



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:33 pm GMT

PDB ID : 3BSX
Title : Crystal Structure of Human Pumilio 1 in complex with Puf5 RNA
Authors : Gupta, Y.K.; Nair, D.T.; Wharton, R.P.; Aggarwal, A.K.
Deposited on : 2007-12-26
Resolution : 2.32 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

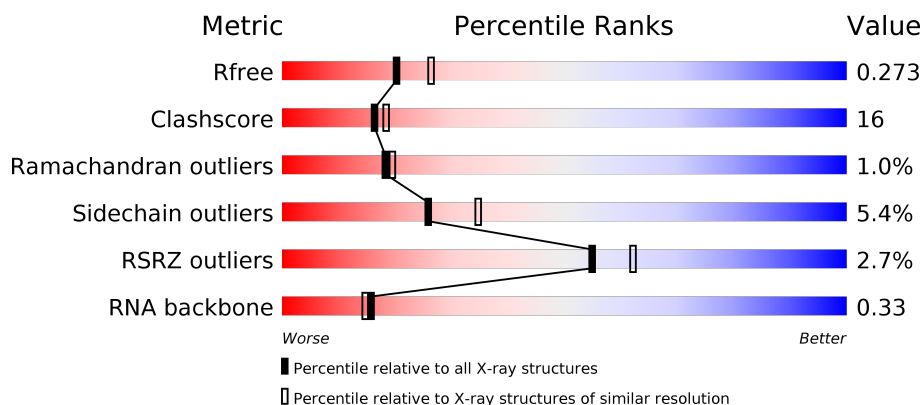
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	100719	4787 (2.34-2.30)
Clashscore	112137	5439 (2.34-2.30)
Ramachandran outliers	110173	5386 (2.34-2.30)
Sidechain outliers	110143	5385 (2.34-2.30)
RSRZ outliers	101464	4814 (2.34-2.30)
RNA backbone	2435	1057 (2.80-1.86)

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	C	11	
1	D	11	
2	A	343	
2	B	343	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6109 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*GP*UP*AP*AP*UP*AP*UP*UP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	10	Total	C	N	O	P	0	0	0
			206	94	32	71	9			
1	D	9	Total	C	N	O	P	0	0	0
			186	85	30	63	8			

- Molecule 2 is a protein called Pumilio homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	341	Total	C	N	O	S	0	0	0
			2749	1744	491	497	17			
2	B	340	Total	C	N	O	S	0	0	0
			2722	1727	489	489	17			

- Molecule 3 is water.

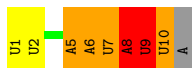
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total	O	0	0
			118	118		
3	B	97	Total	O	0	0
			97	97		
3	C	19	Total	O	0	0
			19	19		
3	D	12	Total	O	0	0
			12	12		

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.

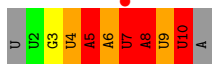
- Molecule 1: 5'-R(*UP*UP*GP*UP*AP*AP*UP*AP*UP*UP*A)-3'

Chain C: 



- Molecule 1: 5'-R(*UP*UP*GP*UP*AP*AP*UP*AP*UP*UP*A)-3'

Chain D: 



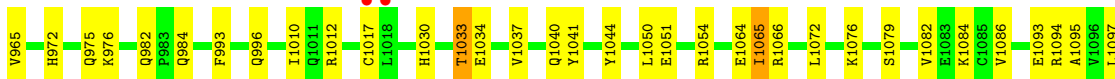
- Molecule 2: Pumilio homolog 1

Chain A: 



- Molecule 2: Pumilio homolog 1

Chain B: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	35.84Å 65.64Å 313.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.93 – 2.32 40.92 – 2.32	Depositor EDS
% Data completeness (in resolution range)	93.8 (40.93-2.32) 93.8 (40.92-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.212 , 0.277 0.208 , 0.273	Depositor DCC
R_{free} test set	3129 reflections (11.13%)	DCC
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6109	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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	C	1.39	1/229 (0.4%)	1.95	5/354 (1.4%)
1	D	1.65	5/207 (2.4%)	2.05	9/320 (2.8%)
2	A	0.78	1/2803 (0.0%)	0.74	1/3785 (0.0%)
2	B	0.72	1/2775 (0.0%)	0.72	0/3749
All	All	0.83	8/6014 (0.1%)	0.90	15/8208 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	828	GLY	N-CA	8.42	1.58	1.46
2	A	1017	CYS	CB-SG	7.53	1.95	1.82
1	D	10	U	N1-C6	6.74	1.44	1.38
1	D	10	U	O4'-C1'	6.40	1.50	1.41
1	D	10	U	N3-C4	6.34	1.44	1.38
1	D	4	U	C3'-O3'	5.61	1.50	1.42
1	D	9	U	C4-C5	5.35	1.48	1.43
1	C	10	U	N1-C6	5.02	1.42	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	9	U	O4'-C1'-N1	9.84	116.07	108.20
1	C	1	U	P-O3'-C3'	9.18	130.72	119.70
1	D	7	U	P-O3'-C3'	9.09	130.61	119.70
1	D	7	U	O4'-C1'-N1	7.52	114.22	108.20
1	D	5	A	P-O3'-C3'	7.25	128.40	119.70
1	C	6	A	P-O3'-C3'	7.19	128.33	119.70
1	D	3	G	O4'-C1'-N9	6.91	113.73	108.20
1	D	9	U	C4'-C3'-C2'	-6.90	95.70	102.60
1	D	9	U	C1'-O4'-C4'	-6.75	104.50	109.90
1	C	9	U	P-O3'-C3'	5.97	126.87	119.70
1	D	7	U	N3-C2-O2	-5.57	118.30	122.20
1	C	8	A	N1-C2-N3	-5.48	126.56	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	U	N3-C2-O2	-5.46	118.38	122.20
1	D	8	A	C3'-C2'-C1'	-5.18	97.36	101.50
2	A	936	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	C	206	0	106	4	0
1	D	186	0	96	11	0
2	A	2749	0	2742	87	0
2	B	2722	0	2712	89	0
3	A	118	0	0	20	0
3	B	97	0	0	25	0
3	C	19	0	0	0	0
3	D	12	0	0	3	0
All	All	6109	0	5656	184	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 16.

All (184) 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:B:975:GLN:HB3	3:B:202:HOH:O	1.34	1.22
2:A:904:LYS:HE2	3:A:93:HOH:O	1.36	1.22
2:A:1117:LYS:HA	3:A:138:HOH:O	1.45	1.16
2:A:1109:HIS:HB2	3:A:141:HOH:O	1.48	1.13
2:A:1062:VAL:HB	3:A:237:HOH:O	1.66	0.95
2:B:1095:ALA:HA	3:B:147:HOH:O	1.68	0.92
2:B:982:GLN:HB2	3:B:215:HOH:O	1.72	0.88
2:A:1154:TYR:O	2:A:1158:LYS:HE3	1.72	0.87
2:A:1094:ARG:HD2	2:A:1131:VAL:HG23	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1117:LYS:HE3	2:B:1154:TYR:HE1	1.40	0.85
2:A:908:PHE:HE1	3:A:145:HOH:O	1.60	0.83
2:B:832:LEU:HB2	3:B:78:HOH:O	1.79	0.81
2:A:894:VAL:HB	2:A:931:GLN:HE22	1.49	0.78
2:B:1082:VAL:HG13	3:B:212:HOH:O	1.83	0.77
2:A:854:MET:CE	2:A:888:ALA:HB3	2.15	0.77
2:A:1143:LYS:HG2	3:A:186:HOH:O	1.84	0.77
2:B:1103:THR:HG22	3:B:184:HOH:O	1.86	0.76
2:B:892:LEU:HB2	2:B:902:ILE:HD11	1.68	0.76
2:B:829:ARG:HH12	2:B:837:ARG:HG2	1.53	0.73
2:A:854:MET:HE3	2:A:888:ALA:HB3	1.70	0.73
2:A:892:LEU:CB	2:A:902:ILE:HD11	2.20	0.72
2:A:892:LEU:HB3	2:A:902:ILE:HD11	1.71	0.72
1:D:7:U:O2'	1:D:8:A:OP1	2.08	0.71
2:A:879:GLN:HE21	2:A:883:ASN:HD21	1.39	0.70
2:B:833:LEU:HB2	3:B:148:HOH:O	1.90	0.70
2:A:880:LEU:HB2	3:A:158:HOH:O	1.91	0.70
2:A:1158:LYS:H	2:A:1158:LYS:HE2	1.57	0.70
2:B:1106:ASP:O	2:B:1108:PRO:HD2	1.92	0.68
2:B:1012:ARG:HG3	3:B:202:HOH:O	1.94	0.68
2:B:840:ARG:CB	3:B:235:HOH:O	2.40	0.68
2:A:1136:GLN:O	2:A:1140:VAL:HG23	1.93	0.68
2:B:847:ARG:HD2	3:B:251:HOH:O	1.92	0.68
2:B:982:GLN:CB	3:B:215:HOH:O	2.33	0.68
2:B:1117:LYS:HE3	2:B:1154:TYR:CE1	2.27	0.67
2:A:1033:THR:HG21	3:A:94:HOH:O	1.95	0.67
2:A:1061:ILE:O	2:A:1065:ILE:HD13	1.94	0.66
2:B:919:GLU:HB2	3:B:211:HOH:O	1.96	0.66
2:B:1157:GLY:O	2:B:1161:LEU:HB2	1.96	0.66
2:B:841:TYR:CD2	3:B:235:HOH:O	2.49	0.65
2:B:1051:GLU:OE1	2:B:1084:LYS:HE2	1.96	0.65
2:B:1098:ILE:HD12	3:B:147:HOH:O	1.97	0.65
2:B:1127:LYS:O	2:B:1131:VAL:HG22	1.97	0.64
2:A:1154:TYR:O	2:A:1158:LYS:CE	2.44	0.64
1:D:9:U:H2'	2:B:900:TYR:OH	1.98	0.63
2:A:1062:VAL:CG1	3:A:237:HOH:O	2.45	0.62
2:A:880:LEU:HD23	2:A:880:LEU:C	2.20	0.62
2:A:954:VAL:HG22	2:A:988:PHE:HZ	1.64	0.62
2:B:1033:THR:HG21	3:B:105:HOH:O	1.98	0.62
2:B:897:PHE:HD1	3:B:177:HOH:O	1.81	0.62
1:D:7:U:O2	1:D:7:U:H2'	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:880:LEU:HD23	2:A:880:LEU:O	2.00	0.61
2:A:879:GLN:HE21	2:A:883:ASN:ND2	1.99	0.60
2:B:1165:GLU:O	2:B:1166:LYS:O	2.20	0.60
2:A:894:VAL:CB	2:A:931:GLN:HE22	2.15	0.59
2:B:829:ARG:HH12	2:B:837:ARG:CG	2.15	0.59
2:B:1105:ASN:O	2:B:1107:GLY:N	2.33	0.58
2:A:880:LEU:C	2:A:880:LEU:CD2	2.72	0.58
2:A:833:LEU:HD22	2:A:855:GLU:HG2	1.86	0.58
2:B:1033:THR:HG21	2:B:1064:GLU:HG3	1.85	0.57
2:A:976:LYS:HD2	2:A:980:CYS:SG	2.44	0.57
2:A:1112:LEU:O	2:A:1116:MET:HG3	2.04	0.57
2:A:1119:GLN:NE2	3:A:252:HOH:O	2.38	0.56
2:B:837:ARG:HE	2:B:861:HIS:HD2	1.53	0.56
2:A:1157:GLY:N	3:A:138:HOH:O	2.39	0.56
1:D:6:A:H2'	3:D:20:HOH:O	2.06	0.56
2:A:1060:LYS:O	2:A:1064:GLU:HG2	2.05	0.55
2:B:1124:VAL:O	2:B:1128:MET:HG3	2.07	0.55
2:A:854:MET:HE1	2:A:888:ALA:HB3	1.88	0.54
2:A:1138:LYS:HA	2:A:1141:MET:HE2	1.89	0.54
2:A:874:THR:OG1	2:A:877:GLU:HG3	2.06	0.54
2:B:1050:LEU:HD13	2:B:1084:LYS:HB3	1.89	0.54
2:B:1104:MET:HE1	3:B:127:HOH:O	2.06	0.54
2:A:902:ILE:HD12	2:A:902:ILE:N	2.22	0.54
2:A:1070:LEU:HD13	2:A:1111:ALA:HB1	1.89	0.54
2:B:1082:VAL:CG1	3:B:212:HOH:O	2.49	0.54
2:A:1062:VAL:CB	3:A:237:HOH:O	2.35	0.54
2:B:1093:GLU:O	2:B:1097:LEU:HG	2.08	0.53
2:B:1148:ILE:HG23	2:B:1161:LEU:HD11	1.91	0.53
2:A:892:LEU:HB2	2:A:902:ILE:HD11	1.89	0.53
2:A:946:PRO:HB2	2:A:949:GLN:NE2	2.24	0.53
2:B:1030:HIS:O	2:B:1033:THR:HG22	2.09	0.53
2:B:1054:ARG:HD2	3:B:209:HOH:O	2.09	0.52
2:A:902:ILE:HD12	2:A:902:ILE:H	1.74	0.52
2:B:1012:ARG:HD2	3:B:202:HOH:O	2.08	0.52
1:C:5:A:H3'	3:A:248:HOH:O	2.09	0.52
2:A:903:GLN:O	2:A:907:GLU:HG3	2.10	0.51
2:A:990:ILE:HG13	2:A:1021:GLN:HB3	1.91	0.51
2:B:892:LEU:HB2	2:B:902:ILE:CD1	2.40	0.51
2:B:860:GLN:HG3	2:B:897:PHE:CE2	2.46	0.51
2:B:854:MET:HB2	3:B:25:HOH:O	2.11	0.51
2:B:1130:ASP:OD2	2:B:1163:LYS:HE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:910:SER:H	2:B:913:GLN:NE2	2.10	0.50
2:B:996:GLN:OE1	2:B:996:GLN:HA	2.11	0.50
2:A:1033:THR:O	2:A:1037:VAL:HG13	2.11	0.50
2:A:1158:LYS:CE	2:A:1158:LYS:H	2.23	0.50
2:A:946:PRO:HB2	2:A:949:GLN:HE21	1.77	0.49
1:D:4:U:H2'	2:B:1044:TYR:OH	2.11	0.49
2:A:951:ASN:O	2:A:955:ARG:HG3	2.12	0.49
1:D:6:A:C2	2:B:972:HIS:CE1	3.01	0.49
2:A:894:VAL:CG1	2:A:931:GLN:HE22	2.25	0.49
2:A:875:PRO:HG3	2:B:1156:TYR:OH	2.12	0.49
2:B:1154:TYR:HD2	2:B:1154:TYR:N	2.11	0.48
2:B:887:GLN:HB2	3:B:113:HOH:O	2.12	0.48
2:A:1095:ALA:O	2:A:1099:ASP:HB2	2.14	0.48
2:A:1118:ASP:HB3	2:A:1121:ALA:HB3	1.94	0.48
2:B:1079:SER:O	2:B:1082:VAL:HG22	2.13	0.48
2:B:1138:LYS:NZ	3:B:50:HOH:O	2.47	0.48
2:A:1092:THR:O	2:A:1096:VAL:HG23	2.14	0.48
2:A:1094:ARG:CD	2:A:1131:VAL:HG23	2.36	0.48
2:B:1153:LYS:HG3	2:B:1154:TYR:CD2	2.49	0.48
2:A:954:VAL:HG21	2:A:986:LEU:CD1	2.45	0.47
2:B:1154:TYR:CD2	2:B:1154:TYR:N	2.80	0.47
2:A:1143:LYS:CE	3:A:186:HOH:O	2.63	0.47
2:B:867:GLN:HA	2:B:904:LYS:HD2	1.97	0.47
2:A:903:GLN:HB3	2:A:940:LYS:HD2	1.97	0.47
2:B:1051:GLU:OE1	2:B:1084:LYS:CE	2.63	0.47
2:B:1167:TYR:HE2	3:B:124:HOH:O	1.97	0.47
2:B:829:ARG:HH12	2:B:837:ARG:CB	2.28	0.46
1:D:9:U:H2'	2:B:900:TYR:HH	1.80	0.46
2:B:832:LEU:HD12	2:B:852:HIS:CD2	2.50	0.46
2:A:993:PHE:CE2	2:A:1010:ILE:HD13	2.50	0.46
2:A:1126:GLN:HB3	2:A:1163:LYS:HD2	1.98	0.46
2:B:837:ARG:HE	2:B:861:HIS:CD2	2.33	0.46
2:A:943:GLU:HB2	2:A:976:LYS:NZ	2.31	0.46
2:B:1034:GLU:O	2:B:1037:VAL:HG22	2.16	0.46
2:A:1089:ALA:HB1	2:A:1093:GLU:HB3	1.97	0.46
2:B:1012:ARG:CD	3:B:202:HOH:O	2.64	0.46
2:B:829:ARG:NH1	2:B:837:ARG:HG2	2.24	0.46
2:A:838:ASN:O	2:A:840:ARG:N	2.50	0.46
2:B:1153:LYS:HG3	2:B:1154:TYR:HD2	1.81	0.46
2:A:1034:GLU:O	2:A:1037:VAL:HG22	2.16	0.45
2:A:1158:LYS:HE2	2:A:1158:LYS:N	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1030:HIS:HA	2:A:1033:THR:CG2	2.47	0.45
2:A:873:ALA:HB1	2:A:877:GLU:HB2	1.97	0.45
2:B:1050:LEU:CD1	2:B:1084:LYS:HB3	2.46	0.45
2:A:963:LYS:HD2	3:A:254:HOH:O	2.16	0.45
2:A:1071:VAL:HG21	3:A:250:HOH:O	2.16	0.45
2:A:896:VAL:HG13	2:A:897:PHE:CD1	2.52	0.45
2:B:1065:ILE:CD1	2:B:1065:ILE:N	2.80	0.45
2:A:920:ARG:HG2	2:A:920:ARG:HH11	1.83	0.44
2:A:962:LEU:HD23	3:A:223:HOH:O	2.17	0.44
2:B:912:GLU:H	2:B:912:GLU:CD	2.20	0.44
2:B:1033:THR:CG2	2:B:1064:GLU:HG3	2.47	0.44
2:A:980:CYS:HB3	2:B:1108:PRO:HG3	1.99	0.44
2:A:1008:ARG:NH2	3:A:248:HOH:O	2.38	0.44
2:B:993:PHE:CE2	2:B:1010:ILE:HD11	2.53	0.43
2:A:1158:LYS:CD	2:A:1158:LYS:H	2.32	0.43
2:A:878:ARG:HD3	3:A:128:HOH:O	2.17	0.43
2:B:892:LEU:CB	2:B:902:ILE:CD1	2.97	0.43
2:B:933:TYR:O	2:B:936:ARG:HB2	2.18	0.43
2:B:1076:LYS:HD2	2:B:1120:TYR:OH	2.18	0.43
2:A:1071:VAL:CG2	3:A:250:HOH:O	2.66	0.43
2:B:833:LEU:O	2:B:837:ARG:HB2	2.19	0.43
1:D:10:U:C3'	3:D:12:HOH:O	2.67	0.42
1:C:9:U:O2'	1:C:10:U:H5'	2.19	0.42
2:A:1147:HIS:O	2:A:1151:LEU:HG	2.19	0.42
2:B:993:PHE:HE2	2:B:1010:ILE:HD11	1.85	0.42
2:B:1040:GLN:HG3	2:B:1041:TYR:CD1	2.54	0.42
2:A:993:PHE:HE2	2:A:1010:ILE:CD1	2.33	0.42
1:D:5:A:O2'	2:B:1041:TYR:HE2	2.03	0.41
2:B:870:LEU:HD22	2:B:878:ARG:HG2	2.02	0.41
1:D:5:A:H3'	3:D:16:HOH:O	2.20	0.41
1:D:8:A:H8	1:D:8:A:H5''	1.84	0.41
2:A:1026:LEU:HD23	2:A:1026:LEU:HA	1.93	0.41
2:A:1029:LEU:HD21	2:A:1045:VAL:HG11	2.02	0.41
2:B:1086:VAL:O	2:B:1094:ARG:HD3	2.20	0.41
2:B:1094:ARG:O	2:B:1098:ILE:HG13	2.21	0.41
2:B:1130:ASP:CG	2:B:1163:LYS:HE2	2.40	0.41
2:B:879:GLN:O	2:B:883:ASN:HB2	2.20	0.41
2:A:1071:VAL:HG23	2:A:1072:LEU:N	2.36	0.41
2:A:1157:GLY:O	2:A:1161:LEU:HD22	2.21	0.41
2:B:1112:LEU:O	2:B:1116:MET:HG3	2.20	0.41
1:C:7:U:O2'	1:C:8:A:OP1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1130:ASP:OD1	2:B:1163:LYS:HE2	2.21	0.41
2:A:1058:LYS:NZ	2:A:1088:HIS:HB3	2.36	0.41
2:A:1069:VAL:HG11	2:A:1101:VAL:CG1	2.51	0.40
2:A:1143:LYS:O	2:A:1146:PRO:HD2	2.21	0.40
2:B:1156:TYR:O	2:B:1158:LYS:N	2.54	0.40
2:B:892:LEU:CB	2:B:902:ILE:HD11	2.42	0.40
2:B:961:VAL:O	2:B:965:VAL:HG23	2.21	0.40
2:B:1072:LEU:HD23	2:B:1072:LEU:HA	1.92	0.40
2:A:1094:ARG:HH11	2:A:1094:ARG:HB2	1.86	0.40
1:C:6:A:P	1:C:6:A:H3'	2.61	0.40
2:A:1047:GLN:HG3	2:A:1081:VAL:HG22	2.03	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	339/343 (99%)	331 (98%)	7 (2%)	1 (0%)	44	54
2	B	338/343 (98%)	315 (93%)	17 (5%)	6 (2%)	10	8
All	All	677/686 (99%)	646 (95%)	24 (4%)	7 (1%)	18	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	839	ASN
2	B	1106	ASP
2	B	1166	LYS
2	B	840	ARG
2	B	1157	GLY
2	B	829	ARG
2	B	1134	PRO

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	
2	A	299/306 (98%)	284 (95%)	15 (5%)	28	39
2	B	294/306 (96%)	277 (94%)	17 (6%)	23	31
All	All	593/612 (97%)	561 (95%)	32 (5%)	26	35

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

Mol	Chain	Res	Type
2	A	880	LEU
2	A	957	LEU
2	A	976	LYS
2	A	986	LEU
2	A	987	GLN
2	A	1017	CYS
2	A	1033	THR
2	A	1092	THR
2	A	1094	ARG
2	A	1099	ASP
2	A	1133	GLU
2	A	1150	THR
2	A	1158	LYS
2	A	1161	LEU
2	A	1163	LYS
2	B	832	LEU
2	B	904	LYS
2	B	919	GLU
2	B	920	ARG
2	B	932	MET
2	B	940	LYS
2	B	976	LYS
2	B	984	GLN
2	B	1017	CYS
2	B	1033	THR
2	B	1065	ILE
2	B	1066	ARG

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Mol	Chain	Res	Type
2	B	1110	SER
2	B	1138	LYS
2	B	1143	LYS
2	B	1154	TYR
2	B	1167	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	839	ASN
2	A	883	ASN
2	A	887	GLN
2	A	913	GLN
2	A	931	GLN
2	A	949	GLN
2	A	960	HIS
2	A	1031	GLN
2	A	1032	HIS
2	B	852	HIS
2	B	858	GLN
2	B	861	HIS
2	B	891	GLN
2	B	913	GLN
2	B	949	GLN
2	B	968	GLN
2	B	972	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	9/11 (81%)	5 (55%)	0
1	D	8/11 (72%)	5 (62%)	0
All	All	17/22 (77%)	10 (58%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	U
1	C	5	A
1	C	7	U

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Mol	Chain	Res	Type
1	C	8	A
1	C	9	U
1	D	5	A
1	D	6	A
1	D	7	U
1	D	8	A
1	D	10	U

There are no RNA pucker outliers to report.

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

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	C	10/11 (90%)	0.12	0 100 100	28, 44, 61, 68	0
1	D	9/11 (81%)	1.00	1 (11%) 6 9	36, 61, 79, 86	0
2	A	341/343 (99%)	-0.13	5 (1%) 74 79	21, 35, 60, 73	0
2	B	340/343 (99%)	0.09	13 (3%) 41 48	26, 41, 66, 79	0
All	All	700/708 (98%)	-0.00	19 (2%) 55 62	21, 38, 64, 86	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1154	TYR	7.9
2	B	1104	MET	4.7
1	D	7	U	4.4
2	B	1106	ASP	4.3
2	A	1108	PRO	3.4
2	B	828	GLY	3.0
2	B	1167	TYR	2.9
2	A	1091	ARG	2.9
2	B	1155	THR	2.9
2	B	1105	ASN	2.7
2	B	1161	LEU	2.5
2	B	830	SER	2.4
2	B	838	ASN	2.4
2	B	1156	TYR	2.4
2	B	1018	LEU	2.3
2	B	1017	CYS	2.2
2	A	829	ARG	2.1
2	A	839	ASN	2.1
2	A	908	PHE	2.1

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.