1030:LEU:CB	1:A:1031:ASP:HA	2.29	0.52
1:A:1226:PHE:O	1:A:1228:HIS:HD2	1.91	0.52
1:A:671:PRO:HD2	1:A:1280:ARG:HH21	1.74	0.52
1:A:1106:LYS:HE3	1:A:1260:TYR:OH	2.10	0.52
1:A:582:PRO:HD2	1:A:1110:LEU:HD13	1.92	0.52
1:A:1083:ALA:HA	1:A:1086:ARG:HD2	1.91	0.52
1:B:963:TRP:HB2	1:B:966:LEU:HB3	1.91	0.52
1:A:678:LYS:O	1:A:682:GLN:HB2	2.10	0.51
1:B:591:TRP:H	1:B:663:GLN:NE2	2.08	0.51
1:B:1186:GLY:HA3	1:B:1262:SER:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:961:ASN:HA	1:B:963:TRP:NE1	2.24	0.51
1:A:749:ILE:HG22	1:A:774:SER:HB2	1.92	0.51
1:A:820:VAL:HB	1:A:821:GLY:CA	2.40	0.51
1:B:1032:ARG:HB3	1:B:1033:GLU:C	2.31	0.51
1:A:915:GLN:HB2	1:A:1069:VAL:HG12	1.92	0.51
1:A:1158:VAL:HG12	1:A:1221:ALA:HB1	1.92	0.50
1:B:977:ASP:HB2	1:B:980:GLY:HA2	1.92	0.50
1:B:1196:GLY:O	1:B:1197:GLY:C	2.51	0.49
1:B:946:TYR:HB2	1:B:950:GLN:HE21	1.77	0.49
1:B:1151:ASP:HB3	1:B:1154:MET:HB2	1.94	0.49
1:B:864:LEU:HB3	1:B:1021:ASN:HD21	1.77	0.49
1:A:939:ILE:HG21	1:A:985:LEU:CD2	2.43	0.49
1:B:827:TYR:HB2	1:B:828:PRO:HD3	1.94	0.49
1:A:815:PRO:CG	1:A:972:ASN:HB3	2.39	0.49
1:B:843:GLY:H	1:B:846:GLN:NE2	2.08	0.49
1:B:575:LEU:HB3	1:B:576:GLY:CA	2.39	0.49
1:B:578:SER:HB3	2:B:40:HOH:O	2.12	0.49
1:A:1155:ASN:O	1:A:1158:VAL:HG22	2.12	0.49
1:B:1140:GLU:HB3	1:B:1212:PHE:HZ	1.78	0.49
1:B:1032:ARG:HB2	1:B:1035:GLN:CG	2.43	0.48
1:B:861:ARG:HD3	1:B:1003:ASP:OD1	2.12	0.48
1:B:899:ASN:C	1:B:901:ARG:N	2.66	0.48
1:A:1000:GLY:HA2	1:A:1022:ILE:HG12	1.96	0.48
1:B:634:MET:HE1	1:B:668:LEU:HD13	1.94	0.48
1:B:912:VAL:HA	1:B:1066:PRO:HD2	1.96	0.48
1:A:817:SER:HB3	1:A:818:ASN:CA	2.44	0.48
1:A:898:ILE:H	1:A:901:ARG:HE	1.60	0.48
1:A:1240:VAL:HG11	1:A:1260:TYR:HD1	1.78	0.47
1:B:937:THR:HB	1:B:1035:GLN:NE2	2.29	0.47
1:B:768:TRP:HD1	1:B:768:TRP:N	2.10	0.47
1:B:981:ALA:HB1	1:B:984:LYS:HB3	1.96	0.47
1:A:979:ASN:CB	1:A:980:GLY:HA3	2.44	0.47
1:B:1130:GLU:N	1:B:1131:ASN:CA	2.73	0.47
1:A:963:TRP:HB2	1:A:966:LEU:HB3	1.96	0.47
1:B:1158:VAL:HG12	1:B:1221:ALA:HB1	1.97	0.47
1:A:768:TRP:N	1:A:768:TRP:HD1	2.11	0.47
1:B:1134:SER:OG	1:B:1135:GLU:HA	2.14	0.47
1:A:895:ALA:CB	1:A:896:MET:HA	2.45	0.47
1:B:632:GLY:CA	1:B:692:ARG:HG3	2.44	0.47
1:A:592:THR:OG1	1:A:595:VAL:HG23	2.15	0.46
1:A:763:PRO:HA	1:A:764:ALA:HA	1.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1028:GLU:CG	1:B:1029:LYS:HG2	2.42	0.46
1:B:1102:PRO:HA	1:B:1103:PRO:HD3	1.77	0.46
1:B:921:ILE:HG21	1:B:981:ALA:O	2.16	0.46
1:A:827:TYR:HB2	1:A:828:PRO:HD3	1.96	0.46
1:B:1194:ARG:CG	1:B:1194:ARG:NH1	2.72	0.46
1:B:749:ILE:HD11	1:B:800:LEU:HB2	1.98	0.46
1:B:1133:VAL:N	1:B:1134:SER:CA	2.64	0.46
1:A:1060:VAL:HG22	1:A:1065:ILE:HG13	1.97	0.46
1:A:910:ARG:HE	1:A:1036:LYS:HG3	1.80	0.46
1:A:979:ASN:HD22	1:A:984:LYS:HD2	1.81	0.46
1:B:936:LEU:HD13	1:B:1038:VAL:HG23	1.96	0.46
1:A:701:GLU:HG2	1:A:1101:THR:HG23	1.97	0.46
1:B:1030:LEU:HB3	1:B:1031:ASP:HB2	1.96	0.45
1:A:1030:LEU:HB3	1:A:1031:ASP:CB	2.45	0.45
1:A:807:GLU:HG3	1:A:1006:VAL:HG23	1.97	0.45
1:A:893:PHE:HD1	1:A:1077:GLN:HA	1.81	0.45
1:B:817:SER:HB3	1:B:818:ASN:C	2.36	0.45
1:A:670:LEU:HD23	1:A:673:MET:SD	2.57	0.45
1:A:819:GLN:HA	1:A:820:VAL:HA	1.79	0.45
1:A:919:LYS:HB2	1:A:919:LYS:HE3	1.73	0.45
1:A:905:CYS:HA	1:A:909:TYR:HB2	1.98	0.45
1:B:1030:LEU:CB	1:B:1031:ASP:HA	2.41	0.45
1:A:946:TYR:O	1:A:950:GLN:HB3	2.17	0.45
1:A:768:TRP:HD1	1:A:768:TRP:H	1.59	0.45
1:A:789:MET:HE2	1:A:824:TYR:HD2	1.81	0.45
1:B:631:GLN:HE22	1:B:692:ARG:HA	1.81	0.45
1:B:777:LEU:HB3	1:B:778:PRO:HD3	1.99	0.45
1:B:1032:ARG:CA	1:B:1033:GLU:CB	2.90	0.45
1:A:864:LEU:HB3	1:A:1021:ASN:HD21	1.82	0.44
1:B:817:SER:CB	1:B:971:PHE:HE2	2.17	0.44
1:B:1122:GLU:HG2	1:B:1232:ASP:HA	2.00	0.44
1:A:977:ASP:HB3	1:A:980:GLY:O	2.17	0.44
1:B:1113:PHE:O	1:B:1252:ARG:HA	2.18	0.44
1:B:1127:PRO:O	1:B:1129:LEU:N	2.48	0.44
1:B:1138:ARG:HG3	1:B:1139:GLU:N	2.33	0.44
1:B:1154:MET:HG2	1:B:1175:ARG:HG2	1.98	0.44
1:B:964:LYS:HG2	2:B:36:HOH:O	2.16	0.44
1:B:1191:TRP:CE2	1:B:1203:GLN:HB2	2.52	0.44
1:B:1223:HIS:CE1	1:B:1224:LEU:HD13	2.52	0.44
1:A:961:ASN:C	1:A:961:ASN:ND2	2.69	0.44
1:B:814:SER:CB	1:B:815:PRO:CD	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1054:ARG:HB2	1:B:1055:PRO:HD2	1.98	0.44
1:A:631:GLN:C	1:A:631:GLN:HE21	2.19	0.44
1:B:776:LEU:HB3	1:B:780:LEU:HD13	1.99	0.44
1:B:1129:LEU:HG	1:B:1131:ASN:HB2	2.00	0.44
1:B:912:VAL:HG23	1:B:1066:PRO:HG2	2.00	0.44
1:A:817:SER:HB3	1:A:818:ASN:C	2.39	0.44
1:B:749:ILE:HG22	1:B:774:SER:HB2	2.00	0.43
1:B:955:GLN:HG3	1:B:960:SER:OG	2.18	0.43
1:A:575:LEU:CB	1:A:576:GLY:HA2	2.27	0.43
1:A:585:ILE:HG22	1:A:630:ARG:HD2	1.99	0.43
1:A:1054:ARG:HB2	1:A:1055:PRO:HD2	2.00	0.43
1:A:1245:LEU:O	1:A:1249:GLN:HG3	2.19	0.43
1:B:895:ALA:HB1	1:B:896:MET:HB3	1.99	0.43
1:A:830:THR:O	1:A:834:MET:HG3	2.18	0.43
1:A:946:TYR:CD1	1:A:950:GLN:NE2	2.84	0.43
1:B:1026:ALA:O	1:B:1030:LEU:HB2	2.17	0.43
1:B:915:GLN:HE21	1:B:1069:VAL:HG12	1.84	0.43
1:A:588:GLU:HG3	2:A:188:HOH:O	2.18	0.43
1:A:706:THR:HG22	1:A:707:SER:N	2.34	0.43
1:B:977:ASP:HA	1:B:978:ILE:CG2	2.47	0.43
1:B:1193:ARG:HD2	1:B:1195:GLU:OE1	2.18	0.43
1:B:818:ASN:ND2	1:B:824:TYR:H	2.17	0.43
1:A:653:ARG:CZ	2:A:219:HOH:O	2.57	0.43
1:A:1004:ASN:HD22	1:A:1004:ASN:HA	1.70	0.43
1:B:896:MET:N	1:B:897:SER:HA	2.34	0.42
1:A:777:LEU:HB3	1:A:778:PRO:HD3	2.00	0.42
1:B:825:GLU:O	1:B:828:PRO:HD2	2.19	0.42
1:B:1134:SER:CB	1:B:1135:GLU:HA	2.50	0.42
1:B:816:TYR:HA	1:B:817:SER:HA	1.62	0.42
1:B:807:GLU:HG3	1:B:1006:VAL:HG23	2.01	0.42
1:B:1135:GLU:O	1:B:1137:LEU:HB3	2.20	0.42
1:A:706:THR:HG22	1:A:707:SER:O	2.19	0.42
1:A:979:ASN:OD1	1:A:979:ASN:N	2.52	0.42
1:A:910:ARG:HH22	1:A:1034:GLY:H	1.67	0.42
1:A:1113:PHE:O	1:A:1252:ARG:HA	2.19	0.42
1:B:1011:ASN:HD22	1:B:1013:TYR:H	1.67	0.42
1:B:1145:ILE:HG13	1:B:1237:ILE:HG21	2.01	0.42
1:B:1195:GLU:HB2	1:B:1199:GLU:HB3	2.02	0.41
1:B:820:VAL:HB	1:B:821:GLY:HA2	2.02	0.41
1:B:1192:TRP:CZ2	1:B:1278:LYS:HB2	2.55	0.41
1:A:587:LEU:HD21	1:A:630:ARG:HD3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:GLU:H	1:A:766:GLU:HG2	1.59	0.41
1:B:954:SER:HA	1:B:957:LEU:HD22	2.01	0.41
1:A:977:ASP:CA	1:A:978:ILE:C	2.84	0.41
1:A:1126:LEU:HB3	1:A:1127:PRO:HD3	2.03	0.41
1:A:1281:LEU:HB3	1:A:1282:THR:H	1.59	0.41
1:B:819:GLN:HA	1:B:820:VAL:HA	1.91	0.41
1:B:830:THR:O	1:B:834:MET:HG3	2.20	0.41
1:B:893:PHE:CE1	1:B:904:LYS:HD2	2.56	0.41
1:B:1193:ARG:NH1	1:B:1195:GLU:OE1	2.37	0.41
1:A:978:ILE:HA	1:A:979:ASN:HA	1.52	0.41
1:A:1026:ALA:O	1:A:1030:LEU:HB2	2.20	0.41
1:B:749:ILE:HD13	1:B:749:ILE:HA	1.88	0.41
1:A:1223:HIS:NE2	1:A:1224:LEU:HD13	2.36	0.40
1:B:937:THR:HB	1:B:1035:GLN:HE22	1.85	0.40
1:B:927:ASN:O	1:B:931:PHE:HB2	2.21	0.40
1:B:763:PRO:HA	1:B:766:GLU:CD	2.42	0.40
1:B:814:SER:O	1:B:815:PRO:O	2.38	0.40
1:B:1035:GLN:HE21	1:B:1035:GLN:HA	1.87	0.40
1:B:1155:ASN:O	1:B:1158:VAL:HG22	2.20	0.40
1:A:706:THR:CG2	1:A:707:SER:N	2.84	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	709/746 (95%)	647 (91%)	49 (7%)	13 (2%)	8	16
1	B	709/746 (95%)	629 (89%)	63 (9%)	17 (2%)	6	10
All	All	1418/1492 (95%)	1276 (90%)	112 (8%)	30 (2%)	7	13

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	961	ASN
1	A	978	ILE
1	B	814	SER
1	B	815	PRO
1	B	1133	VAL
1	B	1213	ALA
1	A	1032	ARG
1	A	1137	LEU
1	A	1213	ALA
1	A	1283	ARG
1	B	825	GLU
1	B	961	ASN
1	B	1229	ASP
1	A	1265	GLY
1	B	900	GLU
1	B	980	GLY
1	B	1031	ASP
1	B	1138	ARG
1	A	821	GLY
1	A	1090	GLU
1	B	978	ILE
1	B	1028	GLU
1	B	1265	GLY
1	A	1028	GLU
1	A	1031	ASP
1	A	1281	LEU
1	B	1032	ARG
1	B	1128	LEU
1	A	815	PRO
1	B	935	GLY

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	616/646 (95%)	560 (91%)	56 (9%)	9	18
1	B	616/646 (95%)	563 (91%)	53 (9%)	10	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1232/1292 (95%)	1123 (91%)	109 (9%)	10	19

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	588	GLU
1	A	596	LEU
1	A	605	LYS
1	A	618	LEU
1	A	631	GLN
1	A	637	LEU
1	A	668	LEU
1	A	672	GLU
1	A	758	ASN
1	A	766	GLU
1	A	818	ASN
1	A	819	GLN
1	A	826	LEU
1	A	851	ARG
1	A	859	SER
1	A	861	ARG
1	A	867	ASN
1	A	893	PHE
1	A	896	MET
1	A	899	ASN
1	A	907	ASN
1	A	937	THR
1	A	957	LEU
1	A	958	GLN
1	A	961	ASN
1	A	965	THR
1	A	975	LYS
1	A	979	ASN
1	A	985	LEU
1	A	986	LEU
1	A	991	ASP
1	A	993	ASN
1	A	1004	ASN
1	A	1029	LYS
1	A	1036	LYS
1	A	1060	VAL
1	A	1079	LEU

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Mol	Chain	Res	Type
1	A	1092	THR
1	A	1104	GLN
1	A	1115	LEU
1	A	1135	GLU
1	A	1144	LYS
1	A	1146	ASP
1	A	1154	MET
1	A	1157	LEU
1	A	1161	GLU
1	A	1177	LYS
1	A	1194	ARG
1	A	1198	MET
1	A	1224	LEU
1	A	1230	GLN
1	A	1231	LEU
1	A	1266	ASN
1	A	1270	LEU
1	A	1282	THR
1	A	1285	LEU
1	B	575	LEU
1	B	588	GLU
1	B	596	LEU
1	B	605	LYS
1	B	618	LEU
1	B	631	GLN
1	B	637	LEU
1	B	652	GLU
1	B	668	LEU
1	B	670	LEU
1	B	678	LYS
1	B	706	THR
1	B	768	TRP
1	B	794	ARG
1	B	819	GLN
1	B	826	LEU
1	B	851	ARG
1	B	859	SER
1	B	861	ARG
1	B	867	ASN
1	B	896	MET
1	B	901	ARG
1	B	931	PHE

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Mol	Chain	Res	Type
1	B	937	THR
1	B	958	GLN
1	B	961	ASN
1	B	978	ILE
1	B	985	LEU
1	B	986	LEU
1	B	993	ASN
1	B	1004	ASN
1	B	1028	GLU
1	B	1029	LYS
1	B	1036	LYS
1	B	1079	LEU
1	B	1092	THR
1	B	1104	GLN
1	B	1106	LYS
1	B	1115	LEU
1	B	1129	LEU
1	B	1134	SER
1	B	1140	GLU
1	B	1144	LYS
1	B	1146	ASP
1	B	1154	MET
1	B	1157	LEU
1	B	1161	GLU
1	B	1177	LYS
1	B	1181	LEU
1	B	1194	ARG
1	B	1224	LEU
1	B	1266	ASN
1	B	1270	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	631	GLN
1	A	663	GLN
1	A	758	ASN
1	A	785	GLN
1	A	839	GLN
1	A	846	GLN
1	A	907	ASN
1	A	915	GLN

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Mol	Chain	Res	Type
1	A	926	ASN
1	A	934	ASN
1	A	958	GLN
1	A	961	ASN
1	A	972	ASN
1	A	1004	ASN
1	A	1011	ASN
1	A	1021	ASN
1	A	1131	ASN
1	A	1203	GLN
1	A	1228	HIS
1	A	1251	ASN
1	B	631	GLN
1	B	663	GLN
1	B	785	GLN
1	B	818	ASN
1	B	839	GLN
1	B	846	GLN
1	B	907	ASN
1	B	915	GLN
1	B	926	ASN
1	B	950	GLN
1	B	961	ASN
1	B	972	ASN
1	B	1004	ASN
1	B	1011	ASN
1	B	1021	ASN
1	B	1035	GLN
1	B	1131	ASN
1	B	1228	HIS
1	B	1251	ASN
1	B	1266	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	711/746 (95%)	0.17	32 (4%) 33 26	45, 60, 77, 99	0
1	B	711/746 (95%)	0.13	28 (3%) 39 32	38, 52, 69, 95	0
All	All	1422/1492 (95%)	0.15	60 (4%) 36 29	38, 57, 75, 99	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1282	THR	6.0
1	A	1282	THR	6.0
1	A	576	GLY	5.5
1	A	821	GLY	5.5
1	A	1284	ALA	5.3
1	A	908	THR	4.8
1	A	822	GLY	4.7
1	B	1283	ARG	4.4
1	B	576	GLY	4.2
1	A	820	VAL	4.2
1	A	1234	THR	4.0
1	B	1032	ARG	3.9
1	A	1210	PHE	3.8
1	B	822	GLY	3.7
1	A	1143	GLN	3.7
1	B	882	ALA	3.7
1	A	819	GLN	3.6
1	A	1235	ILE	3.6
1	B	819	GLN	3.5
1	B	1285	LEU	3.3
1	B	1233	THR	3.2
1	A	1157	LEU	3.2
1	B	1214	GLY	3.2
1	B	820	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1281	LEU	3.1
1	A	1285	LEU	3.1
1	B	821	GLY	2.9
1	A	907	ASN	2.9
1	A	1231	LEU	2.8
1	B	893	PHE	2.8
1	A	824	TYR	2.7
1	B	1128	LEU	2.6
1	A	891	GLU	2.6
1	B	1231	LEU	2.6
1	B	817	SER	2.5
1	A	1233	THR	2.5
1	A	931	PHE	2.5
1	A	978	ILE	2.4
1	A	1141	LEU	2.4
1	A	1079	LEU	2.4
1	A	1134	SER	2.3
1	B	1234	THR	2.3
1	A	1032	ARG	2.3
1	B	1133	VAL	2.3
1	A	1283	ARG	2.3
1	B	1284	ALA	2.3
1	B	996	PHE	2.3
1	B	1040	PHE	2.3
1	B	1078	PHE	2.3
1	B	823	PRO	2.2
1	B	1070	VAL	2.2
1	A	1132	SER	2.2
1	B	1281	LEU	2.2
1	B	939	ILE	2.1
1	B	909	TYR	2.1
1	A	826	LEU	2.1
1	B	946	TYR	2.1
1	A	1034	GLY	2.1
1	A	603	ILE	2.0
1	A	1238	LEU	2.0

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

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.