Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:48 pm BST

PDB ID	:	3Q0M
Title	:	Crystal structure of the PUMILIO-homology domain from Human PUMILIO1 in complex with p38alpha NREb
Authors	:	Lu, G.; Hall, T.M.T.
Deposited on	:	2010-12-15
Resolution	:	2.71 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

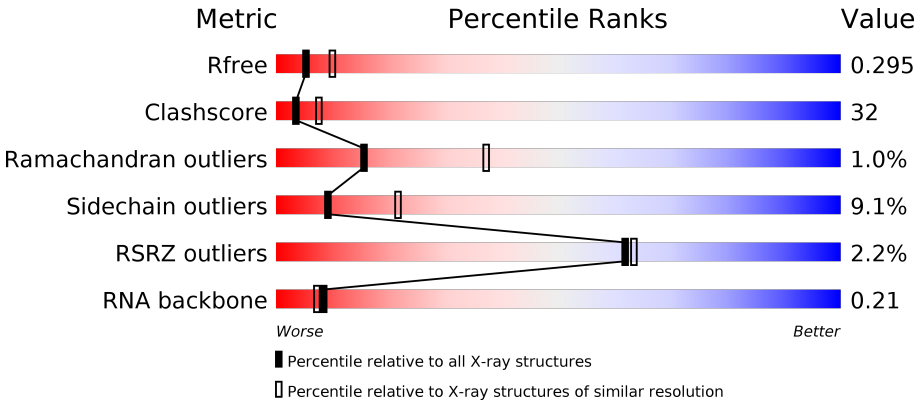
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.71 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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 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 <=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	349	3% 49% 42% 5%
1	B	349	% 43% 48% 6%
2	C	8	38% 13% 13% 38%
2	D	8	25% 25% 50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5912 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 Pumilio homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2738	1732	496	493	17			
1	B	338	Total	C	N	O	S	0	0	0
			2748	1741	495	495	17			

- Molecule 2 is a RNA chain called 5'-R(UP*GP*UP*AP*GP*AP*UP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			169	77	31	54	7			
2	D	8	Total	C	N	O	P	0	0	0
			169	77	31	54	7			

- Molecule 3 is water.

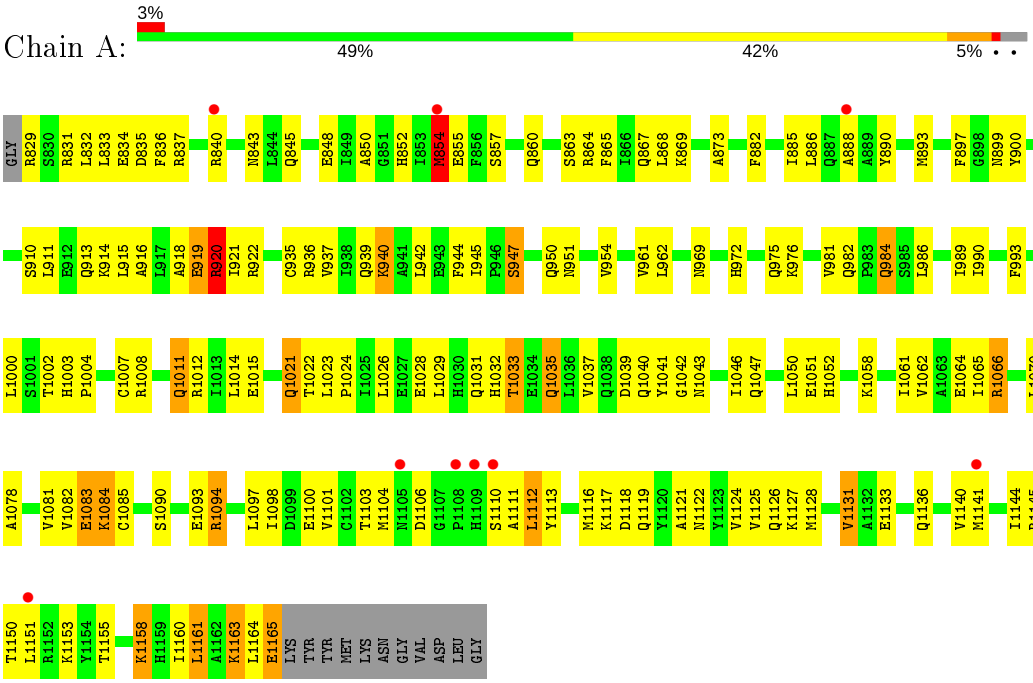
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	39	Total	O	0	0
			39	39		
3	C	4	Total	O	0	0
			4	4		
3	D	6	Total	O	0	0
			6	6		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

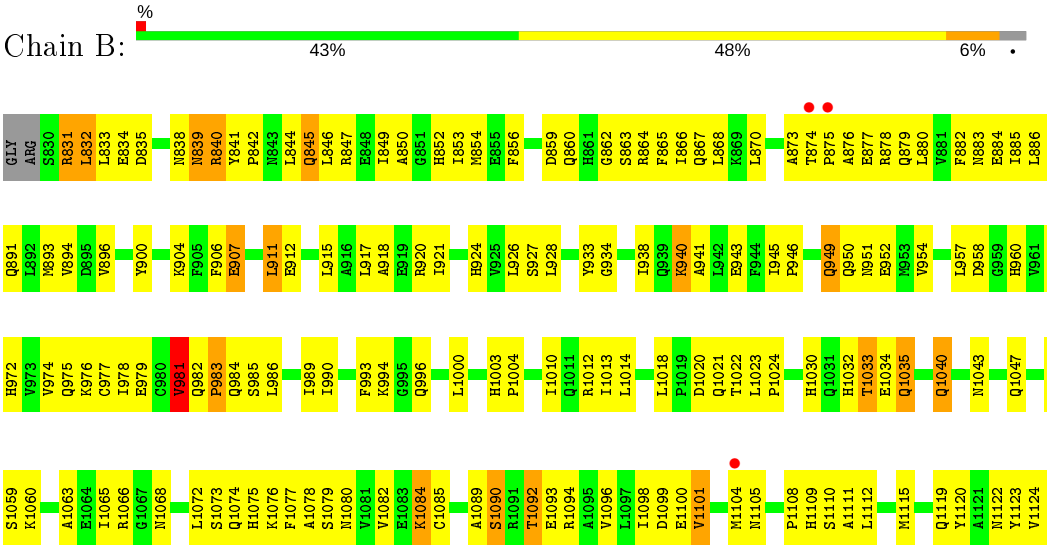
- Molecule 1: Pumilio homolog 1

Chain A:



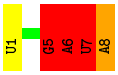
- Molecule 1: Pumilio homolog 1

Chain B:



• Molecule 2: 5'-R(UP*GP*UP*AP*GP*AP*UP*A)-3'

Chain C:



• Molecule 2: 5'-R(UP*GP*UP*AP*GP*AP*UP*A)-3'

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	35.86Å 59.65Å 333.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 2.71 29.83 – 2.71	Depositor EDS
% Data completeness (in resolution range)	78.7 (29.80-2.71) 79.3 (29.83-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.60 (at 2.72Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_6)	Depositor
R, R_{free}	0.212 , 0.298 0.212 , 0.295	Depositor DCC
R_{free} test set	805 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5912	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/2790	0.60	0/3763
1	B	0.42	0/2801	0.58	1/3778 (0.0%)
2	C	0.85	0/189	1.69	5/293 (1.7%)
2	D	0.82	0/189	1.98	7/293 (2.4%)
All	All	0.46	0/5969	0.76	13/8127 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	7	U	O4'-C1'-N1	9.95	116.16	108.20
2	C	6	A	P-O3'-C3'	-7.21	111.05	119.70
2	D	5	G	P-O3'-C3'	6.86	127.93	119.70
2	C	5	G	P-O3'-C3'	6.80	127.86	119.70
2	C	7	U	O5'-P-OP2	-6.68	99.69	105.70
2	D	7	U	N1-C1'-C2'	-6.27	105.11	112.00
2	D	1	U	O4'-C1'-N1	-6.13	103.30	108.20
2	D	6	A	N9-C1'-C2'	-5.62	105.81	112.00
2	D	6	A	C3'-C2'-C1'	5.59	105.97	101.50
2	C	7	U	N1-C1'-C2'	-5.58	105.86	112.00
2	C	7	U	C3'-C2'-C1'	5.37	105.80	101.50
2	D	6	A	P-O5'-C5'	-5.16	112.64	120.90
1	B	981	VAL	CB-CA-C	-5.01	101.88	111.40

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	2738	0	2756	178	0
1	B	2748	0	2765	182	0
2	C	169	0	87	8	0
2	D	169	0	87	12	0
3	A	39	0	0	4	0
3	B	39	0	0	10	0
3	C	4	0	0	1	0
3	D	6	0	0	0	0
All	All	5912	0	5695	370	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 32.

All (370) 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:863:SER:O	1:B:867:GLN:HG3	1.52	1.09
1:B:874:THR:HA	1:B:878:ARG:HD3	1.31	1.07
1:A:990:ILE:HG13	1:A:1021:GLN:HB3	1.43	0.99
2:D:2:G:OP1	2:D:2:G:H4'	1.66	0.95
1:B:1075:HIS:HB3	1:B:1078:ALA:HB3	1.48	0.95
1:A:1040:GLN:OE1	1:B:876:ALA:HB2	1.66	0.95
1:A:1047:GLN:HG3	1:A:1081:VAL:HG22	1.50	0.94
1:A:890:TYR:HA	1:A:893:MET:HE2	1.48	0.94
2:D:1:U:H3'	2:D:2:G:H5"	1.49	0.93
1:B:890:TYR:HB2	1:B:920:ARG:HH21	1.35	0.90
1:B:890:TYR:HB2	1:B:920:ARG:NH2	1.87	0.89
1:B:854:MET:CE	1:B:888:ALA:HB3	2.03	0.88
1:A:890:TYR:HA	1:A:893:MET:CE	2.04	0.88
1:A:1094:ARG:HH11	1:A:1094:ARG:HG3	1.40	0.86
1:A:1161:LEU:O	1:A:1161:LEU:HD22	1.77	0.85
1:A:945:ILE:HG13	1:A:950:GLN:HG3	1.57	0.84
1:B:1043:ASN:O	1:B:1047:GLN:HG3	1.78	0.83
1:A:1007:CYS:O	1:A:1011:GLN:HG2	1.79	0.83
1:A:1075:HIS:HB3	1:A:1078:ALA:HB3	1.61	0.83
2:D:1:U:H3'	2:D:2:G:C5'	2.10	0.81
1:A:1104:MET:O	1:A:1104:MET:HG2	1.80	0.81
1:B:854:MET:HE2	1:B:888:ALA:HB3	1.62	0.80
1:A:854:MET:SD	1:A:888:ALA:HB3	2.22	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:LEU:O	1:A:1058:LYS:HE2	1.81	0.80
1:B:984:GLN:H	1:B:984:GLN:CD	1.84	0.80
1:A:1094:ARG:HH11	1:A:1094:ARG:CG	1.94	0.80
1:A:1161:LEU:O	1:A:1161:LEU:CD2	2.30	0.79
1:B:945:ILE:HD12	1:B:949:GLN:HB3	1.65	0.78
1:A:1021:GLN:O	1:A:1024:PRO:HD2	1.84	0.78
1:A:860:GLN:HG2	1:A:864:ARG:HH12	1.50	0.77
1:B:874:THR:HA	1:B:878:ARG:CD	2.13	0.77
1:A:1062:VAL:HG13	1:A:1097:LEU:HD11	1.67	0.77
1:B:1021:GLN:O	1:B:1024:PRO:HD2	1.85	0.76
1:B:1151:LEU:HD22	1:B:1161:LEU:HB2	1.66	0.76
1:A:950:GLN:O	1:A:954:VAL:HG23	1.85	0.75
1:B:1023:LEU:HB3	1:B:1024:PRO:HD3	1.68	0.75
1:A:1155:THR:HA	1:A:1158:LYS:NZ	2.01	0.75
1:B:911:LEU:HD13	1:B:915:LEU:HD11	1.68	0.75
1:A:1090:SER:HB3	1:A:1093:GLU:HG3	1.70	0.74
1:A:1098:ILE:HG12	1:A:1128:MET:HE2	1.68	0.74
1:B:835:ASP:HB3	1:B:840:ARG:HB2	1.70	0.74
1:A:993:PHE:CE2	1:A:1000:LEU:HD13	2.23	0.74
1:B:986:LEU:HB3	1:B:989:ILE:HD12	1.69	0.74
1:A:1122:ASN:HB2	1:A:1160:ILE:HD11	1.68	0.73
1:B:1092:THR:O	1:B:1096:VAL:HG23	1.89	0.73
1:B:840:ARG:HH11	1:B:840:ARG:HG2	1.53	0.73
1:B:912:GLU:HA	1:B:915:LEU:HD12	1.70	0.73
1:B:934:GLY:O	1:B:938:ILE:HG12	1.88	0.72
1:A:1155:THR:HA	1:A:1158:LYS:HZ3	1.54	0.72
1:B:1105:ASN:HA	1:B:1110:SER:HA	1.69	0.72
1:B:1073:SER:HB2	1:B:1124:VAL:HG21	1.71	0.72
1:A:1144:ILE:HG22	1:A:1164:LEU:HD21	1.71	0.71
1:B:835:ASP:HB2	1:B:841:TYR:CE2	2.24	0.71
1:B:840:ARG:HG2	1:B:840:ARG:NH1	2.05	0.71
1:B:860:GLN:O	1:B:864:ARG:HG3	1.90	0.71
1:A:903:GLN:HB3	1:A:940:LYS:NZ	2.06	0.70
1:B:911:LEU:O	1:B:915:LEU:HG	1.92	0.70
1:B:846:LEU:HD23	1:B:849:ILE:HD11	1.73	0.69
1:B:1140:VAL:O	1:B:1144:ILE:HG13	1.92	0.69
1:A:982:GLN:HB3	1:A:984:GLN:NE2	2.06	0.69
1:B:874:THR:O	1:B:878:ARG:HB2	1.94	0.68
1:B:943:GLU:HB2	1:B:976:LYS:HZ1	1.59	0.68
1:B:1139:ILE:O	1:B:1143:LYS:HG2	1.93	0.68
1:A:903:GLN:OE1	1:A:940:LYS:NZ	2.26	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:882:PHE:HA	1:B:885:ILE:HG12	1.76	0.67
1:B:1079:SER:O	1:B:1082:VAL:HG22	1.95	0.67
1:B:864:ARG:O	1:B:868:LEU:HG	1.95	0.67
1:A:998:PHE:O	1:A:1002:THR:HG23	1.95	0.66
1:A:1022:THR:O	1:A:1026:LEU:HG	1.96	0.66
1:A:1113:TYR:O	1:A:1117:LYS:HG3	1.96	0.66
1:A:899:ASN:O	1:A:903:GLN:HG3	1.96	0.65
1:A:1008:ARG:HA	1:A:1011:GLN:HG3	1.79	0.65
1:A:867:GLN:HB3	1:A:904:LYS:HE2	1.79	0.64
1:A:993:PHE:HE2	1:A:1000:LEU:HD13	1.62	0.64
1:A:903:GLN:HB3	1:A:940:LYS:HZ2	1.61	0.64
1:B:900:TYR:O	1:B:904:LYS:HG2	1.98	0.64
1:A:1003:HIS:CG	1:A:1004:PRO:HD2	2.33	0.63
1:B:873:ALA:HB3	1:B:877:GLU:CD	2.18	0.63
1:A:1136:GLN:O	1:A:1140:VAL:HG23	1.97	0.63
1:B:859:ASP:HB3	1:B:862:GLY:HA3	1.80	0.63
1:A:1031:GLN:HB3	1:A:1032:HIS:CD2	2.34	0.63
1:B:874:THR:HB	1:B:875:PRO:HD3	1.80	0.63
1:A:906:PHE:O	1:A:914:LYS:HE2	1.98	0.62
1:A:989:ILE:O	1:A:993:PHE:HD1	1.83	0.62
1:B:1010:ILE:O	1:B:1014:LEU:HG	2.00	0.62
1:B:911:LEU:HB3	1:B:912:GLU:OE2	2.01	0.61
1:A:1122:ASN:O	1:A:1126:GLN:HG3	2.00	0.61
1:B:984:GLN:N	1:B:984:GLN:CD	2.53	0.61
1:B:981:VAL:HG12	1:B:982:GLN:H	1.66	0.61
1:A:1119:GLN:HG2	3:A:69:HOH:O	1.99	0.61
1:A:984:GLN:H	1:A:984:GLN:CD	2.03	0.61
1:B:890:TYR:O	1:B:894:VAL:HG22	2.00	0.60
1:B:846:LEU:HD12	1:B:877:GLU:OE2	2.02	0.60
1:A:990:ILE:HG13	1:A:1021:GLN:CB	2.26	0.60
1:A:1118:ASP:HB3	1:A:1121:ALA:HB3	1.83	0.60
1:A:975:GLN:OE1	1:A:1012:ARG:NH1	2.32	0.60
1:B:862:GLY:O	1:B:866:ILE:HG13	2.02	0.59
1:A:916:ALA:O	1:A:919:GLU:HB3	2.02	0.59
1:B:943:GLU:HB2	1:B:976:LYS:NZ	2.17	0.59
1:B:1119:GLN:HB2	1:B:1156:TYR:CE1	2.37	0.59
1:B:1159:HIS:HB3	3:B:81:HOH:O	2.02	0.59
1:A:1147:HIS:O	1:A:1150:THR:HB	2.02	0.59
1:B:854:MET:HE1	1:B:888:ALA:HB3	1.81	0.59
1:B:975:GLN:OE1	1:B:1012:ARG:NH1	2.36	0.59
1:B:920:ARG:HD2	3:B:22:HOH:O	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1112:LEU:HD21	1:B:1140:VAL:HG13	1.85	0.58
2:D:2:G:C4'	2:D:2:G:OP1	2.47	0.58
1:A:1039:ASP:O	1:A:1043:ASN:ND2	2.35	0.58
1:A:882:PHE:CD2	1:A:885:ILE:HD11	2.39	0.58
1:B:1056:GLU:O	1:B:1059:SER:HB2	2.03	0.58
1:A:1040:GLN:CD	1:B:876:ALA:HB2	2.23	0.58
1:A:1125:VAL:HA	1:A:1128:MET:HG3	1.85	0.58
1:A:1094:ARG:NH1	1:A:1094:ARG:HB2	2.19	0.58
1:A:1033:THR:O	1:A:1037:VAL:HG13	2.04	0.58
1:B:990:ILE:HG13	1:B:1021:GLN:HB3	1.86	0.58
1:A:1065:ILE:HG21	1:A:1082:VAL:HG12	1.84	0.57
1:A:1023:LEU:N	1:A:1024:PRO:CD	2.66	0.57
1:A:863:SER:O	1:A:867:GLN:HG3	2.04	0.57
1:B:852:HIS:HD2	3:B:61:HOH:O	1.86	0.57
1:B:1140:VAL:O	1:B:1143:LYS:HB2	2.04	0.57
1:B:912:GLU:CD	1:B:912:GLU:N	2.58	0.57
1:B:982:GLN:HB3	1:B:984:GLN:NE2	2.20	0.56
1:A:867:GLN:NE2	1:A:900:TYR:HB2	2.20	0.56
1:A:939:GLN:HE22	2:C:6:A:H2	1.53	0.56
1:B:1047:GLN:NE2	1:B:1080:ASN:HB3	2.20	0.56
1:B:831:ARG:HD2	1:B:832:LEU:N	2.20	0.56
1:A:829:ARG:HD3	1:A:833:LEU:HD23	1.86	0.56
1:A:1110:SER:OG	1:A:1111:ALA:N	2.37	0.56
1:A:890:TYR:CA	1:A:893:MET:HE2	2.31	0.56
1:A:986:LEU:HD22	1:A:989:ILE:HD11	1.86	0.56
1:B:1018:LEU:O	1:B:1022:THR:HG23	2.06	0.55
1:B:1089:ALA:HB1	1:B:1093:GLU:HB2	1.88	0.55
1:B:834:GLU:O	1:B:838:ASN:OD1	2.25	0.55
1:A:882:PHE:O	1:A:885:ILE:HG13	2.06	0.55
1:B:982:GLN:HB3	1:B:984:GLN:HE22	1.72	0.55
1:A:1094:ARG:HH11	1:A:1094:ARG:HB2	1.72	0.55
1:A:869:LYS:O	1:A:873:ALA:HB2	2.06	0.55
1:B:844:LEU:HD12	1:B:845:GLN:H	1.72	0.55
1:B:866:ILE:O	1:B:870:LEU:HG	2.07	0.55
1:B:983:PRO:O	1:B:986:LEU:N	2.37	0.55
2:D:7:U:H4'	2:D:7:U:OP1	2.06	0.55
1:B:847:ARG:HA	1:B:847:ARG:HE	1.71	0.55
1:A:1161:LEU:HD23	1:A:1164:LEU:HD12	1.89	0.54
1:A:854:MET:O	1:A:857:SER:N	2.40	0.54
1:B:1020:ASP:HB2	3:B:74:HOH:O	2.07	0.54
1:B:1137:ARG:O	1:B:1141:MET:HG2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:ARG:HH11	1:A:1094:ARG:CB	2.19	0.54
1:B:1084:LYS:HD2	1:B:1084:LYS:N	2.22	0.54
1:A:1014:LEU:HD22	1:A:1026:LEU:HD21	1.90	0.54
1:B:983:PRO:CB	1:B:1018:LEU:HG	2.38	0.54
1:A:961:VAL:HG12	1:A:962:LEU:HD23	1.89	0.54
1:B:1052:HIS:HB2	3:B:50:HOH:O	2.08	0.54
1:B:918:ALA:HA	1:B:921:ILE:HD12	1.90	0.54
1:B:950:GLN:O	1:B:954:VAL:HG23	2.07	0.54
1:A:860:GLN:HG2	1:A:864:ARG:NH1	2.21	0.53
1:A:982:GLN:HB3	1:A:984:GLN:HE21	1.71	0.53
1:B:840:ARG:HH11	1:B:840:ARG:CG	2.18	0.53
1:A:1033:THR:HB	1:A:1064:GLU:HG3	1.91	0.53
1:A:1112:LEU:O	1:A:1116:MET:HG3	2.09	0.53
1:A:1144:ILE:HG22	1:A:1144:ILE:O	2.08	0.53
1:A:1161:LEU:HA	1:A:1164:LEU:HD12	1.89	0.53
1:A:882:PHE:CD1	1:A:913:GLN:HG2	2.44	0.53
1:A:1161:LEU:O	1:A:1161:LEU:HD23	2.08	0.53
1:B:1143:LYS:HB3	1:B:1143:LYS:HZ3	1.74	0.53
1:B:863:SER:OG	1:B:867:GLN:NE2	2.42	0.53
1:B:1030:HIS:HA	1:B:1033:THR:OG1	2.09	0.52
1:B:1076:LYS:HG3	1:B:1120:TYR:CZ	2.45	0.52
1:B:860:GLN:NE2	2:D:8:A:O2'	2.42	0.52
1:A:1125:VAL:HA	1:A:1128:MET:CG	2.39	0.52
1:A:935:CYS:SG	1:A:969:ASN:HB3	2.49	0.52
1:A:947:SER:HA	1:A:950:GLN:HB2	1.91	0.52
1:B:1075:HIS:CB	1:B:1078:ALA:HB3	2.31	0.52
1:B:1099:ASP:N	1:B:1136:GLN:HE22	2.08	0.51
1:B:1077:PHE:HE2	2:D:3:U:H1'	1.74	0.51
1:A:1075:HIS:HE1	1:A:1077:PHE:HD1	1.58	0.51
1:A:850:ALA:O	1:A:852:HIS:HD2	1.93	0.51
1:B:989:ILE:O	1:B:993:PHE:HD1	1.93	0.51
1:A:1051:GLU:HB2	1:A:1052:HIS:CD2	2.45	0.51
1:A:1014:LEU:CD2	1:A:1026:LEU:HD21	2.41	0.51
1:A:981:VAL:HG12	1:A:982:GLN:O	2.09	0.51
1:B:977:CYS:O	1:B:981:VAL:HG23	2.10	0.51
1:A:1098:ILE:HG12	1:A:1128:MET:CE	2.39	0.51
1:B:1023:LEU:HB3	1:B:1024:PRO:CD	2.39	0.51
1:B:1159:HIS:H	1:B:1159:HIS:CD2	2.28	0.51
1:B:1072:LEU:HD22	1:B:1078:ALA:HB1	1.92	0.51
1:B:983:PRO:HB2	1:B:1018:LEU:HG	1.91	0.51
1:B:1003:HIS:CG	1:B:1004:PRO:HD2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:951:ASN:O	1:B:954:VAL:HB	2.10	0.51
1:A:1082:VAL:O	1:A:1085:CYS:HB2	2.11	0.50
1:B:1090:SER:HB3	1:B:1093:GLU:HG3	1.93	0.50
1:B:1074:GLN:O	1:B:1120:TYR:HD1	1.95	0.50
1:B:1120:TYR:O	1:B:1123:TYR:HB2	2.12	0.50
1:A:1128:MET:HA	1:A:1128:MET:HE2	1.92	0.50
1:B:1148:ILE:HA	1:B:1151:LEU:HB2	1.93	0.50
1:A:993:PHE:CE2	1:A:1000:LEU:CD1	2.93	0.50
1:B:952:GLU:HB2	3:B:29:HOH:O	2.11	0.50
1:A:1163:LYS:C	1:A:1165:GLU:H	2.14	0.50
1:A:835:ASP:OD1	1:A:840:ARG:CZ	2.60	0.50
1:B:1032:HIS:O	1:B:1034:GLU:N	2.45	0.50
1:B:847:ARG:NE	1:B:847:ARG:HA	2.27	0.50
1:A:1075:HIS:HE1	1:A:1077:PHE:CD1	2.30	0.49
1:A:1047:GLN:OE1	1:A:1084:LYS:HD3	2.11	0.49
1:B:941:ALA:O	1:B:945:ILE:HG12	2.12	0.49
1:A:1024:PRO:O	1:A:1028:GLU:HG3	2.12	0.49
1:B:1030:HIS:CE1	1:B:1060:LYS:HB2	2.47	0.49
1:B:906:PHE:HB3	1:B:940:LYS:HG3	1.94	0.49
1:A:1032:HIS:HB3	1:A:1035:GLN:OE1	2.13	0.49
1:A:1061:ILE:O	1:A:1064:GLU:N	2.45	0.49
1:A:845:GLN:HB2	1:A:848:GLU:HG3	1.93	0.49
1:A:1147:HIS:O	1:A:1151:LEU:HG	2.13	0.49
1:B:1023:LEU:CB	1:B:1024:PRO:HD3	2.41	0.49
1:A:1065:ILE:CG2	1:A:1082:VAL:HG12	2.43	0.49
1:A:1158:LYS:HB2	1:A:1158:LYS:NZ	2.28	0.49
1:B:865:PHE:CD2	1:B:865:PHE:C	2.85	0.49
2:D:6:A:C2'	2:D:7:U:O5'	2.61	0.48
2:D:5:G:O2'	2:D:6:A:H5"	2.13	0.48
1:A:1094:ARG:NH1	1:A:1094:ARG:CB	2.76	0.48
1:A:1161:LEU:C	1:A:1161:LEU:CD2	2.80	0.48
1:A:882:PHE:CE1	1:A:913:GLN:HG2	2.48	0.48
1:A:860:GLN:HB2	1:A:897:PHE:CZ	2.49	0.48
1:B:889:ALA:HB1	1:B:893:MET:CE	2.44	0.48
1:B:972:HIS:CE1	2:D:5:G:C8	3.01	0.48
1:B:1063:ALA:HA	1:B:1066:ARG:CZ	2.44	0.48
1:B:1073:SER:HB3	1:B:1082:VAL:HG21	1.96	0.48
1:B:978:ILE:HA	1:B:986:LEU:CD1	2.44	0.48
1:B:996:GLN:NE2	3:B:5:HOH:O	2.47	0.47
1:B:1143:LYS:HB3	1:B:1143:LYS:NZ	2.30	0.47
1:A:1141:MET:HE2	1:A:1141:MET:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:HIS:CD2	1:B:1004:PRO:HD2	2.50	0.47
1:B:1065:ILE:HG13	1:B:1085:CYS:SG	2.54	0.47
1:B:1164:LEU:HD23	1:B:1164:LEU:HA	1.72	0.47
1:A:1002:THR:HB	1:A:1039:ASP:OD2	2.15	0.47
1:A:1104:MET:HE1	3:A:35:HOH:O	2.15	0.47
1:B:1099:ASP:H	1:B:1136:GLN:HE22	1.63	0.47
1:A:1003:HIS:CD2	1:A:1004:PRO:HD2	2.49	0.47
1:B:1018:LEU:HB2	1:B:1021:GLN:OE1	2.15	0.47
1:A:1104:MET:O	1:A:1111:ALA:HB2	2.15	0.46
1:A:854:MET:O	1:A:855:GLU:C	2.53	0.46
1:B:940:LYS:HB2	1:B:940:LYS:HE2	1.55	0.46
2:C:8:A:H4'	3:C:65:HOH:O	2.15	0.46
1:A:1145:ARG:N	1:A:1146:PRO:CD	2.79	0.46
1:B:994:LYS:NZ	1:B:1024:PRO:HG2	2.31	0.46
1:B:850:ALA:HB2	1:B:880:LEU:HD11	1.98	0.46
1:A:939:GLN:NE2	2:C:6:A:C2	2.79	0.46
1:A:1113:TYR:CE2	1:A:1117:LYS:HD2	2.50	0.46
1:B:1013:ILE:HG22	1:B:1014:LEU:N	2.29	0.46
1:A:1144:ILE:CG2	1:A:1164:LEU:HD21	2.42	0.46
1:A:831:ARG:HA	1:A:834:GLU:HB2	1.97	0.46
1:A:1022:THR:O	1:A:1026:LEU:CG	2.63	0.46
1:A:919:GLU:HA	1:A:922:ARG:CZ	2.46	0.46
1:B:1099:ASP:CG	1:B:1136:GLN:HE21	2.18	0.46
1:A:1029:LEU:HA	1:A:1029:LEU:HD23	1.75	0.46
1:A:1002:THR:HA	1:A:1039:ASP:OD2	2.16	0.46
1:B:946:PRO:O	1:B:950:GLN:HG3	2.16	0.46
1:A:835:ASP:OD1	1:A:840:ARG:HD2	2.16	0.45
1:A:962:LEU:HD11	1:A:996:GLN:HG3	1.98	0.45
1:B:1072:LEU:HD22	1:B:1078:ALA:CB	2.46	0.45
1:B:1136:GLN:O	1:B:1140:VAL:HG23	2.17	0.45
1:A:1125:VAL:O	1:A:1128:MET:HB2	2.16	0.45
2:D:7:U:O2'	2:D:8:A:H5'	2.17	0.45
1:A:1141:MET:CE	1:A:1141:MET:HA	2.46	0.45
1:B:906:PHE:CZ	1:B:921:ILE:HD11	2.50	0.45
1:A:1061:ILE:O	1:A:1064:GLU:HB2	2.16	0.45
1:A:1065:ILE:O	1:A:1066:ARG:C	2.54	0.45
1:B:1124:VAL:O	1:B:1128:MET:HG3	2.16	0.45
1:B:975:GLN:O	1:B:979:GLU:HG3	2.16	0.45
1:A:854:MET:HB3	1:A:854:MET:HE3	1.89	0.45
1:B:912:GLU:CD	1:B:912:GLU:H	2.18	0.45
1:B:978:ILE:HA	1:B:986:LEU:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:LEU:O	1:A:915:LEU:HG	2.17	0.45
1:B:1122:ASN:CG	1:B:1123:TYR:N	2.69	0.45
1:B:1073:SER:CB	1:B:1124:VAL:HG21	2.43	0.45
1:B:896:VAL:HA	1:B:933:TYR:CD2	2.52	0.45
1:A:1127:LYS:O	1:A:1128:MET:C	2.55	0.44
1:A:1148:ILE:C	1:A:1150:THR:H	2.21	0.44
1:A:1161:LEU:HD23	1:A:1164:LEU:CD1	2.47	0.44
1:A:986:LEU:HD22	1:A:989:ILE:CD1	2.46	0.44
1:B:1104:MET:HB3	1:B:1111:ALA:HB2	1.98	0.44
1:B:957:LEU:HA	1:B:957:LEU:HD23	1.73	0.44
1:A:936:ARG:HG3	2:C:7:U:C4	2.52	0.44
1:A:972:HIS:O	1:A:976:LYS:HB2	2.17	0.44
1:B:832:LEU:O	1:B:833:LEU:C	2.56	0.44
1:B:886:LEU:HG	1:B:886:LEU:O	2.17	0.44
1:A:1008:ARG:HG3	2:C:5:G:C8	2.53	0.44
1:A:939:GLN:NE2	2:C:6:A:H2	2.16	0.44
1:A:854:MET:SD	1:A:888:ALA:CB	3.01	0.44
1:A:1163:LYS:O	1:A:1165:GLU:N	2.40	0.44
1:A:954:VAL:HG21	1:A:981:VAL:HG21	2.00	0.44
1:B:879:GLN:HE21	1:B:883:ASN:ND2	2.16	0.44
1:B:974:VAL:O	1:B:977:CYS:HB2	2.17	0.44
1:B:1099:ASP:N	1:B:1136:GLN:NE2	2.65	0.44
1:B:1068:ASN:O	1:B:1072:LEU:HB2	2.17	0.44
1:B:840:ARG:C	1:B:842:PRO:HD3	2.38	0.44
1:B:890:TYR:HD1	1:B:890:TYR:O	2.01	0.44
1:B:949:GLN:C	3:B:29:HOH:O	2.56	0.44
1:A:1046:ILE:HG23	1:A:1061:ILE:HD13	1.99	0.44
1:B:962:LEU:HD22	1:B:1000:LEU:HD11	2.00	0.44
2:D:1:U:O5'	2:D:2:G:C5'	2.66	0.43
1:B:852:HIS:HB3	1:B:856:PHE:CD1	2.53	0.43
1:B:874:THR:CB	1:B:875:PRO:HD3	2.48	0.43
1:A:918:ALA:O	1:A:921:ILE:N	2.44	0.43
1:B:1003:HIS:HA	1:B:1004:PRO:HD3	1.82	0.43
1:B:1040:GLN:CD	1:B:1040:GLN:H	2.16	0.43
1:B:1157:GLY:C	1:B:1159:HIS:H	2.21	0.43
1:A:920:ARG:HD2	1:A:920:ARG:HA	1.52	0.43
1:A:1113:TYR:CZ	1:A:1117:LYS:HD2	2.54	0.43
1:A:989:ILE:HG22	1:A:993:PHE:HE1	1.83	0.43
1:A:919:GLU:HG2	1:A:922:ARG:HH22	1.84	0.43
1:B:1099:ASP:CG	1:B:1136:GLN:NE2	2.73	0.43
1:A:1039:ASP:HB3	1:A:1042:GLY:HA3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:ARG:HD3	1:A:1131:VAL:HG23	2.01	0.42
1:A:947:SER:HB3	3:A:87:HOH:O	2.19	0.42
1:A:1104:MET:CE	3:A:35:HOH:O	2.66	0.42
1:B:966:LYS:HA	1:B:1003:HIS:CE1	2.54	0.42
1:B:1127:LYS:HA	1:B:1127:LYS:HD3	1.74	0.42
1:B:1098:ILE:HG12	1:B:1128:MET:HB3	2.02	0.42
1:B:879:GLN:HE21	1:B:883:ASN:HD21	1.66	0.42
1:B:907:GLU:HG3	1:B:940:LYS:HD2	2.01	0.42
1:B:882:PHE:HE2	1:B:917:LEU:HG	1.85	0.42
2:C:6:A:H8	2:C:6:A:H5'	1.84	0.42
1:A:1082:VAL:HG23	1:A:1124:VAL:CG2	2.50	0.42
1:A:829:ARG:NH2	1:A:837:ARG:HH12	2.18	0.42
1:B:1098:ILE:O	1:B:1101:VAL:HG23	2.19	0.42
1:B:1155:THR:C	1:B:1157:GLY:H	2.23	0.42
1:A:910:SER:H	1:A:913:GLN:HE21	1.68	0.42
1:B:880:LEU:HD12	1:B:880:LEU:O	2.19	0.42
1:A:1039:ASP:HB3	1:A:1042:GLY:H	1.84	0.42
1:B:1151:LEU:HD21	1:B:1160:ILE:HB	2.02	0.42
1:B:1072:LEU:O	1:B:1075:HIS:HB3	2.19	0.42
1:A:1100:GLU:CG	1:A:1104:MET:HE3	2.49	0.41
1:A:1161:LEU:C	1:A:1161:LEU:HD22	2.39	0.41
1:A:940:LYS:HD2	1:A:944:PHE:HE1	1.85	0.41
2:C:1:U:O5'	2:C:1:U:H6	2.02	0.41
1:A:1023:LEU:N	1:A:1024:PRO:HD2	2.35	0.41
1:A:1082:VAL:O	1:A:1083:GLU:C	2.57	0.41
1:A:1094:ARG:NH1	1:A:1094:ARG:CG	2.64	0.41
1:B:1018:LEU:N	1:B:1021:GLN:OE1	2.53	0.41
1:B:877:GLU:O	1:B:880:LEU:HB3	2.19	0.41
1:B:926:LEU:HD22	1:B:960:HIS:CD2	2.56	0.41
1:A:1124:VAL:O	1:A:1128:MET:HG2	2.20	0.41
1:A:1163:LYS:C	1:A:1165:GLU:N	2.73	0.41
1:A:913:GLN:HE21	1:A:913:GLN:HB2	1.61	0.41
1:B:1108:PRO:HB2	1:B:1109:HIS:CD2	2.55	0.41
1:B:1109:HIS:CD2	3:B:79:HOH:O	2.72	0.41
1:A:910:SER:H	1:A:913:GLN:NE2	2.18	0.41
1:A:919:GLU:HA	1:A:922:ARG:NH2	2.35	0.41
1:B:1100:GLU:O	1:B:1104:MET:HB2	2.21	0.41
1:B:1157:GLY:O	1:B:1159:HIS:N	2.53	0.41
1:A:1011:GLN:O	1:A:1015:GLU:HG3	2.20	0.41
1:A:860:GLN:CG	1:A:864:ARG:HH12	2.26	0.41
1:B:1094:ARG:NH2	3:B:94:HOH:O	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1023:LEU:HA	1:B:1023:LEU:HD12	1.80	0.41
1:B:1101:VAL:HG11	1:B:1115:MET:SD	2.61	0.41
1:B:853:ILE:HG13	1:B:884:GLU:CD	2.40	0.41
1:A:1035:GLN:HG3	1:A:1035:GLN:H	1.68	0.41
1:B:1125:VAL:O	1:B:1126:GLN:C	2.59	0.41
1:A:832:LEU:HA	1:A:832:LEU:HD12	1.81	0.40
1:A:836:PHE:CZ	1:A:865:PHE:HB2	2.56	0.40
1:B:896:VAL:HG23	1:B:933:TYR:CE2	2.56	0.40
1:A:1094:ARG:NH1	1:A:1094:ARG:HG3	2.18	0.40
1:A:951:ASN:HD22	1:A:951:ASN:HA	1.65	0.40
1:B:839:ASN:HA	1:B:839:ASN:HD22	1.62	0.40
1:B:847:ARG:CA	1:B:847:ARG:NE	2.85	0.40
1:B:924:HIS:O	1:B:928:LEU:HG	2.20	0.40
1:A:882:PHE:CG	1:A:913:GLN:HG2	2.56	0.40
1:B:1032:HIS:HB3	1:B:1035:GLN:HG3	2.03	0.40
1:A:1101:VAL:O	1:A:1111:ALA:HB3	2.22	0.40
1:A:989:ILE:HG22	1:A:993:PHE:CE1	2.57	0.40
1:A:886:LEU:HA	1:A:886:LEU:HD12	1.91	0.40
1:B:907:GLU:CG	1:B:940:LYS:HD2	2.51	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	335/349 (96%)	292 (87%)	40 (12%)	3 (1%)	17 40
1	B	336/349 (96%)	285 (85%)	47 (14%)	4 (1%)	13 32
All	All	671/698 (96%)	577 (86%)	87 (13%)	7 (1%)	15 37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1033	THR
1	A	854	MET
1	A	919	GLU
1	A	920	ARG
1	B	1158	LYS
1	B	981	VAL
1	B	983	PRO

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	301/310 (97%)	271 (90%)	30 (10%)	7 18
1	B	302/310 (97%)	277 (92%)	25 (8%)	11 25
All	All	603/620 (97%)	548 (91%)	55 (9%)	9 21

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	843	ASN
1	A	854	MET
1	A	868	LEU
1	A	920	ARG
1	A	937	VAL
1	A	940	LYS
1	A	942	LEU
1	A	947	SER
1	A	984	GLN
1	A	1011	GLN
1	A	1021	GLN
1	A	1033	THR
1	A	1035	GLN
1	A	1041	TYR
1	A	1066	ARG
1	A	1070	LEU
1	A	1083	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1084	LYS
1	A	1094	ARG
1	A	1103	THR
1	A	1106	ASP
1	A	1112	LEU
1	A	1131	VAL
1	A	1133	GLU
1	A	1147	HIS
1	A	1153	LYS
1	A	1158	LYS
1	A	1161	LEU
1	A	1163	LYS
1	A	1165	GLU
1	B	831	ARG
1	B	832	LEU
1	B	839	ASN
1	B	840	ARG
1	B	845	GLN
1	B	887	GLN
1	B	890	TYR
1	B	891	GLN
1	B	907	GLU
1	B	911	LEU
1	B	927	SER
1	B	940	LYS
1	B	949	GLN
1	B	958	ASP
1	B	985	SER
1	B	1035	GLN
1	B	1040	GLN
1	B	1084	LYS
1	B	1090	SER
1	B	1092	THR
1	B	1101	VAL
1	B	1148	ILE
1	B	1151	LEU
1	B	1159	HIS
1	B	1163	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	838	ASN
1	A	852	HIS
1	A	879	GLN
1	A	883	ASN
1	A	913	GLN
1	A	939	GLN
1	A	951	ASN
1	A	1031	GLN
1	A	1052	HIS
1	A	1119	GLN
1	A	1159	HIS
1	B	838	ASN
1	B	839	ASN
1	B	845	GLN
1	B	852	HIS
1	B	860	GLN
1	B	883	ASN
1	B	887	GLN
1	B	939	GLN
1	B	950	GLN
1	B	960	HIS
1	B	984	GLN
1	B	996	GLN
1	B	1031	GLN
1	B	1088	HIS
1	B	1109	HIS
1	B	1136	GLN
1	B	1147	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	7/8 (87%)	4 (57%)	3 (42%)
2	D	8/8 (100%)	5 (62%)	5 (62%)
All	All	15/16 (93%)	9 (60%)	8 (53%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	5	G
2	C	6	A
2	C	7	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	8	A
2	D	2	G
2	D	4	A
2	D	6	A
2	D	7	U
2	D	8	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	5	G
2	C	6	A
2	C	7	U
2	D	1	U
2	D	2	G
2	D	5	G
2	D	6	A
2	D	7	U

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	337/349 (96%)	-0.18	10 (2%) 50 51	23, 27, 84, 178	0
1	B	338/349 (96%)	-0.24	5 (1%) 73 76	23, 29, 76, 239	0
2	C	8/8 (100%)	-0.93	0 100 100	25, 27, 32, 34	0
2	D	8/8 (100%)	-0.44	0 100 100	24, 25, 29, 34	0
All	All	691/714 (96%)	-0.22	15 (2%) 62 63	23, 28, 79, 239	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1108	PRO	6.8
1	B	1104	MET	5.1
1	B	1152	ARG	5.0
1	A	1151	LEU	4.7
1	A	1148	ILE	4.1
1	A	1109	HIS	3.6
1	B	875	PRO	2.9
1	A	1105	ASN	2.6
1	B	1165	GLU	2.6
1	A	1141	MET	2.6
1	A	888	ALA	2.5
1	A	1110	SER	2.4
1	A	840	ARG	2.4
1	B	874	THR	2.2
1	A	854	MET	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.