



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:11 AM UTC

PDB ID : 3Q0M / pdb_00003q0m
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 types of validation reports are described at

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

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

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

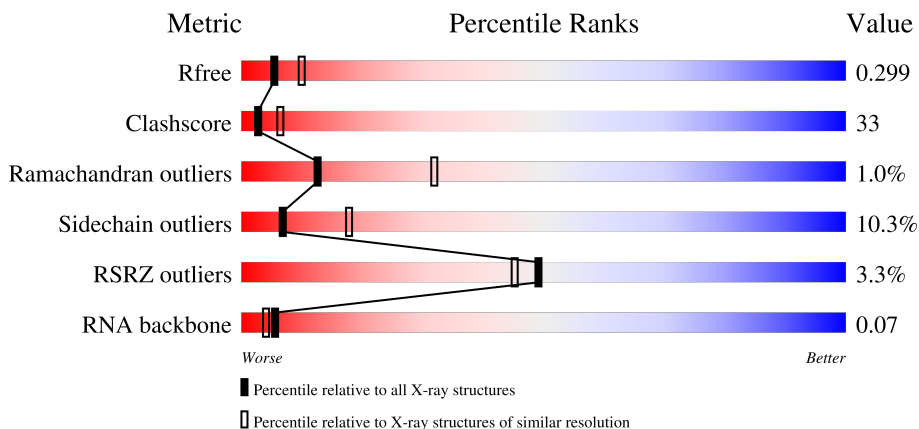
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

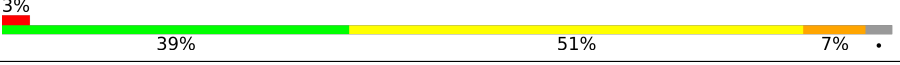
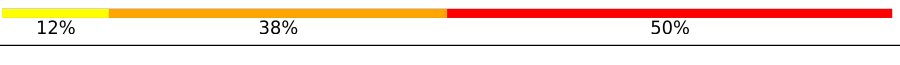
The reported resolution of this entry is 2.71 Å.

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	349	
1	B	349	
2	C	8	
2	D	8	

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.

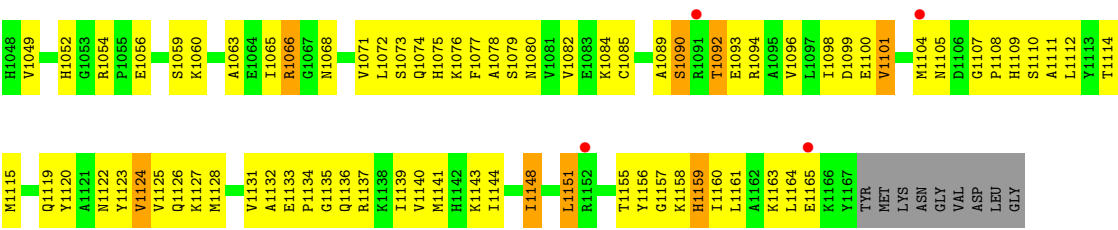
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2738	1732	496	493	17			
1	B	338	Total	C	N	O	S	0	0	0
			2748	1741	495	495	17			

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

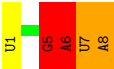
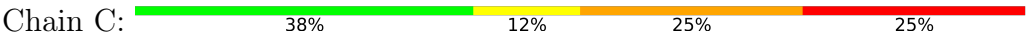
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			169	77	31	54	7			
2	D	8	Total	C	N	O	P	0	0	0
			169	77	31	54	7			

- 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		



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



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



4 Data and refinement statistics

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 29.80 – 2.71	Depositor EDS
% Data completeness (in resolution range)	78.7 (29.80-2.71) 79.2 (29.80-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.72Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_6)	Depositor
R, R_{free}	0.212 , 0.298 0.215 , 0.299	Depositor DCC
R_{free} test set	805 reflections (3.90%)	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)	0.33 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	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.*

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

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	0.54	0/2790	0.92	8/3763 (0.2%)
1	B	0.52	0/2801	0.95	14/3778 (0.4%)
2	C	0.50	0/189	1.36	2/293 (0.7%)
2	D	0.51	0/189	1.50	4/293 (1.4%)
All	All	0.53	0/5969	0.98	28/8127 (0.3%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1003	HIS	CA-C-N	6.86	126.66	119.05
1	B	1003	HIS	C-N-CA	6.86	126.66	119.05
1	B	1165	GLU	N-CA-C	-6.83	103.31	112.94
1	A	841	TYR	CA-C-N	6.50	125.93	118.85
1	A	841	TYR	C-N-CA	6.50	125.93	118.85
1	B	1107	GLY	CA-C-N	6.46	126.15	119.56
1	B	1107	GLY	C-N-CA	6.46	126.15	119.56
1	A	1164	LEU	N-CA-C	-6.23	101.04	110.70
2	C	6	A	P-O3'-C3'	-6.10	111.05	120.20
1	A	886	LEU	N-CA-C	6.05	117.55	111.07
1	A	936	ARG	N-CA-C	-5.80	104.87	111.14
1	B	981	VAL	CB-CA-C	-5.74	101.88	111.29
1	B	1018	LEU	CA-C-N	5.73	125.41	119.05
1	B	1018	LEU	C-N-CA	5.73	125.41	119.05
1	A	1111	ALA	N-CA-C	5.71	117.37	111.03
1	B	1124	VAL	CB-CA-C	-5.69	104.58	112.04
2	D	6	A	P-O5'-C5'	-5.51	112.64	120.90
1	A	1023	LEU	CA-C-N	5.38	125.20	119.28
1	A	1023	LEU	C-N-CA	5.38	125.20	119.28
1	B	1054	ARG	CA-C-N	5.37	126.55	119.84
1	B	1054	ARG	C-N-CA	5.37	126.55	119.84
1	B	1049	VAL	CB-CA-C	-5.28	105.12	111.88
2	D	2	G	O4'-C4'-C3'	5.21	109.21	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1133	GLU	CA-C-N	5.17	125.22	119.32
1	B	1133	GLU	C-N-CA	5.17	125.22	119.32
2	D	5	G	P-O3'-C3'	5.15	127.93	120.20
2	D	7	U	O4'-C1'-N1	5.11	116.16	108.50
2	C	5	G	P-O3'-C3'	5.11	127.86	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2738	0	2756	179	0
1	B	2748	0	2765	192	0
2	C	169	0	87	8	0
2	D	169	0	87	12	0
3	A	39	0	0	3	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	381	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 33.

All (381) 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
1:B:854:MET:HE2	1:B:888:ALA:HB3	1.44	0.96
2:D:2:G:H4'	2:D:2:G:OP1	1.66	0.95
1:A:1040:GLN:OE1	1:B:876:ALA:HB2	1.66	0.95
1:B:1075:HIS:HB3	1:B:1078:ALA:HB3	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:GLN:HG3	1:A:1081:VAL:HG22	1.50	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:B:889:ALA:HB1	1:B:893:MET:HE3	1.58	0.86
1:A:1161:LEU:O	1:A:1161:LEU:HD22	1.77	0.85
1:B:984:GLN:H	1:B:984:GLN:CD	1.84	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:HG2	1:A:1104:MET:O	1.80	0.81
1:A:854:MET:SD	1:A:888:ALA:HB3	2.22	0.80
1:A:1050:LEU:O	1:A:1058:LYS:HE2	1.81	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:B:943:GLU:HB2	1:B:976:LYS:HZ1	1.49	0.78
1:A:1021:GLN:O	1:A:1024:PRO:HD2	1.84	0.78
1:A:1141:MET:HE2	1:A:1141:MET:HA	1.65	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:890:TYR:HA	1:A:893:MET:HE3	1.67	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: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:HG2	1:B:840:ARG:HH11	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1098:ILE:HG12	1:A:1128:MET:HE2	1.72	0.70
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:A:1112:LEU:HG	1:A:1116:MET:HE3	1.72	0.69
1:B:846:LEU:HD23	1:B:849:ILE:HD11	1.73	0.69
1:A:982:GLN:HB3	1:A:984:GLN:NE2	2.06	0.69
1:B:1140:VAL:O	1:B:1144:ILE:HG13	1.92	0.69
1:B:874:THR:O	1:B:878:ARG:HB2	1.94	0.68
1:B:873:ALA:HB3	1:B:877:GLU:CD	2.18	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
1:B:882:PHE:HA	1:B:885:ILE:HG12	1.76	0.67
1:B:864:ARG:O	1:B:868:LEU:HG	1.95	0.67
1:B:1079:SER:O	1:B:1082:VAL:HG22	1.95	0.67
1:A:998:PHE:O	1:A:1002:THR:HG23	1.95	0.66
1:A:890:TYR:HA	1:A:893:MET:HE2	1.77	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:984:GLN:CD	1:A:984:GLN:H	2.03	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:B:984:GLN:CD	1:B:984:GLN:N	2.53	0.65
1:A:867:GLN:HB3	1:A:904:LYS:HE2	1.79	0.64
1:A:903:GLN:HB3	1:A:940:LYS:HZ3	1.62	0.64
1:A:993:PHE:HE2	1:A:1000:LEU:HD13	1.62	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: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:1040:GLN:CD	1:B:876:ALA:HB2	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1143:LYS:HB3	1:B:1143:LYS:HZ3	1.63	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:B:912:GLU:N	1:B:912:GLU:CD	2.58	0.61
1:A:1122:ASN:O	1:A:1126:GLN:HG3	2.00	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: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: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
1:B:1112:LEU:HD21	1:B:1140:VAL:HG13	1.85	0.58
2:D:2:G:OP1	2:D:2:G:C4'	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: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: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:831:ARG:HD2	1:B:832:LEU:N	2.20	0.56
1:B:1047:GLN:NE2	1:B:1080:ASN:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:ARG:HD3	1:A:833:LEU:HD23	1.86	0.56
1:A:986:LEU:HD22	1:A:989:ILE:HD11	1.86	0.56
1:A:1110:SER:OG	1:A:1111:ALA:N	2.37	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:869:LYS:O	1:A:873:ALA:HB2	2.06	0.55
1:A:1094:ARG:HH11	1:A:1094:ARG:HB2	1.72	0.55
1:A:1163:LYS:C	1:A:1165:GLU:H	2.14	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:HE	1:B:847:ARG:HA	1.71	0.55
1:A:854:MET:O	1:A:857:SER:N	2.40	0.54
1:A:1161:LEU:HD23	1:A:1164:LEU:HD12	1.89	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
1:A:1094:ARG:HH11	1:A:1094:ARG:CB	2.19	0.54
1:B:1084:LYS:N	1:B:1084:LYS:HD2	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:A:1128:MET:HE2	1:A:1128:MET:HA	1.88	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:B:865:PHE:C	1:B:865:PHE:CD2	2.85	0.53
1:A:1033:THR:HB	1:A:1064:GLU:HG3	1.91	0.53
1:A:1161:LEU:CD2	1:A:1161:LEU:C	2.80	0.53
1:A:882:PHE:CD1	1:A:913:GLN:HG2	2.44	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:B:1040:GLN:CD	1:B:1040:GLN:H	2.16	0.53
1:A:1161:LEU:O	1:A:1161:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:SER:OG	1:B:867:GLN:NE2	2.42	0.53
1:B:860:GLN:NE2	2:D:8:A:O2'	2.42	0.52
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:A:935:CYS:SG	1:A:969:ASN:HB3	2.49	0.52
1:A:1125:VAL:HA	1:A:1128:MET:CG	2.39	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:1077:PHE:HE2	2:D:3:U:H1'	1.74	0.51
1:B:1099:ASP:N	1:B:1136:GLN:HE22	2.08	0.51
1:A:850:ALA:O	1:A:852:HIS:HD2	1.93	0.51
1:A:1075:HIS:HE1	1:A:1077:PHE:HD1	1.58	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:854:MET:O	1:A:855:GLU:C	2.53	0.51
1:A:981:VAL:HG12	1:A:982:GLN:O	2.09	0.51
1:A:1014:LEU:CD2	1:A:1026:LEU:HD21	2.41	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:983:PRO:HB2	1:B:1018:LEU:HG	1.91	0.51
1:B:1072:LEU:HD22	1:B:1078:ALA:HB1	1.92	0.51
1:B:951:ASN:O	1:B:954:VAL:HB	2.10	0.51
1:B:1003:HIS:CG	1:B:1004:PRO:HD2	2.46	0.51
1:A:1082:VAL:O	1:A:1085:CYS:HB2	2.11	0.50
1:B:1099:ASP:CG	1:B:1136:GLN:HE21	2.18	0.50
1:B:1074:GLN:O	1:B:1120:TYR:HD1	1.95	0.50
1:B:1090:SER:HB3	1:B:1093:GLU:HG3	1.93	0.50
1:B:1120:TYR:O	1:B:1123:TYR:HB2	2.12	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: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:A:1065:ILE:O	1:A:1066:ARG:C	2.54	0.50
1:B:847:ARG:HA	1:B:847:ARG:NE	2.27	0.50
1:A:1047:GLN:OE1	1:A:1084:LYS:HD3	2.11	0.49
1:A:1075:HIS:HE1	1:A:1077:PHE:CD1	2.30	0.49
1:B:912:GLU:CD	1:B:912:GLU:H	2.18	0.49
1:B:941:ALA:O	1:B:945:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:PRO:O	1:A:1028:GLU:HG3	2.12	0.49
1:B:906:PHE:HB3	1:B:940:LYS:HG3	1.94	0.49
1:B:1030:HIS:CE1	1:B:1060:LYS:HB2	2.47	0.49
1:B:1122:ASN:CG	1:B:1123:TYR:N	2.69	0.49
1:A:845:GLN:HB2	1:A:848:GLU:HG3	1.93	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:B:949:GLN:C	3:B:29:HOH:O	2.56	0.49
1:A:1127:LYS:O	1:A:1128:MET:C	2.55	0.49
1:A:1147:HIS:O	1:A:1151:LEU:HG	2.13	0.49
1:A:1148:ILE:C	1:A:1150:THR:H	2.21	0.49
1:B:1023:LEU:CB	1:B:1024:PRO:HD3	2.41	0.49
1:B:832:LEU:O	1:B:833:LEU:C	2.56	0.49
1:A:1065:ILE:CG2	1:A:1082:VAL:HG12	2.43	0.49
1:A:1158:LYS:NZ	1:A:1158:LYS:HB2	2.28	0.49
1:B:840:ARG:C	1:B:842:PRO:HD3	2.38	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:860:GLN:HB2	1:A:897:PHE:CZ	2.49	0.48
1:A:882:PHE:CE1	1:A:913:GLN:HG2	2.48	0.48
1:B:972:HIS:CE1	2:D:5:G:C8	3.01	0.48
1:B:978:ILE:HA	1:B:986:LEU:CD1	2.44	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:1157:GLY:C	1:B:1159:HIS:H	2.21	0.48
1:B:996:GLN:NE2	3:B:5:HOH:O	2.47	0.47
1:B:1099:ASP:CG	1:B:1136:GLN:NE2	2.73	0.47
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:B:1155:THR:C	1:B:1157:GLY:H	2.23	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:1161:LEU:HD22	1:A:1161:LEU:C	2.39	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:1082:VAL:O	1:A:1083:GLU:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:ARG:N	1:A:1146:PRO:CD	2.79	0.46
1:B:850:ALA:HB2	1:B:880:LEU:HD11	1.98	0.46
1:B:994:LYS:NZ	1:B:1024:PRO:HG2	2.31	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:831:ARG:HA	1:A:834:GLU:HB2	1.97	0.46
1:A:1144:ILE:CG2	1:A:1164:LEU:HD21	2.42	0.46
1:A:919:GLU:HA	1:A:922:ARG:CZ	2.46	0.46
1:A:1022:THR:O	1:A:1026:LEU:CG	2.63	0.46
1:A:1002:THR:HA	1:A:1039:ASP:OD2	2.16	0.46
1:A:1029:LEU:HD23	1:A:1029:LEU:HA	1.75	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:853:ILE:HG13	1:B:884:GLU:CD	2.40	0.45
1:B:1072:LEU:HD22	1:B:1078:ALA:CB	2.46	0.45
1:B:1125:VAL:O	1:B:1126:GLN:C	2.59	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: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:B:975:GLN:O	1:B:979:GLU:HG3	2.16	0.45
1:B:1124:VAL:O	1:B:1128:MET:HG3	2.16	0.45
1:B:978:ILE:HA	1:B:986:LEU:HD11	1.99	0.45
1:A:919:GLU:O	1:A:920:ARG:C	2.60	0.45
1:A:911:LEU:O	1:A:915:LEU:HG	2.17	0.45
1:B:896:VAL:HA	1:B:933:TYR:CD2	2.52	0.45
1:B:1073:SER:CB	1:B:1124:VAL:HG21	2.43	0.45
1:A:936:ARG:HG3	2:C:7:U:C4	2.52	0.44
1:A:986:LEU:HD22	1:A:989:ILE:CD1	2.46	0.44
1:A:1161:LEU:HD23	1:A:1164:LEU:CD1	2.47	0.44
1:B:957:LEU:HD23	1:B:957:LEU:HA	1.73	0.44
1:B:962:LEU:O	1:B:963:LYS:C	2.60	0.44
1:B:1104:MET:HB3	1:B:1111:ALA:HB2	1.98	0.44
1:A:972:HIS:O	1:A:976:LYS:HB2	2.17	0.44
1:B:886:LEU:HG	1:B:886:LEU:O	2.17	0.44
1:A:939:GLN:NE2	2:C:6:A:H2	2.16	0.44
1:A:1008:ARG:HG3	2:C:5:G:C8	2.53	0.44
1:A:854:MET:SD	1:A:888:ALA:CB	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:VAL:HG21	1:A:981:VAL:HG21	2.00	0.44
1:A:1163:LYS:O	1:A:1165:GLU:N	2.40	0.44
1:B:879:GLN:HE21	1:B:883:ASN:ND2	2.16	0.44
1:B:953:MET:O	1:B:954:VAL:C	2.61	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:890:TYR:O	1:B:890:TYR:HD1	2.01	0.44
1:B:1068:ASN:O	1:B:1072:LEU:HB2	2.17	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
1:B:1100:GLU:HG2	1:B:1104:MET:HE3	2.00	0.44
2:D:1:U:O5'	2:D:2:G:C5'	2.66	0.43
1:A:1163:LYS:C	1:A:1165:GLU:N	2.73	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:947:SER:HA	1:B:950:GLN:CD	2.43	0.43
1:B:1003:HIS:HA	1:B:1004:PRO:HD3	1.82	0.43
1:A:920:ARG:HD2	1:A:920:ARG:HA	1.52	0.43
1:A:989:ILE:HG22	1:A:993:PHE:HE1	1.83	0.43
1:A:1113:TYR:CZ	1:A:1117:LYS:HD2	2.54	0.43
1:A:919:GLU:HG2	1:A:922:ARG:HH22	1.84	0.43
1:B:1032:HIS:C	1:B:1034:GLU:N	2.76	0.43
1:A:947:SER:HB3	3:A:87:HOH:O	2.19	0.42
1:A:1039:ASP:HB3	1:A:1042:GLY:HA3	2.00	0.42
1:A:1094:ARG:HD3	1:A:1131:VAL:HG23	2.01	0.42
1:A:1104:MET:CE	3:A:35:HOH:O	2.66	0.42
1:A:854:MET:HE3	1:A:854:MET:HB3	1.64	0.42
1:B:879:GLN:HE21	1:B:883:ASN:HD21	1.66	0.42
1:B:966:LYS:HA	1:B:1003:HIS:CE1	2.54	0.42
1:B:1032:HIS:C	1:B:1034:GLU:H	2.27	0.42
1:B:1098:ILE:HG12	1:B:1128:MET:HB3	2.02	0.42
1:B:1127:LYS:HD3	1:B:1127:LYS:HA	1.74	0.42
1:B:882:PHE:HE2	1:B:917:LEU:HG	1.85	0.42
1:B:907:GLU:HG3	1:B:940:LYS:HD2	2.01	0.42
2:C:6:A:H5'	2:C:6:A:H8	1.84	0.42
1:A:829:ARG:NH2	1:A:837:ARG:HH12	2.18	0.42
1:A:1082:VAL:HG23	1:A:1124:VAL:CG2	2.50	0.42
1:B:1098:ILE:O	1:B:1101:VAL:HG23	2.19	0.42
1:A:882:PHE:O	1:A:883:ASN:C	2.62	0.42
1:A:910:SER:H	1:A:913:GLN:HE21	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:880:LEU:HD12	1:B:880:LEU:O	2.19	0.42
1:B:1078:ALA:O	1:B:1079:SER:C	2.61	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:940:LYS:HD2	1:A:944:PHE:HE1	1.85	0.41
2:C:1:U:H6	2:C:1:U:O5'	2.02	0.41
1:A:1023:LEU:N	1:A:1024:PRO:HD2	2.35	0.41
1:A:1094:ARG:CG	1:A:1094:ARG:NH1	2.64	0.41
1:A:1116:MET:HE2	1:A:1144:ILE:HD13	2.02	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:B:1018:LEU:N	1:B:1021:GLN:OE1	2.53	0.41
1:A:913:GLN:HE21	1:A:913:GLN:HB2	1.61	0.41
1:A:1124:VAL:O	1:A:1128:MET:HG2	2.20	0.41
1:B:1108:PRO:HB2	1:B:1109:HIS:CD2	2.55	0.41
1:B:1022:THR:O	1:B:1023:LEU:C	2.64	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:860:GLN:CG	1:A:864:ARG:HH12	2.26	0.41
1:A:1011:GLN:O	1:A:1015:GLU:HG3	2.20	0.41
1:B:921:ILE:HD13	1:B:953:MET:HE1	2.01	0.41
1:B:1094:ARG:NH2	3:B:94:HOH:O	2.52	0.41
1:B:1131:VAL:O	1:B:1132:ALA:C	2.63	0.41
1:B:1023:LEU:HD12	1:B:1023:LEU:HA	1.80	0.41
1:B:1101:VAL:HG11	1:B:1115:MET:SD	2.61	0.41
1:A:1035:GLN:H	1:A:1035:GLN:HG3	1.68	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:951:ASN:HD22	1:A:951:ASN:HA	1.65	0.40
1:A:1094:ARG:HG3	1:A:1094:ARG:NH1	2.18	0.40
1:B:839:ASN:HD22	1:B:839:ASN:HA	1.62	0.40
1:B:847:ARG:NE	1:B:847:ARG:CA	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:B:1134:PRO:O	1:B:1135:GLY:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:ILE:HG22	1:A:993:PHE:CE1	2.57	0.40
1:A:1101:VAL:O	1:A:1111:ALA:HB3	2.22	0.40
1:B:1161:LEU:C	1:B:1161:LEU:HD23	2.46	0.40
1:A:886:LEU:HD12	1:A:886:LEU:HA	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%)	14	35
1	B	336/349 (96%)	285 (85%)	47 (14%)	4 (1%)	10	27
All	All	671/698 (96%)	577 (86%)	87 (13%)	7 (1%)	12	32

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%)	266 (88%)	35 (12%)	5	13
1	B	302/310 (97%)	275 (91%)	27 (9%)	9	23
All	All	603/620 (97%)	541 (90%)	62 (10%)	7	18

All (62) 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	1071	VAL
1	A	1083	GLU
1	A	1084	LYS
1	A	1094	ARG
1	A	1096	VAL
1	A	1103	THR
1	A	1106	ASP
1	A	1112	LEU
1	A	1128	MET
1	A	1131	VAL
1	A	1133	GLU
1	A	1143	LYS
1	A	1147	HIS
1	A	1153	LYS
1	A	1158	LYS
1	A	1160	ILE
1	A	1161	LEU

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Mol	Chain	Res	Type
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	881	VAL
1	B	891	GLN
1	B	904	LYS
1	B	907	GLU
1	B	911	LEU
1	B	949	GLN
1	B	981	VAL
1	B	985	SER
1	B	1035	GLN
1	B	1037	VAL
1	B	1038	GLN
1	B	1040	GLN
1	B	1066	ARG
1	B	1071	VAL
1	B	1090	SER
1	B	1092	THR
1	B	1101	VAL
1	B	1114	THR
1	B	1148	ILE
1	B	1151	LEU
1	B	1159	HIS
1	B	1163	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	852	HIS
1	A	858	GLN
1	A	879	GLN
1	A	883	ASN
1	A	891	GLN
1	A	913	GLN
1	A	939	GLN
1	A	951	ASN
1	A	960	HIS

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Mol	Chain	Res	Type
1	A	982	GLN
1	A	1031	GLN
1	A	1052	HIS
1	A	1074	GLN
1	A	1119	GLN
1	A	1126	GLN
1	A	1159	HIS
1	B	838	ASN
1	B	839	ASN
1	B	845	GLN
1	B	860	GLN
1	B	879	GLN
1	B	883	ASN
1	B	887	GLN
1	B	903	GLN
1	B	939	GLN
1	B	949	GLN
1	B	950	GLN
1	B	960	HIS
1	B	996	GLN
1	B	1016	HIS
1	B	1030	HIS
1	B	1031	GLN
1	B	1088	HIS
1	B	1109	HIS
1	B	1136	GLN
1	B	1147	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	7/8 (87%)	4 (57%)	3 (42%)
2	D	8/8 (100%)	6 (75%)	5 (62%)
All	All	15/16 (93%)	10 (66%)	8 (53%)

All (10) RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
2	C	8	A
2	D	2	G
2	D	3	U
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	337/349 (96%)	-0.06	14 (4%) 40 37	23, 27, 84, 178	0
1	B	338/349 (96%)	-0.17	9 (2%) 56 53	23, 29, 76, 239	0
2	C	8/8 (100%)	-0.73	0 100 100	25, 26, 32, 34	0
2	D	8/8 (100%)	-0.61	0 100 100	24, 25, 29, 34	0
All	All	691/714 (96%)	-0.13	23 (3%) 49 45	23, 28, 79, 239	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1149	ALA	4.4
1	A	1151	LEU	4.4
1	B	875	PRO	4.0
1	A	888	ALA	3.9
1	A	1148	ILE	3.6
1	B	1104	MET	3.3
1	A	1110	SER	3.3
1	A	1108	PRO	3.2
1	A	1105	ASN	3.1
1	A	1103	THR	2.9
1	B	947	SER	2.8
1	A	1041	TYR	2.8
1	B	873	ALA	2.7
1	A	839	ASN	2.6
1	A	1106	ASP	2.5
1	B	1091	ARG	2.4
1	A	1109	HIS	2.3
1	B	1152	ARG	2.3
1	A	1040	GLN	2.3
1	B	929	ALA	2.3
1	A	912	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	891	GLN	2.2
1	B	1165	GLU	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.