



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:18 AM GMT

PDB ID : 3HX6
Title : Crystal structure of Pseudomonas aeruginosa PilY1 C-terminal domain
Authors : Redinbo, M.R.; Orans, J.
Deposited on : 2009-06-19
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

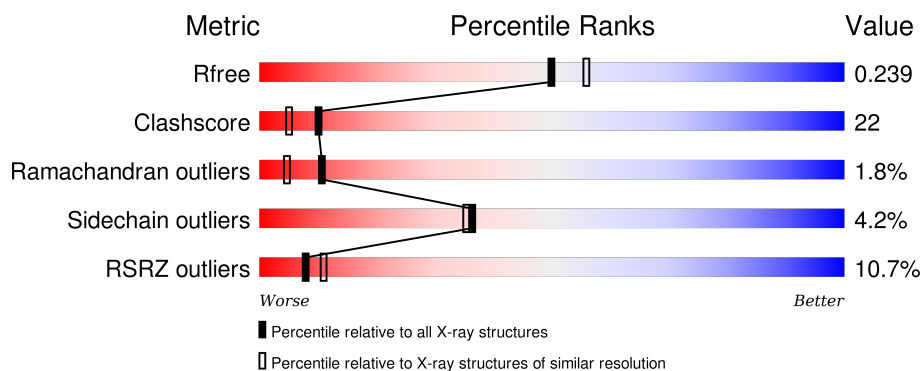
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	570	<div> <div>8%</div> <div>58%</div> <div>26%</div> <div>•</div> <div>14%</div> </div>
1	B	570	<div> <div>10%</div> <div>56%</div> <div>26%</div> <div>•</div> <div>15%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8125 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 Type 4 fimbrial biogenesis protein PilY1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3700	2320	641	730	9			
1	B	486	Total	C	N	O	S	0	0	0
			3663	2299	633	723	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	594	MET	-	EXPRESSION TAG	UNP Q9HVM8
A	595	GLY	-	EXPRESSION TAG	UNP Q9HVM8
A	596	SER	-	EXPRESSION TAG	UNP Q9HVM8
A	597	SER	-	EXPRESSION TAG	UNP Q9HVM8
A	598	HIS	-	EXPRESSION TAG	UNP Q9HVM8
A	599	HIS	-	EXPRESSION TAG	UNP Q9HVM8
A	600	HIS	-	EXPRESSION TAG	UNP Q9HVM8
A	601	HIS	-	EXPRESSION TAG	UNP Q9HVM8
A	602	HIS	-	EXPRESSION TAG	UNP Q9HVM8
A	603	HIS	-	EXPRESSION TAG	UNP Q9HVM8
A	604	SER	-	EXPRESSION TAG	UNP Q9HVM8
A	605	SER	-	EXPRESSION TAG	UNP Q9HVM8
A	606	GLY	-	EXPRESSION TAG	UNP Q9HVM8
A	607	LEU	-	EXPRESSION TAG	UNP Q9HVM8
A	608	VAL	-	EXPRESSION TAG	UNP Q9HVM8
A	609	PRO	-	EXPRESSION TAG	UNP Q9HVM8
A	610	ARG	-	EXPRESSION TAG	UNP Q9HVM8
A	611	GLY	-	EXPRESSION TAG	UNP Q9HVM8
A	612	SER	-	EXPRESSION TAG	UNP Q9HVM8
A	613	HIS	-	EXPRESSION TAG	UNP Q9HVM8
A	614	MET	-	EXPRESSION TAG	UNP Q9HVM8
A	712	MET	LEU	ENGINEERED	UNP Q9HVM8
A	812	MET	LEU	ENGINEERED	UNP Q9HVM8
A	823	MET	LEU	ENGINEERED	UNP Q9HVM8
B	594	MET	-	EXPRESSION TAG	UNP Q9HVM8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	595	GLY	-	EXPRESSION TAG	UNP Q9HVM8
B	596	SER	-	EXPRESSION TAG	UNP Q9HVM8
B	597	SER	-	EXPRESSION TAG	UNP Q9HVM8
B	598	HIS	-	EXPRESSION TAG	UNP Q9HVM8
B	599	HIS	-	EXPRESSION TAG	UNP Q9HVM8
B	600	HIS	-	EXPRESSION TAG	UNP Q9HVM8
B	601	HIS	-	EXPRESSION TAG	UNP Q9HVM8
B	602	HIS	-	EXPRESSION TAG	UNP Q9HVM8
B	603	HIS	-	EXPRESSION TAG	UNP Q9HVM8
B	604	SER	-	EXPRESSION TAG	UNP Q9HVM8
B	605	SER	-	EXPRESSION TAG	UNP Q9HVM8
B	606	GLY	-	EXPRESSION TAG	UNP Q9HVM8
B	607	LEU	-	EXPRESSION TAG	UNP Q9HVM8
B	608	VAL	-	EXPRESSION TAG	UNP Q9HVM8
B	609	PRO	-	EXPRESSION TAG	UNP Q9HVM8
B	610	ARG	-	EXPRESSION TAG	UNP Q9HVM8
B	611	GLY	-	EXPRESSION TAG	UNP Q9HVM8
B	612	SER	-	EXPRESSION TAG	UNP Q9HVM8
B	613	HIS	-	EXPRESSION TAG	UNP Q9HVM8
B	614	MET	-	EXPRESSION TAG	UNP Q9HVM8
B	712	MET	LEU	ENGINEERED	UNP Q9HVM8
B	812	MET	LEU	ENGINEERED	UNP Q9HVM8
B	823	MET	LEU	ENGINEERED	UNP Q9HVM8

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	432	Total O 432 432	0	0
3	B	328	Total O 328 328	0	0

Q1108	N1109	V1110	E1116	Q1117	K1118	G1119	L1120	G1121	G1122	L1123	T1124	L1125	S1126	T1127	N1128	E1129	Q1130	G1131	N1132	P1133	E1134	V1135	C1136	S1137	S1138	C1141	L1142	T1143	P1146	G1147	P1148	ASN	THR	ARG	GLY	ARG	GLN	ASN	TRP	ARG	PRO	ILE	GLU	GLY	LYS	ASN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.00Å 108.00Å 159.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 47.58 – 2.09	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 96.5 (47.58-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.08Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.235 0.201 , 0.239	Depositor DCC
R_{free} test set	6250 reflections (9.85%)	DCC
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 123850 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8125	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.33	0/3781	0.65	0/5144
1	B	0.32	0/3743	0.62	0/5093
All	All	0.32	0/7524	0.64	0/10237

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	3700	0	3560	160	0
1	B	3663	0	3529	164	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	432	0	0	24	0
3	B	328	0	0	24	0
All	All	8125	0	7089	317	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 22.

All (317) 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:857:VAL:HG21	1:A:888:ARG:HD3	1.36	1.08
1:A:680:ARG:HE	1:A:700:THR:HG21	1.23	1.01
1:A:1040:GLU:OE2	1:A:1057:THR:HG21	1.60	0.99
1:B:857:VAL:HG21	1:B:888:ARG:HD3	1.43	0.98
1:A:1080:THR:HG23	1:A:1082:GLY:H	1.31	0.94
1:A:1083:ARG:HD3	1:A:1110:VAL:HG13	1.46	0.93
1:B:1128:ASN:HD21	1:B:1132:ASN:HB2	1.35	0.91
1:B:1080:THR:HG23	1:B:1082:GLY:H	1.37	0.89
1:B:1128:ASN:HB2	1:B:1130:GLN:HE21	1.36	0.87
1:B:687:ASP:HB3	1:B:755:GLY:H	1.40	0.87
1:B:753:ARG:HH21	1:B:788:PHE:HA	1.41	0.85
1:B:680:ARG:HE	1:B:700:THR:HG21	1.44	0.82
1:A:644:SER:HB3	1:A:645:PRO:HD3	1.64	0.80
1:B:1132:ASN:HB3	3:B:1246:HOH:O	1.83	0.78
1:B:1121:GLY:HA3	1:B:1138:SER:HB2	1.65	0.78
1:B:731:GLY:HA2	1:B:753:ARG:HH11	1.48	0.77
1:A:686:ASN:ND2	1:A:687:ASP:H	1.83	0.77
1:B:1043:ILE:HD13	3:B:329:HOH:O	1.85	0.76
1:A:981:THR:HG22	1:A:983:GLY:H	1.51	0.75
1:A:681:VAL:HB	1:A:694:ASP:HB2	1.69	0.75
1:A:729:VAL:O	1:A:753:ARG:HD3	1.86	0.74
1:B:959:GLN:HG3	1:B:1041:MET:HB3	1.70	0.74
1:B:758:GLY:HA2	1:B:784:LEU:HD21	1.70	0.74
1:A:901:VAL:HG11	3:A:1256:HOH:O	1.87	0.73
1:B:941:GLY:HA3	1:B:1042:LEU:HD22	1.69	0.73
1:A:1043:ILE:HD13	3:A:35:HOH:O	1.87	0.73
1:B:1060:PRO:O	1:B:1061:ASN:HB3	1.88	0.72
1:A:1130:GLN:HG3	1:A:1132:ASN:ND2	2.03	0.72
1:B:1033:VAL:HG12	3:B:145:HOH:O	1.90	0.72
1:A:709:PHE:HA	1:A:712:MET:HE3	1.70	0.71
1:A:988:GLN:HE22	1:A:1011:ASN:H	1.38	0.71
1:B:1118:LYS:N	1:B:1118:LYS:HE2	2.05	0.70
1:A:730:ASP:O	1:A:753:ARG:HD2	1.91	0.70
1:B:1047:ILE:HD13	1:B:1125:LEU:HB2	1.74	0.70
1:A:686:ASN:HD22	1:A:686:ASN:N	1.88	0.70
1:A:1129:GLU:OE1	1:B:1127:THR:HB	1.92	0.69
1:B:764:VAL:HG12	1:B:764:VAL:O	1.91	0.69
1:B:705:PRO:HG2	1:B:708:VAL:HG23	1.74	0.69
1:B:1090:ASP:HB3	1:B:1143:THR:HG23	1.75	0.68
1:A:680:ARG:NE	1:A:700:THR:HG21	2.05	0.68
1:B:727:PHE:HE1	1:B:1121:GLY:HA2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:THR:HG23	3:A:33:HOH:O	1.94	0.67
1:B:731:GLY:HA2	1:B:753:ARG:NH1	2.09	0.67
1:A:1120:LEU:HD23	3:A:334:HOH:O	1.94	0.67
1:B:753:ARG:NH2	1:B:788:PHE:HA	2.09	0.67
1:B:942:THR:HG22	1:B:959:GLN:HB3	1.76	0.67
1:B:687:ASP:HB3	1:B:755:GLY:N	2.10	0.67
1:B:880:VAL:HG13	1:B:885:PRO:HA	1.76	0.67
1:A:1106:ASN:HB2	3:A:71:HOH:O	1.94	0.66
1:A:781:GLU:OE1	1:A:831:LYS:HE2	1.95	0.66
1:B:1071:ASN:OD1	1:B:1119:GLY:HA2	1.94	0.66
1:B:1070:SER:HA	3:B:1240:HOH:O	1.96	0.66
1:B:708:VAL:O	1:B:711:LYS:HG2	1.96	0.66
1:B:942:THR:HG23	1:B:959:GLN:OE1	1.96	0.65
1:A:959:GLN:HG3	1:A:1041:MET:HB3	1.79	0.65
1:B:1043:ILE:HG22	3:B:1237:HOH:O	1.97	0.65
1:A:999:ALA:HB2	1:A:1092:ALA:HB1	1.77	0.65
1:B:670:PHE:O	1:B:674:GLN:HG2	1.98	0.64
1:A:764:VAL:O	1:A:764:VAL:HG13	1.97	0.64
1:A:672:GLU:HG3	1:B:1093:ARG:NH1	2.12	0.64
1:A:660:PRO:HB2	3:A:1226:HOH:O	1.98	0.63
1:B:702:ALA:HB2	3:B:416:HOH:O	1.99	0.63
1:B:1083:ARG:HD3	1:B:1110:VAL:HG22	1.79	0.62
1:A:1033:VAL:HG12	3:A:192:HOH:O	1.98	0.62
1:A:670:PHE:O	1:A:674:GLN:HG2	1.99	0.62
1:A:1122:GLY:O	1:A:1137:SER:HA	1.99	0.62
1:B:1098:ASP:OD1	1:B:1100:LYS:HB2	2.00	0.61
1:A:788:PHE:N	1:A:789:PRO:CD	2.63	0.61
1:A:1120:LEU:H	1:A:1120:LEU:HD12	1.65	0.61
1:B:834:VAL:HG13	1:B:871:TRP:CZ2	2.35	0.61
1:B:1080:THR:HG21	3:B:1214:HOH:O	1.99	0.61
1:B:736:ALA:HB1	3:B:1219:HOH:O	2.02	0.60
1:B:1128:ASN:OD1	1:B:1130:GLN:HG2	2.01	0.59
1:B:749:ILE:N	1:B:749:ILE:HD12	2.17	0.59
1:A:751:SER:HB2	1:A:787:SER:HB2	1.84	0.59
1:B:932:THR:O	1:B:933:ARG:HB2	2.02	0.59
1:B:788:PHE:N	1:B:789:PRO:CD	2.66	0.59
1:A:709:PHE:HA	1:A:712:MET:CE	2.32	0.59
1:A:693:PHE:HB2	1:A:698:ASN:O	2.02	0.59
1:B:999:ALA:HB2	1:B:1092:ALA:HB1	1.85	0.58
1:A:918:ALA:O	1:A:957:ARG:NH2	2.28	0.58
1:B:781:GLU:OE1	1:B:831:LYS:HE2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:ALA:HB1	3:A:470:HOH:O	2.04	0.58
1:A:776:ILE:HD12	1:A:821:ILE:HD13	1.85	0.58
1:B:888:ARG:HD2	3:B:199:HOH:O	2.02	0.58
1:A:1118:LYS:HA	3:A:428:HOH:O	2.04	0.58
1:B:1080:THR:HG23	1:B:1082:GLY:N	2.14	0.57
1:B:1090:ASP:CB	1:B:1143:THR:HG23	2.34	0.57
1:A:1056:GLN:HB2	1:A:1123:LEU:HG	1.85	0.57
1:A:888:ARG:HD2	3:A:562:HOH:O	2.03	0.57
1:B:1061:ASN:HA	3:B:1236:HOH:O	2.04	0.57
1:A:1033:VAL:O	1:A:1036:THR:HG22	2.04	0.57
1:A:980:LEU:HD22	1:A:980:LEU:N	2.20	0.57
1:A:1130:GLN:CD	1:B:654:LEU:HD21	2.25	0.57
1:A:757:LYS:HE3	3:A:412:HOH:O	2.05	0.57
1:B:941:GLY:HA3	1:B:1042:LEU:CD2	2.35	0.56
1:A:1033:VAL:O	1:A:1036:THR:CG2	2.53	0.56
1:B:1121:GLY:HA3	1:B:1138:SER:CB	2.34	0.56
1:A:1130:GLN:OE1	1:B:654:LEU:HD21	2.06	0.56
1:A:885:PRO:HG3	1:A:970:LYS:O	2.06	0.56
1:A:1130:GLN:NE2	1:B:654:LEU:HD21	2.21	0.55
1:B:1128:ASN:HB2	1:B:1130:GLN:NE2	2.15	0.55
1:A:686:ASN:HA	1:A:730:ASP:OD1	2.07	0.55
1:B:1080:THR:CG2	1:B:1082:GLY:H	2.16	0.55
1:B:1136:CYS:HA	1:B:1141:CYS:HA	1.87	0.55
1:B:1118:LYS:H	1:B:1118:LYS:HE2	1.70	0.55
1:A:881:ASN:O	1:A:883:ASP:N	2.40	0.55
1:A:749:ILE:N	1:A:749:ILE:HD12	2.21	0.55
1:A:1080:THR:HG23	1:A:1082:GLY:N	2.13	0.54
1:B:759:LEU:HD12	3:B:1221:HOH:O	2.06	0.54
1:A:695:THR:O	1:A:696:ASP:HB2	2.08	0.54
1:B:685:ALA:HB3	1:B:689:MET:HB2	1.90	0.54
1:A:1083:ARG:CD	1:A:1110:VAL:HG13	2.30	0.54
1:A:1080:THR:HG21	3:A:1274:HOH:O	2.08	0.54
1:A:769:ASN:HD21	1:A:771:LYS:HE3	1.72	0.54
1:A:686:ASN:ND2	1:A:686:ASN:N	2.55	0.54
1:A:676:THR:HG23	3:A:1232:HOH:O	2.07	0.54
1:B:1083:ARG:CD	1:B:1110:VAL:HG22	2.38	0.54
1:B:933:ARG:HG3	3:B:1179:HOH:O	2.07	0.53
1:B:946:PHE:CE1	1:B:947:GLU:HG3	2.43	0.53
1:B:727:PHE:CE1	1:B:1121:GLY:HA2	2.42	0.53
1:A:1043:ILE:HD12	1:A:1058:ILE:HG21	1.90	0.53
1:A:1005:ILE:C	1:A:1005:ILE:HD12	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:LEU:O	1:A:702:ALA:HA	2.09	0.53
1:A:648:VAL:HG21	1:A:764:VAL:HG11	1.90	0.52
1:B:764:VAL:HG12	3:B:460:HOH:O	2.08	0.52
1:B:687:ASP:HB3	1:B:752:LEU:O	2.10	0.52
1:A:834:VAL:HG21	1:A:871:TRP:CD2	2.44	0.52
1:B:1004:THR:HG23	1:B:1116:GLU:HB3	1.90	0.52
1:B:1117:GLN:HG2	1:B:1137:SER:OG	2.10	0.52
1:B:1124:THR:HG23	1:B:1136:CYS:HB2	1.92	0.52
1:A:998:PHE:O	1:A:999:ALA:HB3	2.11	0.51
1:B:1006:ARG:HG3	1:B:1072:TRP:CH2	2.46	0.51
1:B:1137:SER:HB2	3:B:322:HOH:O	2.10	0.51
1:B:1143:THR:HG22	3:B:150:HOH:O	2.11	0.51
1:A:1000:SER:HB2	3:B:348:HOH:O	2.11	0.51
1:B:1128:ASN:CB	1:B:1130:GLN:HE21	2.17	0.51
1:B:709:PHE:O	1:B:711:LYS:HG3	2.10	0.51
1:B:769:ASN:HD21	1:B:771:LYS:HE2	1.75	0.51
1:B:1017:ASN:OD1	1:B:1023:LYS:HG3	2.11	0.51
1:B:942:THR:CG2	1:B:959:GLN:OE1	2.59	0.51
1:B:1120:LEU:C	1:B:1120:LEU:HD12	2.32	0.51
1:A:1057:THR:HG22	1:A:1072:TRP:HB2	1.93	0.51
1:A:1129:GLU:O	1:A:1130:GLN:HB3	2.11	0.51
1:B:731:GLY:O	1:B:732:SER:HB2	2.11	0.50
1:A:1120:LEU:H	1:A:1120:LEU:CD1	2.23	0.50
1:A:1088:VAL:HG13	1:A:1089:PHE:CD2	2.46	0.50
1:A:978:PRO:HB2	1:A:980:LEU:HD21	1.93	0.50
1:A:748:LEU:HD23	1:A:748:LEU:C	2.32	0.50
1:A:1043:ILE:HD12	1:A:1058:ILE:CG2	2.41	0.50
1:A:1071:ASN:OD1	1:A:1120:LEU:HA	2.10	0.50
1:A:791:PRO:HB3	1:A:805:THR:HB	1.93	0.50
1:A:981:THR:CG2	1:A:982:ARG:N	2.74	0.50
1:B:850:ALA:HB2	1:B:927:LEU:CD1	2.41	0.50
1:A:1057:THR:CG2	1:A:1072:TRP:HB2	2.41	0.50
1:A:979:ARG:HD3	3:A:503:HOH:O	2.11	0.50
1:A:1034:ASN:HA	3:A:105:HOH:O	2.11	0.50
1:B:884:ASP:OD1	1:B:887:SER:HB2	2.11	0.50
1:A:992:LEU:O	1:A:1006:ARG:HA	2.12	0.49
1:B:1124:THR:CG2	1:B:1136:CYS:HB2	2.43	0.49
1:B:680:ARG:NE	1:B:700:THR:HG21	2.22	0.49
1:A:932:THR:O	1:A:933:ARG:HB2	2.13	0.49
1:B:747:VAL:HG22	1:B:748:LEU:N	2.27	0.49
1:A:747:VAL:HG22	1:A:748:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1128:ASN:ND2	1:B:1132:ASN:HB2	2.16	0.49
1:B:1049:ILE:O	1:B:1052:VAL:HG12	2.12	0.49
1:A:685:ALA:HB3	1:A:689:MET:HB2	1.94	0.48
1:A:747:VAL:HG21	1:A:823:MET:CE	2.43	0.48
1:B:751:SER:HB2	1:B:787:SER:HB2	1.95	0.48
1:A:681:VAL:HB	1:A:694:ASP:CB	2.40	0.48
1:A:1087:THR:HB	1:A:1102:ASP:OD1	2.14	0.48
1:A:721:GLN:HG2	1:A:722:GLY:H	1.79	0.48
1:A:1077:ASP:HB3	1:A:1080:THR:HG22	1.95	0.48
1:A:1128:ASN:O	1:A:1130:GLN:HG2	2.14	0.47
1:B:984:ASN:HB3	3:B:69:HOH:O	2.12	0.47
1:B:1119:GLY:HA3	3:B:1240:HOH:O	2.13	0.47
1:A:724:ALA:HA	1:A:1120:LEU:HD22	1.95	0.47
1:B:748:LEU:HD23	1:B:748:LEU:C	2.34	0.47
1:A:884:ASP:O	1:A:884:ASP:CG	2.51	0.47
1:A:1058:ILE:HD12	1:A:1120:LEU:HD21	1.95	0.47
1:A:1047:ILE:HD13	1:A:1125:LEU:HB2	1.95	0.47
1:B:1005:ILE:HD12	1:B:1005:ILE:C	2.34	0.47
1:A:701:PHE:HE1	1:A:703:PHE:HB2	1.79	0.47
1:B:877:ALA:HA	1:B:898:SER:OG	2.15	0.47
1:A:690:LEU:HD11	1:A:748:LEU:HD21	1.97	0.47
1:A:798:ASN:HA	1:A:892:GLY:O	2.14	0.47
1:B:646:ALA:HB3	1:B:682:TYR:O	2.15	0.47
1:B:1125:LEU:HD13	1:B:1126:SER:N	2.30	0.47
1:B:1027:TRP:CE3	1:B:1081:GLY:HA3	2.50	0.47
1:A:1110:VAL:HG12	1:A:1111:ALA:O	2.15	0.47
1:A:885:PRO:HB2	3:A:1254:HOH:O	2.15	0.46
1:A:1128:ASN:O	1:A:1130:GLN:N	2.49	0.46
1:B:834:VAL:CG1	1:B:871:TRP:CE2	2.98	0.46
1:A:1098:ASP:OD1	1:A:1100:LYS:HB2	2.15	0.46
1:A:694:ASP:OD1	1:A:695:THR:N	2.46	0.46
1:A:981:THR:HG22	1:A:982:ARG:N	2.30	0.46
1:B:1106:ASN:O	1:B:1108:GLN:NE2	2.48	0.46
1:B:1003:ARG:HD2	1:B:1091:LEU:HB3	1.98	0.46
1:A:1052:VAL:HA	1:A:1078:PRO:HD3	1.96	0.46
1:A:693:PHE:O	1:A:694:ASP:HB2	2.16	0.46
1:A:814:ASP:HB3	1:A:841:PRO:HA	1.98	0.46
1:A:1130:GLN:HB3	1:A:1130:GLN:HE21	1.54	0.46
1:B:1004:THR:HG21	1:B:1116:GLU:OE1	2.16	0.46
1:B:758:GLY:C	1:B:759:LEU:HD22	2.36	0.45
1:B:834:VAL:HG11	1:B:871:TRP:NE1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:ASP:OD2	1:A:887:SER:HB2	2.16	0.45
1:B:651:ALA:HB2	1:B:671:ALA:HA	1.98	0.45
1:A:1058:ILE:CD1	1:A:1120:LEU:HD21	2.47	0.45
1:B:811:SER:O	1:B:812:MET:C	2.55	0.45
1:B:1123:LEU:HD22	1:B:1135:VAL:CG2	2.47	0.45
1:B:1043:ILE:HA	3:B:1237:HOH:O	2.16	0.45
1:A:1069:ALA:N	3:A:231:HOH:O	2.50	0.45
1:B:696:ASP:O	1:B:698:ASN:N	2.49	0.45
1:A:686:ASN:HD21	1:A:689:MET:CE	2.30	0.45
1:B:1117:GLN:HG2	1:B:1137:SER:CB	2.47	0.45
1:B:932:THR:O	1:B:932:THR:HG22	2.16	0.45
1:B:958:ALA:HB2	1:B:1037:LEU:CD2	2.47	0.45
1:A:992:LEU:HD12	1:A:1007:ILE:CD1	2.47	0.45
1:A:690:LEU:HB2	1:A:703:PHE:HB3	1.98	0.45
1:B:1122:GLY:O	1:B:1137:SER:HA	2.17	0.45
1:B:674:GLN:NE2	1:B:677:ARG:HD3	2.31	0.44
1:A:776:ILE:CD1	1:A:821:ILE:HD13	2.46	0.44
1:B:764:VAL:CG1	3:B:460:HOH:O	2.65	0.44
1:B:701:PHE:CG	1:B:702:ALA:N	2.85	0.44
1:A:731:GLY:HA3	1:A:753:ARG:NH1	2.32	0.44
1:A:1033:VAL:HG13	1:A:1033:VAL:O	2.18	0.44
1:B:939:ILE:HA	1:B:962:TYR:O	2.18	0.44
1:B:1119:GLY:O	1:B:1120:LEU:HB3	2.18	0.44
1:B:1134:GLU:HG2	1:B:1141:CYS:HB3	2.00	0.44
1:A:701:PHE:CE1	1:A:703:PHE:HB2	2.53	0.44
1:A:1015:TRP:CB	1:A:1016:LEU:HD22	2.48	0.44
1:B:774:TRP:CE3	1:B:776:ILE:HG12	2.53	0.44
1:B:751:SER:HB2	1:B:787:SER:CB	2.47	0.44
1:B:696:ASP:O	1:B:697:GLY:C	2.56	0.44
1:B:992:LEU:O	1:B:1006:ARG:HA	2.18	0.44
1:A:897:SER:HB3	3:A:1220:HOH:O	2.16	0.44
1:B:1127:THR:CG2	1:B:1131:GLY:HA2	2.48	0.43
1:A:659:GLN:HB3	1:A:660:PRO:HD3	2.00	0.43
1:B:834:VAL:HG11	1:B:871:TRP:CE2	2.53	0.43
1:A:882:GLN:O	1:A:885:PRO:HD3	2.18	0.43
1:A:992:LEU:HD13	1:A:993:GLN:N	2.32	0.43
1:B:1013:VAL:HG23	1:B:1080:THR:OG1	2.18	0.43
1:B:674:GLN:HA	1:B:674:GLN:NE2	2.33	0.43
1:A:747:VAL:HG23	1:A:762:LEU:O	2.18	0.43
1:B:960:THR:HB	1:B:962:TYR:CE1	2.52	0.43
1:B:1006:ARG:HG3	1:B:1072:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1128:ASN:CG	1:B:1130:GLN:HG2	2.39	0.43
1:B:999:ALA:CB	1:B:1092:ALA:HB1	2.47	0.43
1:A:913:ASP:OD2	1:A:917:ALA:HB3	2.19	0.43
1:A:992:LEU:C	1:A:992:LEU:HD13	2.39	0.43
1:B:1033:VAL:HG13	1:B:1033:VAL:O	2.19	0.43
1:B:1117:GLN:HA	1:B:1118:LYS:HE2	2.00	0.43
1:A:1015:TRP:HB2	1:A:1016:LEU:HD22	2.01	0.43
1:A:1120:LEU:N	1:A:1120:LEU:HD12	2.32	0.43
1:B:998:PHE:O	1:B:999:ALA:HB3	2.19	0.43
1:B:1135:VAL:O	1:B:1135:VAL:HG13	2.19	0.43
1:B:687:ASP:CB	1:B:755:GLY:N	2.81	0.42
1:A:686:ASN:ND2	1:A:687:ASP:N	2.58	0.42
1:A:696:ASP:O	1:A:698:ASN:OD1	2.37	0.42
1:A:769:ASN:ND2	1:A:771:LYS:HE3	2.34	0.42
1:B:922:THR:HB	3:B:1237:HOH:O	2.18	0.42
1:A:776:ILE:HD11	1:A:821:ILE:HG21	2.00	0.42
1:A:1007:ILE:HD11	1:A:1103:TYR:CD1	2.54	0.42
1:A:644:SER:C	1:A:646:ALA:H	2.23	0.42
1:B:919:GLN:HB3	1:B:942:THR:CG2	2.49	0.42
1:A:788:PHE:N	1:A:789:PRO:HD3	2.34	0.42
1:B:1055:LEU:C	1:B:1123:LEU:HD11	2.40	0.42
1:A:1093:ARG:NH1	1:B:672:GLU:HG3	2.34	0.42
1:A:1129:GLU:HA	1:A:1129:GLU:OE1	2.20	0.42
1:B:1118:LYS:H	1:B:1118:LYS:CE	2.32	0.42
1:B:646:ALA:CB	1:B:733:PRO:HG2	2.49	0.42
1:A:1131:GLY:HA2	1:B:1131:GLY:HA2	2.02	0.42
1:B:749:ILE:CD1	1:B:749:ILE:N	2.82	0.42
1:A:705:PRO:HB3	3:A:1233:HOH:O	2.19	0.42
1:B:759:LEU:CD2	1:B:784:LEU:HD11	2.50	0.42
1:B:1133:PRO:HG2	1:B:1146:PRO:HG2	2.02	0.42
1:A:724:ALA:HB1	1:A:1120:LEU:HD21	2.01	0.42
1:A:834:VAL:HG13	1:A:871:TRP:CZ2	2.55	0.42
1:B:1083:ARG:CZ	1:B:1110:VAL:HG21	2.50	0.42
1:A:946:PHE:CE1	1:A:947:GLU:HG3	2.55	0.42
1:B:959:GLN:HG3	1:B:1041:MET:CB	2.47	0.41
1:B:747:VAL:HG21	1:B:823:MET:CE	2.50	0.41
1:B:662:GLU:HG3	1:B:739:PHE:CG	2.55	0.41
1:B:686:ASN:O	1:B:687:ASP:C	2.59	0.41
1:A:1129:GLU:O	1:A:1130:GLN:CB	2.67	0.41
1:B:699:GLU:HA	1:B:699:GLU:OE1	2.20	0.41
1:A:710:GLU:O	1:A:713:HIS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:GLY:O	1:A:693:PHE:HB3	2.21	0.41
1:A:674:GLN:HA	1:A:674:GLN:NE2	2.36	0.41
1:A:885:PRO:HA	3:A:1255:HOH:O	2.20	0.41
1:B:659:GLN:HB3	1:B:660:PRO:HD3	2.02	0.41
1:B:922:THR:HG21	3:B:363:HOH:O	2.19	0.41
1:B:710:GLU:O	1:B:711:LYS:C	2.58	0.41
1:A:1034:ASN:HB2	3:A:1216:HOH:O	2.18	0.41
1:A:918:ALA:C	1:A:957:ARG:HH22	2.19	0.41
1:B:650:LYS:HB3	3:B:352:HOH:O	2.19	0.41
1:B:935:GLY:HA2	1:B:969:THR:OG1	2.20	0.41
1:A:881:ASN:HB3	3:A:1255:HOH:O	2.20	0.41
1:B:992:LEU:HD13	1:B:992:LEU:C	2.41	0.41
1:A:680:ARG:HE	1:A:700:THR:CG2	2.12	0.41
1:B:781:GLU:HA	1:B:782:PRO:HD2	1.88	0.41
1:B:960:THR:HG22	1:B:961:LEU:N	2.35	0.41
1:A:651:ALA:HB2	1:A:671:ALA:HA	2.03	0.41
1:A:1006:ARG:HG3	1:A:1072:TRP:CZ3	2.56	0.40
1:B:687:ASP:OD2	1:B:754:ALA:HB3	2.21	0.40
1:B:943:GLY:C	3:B:1237:HOH:O	2.58	0.40
1:A:747:VAL:HG21	1:A:823:MET:HE1	2.03	0.40
1:B:1130:GLN:N	1:B:1130:GLN:CD	2.74	0.40
1:A:721:GLN:CG	1:A:722:GLY:H	2.33	0.40
1:A:864:GLY:HA2	1:A:869:ASN:O	2.21	0.40
1:A:795:ARG:HD3	1:A:801:TRP:CD1	2.56	0.40
1:B:1132:ASN:HA	1:B:1133:PRO:HD3	1.97	0.40
1:B:772:LEU:HD11	1:B:775:GLU:HG3	2.02	0.40
1:A:652:GLN:HB2	3:A:1239:HOH:O	2.19	0.40
1:A:1083:ARG:NH2	3:A:263:HOH:O	2.48	0.40
1:A:647:THR:HB	1:A:681:VAL:HG22	2.03	0.40
1:A:834:VAL:HG11	1:A:871:TRP:CE2	2.57	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	485/570 (85%)	443 (91%)	34 (7%)	8 (2%)	12	6
1	B	480/570 (84%)	451 (94%)	20 (4%)	9 (2%)	10	4
All	All	965/1140 (85%)	894 (93%)	54 (6%)	17 (2%)	11	5

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	882	GLN
1	A	1129	GLU
1	A	1130	GLN
1	B	687	ASP
1	B	732	SER
1	B	1120	LEU
1	A	697	GLY
1	A	1119	GLY
1	B	686	ASN
1	B	697	GLY
1	B	1119	GLY
1	B	1138	SER
1	B	882	GLN
1	B	812	MET
1	A	695	THR
1	A	1121	GLY
1	A	1120	LEU

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	386/453 (85%)	374 (97%)	12 (3%)	47	50
1	B	382/453 (84%)	362 (95%)	20 (5%)	29	25
All	All	768/906 (85%)	736 (96%)	32 (4%)	36	35

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	686	ASN
1	A	759	LEU
1	A	764	VAL
1	A	832	LEU
1	A	834	VAL
1	A	957	ARG
1	A	1036	THR
1	A	1043	ILE
1	A	1055	LEU
1	A	1087	THR
1	A	1108	GLN
1	A	1130	GLN
1	B	676	THR
1	B	710	GLU
1	B	730	ASP
1	B	832	LEU
1	B	881	ASN
1	B	934	LYS
1	B	942	THR
1	B	945	TYR
1	B	957	ARG
1	B	980	LEU
1	B	1004	THR
1	B	1014	ASN
1	B	1016	LEU
1	B	1043	ILE
1	B	1055	LEU
1	B	1110	VAL
1	B	1117	GLN
1	B	1118	LYS
1	B	1130	GLN
1	B	1143	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	674	GLN
1	A	686	ASN
1	A	691	HIS
1	A	698	ASN
1	A	769	ASN

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Mol	Chain	Res	Type
1	A	919	GLN
1	A	967	GLN
1	A	988	GLN
1	A	1011	ASN
1	A	1051	GLN
1	A	1132	ASN
1	B	674	GLN
1	B	698	ASN
1	B	769	ASN
1	B	968	GLN
1	B	987	GLN
1	B	1014	ASN
1	B	1034	ASN
1	B	1106	ASN
1	B	1108	GLN
1	B	1109	ASN
1	B	1117	GLN
1	B	1130	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	491/570 (86%)	0.54	47 (9%) 10 14	11, 23, 63, 87	0
1	B	486/570 (85%)	0.70	58 (11%) 6 8	13, 27, 62, 83	0
All	All	977/1140 (85%)	0.62	105 (10%) 8 11	11, 25, 63, 87	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	694	ASP	11.5
1	A	693	PHE	10.9
1	A	1139	GLY	10.5
1	B	882	GLN	8.3
1	B	730	ASP	8.1
1	B	1120	LEU	7.9
1	A	644	SER	7.5
1	B	686	ASN	7.5
1	B	1119	GLY	7.1
1	A	685	ALA	6.9
1	B	727	PHE	6.8
1	A	1120	LEU	6.8
1	A	698	ASN	6.7
1	A	1118	LYS	6.6
1	B	725	HIS	6.6
1	A	883	ASP	6.4
1	A	882	GLN	6.0
1	A	699	GLU	6.0
1	A	713	HIS	6.0
1	B	726	GLN	5.8
1	B	685	ALA	5.7
1	B	724	ALA	5.7
1	B	729	VAL	5.6
1	B	728	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	1107	LYS	5.1
1	A	709	PHE	4.9
1	B	694	ASP	4.8
1	B	1138	SER	4.8
1	B	687	ASP	4.5
1	B	1061	ASN	4.5
1	A	1119	GLY	4.5
1	B	812	MET	4.5
1	B	723	GLY	4.3
1	A	686	ASN	4.2
1	A	696	ASP	4.2
1	B	710	GLU	4.1
1	A	1138	SER	4.0
1	A	1129	GLU	3.9
1	A	1019	ASP	3.8
1	B	709	PHE	3.8
1	A	880	VAL	3.8
1	A	1130	GLN	3.7
1	B	883	ASP	3.7
1	B	1118	LYS	3.7
1	A	700	THR	3.7
1	B	695	THR	3.7
1	B	697	GLY	3.6
1	A	712	MET	3.6
1	A	691	HIS	3.6
1	B	696	ASP	3.6
1	B	881	ASN	3.6
1	A	881	ASN	3.5
1	B	693	PHE	3.5
1	A	683	VAL	3.5
1	A	697	GLY	3.5
1	A	645	PRO	3.4
1	A	1140	GLU	3.4
1	B	755	GLY	3.4
1	B	945	TYR	3.4
1	A	1128	ASN	3.4
1	B	880	VAL	3.3
1	B	1148	PRO	3.3
1	B	1137	SER	3.3
1	B	952	ARG	3.2
1	A	722	GLY	3.2
1	A	701	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	754	ALA	3.2
1	A	695	THR	3.2
1	A	1121	GLY	3.2
1	B	688	GLY	3.1
1	B	1108	GLN	3.0
1	B	700	THR	3.0
1	B	1069	ALA	3.0
1	B	731	GLY	2.9
1	B	698	ASN	2.8
1	B	1121	GLY	2.8
1	A	704	ILE	2.8
1	B	699	GLU	2.7
1	B	951	ALA	2.7
1	A	681	VAL	2.7
1	B	879	LYS	2.7
1	B	950	ASP	2.6
1	A	1137	SER	2.6
1	B	645	PRO	2.5
1	B	768	ALA	2.5
1	B	752	LEU	2.5
1	A	1131	GLY	2.4
1	A	710	GLU	2.4
1	B	1123	LEU	2.4
1	A	676	THR	2.4
1	A	884	ASP	2.3
1	B	692	GLY	2.3
1	B	691	HIS	2.2
1	B	707	ALA	2.2
1	B	948	ASN	2.2
1	A	687	ASP	2.1
1	A	952	ARG	2.1
1	A	707	ALA	2.1
1	A	768	ALA	2.1
1	B	1033	VAL	2.1
1	A	721	GLN	2.1
1	A	684	GLY	2.1
1	B	933	ARG	2.1
1	B	1106	ASN	2.1
1	B	690	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	B	1	1/1	0.99	0.11	0.32	18,18,18,18	0
2	CA	A	1	1/1	0.99	0.03	-6.19	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.