Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:47 AM GMT

PDB ID : 3Q0L
Title : Crystal structure of the PUMILIO-homology domain from Human PUMILIO1 in complex with p38alpha NREa
Authors : Lu, G.; Hall, T.M.T.
Deposited on : 2010-12-15
Resolution : 2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	trunk26865

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 2.50 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.

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
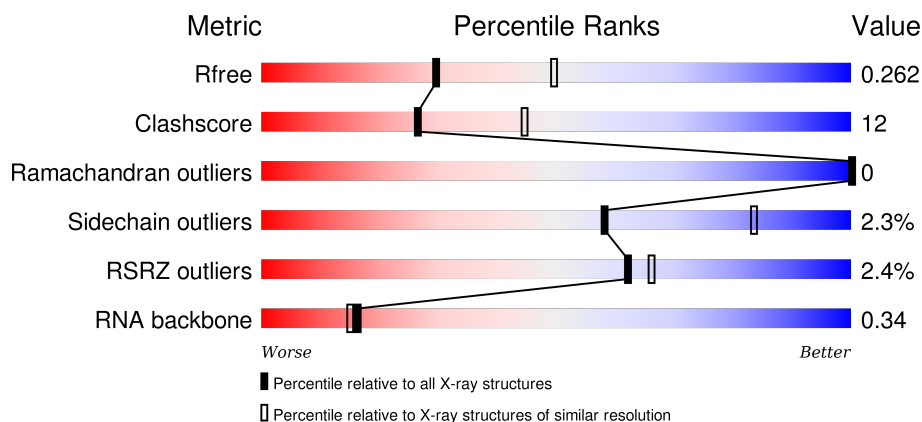
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	349	74% 23%
1	B	349	67% 29%
2	C	8	63% 13% 25%
2	D	8	50% 25% 13% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6019 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	341	Total 2768	C 1756	N 495	O 499	S 18	0	1	0
1	B	340	Total 2727	C 1729	N 486	O 495	S 17	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total 168	C 77	N 31	O 53	P 7	0	0	0
2	D	8	Total 168	C 77	N 31	O 53	P 7	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total 109	O 109	0	0
3	B	69	Total 69	O 69	0	0
3	C	9	Total 9	O 9	0	0
3	D	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Pumilio homolog 1
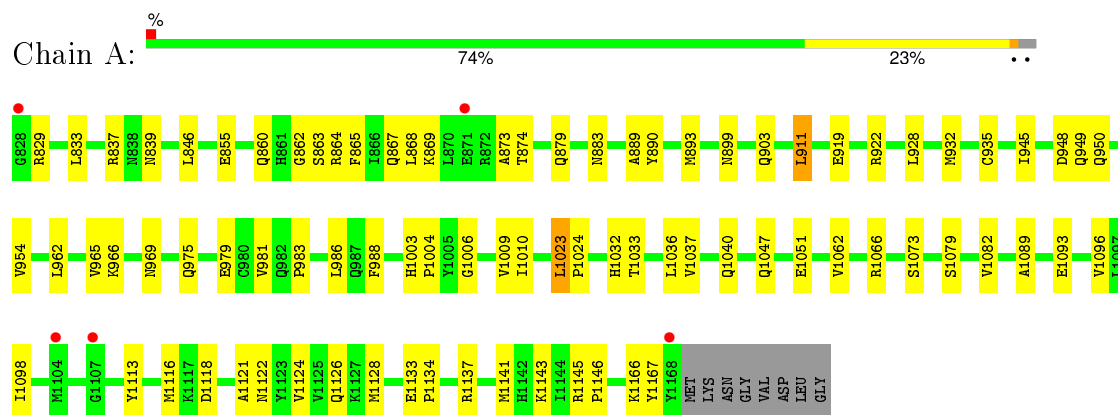
- Molecule 1: Pumilio homolog 1
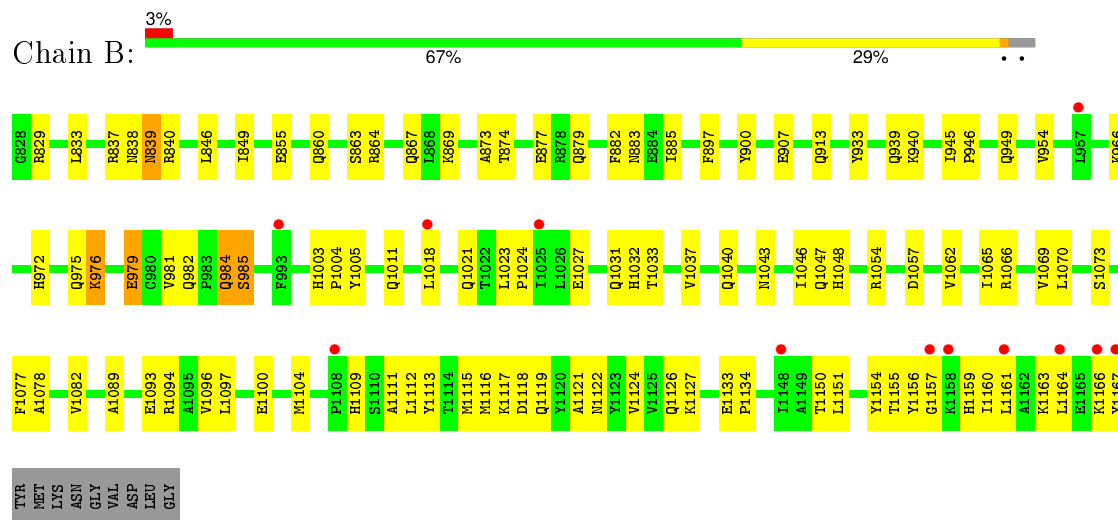
- Molecule 2: 5'-R(UP*GP*UP*AP*AP*AP*UP*A)-3'

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

Chain D:

50%   25%   13%   13%

4   Data and refinement statistics (i)

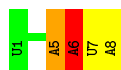| Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	262.30Å 37.37Å 82.54Å 90.00° 102.63° 90.00°	Depositor
Resolution (Å)	28.20 – 2.50 42.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (28.20-2.50) 99.3 (42.66-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.36 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_6)	Depositor
R, R_{free}	0.192 , 0.259 0.200 , 0.262	Depositor DCC
R_{free} test set	1413 reflections (5.42%)	DCC
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 27467 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6019	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

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	0/2825	0.54	0/3811
1	B	0.38	0/2780	0.52	0/3756
2	C	0.61	0/188	1.21	0/291
2	D	0.55	0/188	1.27	2/291 (0.7%)
All	All	0.42	0/5981	0.61	2/8149 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	5	A	P-O3'-C3'	8.44	129.83	119.70
2	D	6	A	C3'-C2'-C1'	5.83	106.16	101.50

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	2768	0	2777	60	0
1	B	2727	0	2711	75	0
2	C	168	0	87	7	0
2	D	168	0	87	4	0
3	A	109	0	0	2	0
3	B	69	0	0	1	0
3	C	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
All	All	6019	0	5662	140	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 12.

All (140) 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:C:5:A:H1'	3:C:16:HOH:O	1.68	0.92
1:A:890:TYR:HA	1:A:893:MET:HE2	1.53	0.90
1:A:879:GLN:HE21	1:A:883:ASN:HD21	1.26	0.80
1:A:975:GLN:HE22	2:C:5:A:H2	1.28	0.79
1:B:1018:LEU:HB2	1:B:1021:GLN:HG3	1.69	0.74
1:B:1023:LEU:HB3	1:B:1024:PRO:HD3	1.67	0.74
1:B:879:GLN:HE21	1:B:883:ASN:HD21	1.35	0.74
1:A:1079:SER:HA	1:A:1082:VAL:HG13	1.70	0.72
1:A:1118:ASP:HB3	1:A:1121:ALA:HB3	1.70	0.72
1:B:984:GLN:H	1:B:984:GLN:NE2	1.86	0.71
1:B:984:GLN:CD	1:B:984:GLN:H	1.92	0.71
1:A:919:GLU:HG2	1:A:922:ARG:HH12	1.57	0.69
1:B:1118:ASP:HB3	1:B:1121:ALA:HB3	1.78	0.66
1:B:833:LEU:HD22	1:B:855:GLU:HG2	1.76	0.65
1:B:1133:GLU:HG2	1:B:1134:PRO:HD2	1.79	0.64
1:B:1066:ARG:CZ	1:B:1096:VAL:HG11	2.26	0.64
1:B:1043:ASN:O	1:B:1047:GLN:HG3	1.96	0.64
1:B:945:ILE:HD12	1:B:949:GLN:HB3	1.79	0.64
1:A:1079:SER:HA	1:A:1082:VAL:CG1	2.27	0.63
1:B:954:VAL:HG21	1:B:981:VAL:HG21	1.79	0.63
1:A:1122:ASN:O	1:A:1126:GLN:HG3	1.98	0.63
1:B:1070:LEU:HD13	1:B:1111:ALA:HB1	1.81	0.62
1:B:933:TYR:HE2	2:D:7:U:HO2'	1.48	0.62
1:B:1062:VAL:O	1:B:1066:ARG:HG3	2.01	0.61
1:A:846:LEU:HG	1:A:869:LYS:HB3	1.83	0.61
2:C:5:A:H8	2:C:5:A:H5"	1.66	0.60
1:A:879:GLN:HE21	1:A:883:ASN:ND2	1.98	0.60
1:A:869:LYS:O	1:A:873:ALA:HB2	2.01	0.60
1:B:946:PRO:HB2	1:B:949:GLN:NE2	2.16	0.60
1:B:981:VAL:HG12	1:B:982:GLN:N	2.17	0.59
2:C:5:A:C8	2:C:5:A:H3'	2.38	0.58
1:B:869:LYS:O	1:B:873:ALA:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:946:PRO:HB2	1:B:949:GLN:HE21	1.69	0.57
1:A:1003:HIS:CG	1:A:1004:PRO:HD2	2.39	0.57
1:A:919:GLU:HG2	1:A:922:ARG:NH1	2.19	0.57
1:A:1066:ARG:CZ	1:A:1096:VAL:HG11	2.35	0.56
1:A:833:LEU:O	1:A:837:ARG:HG3	2.04	0.56
1:B:867:GLN:OE1	1:B:900:TYR:HB3	2.06	0.56
1:B:1150:THR:HG22	1:B:1154:TYR:HE2	1.71	0.55
1:A:889:ALA:O	1:A:893:MET:HG3	2.06	0.55
1:B:860:GLN:HB2	1:B:897:PHE:CE2	2.41	0.55
1:B:1089:ALA:HB1	1:B:1093:GLU:HB2	1.88	0.55
1:B:829:ARG:CZ	1:B:837:ARG:NH1	2.70	0.55
1:A:893:MET:HE1	1:A:928:LEU:HD11	1.88	0.55
1:A:863:SER:O	1:A:867:GLN:HG3	2.07	0.54
1:A:945:ILE:HD12	1:A:949:GLN:HB3	1.89	0.54
1:B:1073:SER:HB2	1:B:1124:VAL:HG21	1.89	0.53
1:B:1150:THR:HG22	1:B:1154:TYR:CE2	2.43	0.53
1:A:1113:TYR:HD1	1:A:1116:MET:HE3	1.74	0.53
1:A:1098:ILE:HG12	1:A:1128:MET:HG2	1.90	0.53
1:A:1133:GLU:HB2	3:A:61:HOH:O	2.09	0.53
1:B:1160:ILE:O	1:B:1164:LEU:HG	2.09	0.53
1:B:1156:TYR:HA	1:B:1159:HIS:CD2	2.45	0.52
1:B:879:GLN:NE2	1:B:883:ASN:HD21	2.06	0.52
1:A:1073:SER:HB2	1:A:1124:VAL:HG21	1.91	0.52
1:A:1033:THR:O	1:A:1037:VAL:HG13	2.09	0.52
2:C:5:A:C8	2:C:5:A:C3'	2.93	0.52
1:A:1003:HIS:ND1	1:A:1004:PRO:HD2	2.26	0.51
1:A:1133:GLU:HG2	1:A:1134:PRO:HD2	1.93	0.51
1:A:911:LEU:HD12	1:A:911:LEU:O	2.11	0.50
1:B:981:VAL:CG1	1:B:982:GLN:N	2.74	0.50
1:B:885:ILE:C	1:B:885:ILE:HD12	2.31	0.50
1:B:1011:GLN:HG2	1:B:1048:HIS:CD2	2.46	0.50
1:B:1156:TYR:HA	1:B:1159:HIS:HD2	1.76	0.50
1:B:863:SER:C	1:B:867:GLN:HE21	2.15	0.50
1:A:954:VAL:HG13	1:A:988:PHE:CE2	2.46	0.50
1:A:1113:TYR:HA	1:A:1116:MET:HE3	1.93	0.50
1:B:1160:ILE:O	1:B:1163:LYS:HB3	2.12	0.50
2:C:6:A:H5'	2:C:7:U:OP2	2.11	0.50
1:A:1003:HIS:CE1	1:A:1004:PRO:HD2	2.47	0.49
1:B:1078:ALA:O	1:B:1082:VAL:HG23	2.12	0.49
1:A:833:LEU:HD22	1:A:855:GLU:HG2	1.93	0.49
1:B:1166:LYS:O	1:B:1167:TYR:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:SER:CA	1:A:1082:VAL:HG13	2.40	0.49
1:B:1027:GLU:HA	1:B:1027:GLU:OE1	2.12	0.49
1:B:1066:ARG:HG2	1:B:1097:LEU:HD21	1.93	0.49
1:B:933:TYR:CE2	2:D:7:U:H1'	2.48	0.49
1:B:907:GLU:HG3	1:B:940:LYS:HD2	1.94	0.49
1:B:975:GLN:O	1:B:979:GLU:HG2	2.12	0.49
1:A:1113:TYR:HA	1:A:1116:MET:CE	2.43	0.48
1:B:939:GLN:HG2	1:B:976:LYS:HG3	1.94	0.48
1:A:1145:ARG:HB3	1:A:1146:PRO:HD3	1.95	0.48
1:A:1032:HIS:O	1:A:1036:LEU:HG	2.13	0.48
1:B:1069:VAL:O	1:B:1073:SER:HB3	2.14	0.48
1:A:1047:GLN:O	1:A:1051:GLU:HG3	2.14	0.48
1:A:975:GLN:O	1:A:979:GLU:HG3	2.14	0.47
1:A:950:GLN:HB3	1:A:981:VAL:HG22	1.96	0.47
1:B:1155:THR:O	1:B:1159:HIS:CD2	2.68	0.47
1:A:962:LEU:HB3	1:A:966:LYS:NZ	2.30	0.47
1:A:935:CYS:SG	1:A:969:ASN:HB3	2.55	0.47
1:B:860:GLN:HB2	1:B:897:PHE:CZ	2.49	0.47
1:B:1040:GLN:HB3	1:B:1077:PHE:CZ	2.49	0.47
1:A:1062:VAL:O	1:A:1066:ARG:HG3	2.16	0.46
1:B:838:ASN:O	1:B:839:ASN:C	2.53	0.46
1:A:948:ASP:HA	3:A:23:HOH:O	2.16	0.46
1:B:1033:THR:O	1:B:1037:VAL:HG13	2.16	0.46
1:B:1155:THR:O	1:B:1159:HIS:HD2	1.98	0.45
1:B:1113:TYR:HA	1:B:1116:MET:CE	2.46	0.45
1:A:983:PRO:HA	1:A:986:LEU:HD12	1.98	0.45
1:A:1166:LYS:HB3	1:A:1167:TYR:CD2	2.52	0.45
1:A:862:GLY:O	1:A:865:PHE:HB3	2.17	0.45
1:B:1119:GLN:HB3	1:B:1156:TYR:CZ	2.51	0.45
1:B:1054:ARG:O	1:B:1057:ASP:HB2	2.17	0.45
1:B:1157:GLY:O	1:B:1161:LEU:HG	2.15	0.45
1:B:982:GLN:O	1:B:985:SER:HB2	2.17	0.45
1:B:1003:HIS:ND1	1:B:1004:PRO:HD2	2.31	0.45
1:B:860:GLN:HE21	1:B:864:ARG:NH1	2.15	0.45
1:B:1151:LEU:HD13	1:B:1161:LEU:HD21	1.97	0.45
1:B:1100:GLU:O	1:B:1104:MET:HB3	2.17	0.45
1:B:1111:ALA:O	1:B:1115:MET:HG3	2.17	0.44
1:B:846:LEU:O	1:B:849:ILE:HG12	2.17	0.44
1:B:882:PHE:CD2	1:B:913:GLN:HG2	2.53	0.44
1:B:1163:LYS:HG3	1:B:1164:LEU:HD23	1.99	0.44
1:B:1117:LYS:HE3	1:B:1117:LYS:HB2	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:GLY:O	1:A:1010:ILE:HG12	2.18	0.43
1:A:1023:LEU:HB3	1:A:1024:PRO:HD3	2.01	0.43
1:B:933:TYR:HE2	2:D:7:U:O2'	1.99	0.43
1:B:966:LYS:O	1:B:1005:TYR:HD1	2.02	0.43
1:A:860:GLN:O	1:A:864:ARG:HG3	2.18	0.43
1:A:975:GLN:NE2	2:C:5:A:H2	2.07	0.43
1:A:846:LEU:HG	1:A:869:LYS:CB	2.47	0.43
1:B:972:HIS:CD2	2:D:6:A:C8	3.07	0.43
1:B:1112:LEU:O	1:B:1116:MET:HE2	2.19	0.43
1:A:899:ASN:O	1:A:903:GLN:HG3	2.20	0.42
1:A:893:MET:CE	1:A:928:LEU:HD11	2.49	0.42
1:B:1037:VAL:HG12	1:B:1046:ILE:HG21	2.00	0.42
1:B:874:THR:OG1	1:B:877:GLU:HG3	2.20	0.41
1:B:1094:ARG:NH1	1:B:1094:ARG:HB2	2.35	0.41
1:A:1003:HIS:CG	1:A:1004:PRO:CD	3.03	0.41
1:A:1089:ALA:HB1	1:A:1093:GLU:HB2	2.02	0.41
1:A:837:ARG:C	1:A:839:ASN:H	2.24	0.41
1:B:1151:LEU:CD1	1:B:1161:LEU:HD21	2.50	0.41
1:B:1127:LYS:HE2	3:B:51:HOH:O	2.19	0.41
1:A:1137:ARG:O	1:A:1141:MET:HG2	2.21	0.41
1:A:846:LEU:HD23	1:A:846:LEU:HA	1.77	0.41
1:A:829:ARG:CZ	1:A:837:ARG:NH1	2.84	0.41
1:A:965:VAL:HG22	1:A:1009:VAL:HG21	2.02	0.41
1:B:1122:ASN:O	1:B:1126:GLN:HG3	2.21	0.41
1:B:1031:GLN:O	1:B:1032:HIS:CG	2.75	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	
1	A	340/349 (97%)	327 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	338/349 (97%)	320 (95%)	18 (5%)	0	100	100
All	All	678/698 (97%)	647 (95%)	31 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	303/310 (98%)	297 (98%)	6 (2%)	63	86
1	B	296/310 (96%)	288 (97%)	8 (3%)	52	79
All	All	599/620 (97%)	585 (98%)	14 (2%)	58	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	868	LEU
1	A	874	THR
1	A	911	LEU
1	A	1023	LEU
1	A	1040	GLN
1	A	1143	LYS
1	B	839	ASN
1	B	840	ARG
1	B	976	LYS
1	B	979	GLU
1	B	984	GLN
1	B	985	SER
1	B	1065	ILE
1	B	1109	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

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Mol	Chain	Res	Type
1	A	883	ASN
1	A	891	GLN
1	A	951	ASN
1	A	1032	HIS
1	A	1119	GLN
1	A	1159	HIS
1	B	839	ASN
1	B	852	HIS
1	B	860	GLN
1	B	867	GLN
1	B	883	ASN
1	B	891	GLN
1	B	949	GLN
1	B	951	ASN
1	B	960	HIS
1	B	984	GLN
1	B	1088	HIS
1	B	1109	HIS
1	B	1119	GLN
1	B	1159	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	7/8 (87%)	2 (28%)	0
2	D	7/8 (87%)	3 (42%)	2 (28%)
All	All	14/16 (87%)	5 (35%)	2 (14%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	6	A
2	C	7	U
2	D	5	A
2	D	6	A
2	D	8	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	5	A
2	D	6	A

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	341/349 (97%)	-0.08	5 (1%)	76	79	21, 32, 55, 84	0
1	B	340/349 (97%)	0.17	12 (3%)	48	53	25, 42, 69, 85	0
2	C	8/8 (100%)	-0.18	0	100	100	30, 36, 51, 52	0
2	D	8/8 (100%)	-0.42	0	100	100	40, 47, 55, 56	0
All	All	697/714 (97%)	0.04	17 (2%)	62	66	21, 37, 62, 85	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1168	TYR	4.2
1	A	828	GLY	3.7
1	B	1164	LEU	3.3
1	A	1107	GLY	3.0
1	B	1167	TYR	2.8
1	B	1157	GLY	2.5
1	B	1018	LEU	2.5
1	B	1148	ILE	2.4
1	A	1104	MET	2.4
1	B	1161	LEU	2.3
1	B	1158	LYS	2.2
1	B	993	PHE	2.2
1	A	871	GLU	2.1
1	B	1025	ILE	2.0
1	B	957	LEU	2.0
1	B	1166	LYS	2.0
1	B	1108	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.