W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:41 AM GMT

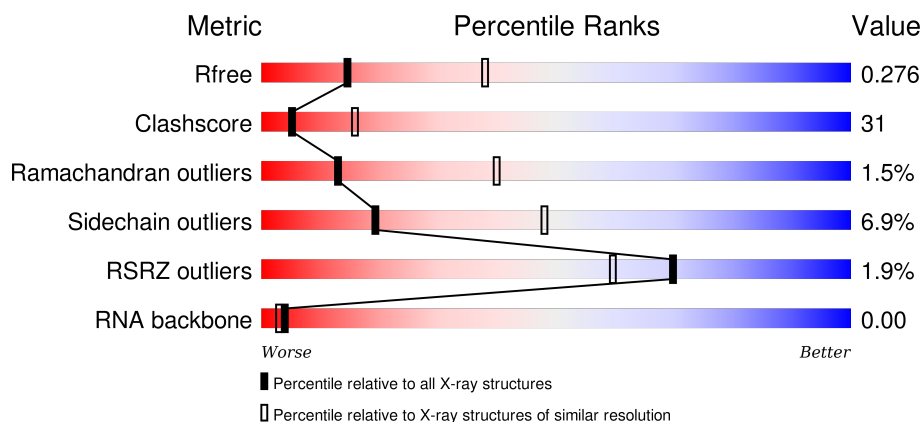|		
PDB ID	:	3BSB
Title	:	Crystal Structure of Human Pumilio1 in Complex with CyclinB reverse RNA
Authors	:	Gupta, Y.K.; Nair, D.T.; Wharton, R.P.; Aggarwal, A.K.
Deposited on	:	2007-12-23
Resolution	:	2.80 Å(reported)

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.276
Clashscore		31
Ramachandran outliers		1.5%
Sidechain outliers		6.9%
RSRZ outliers		1.9%
RNA backbone		0.00

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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 <=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	C	9	11% / 11% ... 89%
2	A	343	2% / 57% ... 39% ··
2	B	343	% / 56% ... 37% ... 6% ··

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5820 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 RNA chain called 5'-R(*UP*UP*UP*AP*AP*UP*GP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	9	Total	C	N	O	P	0	0	0
			184	84	27	65	8			

- Molecule 2 is a protein called Pumilio homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	340	Total	C	N	O	S	0	0	0
			2742	1741	490	494	17			
2	B	341	Total	C	N	O	S	0	0	0
			2749	1743	490	499	17			

- Molecule 3 is water.

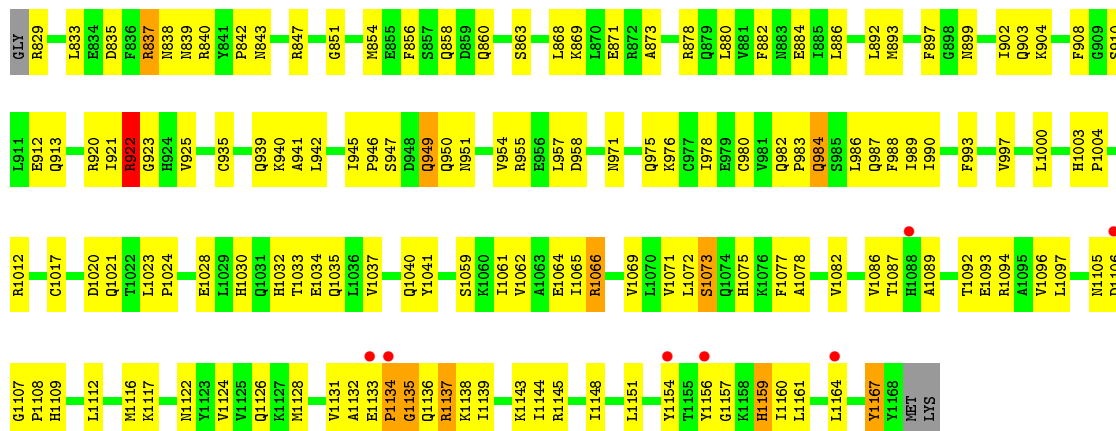| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		
3	B	83	Total	O	0	0
			83	83		
3	C	14	Total	O	0	0
			14	14		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
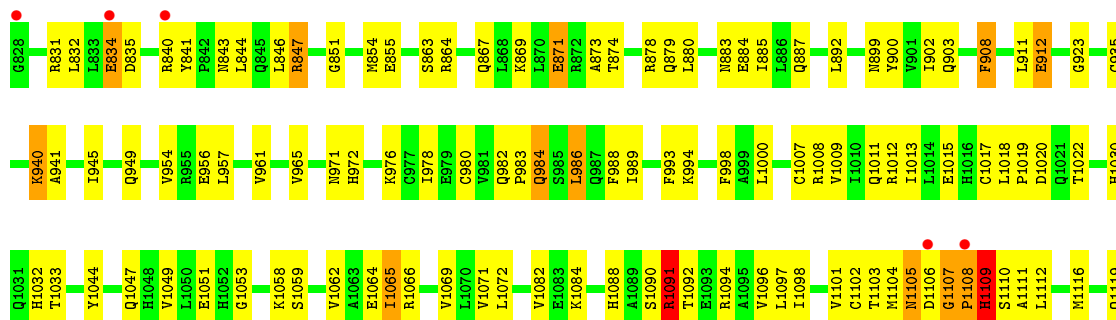
- Molecule 1: 5'-R(*UP*UP*UP*AP*AP*UP*GP*UP*U)-3'

Chain C:

- Molecule 2: Pumilio homolog 1

Chain A:

- Molecule 2: Pumilio homolog 1

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	35.87Å 64.29Å 321.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.87 – 2.80 25.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.3 (25.87-2.80) 89.6 (25.30-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$<I/\sigma(I)>$ [1]	5.08 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.268 0.252 , 0.276	Depositor DCC
R_{free} test set	1329 reflections (7.68%)	DCC
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.934	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Outliers	0 of 17894 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5820	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	C	1.33	1/204 (0.5%)	2.65	24/315 (7.6%)
2	A	0.42	0/2796	0.61	0/3776
2	B	0.59	0/2803	0.81	9/3786 (0.2%)
All	All	0.56	1/5803 (0.0%)	0.88	33/7877 (0.4%)

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	C	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3	U	C3'-O3'	6.25	1.50	1.42

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	8	U	N1-C1'-C2'	-13.22	96.81	114.00
1	C	3	U	P-O3'-C3'	10.59	132.41	119.70
1	C	2	U	O4'-C4'-C3'	-10.28	93.72	104.00
1	C	7	G	N9-C1'-C2'	-9.98	101.02	112.00
2	B	1108	PRO	CA-N-CD	-9.26	98.54	111.50
1	C	6	U	P-O3'-C3'	9.23	130.78	119.70
1	C	4	A	N9-C1'-C2'	-9.07	102.02	112.00
2	B	1167	TYR	CB-CG-CD1	-8.79	115.73	121.00
1	C	6	U	O4'-C4'-C3'	-8.29	95.71	104.00
2	B	1109	HIS	CA-CB-CG	-7.45	100.94	113.60
1	C	4	A	OP1-P-OP2	-7.14	108.88	119.60
1	C	4	A	P-O3'-C3'	7.04	128.15	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2	U	OP1-P-OP2	-6.83	109.36	119.60
1	C	3	U	OP1-P-OP2	-6.76	109.46	119.60
2	B	1134	PRO	CA-N-CD	-6.67	102.16	111.50
1	C	5	A	C8-N9-C4	-6.59	103.16	105.80
1	C	8	U	OP1-P-OP2	-6.36	110.07	119.60
1	C	9	U	OP1-P-OP2	-6.33	110.11	119.60
1	C	5	A	OP1-P-OP2	-6.13	110.41	119.60
1	C	6	U	O3'-P-O5'	-6.08	92.45	104.00
1	C	6	U	OP1-P-OP2	-5.86	110.81	119.60
2	B	834	GLU	CA-C-N	-5.85	104.32	117.20
1	C	5	A	P-O3'-C3'	5.85	126.72	119.70
2	B	1091	ARG	CB-CA-C	-5.84	98.72	110.40
1	C	1	U	O4'-C1'-N1	-5.83	103.54	108.20
1	C	4	A	O4'-C4'-C3'	-5.44	98.56	104.00
1	C	1	U	N1-C1'-C2'	5.43	121.06	114.00
1	C	4	A	C3'-C2'-C1'	-5.39	97.19	101.50
2	B	1158	LYS	CA-C-N	5.25	128.76	117.20
2	B	1152	ARG	C-N-CA	-5.23	108.62	121.70
2	B	1167	TYR	CB-CA-C	5.10	120.60	110.40
1	C	6	U	N1-C1'-C2'	5.03	120.54	114.00
1	C	3	U	P-O5'-C5'	-5.01	112.88	120.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1	U	Sidechain
1	C	4	A	Sidechain
1	C	6	U	Sidechain

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	C	184	0	95	27	0
2	A	2742	0	2737	132	0
2	B	2749	0	2735	203	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	48	0	0	20	0
3	B	83	0	0	64	0
3	C	14	0	0	10	0
All	All	5820	0	5567	343	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 31.

All (343) 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)
2:A:829:ARG:NE	2:A:837:ARG:HH12	1.27	1.28
2:B:982:GLN:HB3	3:B:141:HOH:O	1.26	1.25
2:A:1138:LYS:HG2	3:A:166:HOH:O	1.37	1.22
2:A:829:ARG:NE	2:A:837:ARG:NH1	1.86	1.21
2:B:1098:ILE:HG12	3:B:145:HOH:O	1.43	1.14
2:A:829:ARG:HE	2:A:837:ARG:NH1	1.42	1.11
2:B:1128:MET:HB3	3:B:145:HOH:O	1.56	1.02
2:B:1166:LYS:HG2	2:B:1166:LYS:O	1.61	1.01
2:B:1009:VAL:HG11	3:B:140:HOH:O	1.58	1.00
2:B:1097:LEU:HD23	3:B:148:HOH:O	1.61	1.00
2:B:1129:ILE:HD11	3:B:149:HOH:O	1.62	0.99
2:A:1108:PRO:HG3	2:B:980:CYS:HB3	1.43	0.97
2:B:949:GLN:HG3	3:B:40:HOH:O	1.64	0.96
2:B:1069:VAL:HG21	3:B:148:HOH:O	1.66	0.95
2:B:989:ILE:HA	3:B:150:HOH:O	1.65	0.95
2:B:899:ASN:O	2:B:903:GLN:HG3	1.67	0.92
2:A:833:LEU:O	2:A:837:ARG:HB2	1.69	0.91
2:A:829:ARG:CZ	2:A:837:ARG:HH12	1.85	0.90
2:B:1033:THR:HG21	2:B:1064:GLU:HG3	1.53	0.89
1:C:6:U:H3'	3:C:116:HOH:O	1.73	0.88
2:B:1168:TYR:N	2:B:1168:TYR:CD2	2.31	0.88
2:A:835:ASP:OD1	2:A:840:ARG:CB	2.23	0.87
2:A:1138:LYS:CG	3:A:166:HOH:O	2.06	0.85
2:B:1090:SER:O	2:B:1091:ARG:C	2.13	0.85
2:A:986:LEU:HG	2:A:989:ILE:HD12	1.58	0.85
2:A:829:ARG:HE	2:A:837:ARG:HH12	0.99	0.83
2:B:961:VAL:HG11	3:B:150:HOH:O	1.76	0.83
2:B:1137:ARG:HB2	3:B:119:HOH:O	1.78	0.83
2:A:1138:LYS:HG2	2:A:1167:TYR:OH	1.79	0.82
2:B:1167:TYR:HD1	2:B:1167:TYR:C	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1167:TYR:CD1	2:B:1167:TYR:C	2.53	0.82
1:C:8:U:H4'	3:C:98:HOH:O	1.79	0.81
2:B:1164:LEU:HD12	2:B:1164:LEU:O	1.81	0.81
2:B:854:MET:SD	3:B:133:HOH:O	2.39	0.80
2:B:989:ILE:HG12	3:B:150:HOH:O	1.80	0.80
2:A:1156:TYR:HA	2:A:1159:HIS:NE2	1.97	0.78
2:A:1138:LYS:CD	3:A:166:HOH:O	2.31	0.78
2:B:879:GLN:HE21	2:B:883:ASN:HD21	1.30	0.78
2:B:993:PHE:HZ	3:B:140:HOH:O	1.67	0.77
2:A:1032:HIS:CE1	3:A:144:HOH:O	2.36	0.77
2:A:921:ILE:O	2:A:922:ARG:O	2.03	0.77
2:B:1017:CYS:SG	3:B:115:HOH:O	2.22	0.77
2:B:1017:CYS:SG	3:B:139:HOH:O	2.42	0.77
2:B:1133:GLU:C	3:B:119:HOH:O	2.23	0.76
2:B:841:TYR:HB3	2:B:844:LEU:HB2	1.67	0.76
1:C:2:U:H5'	3:C:109:HOH:O	1.86	0.75
2:B:1125:VAL:CG1	3:B:149:HOH:O	2.34	0.75
2:B:1110:SER:HB2	3:B:142:HOH:O	1.86	0.75
2:B:1159:HIS:O	2:B:1163:LYS:HD2	1.87	0.74
2:B:880:LEU:HD23	3:B:164:HOH:O	1.86	0.74
2:B:1013:ILE:HG12	3:B:139:HOH:O	1.87	0.74
2:B:1168:TYR:N	2:B:1168:TYR:HD2	1.85	0.73
2:B:864:ARG:HG3	3:B:157:HOH:O	1.88	0.73
2:B:1125:VAL:HG12	3:B:149:HOH:O	1.88	0.73
1:C:7:G:N2	2:B:935:CYS:SG	2.61	0.73
2:B:1030:HIS:HA	3:B:120:HOH:O	1.88	0.73
2:B:885:ILE:HG22	3:B:133:HOH:O	1.89	0.72
1:C:9:U:C6	2:B:900:TYR:CZ	2.77	0.72
2:A:1033:THR:HG21	2:A:1064:GLU:HG3	1.72	0.72
2:B:1137:ARG:CB	3:B:119:HOH:O	2.36	0.72
2:B:1098:ILE:HG23	3:B:145:HOH:O	1.89	0.72
2:B:984:GLN:HG2	3:B:141:HOH:O	1.89	0.71
1:C:6:U:H2'	3:C:116:HOH:O	1.90	0.71
2:A:951:ASN:O	2:A:955:ARG:HG3	1.91	0.71
1:C:6:U:C3'	3:C:116:HOH:O	2.32	0.71
2:B:1108:PRO:HD2	2:B:1109:HIS:N	2.05	0.70
2:B:1167:TYR:C	2:B:1168:TYR:CD2	2.65	0.70
2:B:965:VAL:CG2	3:B:140:HOH:O	2.39	0.70
2:B:1097:LEU:HA	3:B:148:HOH:O	1.92	0.69
2:B:986:LEU:HG	2:B:989:ILE:HD12	1.73	0.69
3:C:186:HOH:O	2:B:1158:LYS:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:U:C2'	3:C:116:HOH:O	2.41	0.69
2:B:1160:ILE:O	2:B:1161:LEU:C	2.31	0.69
2:B:1167:TYR:C	2:B:1168:TYR:HD2	1.95	0.69
2:B:1066:ARG:NH1	2:B:1096:VAL:HG11	2.08	0.69
2:A:903:GLN:HB3	2:A:940:LYS:HD2	1.75	0.68
2:B:1051:GLU:OE1	2:B:1084:LYS:NZ	2.26	0.68
2:A:920:ARG:CZ	3:A:163:HOH:O	2.39	0.68
2:B:1092:THR:HB	3:B:88:HOH:O	1.94	0.68
2:B:961:VAL:HG21	3:B:150:HOH:O	1.94	0.68
2:B:1110:SER:CB	3:B:142:HOH:O	2.41	0.68
2:A:893:MET:HG3	2:A:902:ILE:HD13	1.76	0.67
2:A:1034:GLU:HB3	2:A:1035:GLN:HE21	1.60	0.67
1:C:9:U:H1'	2:B:900:TYR:CE1	2.29	0.66
2:A:1073:SER:OG	2:A:1124:VAL:HG21	1.94	0.66
2:A:1105:ASN:HB2	3:A:176:HOH:O	1.95	0.66
2:A:935:CYS:O	2:A:939:GLN:HG3	1.96	0.66
2:A:1136:GLN:O	2:A:1137:ARG:C	2.34	0.66
2:B:961:VAL:CG1	3:B:150:HOH:O	2.37	0.66
2:A:1167:TYR:CD1	2:A:1167:TYR:C	2.69	0.66
2:B:1161:LEU:HB3	3:B:108:HOH:O	1.94	0.66
2:A:1069:VAL:O	2:A:1073:SER:HB2	1.95	0.66
2:A:971:ASN:O	2:A:975:GLN:HG3	1.97	0.65
2:B:1066:ARG:HH11	2:B:1066:ARG:HG2	1.62	0.65
2:A:921:ILE:O	2:A:922:ARG:C	2.36	0.64
2:B:1112:LEU:O	2:B:1116:MET:HG2	1.98	0.64
2:A:1105:ASN:HB2	3:A:152:HOH:O	1.97	0.63
2:B:1058:LYS:HE3	2:B:1088:HIS:HB3	1.79	0.63
2:A:1138:LYS:HD3	3:A:166:HOH:O	1.98	0.63
2:B:965:VAL:HG21	3:B:140:HOH:O	1.96	0.62
2:A:833:LEU:O	2:A:837:ARG:CB	2.45	0.62
2:B:854:MET:HE1	2:B:892:LEU:HG	1.81	0.62
2:B:1160:ILE:O	2:B:1163:LYS:N	2.31	0.62
2:B:1013:ILE:HG23	3:B:139:HOH:O	1.99	0.62
1:C:5:A:H5''	3:B:56:HOH:O	1.99	0.62
2:B:892:LEU:HB2	2:B:902:ILE:HD11	1.82	0.62
2:A:1124:VAL:O	2:A:1128:MET:HG3	1.99	0.62
2:B:1090:SER:O	2:B:1091:ARG:O	2.18	0.61
2:B:1106:ASP:CG	2:B:1107:GLY:H	2.04	0.61
2:A:1107:GLY:N	3:A:176:HOH:O	2.25	0.61
2:A:893:MET:CG	2:A:902:ILE:HD13	2.30	0.61
2:A:892:LEU:HB2	2:A:902:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1167:TYR:C	2:A:1167:TYR:HD1	2.03	0.61
2:B:1107:GLY:C	2:B:1109:HIS:H	2.04	0.61
2:B:1124:VAL:O	2:B:1128:MET:HG3	2.01	0.60
2:B:1168:TYR:HA	3:B:113:HOH:O	2.00	0.60
2:B:1111:ALA:HA	3:B:137:HOH:O	1.99	0.60
2:A:1138:LYS:HD3	3:A:147:HOH:O	2.01	0.60
2:B:879:GLN:NE2	2:B:883:ASN:HD21	1.97	0.60
2:A:1059:SER:HA	2:A:1062:VAL:HG12	1.82	0.60
2:A:1108:PRO:HG3	2:B:980:CYS:CB	2.25	0.60
2:B:1033:THR:HB	3:B:120:HOH:O	2.02	0.60
2:A:941:ALA:O	2:A:945:ILE:HG12	2.02	0.59
2:B:1069:VAL:CG2	3:B:148:HOH:O	2.38	0.59
2:A:829:ARG:CD	2:A:837:ARG:NH1	2.65	0.59
2:B:1165:GLU:O	2:B:1167:TYR:N	2.35	0.59
2:B:1104:MET:HG2	2:B:1105:ASN:N	2.18	0.59
2:A:869:LYS:O	2:A:873:ALA:HB2	2.04	0.58
2:A:1145:ARG:HA	2:A:1164:LEU:HD11	1.85	0.58
2:A:1108:PRO:CG	2:B:980:CYS:HB3	2.26	0.58
2:A:1034:GLU:HB3	2:A:1035:GLN:NE2	2.18	0.58
2:B:940:LYS:HA	2:B:940:LYS:HE3	1.86	0.58
1:C:4:A:H1'	2:B:1044:TYR:CE2	2.38	0.58
2:B:831:ARG:O	2:B:835:ASP:CG	2.42	0.58
2:A:976:LYS:CD	3:A:110:HOH:O	2.50	0.58
2:B:912:GLU:CD	2:B:912:GLU:H	2.07	0.57
2:B:884:GLU:HG3	3:B:164:HOH:O	2.03	0.57
2:A:833:LEU:O	2:A:837:ARG:N	2.32	0.57
2:A:1032:HIS:HE1	3:A:144:HOH:O	1.76	0.57
2:A:1092:THR:O	2:A:1096:VAL:HG23	2.04	0.57
2:A:1148:ILE:HG23	2:A:1161:LEU:HD11	1.87	0.57
2:A:976:LYS:HD3	3:A:110:HOH:O	2.04	0.57
2:B:961:VAL:O	2:B:965:VAL:HG23	2.05	0.57
2:B:885:ILE:C	2:B:885:ILE:HD12	2.25	0.57
2:B:961:VAL:CG2	3:B:150:HOH:O	2.52	0.56
2:A:1112:LEU:CD2	2:A:1143:LYS:HB3	2.35	0.56
2:A:1109:HIS:HB3	3:A:1:HOH:O	2.05	0.56
2:B:1155:THR:C	2:B:1157:GLY:H	2.09	0.56
1:C:9:U:N1	2:B:900:TYR:CZ	2.73	0.56
2:B:984:GLN:NE2	3:B:141:HOH:O	2.24	0.56
2:A:1040:GLN:HA	2:A:1077:PHE:CD2	2.41	0.56
2:B:878:ARG:HG3	2:B:878:ARG:HH11	1.70	0.56
2:B:1102:CYS:SG	2:B:1140:VAL:HG22	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1125:VAL:HG12	2:B:1160:ILE:HD12	1.88	0.56
2:B:887:GLN:HA	2:B:887:GLN:NE2	2.21	0.56
2:A:921:ILE:C	2:A:922:ARG:O	2.42	0.56
2:B:1145:ARG:HB3	2:B:1146:PRO:HD3	1.87	0.55
2:B:1135:GLY:O	2:B:1139:ILE:HG13	2.06	0.55
2:B:879:GLN:HE21	2:B:883:ASN:ND2	2.01	0.55
2:A:842:PRO:HG2	2:A:843:ASN:OD1	2.06	0.55
2:B:1158:LYS:C	3:B:108:HOH:O	2.44	0.55
2:A:984:GLN:H	2:A:984:GLN:CD	2.09	0.55
2:B:1106:ASP:HB3	3:B:137:HOH:O	2.06	0.55
2:B:1066:ARG:NH1	2:B:1096:VAL:CG1	2.69	0.55
2:A:1116:MET:SD	2:A:1144:ILE:HG23	2.46	0.55
1:C:9:U:C6	2:B:900:TYR:OH	2.59	0.55
2:B:1108:PRO:CD	2:B:1109:HIS:N	2.63	0.55
2:A:920:ARG:NH2	3:A:163:HOH:O	2.40	0.55
2:A:1107:GLY:CA	3:A:176:HOH:O	2.53	0.55
2:B:965:VAL:HG22	3:B:140:HOH:O	2.06	0.54
2:A:854:MET:O	2:A:858:GLN:HG3	2.07	0.54
2:A:912:GLU:OE1	2:A:912:GLU:N	2.38	0.54
2:A:910:SER:H	2:A:913:GLN:NE2	2.06	0.54
2:B:840:ARG:HA	2:B:840:ARG:NE	2.23	0.54
2:B:911:LEU:HB3	2:B:912:GLU:OE1	2.08	0.54
2:B:941:ALA:O	2:B:945:ILE:HG12	2.08	0.54
2:B:1059:SER:O	2:B:1062:VAL:HG12	2.07	0.53
2:B:912:GLU:N	2:B:912:GLU:OE1	2.36	0.53
2:B:1103:THR:O	2:B:1103:THR:HG22	2.09	0.53
2:B:1138:LYS:O	2:B:1139:ILE:C	2.44	0.53
2:B:846:LEU:HG	2:B:869:LYS:HB3	1.91	0.53
2:A:1030:HIS:O	2:A:1033:THR:HG22	2.08	0.53
2:B:1018:LEU:O	2:B:1022:THR:HG23	2.09	0.53
1:C:9:U:C4	2:B:900:TYR:CE2	2.96	0.53
2:A:1167:TYR:CD1	2:A:1167:TYR:O	2.62	0.53
2:A:1133:GLU:O	2:A:1135:GLY:N	2.42	0.53
2:A:1094:ARG:HD2	2:A:1131:VAL:HB	1.91	0.53
2:B:1159:HIS:N	3:B:108:HOH:O	2.42	0.52
2:A:860:GLN:HG3	2:A:897:PHE:CE2	2.44	0.52
2:B:1134:PRO:HD3	3:B:156:HOH:O	2.09	0.52
2:B:982:GLN:C	3:B:141:HOH:O	2.47	0.52
2:A:942:LEU:O	2:A:950:GLN:NE2	2.43	0.52
2:A:987:GLN:OE1	2:A:1021:GLN:HG2	2.10	0.52
2:A:1071:VAL:HG23	2:A:1072:LEU:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:871:GLU:HA	2:B:871:GLU:OE1	2.09	0.52
2:A:829:ARG:HG3	2:A:829:ARG:HH11	1.76	0.51
2:B:984:GLN:H	2:B:984:GLN:CD	2.13	0.51
2:B:854:MET:HE3	2:B:892:LEU:HD21	1.92	0.51
2:B:831:ARG:O	2:B:835:ASP:CB	2.59	0.51
2:A:954:VAL:HA	2:A:957:LEU:HD13	1.92	0.51
1:C:9:U:C2	2:B:900:TYR:CE1	2.99	0.51
2:B:1047:GLN:OE1	2:B:1084:LYS:NZ	2.34	0.51
2:B:840:ARG:HA	2:B:840:ARG:HE	1.76	0.51
2:B:1098:ILE:HD13	2:B:1132:ALA:HB2	1.92	0.50
1:C:9:U:C1'	2:B:900:TYR:CE1	2.94	0.50
2:A:829:ARG:HG3	2:A:829:ARG:NH1	2.25	0.50
2:B:1091:ARG:O	2:B:1094:ARG:HB2	2.11	0.50
2:A:1093:GLU:O	2:A:1097:LEU:HG	2.12	0.50
2:B:1106:ASP:CG	2:B:1107:GLY:N	2.63	0.50
2:A:829:ARG:HB3	2:A:833:LEU:HD23	1.92	0.50
2:B:831:ARG:O	2:B:835:ASP:HB2	2.12	0.50
2:A:1003:HIS:CG	2:A:1004:PRO:HD2	2.47	0.50
2:B:1098:ILE:CG2	3:B:145:HOH:O	2.53	0.49
2:B:1129:ILE:CD1	3:B:149:HOH:O	2.37	0.49
2:A:1033:THR:O	2:A:1037:VAL:HG13	2.12	0.49
2:A:1136:GLN:O	2:A:1139:ILE:N	2.44	0.49
2:B:832:LEU:O	2:B:835:ASP:HB2	2.13	0.49
2:B:1141:MET:CB	2:B:1167:TYR:OH	2.61	0.49
1:C:9:U:N1	2:B:900:TYR:CE1	2.79	0.49
1:C:1:U:C4	3:C:186:HOH:O	2.53	0.49
2:B:940:LYS:CE	2:B:940:LYS:HA	2.42	0.49
2:B:874:THR:O	2:B:878:ARG:HG3	2.11	0.49
1:C:4:A:H1'	2:B:1044:TYR:HE2	1.75	0.49
2:A:1126:GLN:HG2	2:A:1160:ILE:HD13	1.94	0.49
2:A:1017:CYS:SG	3:A:68:HOH:O	2.37	0.49
2:B:883:ASN:ND2	3:B:161:HOH:O	2.45	0.49
2:A:1028:GLU:O	2:A:1032:HIS:HD2	1.96	0.49
2:B:878:ARG:HG3	2:B:878:ARG:NH1	2.28	0.49
2:B:976:LYS:HE3	2:B:980:CYS:SG	2.53	0.48
2:B:1148:ILE:O	2:B:1149:ALA:C	2.48	0.48
2:A:1117:LYS:HG3	3:A:138:HOH:O	2.12	0.48
2:B:887:GLN:HA	2:B:887:GLN:HE21	1.78	0.48
1:C:7:G:H2'	1:C:7:G:N3	2.28	0.48
2:B:1130:ASP:OD1	2:B:1163:LYS:NZ	2.47	0.48
2:B:880:LEU:HD23	2:B:880:LEU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1091:ARG:HH21	2:B:1133:GLU:CD	2.16	0.48
2:B:854:MET:HA	3:B:133:HOH:O	2.13	0.48
2:A:1061:ILE:O	2:A:1065:ILE:HD13	2.14	0.48
2:A:1089:ALA:HB1	2:A:1093:GLU:OE2	2.14	0.48
2:B:1011:GLN:O	2:B:1015:GLU:HG3	2.14	0.47
2:A:880:LEU:HD23	2:A:880:LEU:O	2.14	0.47
2:A:982:GLN:HB3	2:A:984:GLN:HE21	1.78	0.47
1:C:5:A:C2	2:B:972:HIS:CE1	3.02	0.47
2:B:993:PHE:CE2	2:B:1000:LEU:HD13	2.50	0.47
2:A:868:LEU:O	2:A:871:GLU:CB	2.62	0.47
2:A:1033:THR:CG2	2:A:1064:GLU:HG3	2.42	0.47
2:B:1107:GLY:C	2:B:1109:HIS:N	2.68	0.47
2:A:946:PRO:HB2	2:A:949:GLN:HE21	1.79	0.47
2:A:1075:HIS:HB3	2:A:1078:ALA:HB3	1.96	0.47
2:B:1012:ARG:NH1	2:B:1012:ARG:HG2	2.30	0.46
2:B:1137:ARG:N	3:B:119:HOH:O	2.38	0.46
2:B:1164:LEU:C	2:B:1164:LEU:HD12	2.36	0.46
2:B:892:LEU:HB2	2:B:902:ILE:CD1	2.44	0.46
1:C:9:U:C5	2:B:900:TYR:CE2	3.04	0.46
2:A:868:LEU:O	2:A:871:GLU:HB2	2.16	0.46
2:B:998:PHE:HB2	2:B:1032:HIS:CD2	2.51	0.46
2:B:1030:HIS:O	2:B:1033:THR:HG22	2.16	0.46
2:A:983:PRO:O	2:A:986:LEU:HB2	2.15	0.45
2:A:1040:GLN:HA	2:A:1077:PHE:CE2	2.51	0.45
2:B:1119:GLN:HG3	2:B:1156:TYR:CZ	2.51	0.45
2:B:1160:ILE:HG12	3:B:14:HOH:O	2.17	0.45
2:B:869:LYS:O	2:B:873:ALA:HB2	2.16	0.45
2:A:878:ARG:HH11	2:A:878:ARG:HG3	1.82	0.45
2:B:978:ILE:HA	2:B:986:LEU:CD2	2.46	0.45
2:A:851:GLY:H	2:A:884:GLU:CD	2.20	0.45
2:A:1138:LYS:HG2	2:A:1167:TYR:HH	1.81	0.45
2:B:1094:ARG:O	2:B:1098:ILE:HG13	2.16	0.45
2:B:1071:VAL:HG23	2:B:1072:LEU:N	2.31	0.45
1:C:1:U:O4	2:B:1159:HIS:HB2	2.17	0.45
2:B:1141:MET:HB3	2:B:1167:TYR:OH	2.17	0.44
2:A:978:ILE:HA	2:A:986:LEU:HD21	1.99	0.44
1:C:9:U:C2	2:B:900:TYR:CD1	3.05	0.44
2:A:1107:GLY:HA2	3:A:176:HOH:O	2.14	0.44
2:A:1145:ARG:O	2:A:1148:ILE:HG13	2.17	0.44
2:B:1007:CYS:O	2:B:1011:GLN:HG3	2.17	0.44
2:A:947:SER:O	2:A:951:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1145:ARG:NH2	3:B:113:HOH:O	2.50	0.44
2:B:851:GLY:H	2:B:884:GLU:CD	2.20	0.44
2:B:899:ASN:OD1	2:B:903:GLN:NE2	2.51	0.44
2:B:1091:ARG:O	2:B:1094:ARG:N	2.50	0.44
2:B:993:PHE:CZ	3:B:140:HOH:O	2.54	0.44
2:B:986:LEU:HG	2:B:989:ILE:CD1	2.44	0.44
2:B:847:ARG:HH11	2:B:880:LEU:HD12	1.83	0.43
2:A:1087:THR:O	2:A:1087:THR:HG22	2.18	0.43
2:B:1091:ARG:HA	2:B:1094:ARG:NH2	2.34	0.43
2:B:923:GLY:H	2:B:956:GLU:CD	2.21	0.43
2:A:1071:VAL:HG23	2:A:1072:LEU:H	1.83	0.43
2:A:1151:LEU:HD22	2:A:1157:GLY:HA2	2.00	0.43
2:B:1106:ASP:CB	3:B:137:HOH:O	2.64	0.43
2:A:1112:LEU:HD23	2:A:1143:LYS:HB3	2.00	0.43
2:A:1106:ASP:O	2:A:1108:PRO:HD2	2.19	0.43
2:A:899:ASN:O	2:A:903:GLN:HG3	2.19	0.43
2:B:863:SER:O	2:B:867:GLN:HG3	2.19	0.43
2:A:958:ASP:HA	2:A:988:PHE:CD1	2.53	0.43
2:B:1128:MET:CG	3:B:145:HOH:O	2.64	0.43
1:C:9:U:H5"	3:C:22:HOH:O	2.19	0.43
2:B:832:LEU:C	2:B:835:ASP:HB2	2.39	0.43
2:A:880:LEU:C	2:A:880:LEU:HD23	2.39	0.43
2:A:1012:ARG:NE	2:A:1012:ARG:HA	2.34	0.43
2:B:1165:GLU:C	2:B:1167:TYR:H	2.22	0.42
2:B:954:VAL:CG1	2:B:988:PHE:HE2	2.32	0.42
2:A:1133:GLU:O	2:A:1134:PRO:C	2.56	0.42
2:B:1153:LYS:HE2	2:B:1153:LYS:HB3	1.45	0.42
2:A:997:VAL:HG21	2:A:1028:GLU:HB2	2.01	0.42
1:C:9:U:P	3:C:175:HOH:O	2.77	0.42
2:B:1007:CYS:SG	2:B:1008:ARG:N	2.93	0.42
2:B:1012:ARG:HH11	2:B:1012:ARG:HG2	1.85	0.42
2:B:1145:ARG:O	2:B:1148:ILE:HG13	2.20	0.42
2:A:835:ASP:C	2:A:838:ASN:H	2.23	0.42
2:A:1040:GLN:HG3	2:A:1041:TYR:CD1	2.55	0.42
2:A:957:LEU:HD12	2:A:957:LEU:N	2.35	0.42
2:A:904:LYS:HG3	2:A:908:PHE:CD1	2.55	0.42
2:A:1122:ASN:O	2:A:1126:GLN:HG3	2.20	0.41
2:B:983:PRO:HG2	2:B:984:GLN:NE2	2.36	0.41
2:A:983:PRO:HG2	2:A:984:GLN:NE2	2.36	0.41
2:A:1117:LYS:HD2	2:A:1154:TYR:HE1	1.86	0.41
2:A:993:PHE:CE2	2:A:1000:LEU:HD13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1129:ILE:HD12	2:B:1163:LYS:HD3	2.03	0.41
2:B:1101:VAL:O	2:B:1111:ALA:HB3	2.20	0.41
2:A:1132:ALA:O	2:A:1137:ARG:NH1	2.54	0.41
2:B:989:ILE:CG1	3:B:150:HOH:O	2.55	0.41
2:B:1049:VAL:O	2:B:1053:GLY:N	2.52	0.41
2:B:1098:ILE:CG1	3:B:145:HOH:O	2.24	0.41
2:B:1168:TYR:CD2	2:B:1168:TYR:C	2.88	0.41
2:A:886:LEU:HD11	3:A:163:HOH:O	2.20	0.41
2:A:1066:ARG:NH2	2:A:1096:VAL:HG11	2.35	0.41
2:B:1134:PRO:HA	3:B:156:HOH:O	2.20	0.41
2:A:882:PHE:CE1	2:A:886:LEU:HD22	2.56	0.41
2:A:990:ILE:HG13	2:A:1021:GLN:HB3	2.03	0.41
2:B:1065:ILE:HA	2:B:1065:ILE:HD12	1.88	0.41
2:B:1145:ARG:N	2:B:1146:PRO:CD	2.84	0.40
2:A:925:VAL:CG1	2:A:957:LEU:HD11	2.51	0.40
2:B:1167:TYR:HD1	2:B:1168:TYR:N	2.19	0.40
2:A:1059:SER:O	2:A:1062:VAL:HG12	2.22	0.40
2:B:1152:ARG:HG2	2:B:1152:ARG:HH11	1.86	0.40
2:A:1082:VAL:O	2:A:1086:VAL:HG23	2.21	0.40
2:B:1096:VAL:O	2:B:1096:VAL:HG12	2.20	0.40
2:A:856:PHE:O	2:A:863:SER:N	2.54	0.40
2:A:1023:LEU:N	2:A:1024:PRO:HD2	2.36	0.40
2:B:978:ILE:HA	2:B:986:LEU:HD21	2.03	0.40
1:C:4:A:C1'	2:B:1044:TYR:CE2	3.04	0.40
2:B:835:ASP:O	2:B:840:ARG:HB2	2.20	0.40
2:B:908:PHE:CD1	2:B:908:PHE:N	2.89	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	
2	A	338/343 (98%)	315 (93%)	18 (5%)	5 (2%)	13	40
2	B	339/343 (99%)	313 (92%)	21 (6%)	5 (2%)	13	40
All	All	677/686 (99%)	628 (93%)	39 (6%)	10 (2%)	13	40

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	922	ARG
2	A	1134	PRO
2	B	1107	GLY
2	B	1134	PRO
2	B	1166	LYS
2	B	1091	ARG
2	A	839	ASN
2	A	923	GLY
2	A	1135	GLY
2	B	1160	ILE

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	
2	A	298/306 (97%)	286 (96%)	12 (4%)	38	73
2	B	299/306 (98%)	270 (90%)	29 (10%)	10	29
All	All	597/612 (98%)	556 (93%)	41 (7%)	19	48

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	837	ARG
2	A	847	ARG
2	A	922	ARG
2	A	949	GLN
2	A	980	CYS
2	A	984	GLN

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Mol	Chain	Res	Type
2	A	1020	ASP
2	A	1066	ARG
2	A	1073	SER
2	A	1137	ARG
2	A	1159	HIS
2	A	1167	TYR
2	B	834	GLU
2	B	843	ASN
2	B	847	ARG
2	B	855	GLU
2	B	871	GLU
2	B	908	PHE
2	B	912	GLU
2	B	940	LYS
2	B	957	LEU
2	B	971	ASN
2	B	984	GLN
2	B	986	LEU
2	B	994	LYS
2	B	1019	PRO
2	B	1020	ASP
2	B	1065	ILE
2	B	1082	VAL
2	B	1105	ASN
2	B	1109	HIS
2	B	1127	LYS
2	B	1134	PRO
2	B	1143	LYS
2	B	1151	LEU
2	B	1153	LYS
2	B	1161	LEU
2	B	1163	LYS
2	B	1166	LYS
2	B	1167	TYR
2	B	1168	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	860	GLN
2	A	883	ASN
2	A	891	GLN

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Mol	Chain	Res	Type
2	A	913	GLN
2	A	949	GLN
2	A	984	GLN
2	A	1031	GLN
2	A	1032	HIS
2	A	1035	GLN
2	A	1136	GLN
2	B	839	ASN
2	B	858	GLN
2	B	860	GLN
2	B	883	ASN
2	B	887	GLN
2	B	891	GLN
2	B	913	GLN
2	B	949	GLN
2	B	968	GLN
2	B	972	HIS
2	B	984	GLN
2	B	1031	GLN
2	B	1032	HIS
2	B	1074	GLN
2	B	1109	HIS
2	B	1119	GLN
2	B	1147	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	9/9 (100%)	8 (88%)	4 (44%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	U
1	C	3	U
1	C	4	A
1	C	5	A
1	C	6	U
1	C	7	G
1	C	8	U
1	C	9	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	1	U
1	C	2	U
1	C	4	A
1	C	6	U

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 carbohydrates 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(Å²)	Q<0.9
1	C	9/9 (100%)	0.95	1 (11%)	7	3	58, 70, 86, 90	0
2	A	340/343 (99%)	0.17	7 (2%)	67	56	25, 47, 73, 87	0
2	B	341/343 (99%)	-0.03	5 (1%)	76	68	19, 37, 69, 87	0
All	All	690/695 (99%)	0.08	13 (1%)	70	59	19, 42, 73, 90	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	828	GLY	3.9
2	A	1156	TYR	3.7
2	B	840	ARG	3.3
2	A	1106	ASP	2.9
2	A	1088	HIS	2.7
2	A	1154	TYR	2.6
1	C	7	G	2.5
2	A	1134	PRO	2.5
2	A	1164	LEU	2.4
2	B	1106	ASP	2.3
2	B	834	GLU	2.2
2	B	1108	PRO	2.2
2	A	1133	GLU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.