



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:35 AM UTC

PDB ID : 2EC5 / pdb_00002ec5
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

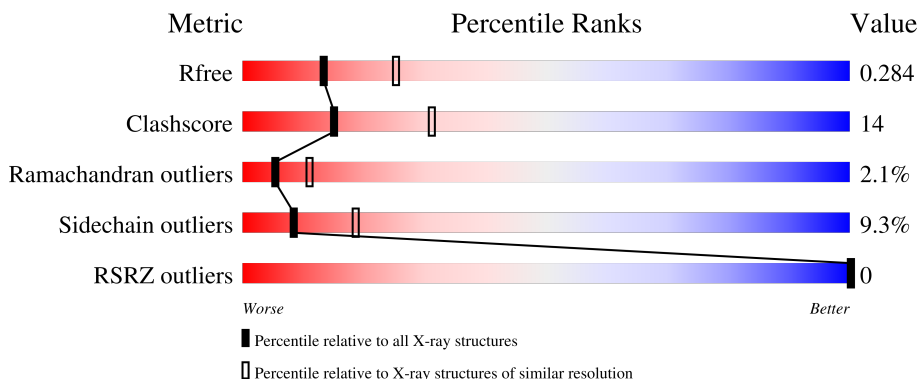
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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	
1	B	746	

2 Entry composition i

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
			Total	C	N	O	S			
1	A	711	5643	3603	939	1075	26	0	0	0
1	B	711	5643	3603	939	1075	26	0	0	0

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.

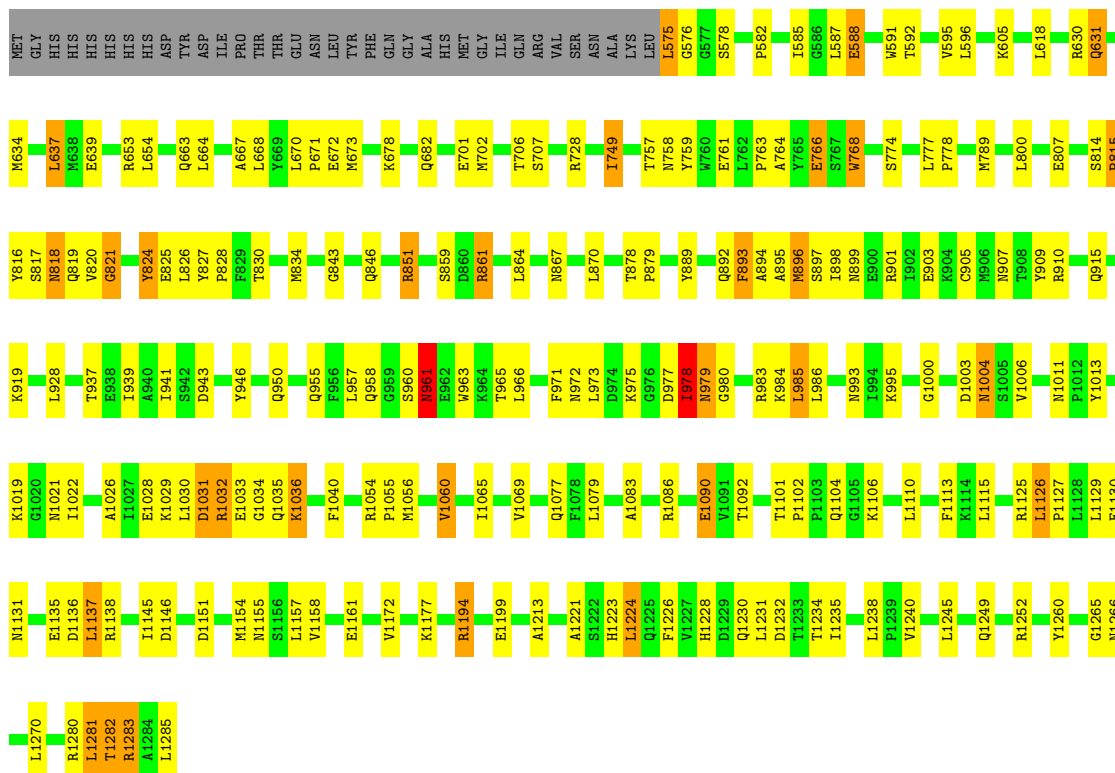
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	119	Total O 119 119	0	0
2	B	123	Total O 123 123	0	0

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.

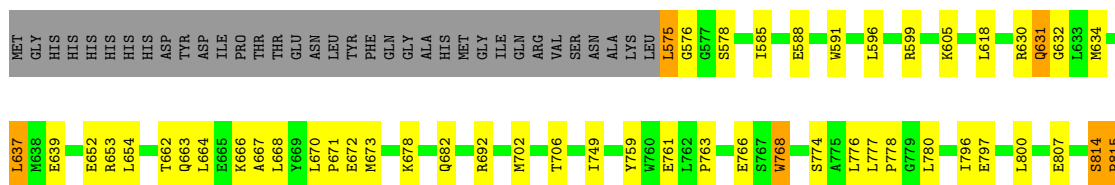
- Molecule 1: Dermonecrotic toxin

Chain A: 



- Molecule 1: Dermonecrotic toxin

Chain B: 



Y816	Y824	Y825	Y826	Y827	Y828	Y829	Y830	Y831	Y835	Y836	Y837	Y838	Y839	Y840	Y846	Y850	Y854	Y855	Y856	Y857	Y858	Y859	Y860	Y861	Y864	Y865	Y866	Y867	Y870	Y889	Y892	Y893	Y894	Y895	Y896	Y897	Y898	Y899	Y900	Y901	Y904	Y905	Y909	Y912	Y915	Y921	Y922	Y926
Y927	Y928	Y929	Y930	Y931	Y935	Y936	Y937	Y946	Y950	Y954	Y955	Y956	Y957	Y958	Y959	Y960	Y961	Y962	Y963	Y964	Y965	Y966	Y971	Y974	Y977	Y978	Y979	Y980	Y981	Y984	Y985	Y986	Y993	Y994	Y995	D1003	D1004	D1005	D1006	D1011	D1012	D1013	D1016	D1021				
A1026	E1027	E1028	L1030	D1031	R1032	E1033	G1034	Q1035	K1036	F1037	V1038	V1039	F1040	R1054	P1055	V1060	I1065	S960	P1066	V1069	D1073	L1079	A1083	R1086	T1092	P1102	P1103	Q1104	F1113	K1114	L1115	E1122	R1125	L1126	P1127	L1128	L1129	E1130	N1131	S1132	V1133	S1134	E1135	D1136	L1137			
R1138	E1139	E1140	K1144	I1145	D1146	A1147	D1151	M1154	M1155	S1156	L1157	V1158	E1161	S1167	K1171	V1172	R1175	L1181	G1186	W1191	W1192	R1193	R1194	E1195	G1196	G1197	M1198	E1199	Q1203	F1212	A1213	A1221	S1222	H1223	L1224	Q1225	F1226	V1227	H1228	D1229	D1232	T1233	T1234	I1235	L1236			
I1237	L1238	F1239	V1240	R1252	S1262	G1265	N1266	L1270	K1278	P1279	R1280	L1281	L1285																																			

4 Data and refinement statistics i

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)	Xtrriage
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 (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.478 for -h-2*1,-k,l	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

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	0.51	0/5769	0.87	4/7811 (0.1%)
1	B	0.56	4/5769 (0.1%)	0.86	5/7811 (0.1%)
All	All	0.54	4/11538 (0.0%)	0.86	9/15622 (0.1%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	926	ASN	CG-ND2	9.26	1.52	1.33
1	B	926	ASN	CG-OD1	7.77	1.38	1.23
1	B	922	ASP	C-O	5.91	1.31	1.24
1	B	1073	ASP	CG-OD2	5.47	1.35	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	654	LEU	N-CA-C	8.42	120.08	111.07
1	A	825	GLU	N-CA-C	6.71	118.51	110.19
1	A	1102	PRO	CA-C-N	6.45	126.20	119.05
1	A	1102	PRO	C-N-CA	6.45	126.20	119.05
1	A	654	LEU	N-CA-C	6.16	117.80	111.14
1	B	926	ASN	OD1-CG-ND2	6.08	128.68	122.60
1	B	1102	PRO	CA-C-N	6.08	125.97	119.28
1	B	1102	PRO	C-N-CA	6.08	125.97	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1240	VAL	N-CA-C	5.20	115.82	110.36

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 [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	5643	0	5575	145	0
1	B	5643	0	5575	164	0
2	A	119	0	0	6	0
2	B	123	0	0	5	0
All	All	11528	0	11150	307	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 14.

All (307) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:768:TRP:H	1:B:768:TRP:CD1	2.02	0.78
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:B:1132:SER:C	1:B:1134:SER:HA	2.11	0.76
1:A:979:ASN:CG	1:A:980:GLY:HA3	2.10	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:A:977:ASP:HA	1:A:978:ILE:C	2.12	0.74
1:A:1130:GLU:HA	1:A:1131:ASN:C	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:H	1:B:768:TRP:HD1	1.38	0.70
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
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:A:1154:MET:HE1	1:A:1172:VAL:HG13	1.76	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:A:673:MET:HE3	1:A:702:MET:HE1	1.73	0.68
1:B:1194:ARG:HH11	1:B:1194:ARG:CG	2.07	0.68
1:B:1136:ASP:HA	1:B:1137:LEU:C	2.19	0.67
1:B:899:ASN:C	1:B:901:ARG:H	2.02	0.67
1:A:961:ASN:C	1:A:961:ASN:HD22	2.02	0.67
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:B:1154:MET:HE1	1:B:1172:VAL:HG13	1.78	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: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:1126:LEU:HB3	1:B:1127:PRO:HD3	1.81	0.62
1:A:653:ARG:HD3	2:A:4:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:ARG:HB2	1:A:1035:GLN:CG	2.30	0.61
1:A:768:TRP:CD1	1:A:768:TRP:H	2.19	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:B:634:MET:HE1	1:B:667:ALA:HB3	1.85	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:CD1	1:B:768:TRP:N	2.69	0.58
1:A:1032:ARG:HB3	1:A:1033:GLU:C	2.29	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
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:B:1032:ARG:HB3	1:B:1033:GLU:C	2.31	0.56
1:A:768:TRP:CD1	1:A:768:TRP:N	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:1196:GLY:O	1:B:1197:GLY:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:865:MET:HE1	1:B:1016:LEU:HD23	1.92	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
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: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:817:SER:HB3	1:B:818:ASN:C	2.36	0.50
1:A:1019:LYS:HG2	1:A:1056:MET:HE2	1.94	0.50
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:B:899:ASN:C	1:B:901:ARG:N	2.66	0.49
1:A:1155:ASN:O	1:A:1158:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1140:GLU:HB3	1:B:1212:PHE:HZ	1.78	0.49
1:A:631:GLN:C	1:A:631:GLN:HE21	2.19	0.48
1:B:673:MET:HE3	1:B:702:MET:HE1	1.95	0.48
1:B:1032:ARG:HB2	1:B:1035:GLN:CG	2.43	0.48
1:A:817:SER:HB3	1:A:818:ASN:C	2.39	0.48
1:B:861:ARG:HD3	1:B:1003:ASP:OD1	2.12	0.48
1:A:1000:GLY:HA2	1:A:1022:ILE:HG12	1.96	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:A:977:ASP:CA	1:A:978:ILE:C	2.84	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
1:A:789:MET:HE2	1:A:824:TYR:HD2	1.80	0.46
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:B:763:PRO:HA	1:B:766:GLU:CD	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:634:MET:HE1	1:A:667:ALA:HB3	1.99	0.45
1:A:946:TYR:O	1:A:950:GLN:HB3	2.17	0.45
1:A:768:TRP:H	1:A:768:TRP:HD1	1.59	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:B:814:SER:CB	1:B:815:PRO:CD	2.86	0.44
1:B:1054:ARG:HB2	1:B:1055:PRO:HD2	1.98	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:1090:GLU:CD	1:B:599:ARG:HH21	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:757:THR:C	1:A:758:ASN:HD22	2.26	0.43
1:B:631:GLN:HE21	1:B:631:GLN:C	2.26	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:961:ASN:C	1:A:961:ASN:ND2	2.69	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
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: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:759:TYR:C	1:B:761:GLU:H	2.28	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:961:ASN:HD22	1:B:961:ASN:C	2.29	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:578:SER:C	2:B:3:HOH:O	2.64	0.41
1:B:749:ILE:HD13	1:B:749:ILE:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:929:THR:C	1:B:931:PHE:H	2.28	0.41
1:A:588:GLU:CD	1:A:588:GLU:H	2.29	0.40
1:A:759:TYR:C	1:A:761:GLU:H	2.30	0.40
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:796:ILE:O	1:B:797:GLU:C	2.64	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

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%)	6 14
1	B	709/746 (95%)	629 (89%)	63 (9%)	17 (2%)	4 9
All	All	1418/1492 (95%)	1276 (90%)	112 (8%)	30 (2%)	5 11

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

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Mol	Chain	Res	Type
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 [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	616/646 (95%)	557 (90%)	59 (10%)	8 17
1	B	616/646 (95%)	561 (91%)	55 (9%)	9 20
All	All	1232/1292 (95%)	1118 (91%)	114 (9%)	8 18

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	575	LEU

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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	749	ILE
1	A	766	GLU
1	A	768	TRP
1	A	818	ASN
1	A	826	LEU
1	A	851	ARG
1	A	859	SER
1	A	861	ARG
1	A	867	ASN
1	A	870	LEU
1	A	893	PHE
1	A	896	MET
1	A	899	ASN
1	A	907	ASN
1	A	928	LEU
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	978	ILE
1	A	979	ASN
1	A	985	LEU
1	A	986	LEU
1	A	993	ASN
1	A	995	LYS
1	A	1004	ASN
1	A	1029	LYS
1	A	1036	LYS
1	A	1060	VAL
1	A	1079	LEU
1	A	1092	THR
1	A	1104	GLN

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Mol	Chain	Res	Type
1	A	1115	LEU
1	A	1126	LEU
1	A	1129	LEU
1	A	1145	ILE
1	A	1146	ASP
1	A	1157	LEU
1	A	1161	GLU
1	A	1177	LYS
1	A	1194	ARG
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	672	GLU
1	B	706	THR
1	B	768	TRP
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	870	LEU
1	B	896	MET
1	B	901	ARG
1	B	937	THR
1	B	958	GLN
1	B	961	ASN
1	B	978	ILE

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Mol	Chain	Res	Type
1	B	985	LEU
1	B	986	LEU
1	B	993	ASN
1	B	995	LYS
1	B	1004	ASN
1	B	1028	GLU
1	B	1029	LYS
1	B	1036	LYS
1	B	1060	VAL
1	B	1079	LEU
1	B	1092	THR
1	B	1104	GLN
1	B	1115	LEU
1	B	1126	LEU
1	B	1129	LEU
1	B	1134	SER
1	B	1137	LEU
1	B	1140	GLU
1	B	1144	LYS
1	B	1145	ILE
1	B	1146	ASP
1	B	1157	LEU
1	B	1161	GLU
1	B	1181	LEU
1	B	1194	ARG
1	B	1224	LEU
1	B	1266	ASN
1	B	1270	LEU
1	B	1281	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	619	GLN
1	A	631	GLN
1	A	648	GLN
1	A	663	GLN
1	A	758	ASN
1	A	785	GLN
1	A	798	ASN
1	A	818	ASN
1	A	846	GLN

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Mol	Chain	Res	Type
1	A	852	ASN
1	A	892	GLN
1	A	907	ASN
1	A	915	GLN
1	A	926	ASN
1	A	958	GLN
1	A	961	ASN
1	A	972	ASN
1	A	1001	HIS
1	A	1004	ASN
1	A	1011	ASN
1	A	1021	ASN
1	A	1112	GLN
1	A	1131	ASN
1	A	1155	ASN
1	A	1228	HIS
1	A	1230	GLN
1	B	622	HIS
1	B	631	GLN
1	B	663	GLN
1	B	785	GLN
1	B	839	GLN
1	B	846	GLN
1	B	907	ASN
1	B	915	GLN
1	B	926	ASN
1	B	927	ASN
1	B	950	GLN
1	B	961	ASN
1	B	972	ASN
1	B	979	ASN
1	B	992	ASN
1	B	1004	ASN
1	B	1011	ASN
1	B	1021	ASN
1	B	1035	GLN
1	B	1112	GLN
1	B	1228	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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 [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, 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%)	-1.08	0 100 100	45, 60, 77, 99	0
1	B	711/746 (95%)	-1.17	0 100 100	38, 52, 69, 95	0
All	All	1422/1492 (95%)	-1.12	0 100 100	38, 57, 75, 99	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.