



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:20 PM UTC

PDB ID : 1M8W / pdb_00001m8w
Title : CRYSTAL STRUCTURE OF THE PUMILIO-HOMOLOGY DOMAIN
FROM HUMAN PUMILIO1 IN COMPLEX WITH NRE1-19 RNA
Authors : Wang, X.; McLachlan, J.; Zamore, P.D.; Hall, T.M.T.
Deposited on : 2002-07-26
Resolution : 2.20 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

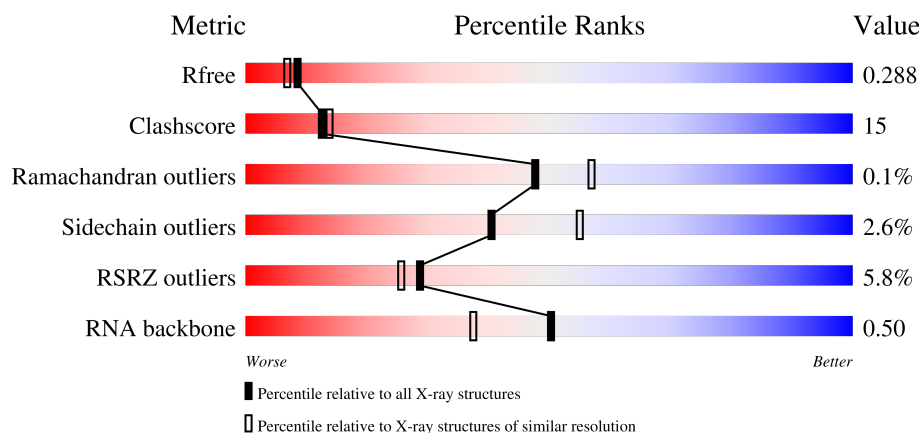
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)
RNA backbone	3983	1052 (2.50-1.90)

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	C	8	14% 50% 25% 25%
2	D	7	14% 57% 29% 14%
3	E	8	25% 25% 50% 25%
4	F	7	14% 57% 29% 14%

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Mol	Chain	Length	Quality of chain
5	A	349	3% 69% 27% ••
5	B	349	7% 62% 34% ••

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6475 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(P*UP*UP*GP*UP*AP*UP*AP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	8	Total	C	N	O	P	0	8	0
			167	75	25	59	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	7	Total	C	N	O	P	0	7	0
			147	66	23	51	7			

- Molecule 3 is a RNA chain called 5'-R(P*UP*UP*GP*UP*CP*CP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	P	0	8	0
			168	75	27	58	8			

- Molecule 4 is a RNA chain called 5'-R(P*UP*GP*UP*CP*CP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	7	Total	C	N	O	P	0	7	0
			148	66	25	50	7			

- Molecule 5 is a protein called Pumilio 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	340	Total	C	N	O	S	0	0	0
			2763	1749	500	497	17			
5	B	341	Total	C	N	O	S	0	0	0
			2775	1758	501	499	17			

- Molecule 6 is water.

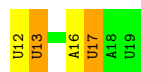
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	5	Total 5	O 5	0	0
6	E	6	Total 6	O 6	0	0
6	F	6	Total 6	O 6	0	0
6	A	205	Total 205	O 205	0	0
6	B	85	Total 85	O 85	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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(P*UP*UP*GP*UP*AP*UP*AP*U)-3'

Chain C: 

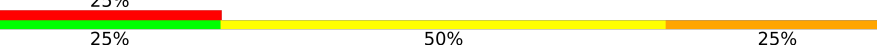


- Molecule 2: 5'-R(P*UP*GP*UP*AP*UP*AP*U)-3'

Chain D: 



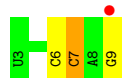
- Molecule 3: 5'-R(P*UP*UP*GP*UP*CP*CP*AP*G)-3'

Chain E: 



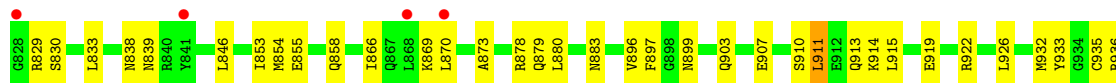
- Molecule 4: 5'-R(P*UP*GP*UP*CP*CP*AP*G)-3'

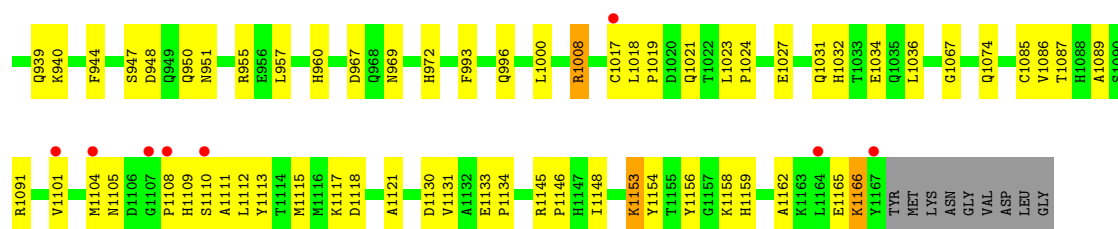
Chain F: 



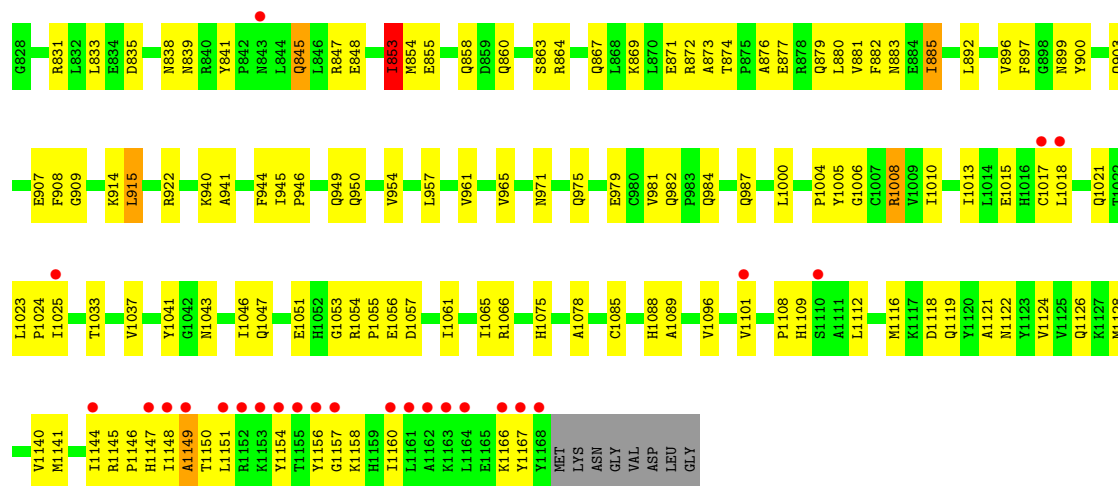
- Molecule 5: Pumilio 1

Chain A: 





• Molecule 5: Pumilio 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	262.73Å 37.73Å 82.52Å 90.00° 102.95° 90.00°	Depositor
Resolution (Å)	42.68 – 2.20 42.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.0 (42.68-2.20) 96.0 (42.68-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.224 , 0.289 0.224 , 0.288	Depositor DCC
R_{free} test set	2447 reflections (5.98%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6475	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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	C	0.46	0/185	0.82	0/285
2	D	0.42	0/163	0.62	0/251
3	E	0.40	0/186	0.63	0/287
4	F	0.41	0/164	0.56	0/253
5	A	0.48	0/2816	0.86	6/3797 (0.2%)
5	B	0.38	0/2829	0.85	3/3815 (0.1%)
All	All	0.43	0/6343	0.84	9/8688 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1067	GLY	N-CA-C	-7.73	105.49	114.69
5	B	853	ILE	N-CA-C	6.86	117.64	110.72
5	A	944	PHE	N-CA-C	6.15	121.72	113.72
5	A	853	ILE	N-CA-C	5.75	115.94	110.42
5	A	1148	ILE	N-CA-C	5.74	116.38	110.36
5	A	1087	THR	N-CA-C	5.54	116.99	111.07
5	A	1130	ASP	N-CA-C	5.34	117.10	111.28
5	B	1166	LYS	N-CA-C	-5.21	107.30	113.97
5	B	944	PHE	N-CA-C	5.03	120.04	112.94

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	167	0	74	4	0
2	D	147	0	66	4	0
3	E	168	0	73	7	0
4	F	148	0	66	3	0
5	A	2763	0	2781	73	0
5	B	2775	0	2790	99	0
6	A	205	0	0	9	0
6	B	85	0	0	3	0
6	C	5	0	0	0	0
6	E	6	0	0	0	0
6	F	6	0	0	0	0
All	All	6475	0	5850	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 15.

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)
5:A:1166:LYS:HD2	5:A:1166:LYS:H	1.23	0.98
5:A:879:GLN:HE21	5:A:883:ASN:HD21	1.22	0.88
5:A:1023:LEU:HB3	5:A:1024:PRO:HD3	1.60	0.84
5:A:1105:ASN:HA	5:A:1110:SER:HA	1.60	0.82
5:A:1101:VAL:HG21	5:A:1115:MET:SD	2.21	0.80
4:F:6[B]:C:H2'	4:F:7[B]:C:H5''	1.64	0.79
5:B:1023:LEU:HB3	5:B:1024:PRO:HD3	1.63	0.79
5:B:845:GLN:HG3	5:B:848:GLU:HG3	1.63	0.79
5:B:1043:ASN:O	5:B:1047:GLN:HG3	1.84	0.76
5:B:1101:VAL:HG12	5:B:1112:LEU:HG	1.69	0.75
5:B:907:GLU:OE2	5:B:940:LYS:HE2	1.87	0.75
5:A:879:GLN:HE21	5:A:883:ASN:ND2	1.85	0.75
5:B:871:GLU:HG2	5:B:908:PHE:CE1	2.22	0.74
5:B:879:GLN:HE21	5:B:883:ASN:HD21	1.35	0.74
5:A:1166:LYS:H	5:A:1166:LYS:CD	1.99	0.74
5:B:1065:ILE:HG13	5:B:1085:CYS:SG	2.28	0.74
3:E:6[B]:C:H2'	3:E:7[B]:C:H5''	1.71	0.73
5:A:870:LEU:HD13	5:A:878:ARG:HG2	1.70	0.72
5:A:1166:LYS:HD2	5:A:1166:LYS:N	2.02	0.72
5:B:1116:MET:HE3	5:B:1151:LEU:HD13	1.72	0.71
5:A:1017:CYS:SG	5:A:1021:GLN:OE1	2.48	0.71
1:C:16[A]:A:H2'	1:C:17[A]:U:H5''	1.72	0.71
5:B:879:GLN:HE21	5:B:883:ASN:ND2	1.87	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1122:ASN:HB2	5:B:1160:ILE:HD11	1.71	0.71
5:A:1017:CYS:SG	5:A:1021:GLN:CD	2.74	0.70
5:B:874:THR:OG1	5:B:877:GLU:HG3	1.91	0.70
5:B:1008:ARG:HA	5:B:1008:ARG:HE	1.55	0.70
5:A:1145:ARG:HB3	5:A:1146:PRO:HD3	1.75	0.68
5:B:833:LEU:HD22	5:B:855:GLU:HG2	1.75	0.68
5:B:1118:ASP:HB3	5:B:1121:ALA:HB3	1.74	0.68
5:B:954:VAL:HG21	5:B:981:VAL:HG21	1.76	0.68
2:D:16[A]:A:H2'	2:D:17[A]:U:H5''	1.76	0.67
5:A:1086:VAL:HG12	5:A:1131:VAL:HG21	1.75	0.67
5:B:1046:ILE:HG23	5:B:1061:ILE:HD13	1.77	0.66
5:B:1066:ARG:CZ	5:B:1096:VAL:HG11	2.25	0.65
5:B:1056:GLU:H	5:B:1056:GLU:CD	2.07	0.63
5:A:951:ASN:O	5:A:955:ARG:HG3	1.99	0.63
5:B:1000:LEU:HB2	5:B:1010:ILE:HD11	1.81	0.62
5:A:1008:ARG:HH11	5:A:1008:ARG:HG3	1.64	0.61
5:B:945:ILE:HD12	5:B:949:GLN:HB3	1.82	0.61
5:B:1150:THR:HG22	5:B:1154:TYR:HE2	1.65	0.61
5:B:1157:GLY:HA2	5:B:1160:ILE:HD13	1.83	0.61
5:B:1054:ARG:HB2	5:B:1057:ASP:OD2	2.01	0.61
5:B:853:ILE:HD12	5:B:881:VAL:HA	1.83	0.61
4:F:6[B]:C:C2'	4:F:7[B]:C:H5''	2.30	0.60
5:B:1055:PRO:HB2	5:B:1056:GLU:OE2	2.02	0.60
5:A:1017:CYS:HG	5:A:1018:LEU:H	1.49	0.60
5:B:1051:GLU:HG2	5:B:1088:HIS:NE2	2.17	0.60
5:A:829:ARG:HG2	5:A:833:LEU:HD23	1.83	0.59
5:A:926:LEU:HD22	5:A:960:HIS:CD2	2.38	0.59
5:B:946:PRO:HB2	5:B:949:GLN:HE21	1.67	0.59
3:E:2[B]:U:H5''	3:E:3[B]:U:OP2	2.04	0.58
5:B:831:ARG:HA	5:B:831:ARG:HE	1.69	0.57
5:A:1108:PRO:HB2	5:A:1109:HIS:ND1	2.19	0.57
5:B:882:PHE:HA	5:B:885:ILE:CD1	2.35	0.57
5:A:899:ASN:O	5:A:903:GLN:HG3	2.05	0.56
5:A:972:HIS:HD2	6:A:227:HOH:O	1.88	0.56
5:A:932:MET:HB2	6:A:249:HOH:O	2.05	0.56
5:B:946:PRO:O	5:B:950:GLN:HG3	2.06	0.55
3:E:6[B]:C:C2'	3:E:7[B]:C:H5''	2.36	0.55
5:B:896:VAL:HG13	5:B:897:PHE:CD1	2.41	0.54
5:B:1145:ARG:CG	5:B:1146:PRO:HD3	2.37	0.54
5:B:1145:ARG:O	5:B:1148:ILE:HG13	2.07	0.54
5:B:946:PRO:HB2	5:B:949:GLN:NE2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:981:VAL:HG12	5:B:982:GLN:N	2.23	0.53
5:B:1160:ILE:N	5:B:1160:ILE:HD12	2.23	0.53
5:B:879:GLN:NE2	5:B:883:ASN:HD21	2.05	0.53
5:B:1141:MET:HG3	5:B:1167:TYR:CD2	2.43	0.53
5:A:869:LYS:O	5:A:873:ALA:HB2	2.09	0.53
5:A:1118:ASP:HB3	5:A:1121:ALA:HB3	1.91	0.53
5:B:971:ASN:O	5:B:975:GLN:HG3	2.09	0.53
1:C:16[A]:A:C2'	1:C:17[A]:U:H5''	2.38	0.53
5:A:932:MET:HE2	5:A:933:TYR:CZ	2.44	0.53
5:A:1101:VAL:HG23	5:A:1111:ALA:HB3	1.90	0.52
5:A:907:GLU:HG2	5:A:940:LYS:HD2	1.92	0.52
5:B:1033:THR:O	5:B:1037:VAL:HG13	2.09	0.52
1:C:12[A]:U:H5''	1:C:13[A]:U:OP2	2.10	0.52
5:A:910:SER:O	5:A:914:LYS:HG3	2.10	0.51
5:B:853:ILE:CD1	5:B:881:VAL:HA	2.40	0.51
5:B:941:ALA:O	5:B:945:ILE:HG12	2.11	0.51
5:B:854:MET:O	5:B:858:GLN:HG3	2.10	0.51
5:B:879:GLN:NE2	5:B:883:ASN:ND2	2.56	0.51
2:D:16[A]:A:C2'	2:D:17[A]:U:H5''	2.38	0.51
5:A:1156:TYR:HA	5:A:1159:HIS:HD2	1.76	0.51
5:B:1053:GLY:HA2	6:B:293:HOH:O	2.10	0.51
5:B:1145:ARG:HG2	5:B:1146:PRO:HD3	1.92	0.51
5:B:1021:GLN:O	5:B:1024:PRO:HD2	2.11	0.50
5:B:885:ILE:HB	5:B:892:LEU:CD1	2.41	0.50
3:E:7[B]:C:C6	5:A:1008:ARG:NH2	2.79	0.50
5:B:871:GLU:HG2	5:B:908:PHE:HE1	1.72	0.50
5:A:910:SER:OG	5:A:913:GLN:HG3	2.11	0.50
5:B:872:ARG:HH11	5:B:872:ARG:HG2	1.77	0.49
5:B:1056:GLU:CD	5:B:1056:GLU:N	2.70	0.49
4:F:9[B]:G:H2'	5:B:900:TYR:OH	2.12	0.49
5:A:1113:TYR:O	5:A:1117:LYS:HD3	2.12	0.49
5:B:961:VAL:O	5:B:965:VAL:HG23	2.11	0.49
5:A:1019:PRO:O	5:A:1023:LEU:HB2	2.13	0.49
5:A:911:LEU:O	5:A:915:LEU:HG	2.12	0.49
5:B:1006:GLY:O	5:B:1010:ILE:HG13	2.14	0.48
5:B:1122:ASN:O	5:B:1126:GLN:HG3	2.13	0.48
5:A:1101:VAL:CG2	5:A:1115:MET:SD	2.98	0.48
5:B:838:ASN:O	5:B:839:ASN:C	2.56	0.48
1:C:17[A]:U:C6	5:A:1008:ARG:NH2	2.82	0.47
5:B:1141:MET:HE3	5:B:1167:TYR:HB2	1.96	0.47
5:B:922:ARG:HD2	6:B:239:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1061:ILE:O	5:B:1065:ILE:HG12	2.15	0.47
5:A:947:SER:HA	5:A:950:GLN:OE1	2.15	0.47
5:A:1101:VAL:HG22	5:A:1101:VAL:O	2.14	0.47
5:B:1108:PRO:HG2	5:B:1109:HIS:ND1	2.29	0.47
5:A:967:ASP:OD1	5:A:969:ASN:N	2.46	0.47
5:A:1113:TYR:CE1	5:A:1117:LYS:HD2	2.50	0.47
5:B:1145:ARG:N	5:B:1146:PRO:HD2	2.30	0.46
5:A:1008:ARG:HG3	5:A:1008:ARG:NH1	2.30	0.46
5:B:1148:ILE:HG22	5:B:1148:ILE:O	2.16	0.46
5:B:847:ARG:HD3	6:B:130:HOH:O	2.15	0.46
5:B:1124:VAL:O	5:B:1128:MET:HG3	2.16	0.46
5:A:879:GLN:NE2	5:A:883:ASN:ND2	2.57	0.46
5:A:1032:HIS:O	5:A:1036:LEU:HG	2.15	0.46
5:B:909:GLY:O	5:B:914:LYS:HE3	2.16	0.46
5:A:858:GLN:NE2	6:A:195:HOH:O	2.38	0.45
5:A:907:GLU:CG	5:A:940:LYS:HD2	2.46	0.45
5:B:882:PHE:HA	5:B:885:ILE:HD13	1.98	0.45
5:B:975:GLN:O	5:B:979:GLU:HG2	2.16	0.45
5:A:1104:MET:HE3	5:A:1104:MET:HA	1.98	0.45
5:B:899:ASN:O	5:B:903:GLN:HG3	2.16	0.45
5:A:993:PHE:CE2	5:A:1000:LEU:HD13	2.51	0.45
5:A:1034:GLU:HG3	6:A:161:HOH:O	2.17	0.45
5:B:1116:MET:SD	5:B:1144:ILE:HG13	2.57	0.45
5:A:1108:PRO:HB2	5:A:1109:HIS:CE1	2.52	0.45
5:A:1101:VAL:HG22	5:A:1112:LEU:HG	1.99	0.45
5:B:1112:LEU:HD11	5:B:1140:VAL:HG13	1.99	0.44
5:A:830:SER:N	5:A:855:GLU:OE1	2.49	0.44
5:A:1154:TYR:O	5:A:1158:LYS:HG3	2.18	0.44
5:A:1162:ALA:O	5:A:1165:GLU:HB2	2.18	0.44
5:B:1147:HIS:C	5:B:1149:ALA:H	2.24	0.44
5:A:1085:CYS:O	5:A:1089:ALA:HB2	2.18	0.44
5:B:1141:MET:HE3	5:B:1167:TYR:CB	2.47	0.44
5:A:1101:VAL:HG23	5:A:1111:ALA:CB	2.47	0.43
3:E:8[B]:A:H2'	5:A:936:ARG:NH2	2.33	0.43
5:B:1112:LEU:O	5:B:1116:MET:HG2	2.19	0.43
5:A:896:VAL:HG13	5:A:897:PHE:CD1	2.53	0.43
5:A:996:GLN:HA	6:A:69:HOH:O	2.17	0.43
5:A:1074:GLN:NE2	6:A:118:HOH:O	2.46	0.43
5:A:1027:GLU:O	5:A:1031:GLN:HG3	2.19	0.43
5:B:1147:HIS:C	5:B:1149:ALA:N	2.77	0.43
5:B:869:LYS:O	5:B:873:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:984:GLN:NE2	5:B:984:GLN:HA	2.33	0.43
5:B:1156:TYR:C	5:B:1158:LYS:H	2.27	0.43
5:B:864:ARG:HD2	5:B:864:ARG:HA	1.88	0.43
2:D:19[A]:U:H2'	5:B:900:TYR:OH	2.19	0.43
5:A:866:ILE:O	5:A:870:LEU:HD23	2.19	0.43
5:B:1013:ILE:HG21	5:B:1025:ILE:CD1	2.49	0.43
5:B:1075:HIS:HB3	5:B:1078:ALA:HB3	2.01	0.42
5:A:838:ASN:O	5:A:839:ASN:HB2	2.19	0.42
5:A:1153:LYS:NZ	5:A:1153:LYS:HB2	2.34	0.42
5:B:860:GLN:HA	5:B:897:PHE:CD2	2.55	0.42
5:A:870:LEU:CD1	5:A:878:ARG:HG2	2.45	0.42
5:A:1008:ARG:NH1	6:A:110:HOH:O	2.52	0.42
5:B:1085:CYS:O	5:B:1089:ALA:HB2	2.20	0.42
3:E:7[B]:C:H5'	6:A:119:HOH:O	2.20	0.42
5:B:835:ASP:HB2	5:B:841:TYR:HE2	1.85	0.42
5:B:915:LEU:HD12	5:B:915:LEU:HA	1.93	0.42
5:B:1108:PRO:C	5:B:1109:HIS:ND1	2.78	0.42
5:A:919:GLU:OE2	5:A:922:ARG:NH2	2.53	0.42
5:B:1004:PRO:HB3	5:B:1041:TYR:CZ	2.55	0.41
5:B:1145:ARG:N	5:B:1146:PRO:CD	2.83	0.41
5:A:854:MET:O	5:A:858:GLN:HG3	2.21	0.41
5:B:1005:TYR:O	5:B:1008:ARG:HB2	2.19	0.41
5:B:1018:LEU:O	5:B:1021:GLN:HB2	2.20	0.41
5:B:876:ALA:O	5:B:880:LEU:HG	2.20	0.41
3:E:8[B]:A:O2'	3:E:9[B]:G:H5'	2.21	0.41
5:A:935:CYS:O	5:A:939:GLN:HG3	2.20	0.41
5:B:1145:ARG:HG3	5:B:1146:PRO:HD3	2.02	0.41
5:A:846:LEU:HD23	5:A:846:LEU:HA	1.93	0.41
2:D:19[A]:U:H2'	5:B:900:TYR:HH	1.85	0.41
5:B:1119:GLN:HB3	5:B:1156:TYR:CZ	2.55	0.41
5:B:863:SER:O	5:B:867:GLN:HG3	2.21	0.41
5:B:885:ILE:HB	5:B:892:LEU:HD12	2.02	0.41
5:A:878:ARG:HD2	6:A:199:HOH:O	2.19	0.40
5:A:1017:CYS:SG	5:A:1021:GLN:CB	3.09	0.40
5:B:847:ARG:HH12	5:B:877:GLU:HG2	1.87	0.40
5:A:1023:LEU:HB3	5:A:1024:PRO:CD	2.40	0.40
5:A:1091:ARG:NH1	5:A:1133:GLU:OE2	2.54	0.40
5:B:1013:ILE:O	5:B:1017:CYS:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	338/349 (97%)	330 (98%)	8 (2%)	0	100	100
5	B	339/349 (97%)	325 (96%)	13 (4%)	1 (0%)	36	42
All	All	677/698 (97%)	655 (97%)	21 (3%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	1149	ALA

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	
5	A	303/310 (98%)	295 (97%)	8 (3%)	40	55
5	B	304/310 (98%)	296 (97%)	8 (3%)	40	55
All	All	607/620 (98%)	591 (97%)	16 (3%)	40	55

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	880	LEU
5	A	911	LEU
5	A	948	ASP
5	A	957	LEU
5	A	1008	ARG

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Mol	Chain	Res	Type
5	A	1134	PRO
5	A	1153	LYS
5	A	1166	LYS
5	B	845	GLN
5	B	853	ILE
5	B	885	ILE
5	B	915	LEU
5	B	957	LEU
5	B	987	GLN
5	B	1008	ARG
5	B	1015	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	858	GLN
5	A	860	GLN
5	A	883	ASN
5	A	891	GLN
5	A	903	GLN
5	A	949	GLN
5	A	951	ASN
5	A	960	HIS
5	A	972	HIS
5	A	1035	GLN
5	A	1074	GLN
5	A	1080	ASN
5	A	1119	GLN
5	A	1159	HIS
5	B	843	ASN
5	B	860	GLN
5	B	861	HIS
5	B	883	ASN
5	B	891	GLN
5	B	903	GLN
5	B	949	GLN
5	B	950	GLN
5	B	951	ASN
5	B	968	GLN
5	B	972	HIS
5	B	975	GLN
5	B	984	GLN

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Mol	Chain	Res	Type
5	B	996	GLN
5	B	1031	GLN
5	B	1032	HIS
5	B	1035	GLN
5	B	1048	HIS
5	B	1119	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	7/8 (87%)	2 (28%)	0
2	D	6/7 (85%)	1 (16%)	0
3	E	7/8 (87%)	2 (28%)	0
4	F	6/7 (85%)	1 (16%)	0
All	All	26/30 (86%)	6 (23%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	13[A]	U
1	C	17[A]	U
2	D	17[A]	U
3	E	3[B]	U
3	E	7[B]	C
4	F	7[B]	C

There are no RNA pucker outliers to report.

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 oligosaccharides 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, 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	8/8 (100%)	0.30	0 100 100	23, 34, 50, 60	8 (100%)
2	D	7/7 (100%)	0.79	1 (14%) 6 4	37, 46, 56, 65	7 (100%)
3	E	8/8 (100%)	0.89	2 (25%) 2 1	10, 15, 19, 22	8 (100%)
4	F	7/7 (100%)	1.68	1 (14%) 6 4	17, 19, 22, 23	7 (100%)
5	A	340/349 (97%)	0.06	12 (3%) 47 44	21, 34, 68, 80	0
5	B	341/349 (97%)	0.65	25 (7%) 21 18	27, 48, 97, 105	0
All	All	711/728 (97%)	0.38	41 (5%) 29 25	10, 41, 72, 105	30 (4%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	9[B]	G	5.8
5	A	1017	CYS	4.3
5	B	1156	TYR	4.2
5	A	1108	PRO	3.9
5	B	1161	LEU	3.9
5	B	1164	LEU	3.6
5	B	1154	TYR	3.6
5	B	1157	GLY	3.4
5	A	1107	GLY	3.3
5	B	1162	ALA	3.3
5	B	1168	TYR	3.1
5	B	843	ASN	3.1
5	B	1151	LEU	3.1
3	E	9[B]	G	3.0
5	B	1160	ILE	3.0
5	B	1166	LYS	3.0
5	B	1147	HIS	2.9
5	B	1148	ILE	2.9
5	A	870	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
5	B	1152	ARG	2.8
5	B	1153	LYS	2.6
2	D	19[A]	U	2.6
5	A	868	LEU	2.5
5	B	1163	LYS	2.5
5	B	1155	THR	2.4
5	B	1167	TYR	2.3
5	A	841	TYR	2.3
5	B	1101	VAL	2.3
5	A	828	GLY	2.3
5	B	1149	ALA	2.3
5	B	1144	ILE	2.2
5	A	1104	MET	2.2
5	B	1110	SER	2.2
5	B	1025	ILE	2.1
5	B	1017	CYS	2.1
5	A	1110	SER	2.1
3	E	7[B]	C	2.1
5	B	1018	LEU	2.1
5	A	1167	TYR	2.0
5	A	1101	VAL	2.0
5	A	1164	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.