Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:13 am BST

PDB ID	:	1M8Y
Title	:	CRYSTAL STRUCTURE OF THE PUMILIO-HOMOLOGY DOMAIN FROM HUMAN PUMILIO1 IN COMPLEX WITH NRE2-10 RNA
Authors	:	Wang, X.; McLachlan, J.; Zamore, P.D.; Hall, T.M.T.
Deposited on	:	2002-07-26
Resolution	:	2.60 Å(reported)

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

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

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

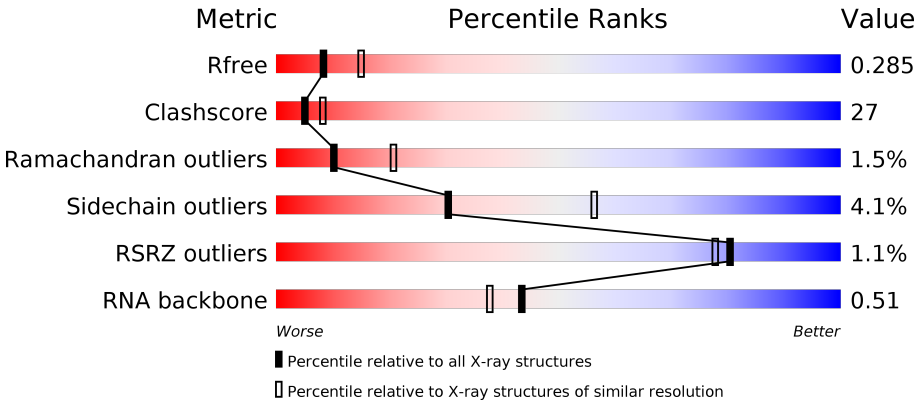
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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

Mol	Chain	Length	Quality of chain
1	C	10	30% 50% 20%
1	D	10	20% 60% 20%
2	A	349	% 62% 34%
2	B	349	2% 46% 46% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6303 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*AP*UP*UP*GP*UP*AP*CP*AP*UP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	10	Total	C	N	O	P	0	0	0
			211	95	36	70	10			
1	D	10	Total	C	N	O	P	0	0	0
			211	95	36	70	10			

- Molecule 2 is a protein called Pumilio 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	341	Total	C	N	O	S	0	0	0
			2768	1752	501	498	17			
2	B	342	Total	C	N	O	S	0	0	0
			2773	1755	502	499	17			

- Molecule 3 is water.

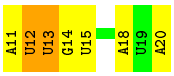
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	30	Total	O	0	0
			30	30		
3	D	16	Total	O	0	0
			16	16		
3	A	190	Total	O	0	0
			190	190		
3	B	104	Total	O	0	0
			104	104		

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.

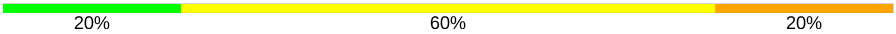
- Molecule 1: 5'-R(P*AP*UP*UP*GP*UP*AP*CP*AP*UP*A)-3'

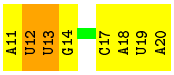
Chain C:



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

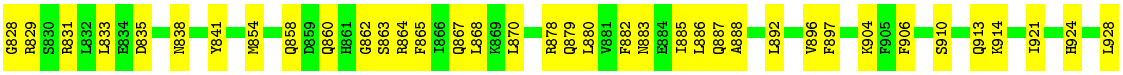
Chain D:

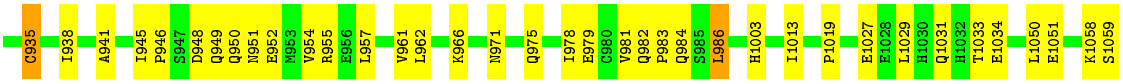


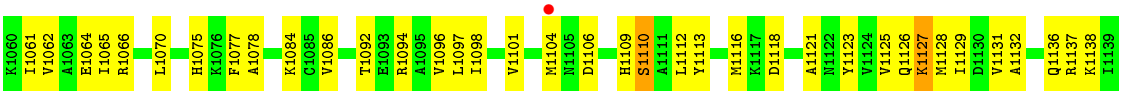


- Molecule 2: Pumilio 1

Chain A:

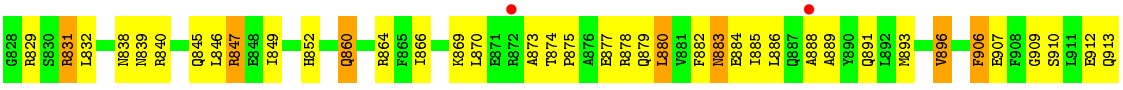


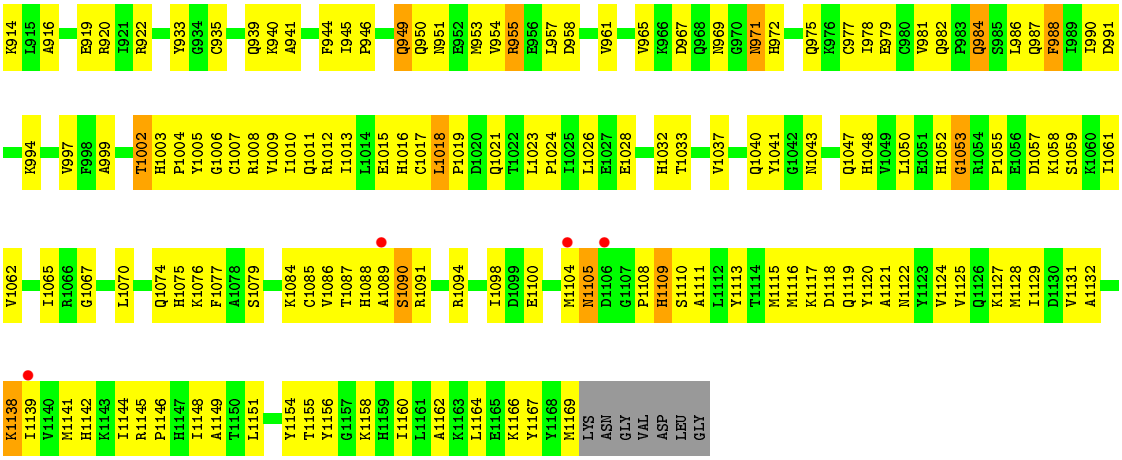




- Molecule 2: Pumilio 1

Chain B:




K914 L915 A916 E919 R920 I921 R922 Y933 G934 C935 Q939 K940 A941 F944 I945 P946 Q949 Q950 N951 E952 M953 V954 R955 E956 L957 D958 V961 V965 K966 D967 Q968 N969 G970 N971 H972 Q975 K976 C977 I978 E979 C980 V981 Q982 P983 Q984 S985 L986 Q987 F988 I989 I990 D991
K994 V997 F998 A999 T1002 H1003 P1004 Y1005 G1006 C1007 R1008 V1009 I1010 Q1011 R1012 I1013 L1014 E1015 H1016 C1017 L1018 P1019 D1020 Q1021 T1022 L1023 P1024 I1025 L1026 E1027 E1028 H1032 T1033 V1037 Q1040 Y1041 G1042 N1043 Q1047 H1048 V1049 L1050 E1051 H1052 G1053 R1054 P1055 E1056 D1057 K1058 S1059 K1060 I1061
V1062 I1065 R1066 G1067 L1070 Q1074 H1075 K1076 F1077 A1078 S1079 K1084 C1085 V1086 T1087 H1088 A1089 S1090 R1091 R1094 I1098 D1099 E1100 M1104 N1105 D1106 G1107 P1108 H1109 S1110 A1111 L1112 Y1113 T1114 M1115 M1116 K1117 D1118 Q1119 Y1120 A1121 N1122 Y1123 V1124 V1125 Q1126 K1127 M1128 I1129 D1130 V1131 A1132
K1138 I1139 Y1140 M1141 H1142 K1143 I1144 R1145 P1146 H1147 I1148 A1149 T1150 L1151 Y1154 T1155 Y1156 G1157 K1158 H1159 I1160 L1161 A1162 K1163 L1164 E1165 K1166 Y1167 Y1168 M1169 LYS ASN GLY VAL ASP LEU GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	35.84Å 59.73Å 340.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.74 – 2.60 37.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	83.4 (37.74-2.60) 83.4 (37.74-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.286 0.214 , 0.285	Depositor DCC
R_{free} test set	1193 reflections (5.84%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6303	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	C	0.55	0/235	0.79	0/363
1	D	0.48	0/235	0.73	0/363
2	A	0.39	0/2821	0.60	0/3804
2	B	0.37	0/2826	0.60	0/3811
All	All	0.39	0/6117	0.61	0/8341

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	19	U	Sidechain

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	211	0	107	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	211	0	107	7	0
2	A	2768	0	2783	117	0
2	B	2773	0	2785	192	0
3	A	190	0	0	4	0
3	B	104	0	0	6	0
3	C	30	0	0	0	0
3	D	16	0	0	0	0
All	All	6303	0	5782	317	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 27.

All (317) 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:831:ARG:HD3	2:B:831:ARG:H	1.21	1.04
2:A:1141:MET:HE1	2:A:1164:LEU:HA	1.40	1.00
2:B:975:GLN:HG3	2:B:1012:ARG:HG3	1.45	0.96
1:D:11:A:H5'	1:D:14:G:OP2	1.67	0.95
1:C:11:A:H5'	1:C:12:U:H3'	1.50	0.92
2:B:951:ASN:HB3	2:B:955:ARG:HH22	1.37	0.87
2:B:1089:ALA:HB3	2:B:1094:ARG:HB2	1.58	0.85
2:B:831:ARG:N	2:B:831:ARG:HD3	1.96	0.80
2:B:1138:LYS:NZ	2:B:1138:LYS:HB3	1.98	0.78
2:A:1113:TYR:HA	2:A:1116:MET:HE2	1.65	0.78
2:B:919:GLU:HG2	2:B:922:ARG:NH2	1.99	0.77
2:A:864:ARG:O	2:A:868:LEU:HG	1.84	0.77
2:B:1144:ILE:HG23	2:B:1164:LEU:HD11	1.69	0.73
2:A:829:ARG:HD3	2:A:833:LEU:HD23	1.69	0.73
2:A:885:ILE:HD12	2:A:886:LEU:N	2.04	0.73
2:B:990:ILE:HG22	2:B:994:LYS:HE3	1.71	0.73
1:C:11:A:H5"	1:C:12:U:C6	2.24	0.73
2:A:966:LYS:HE3	3:A:92:HOH:O	1.89	0.72
2:B:1094:ARG:HD3	2:B:1131:VAL:HG23	1.70	0.72
2:B:1166:LYS:HA	2:B:1169:MET:O	1.89	0.71
2:B:866:ILE:O	2:B:870:LEU:HB2	1.91	0.71
2:B:1018:LEU:H	2:B:1021:GLN:NE2	1.89	0.71
2:B:946:PRO:HB2	2:B:949:GLN:NE2	2.06	0.70
2:A:952:GLU:HA	2:A:955:ARG:HH11	1.56	0.70
2:B:949:GLN:H	2:B:949:GLN:NE2	1.89	0.70
2:B:1084:LYS:HA	2:B:1087:THR:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:910:SER:OG	2:B:913:GLN:HG3	1.93	0.69
2:B:874:THR:O	2:B:878:ARG:HG3	1.93	0.69
2:A:1050:LEU:HD13	2:A:1084:LYS:HB3	1.73	0.69
2:A:882:PHE:CD2	2:A:885:ILE:HD11	2.29	0.68
2:B:1125:VAL:O	2:B:1129:ILE:HG13	1.93	0.68
2:B:1033:THR:O	2:B:1037:VAL:HG13	1.94	0.68
2:B:883:ASN:HD22	2:B:883:ASN:C	1.97	0.67
1:C:20:A:H1'	2:A:897:PHE:HE2	1.60	0.67
2:A:1109:HIS:HD2	2:A:1110:SER:H	1.42	0.67
1:D:20:A:H1'	2:B:860:GLN:HE21	1.60	0.67
2:A:1118:ASP:HB3	2:A:1121:ALA:HB3	1.75	0.67
1:C:12:U:O2'	1:C:13:U:OP1	2.12	0.67
2:B:831:ARG:H	2:B:831:ARG:CD	2.03	0.66
2:B:949:GLN:HE21	2:B:949:GLN:H	1.41	0.66
2:B:874:THR:OG1	2:B:877:GLU:HG3	1.95	0.66
2:B:1116:MET:HB2	2:B:1151:LEU:HD21	1.76	0.66
2:B:847:ARG:H	2:B:847:ARG:HD3	1.60	0.66
2:A:1152:ARG:NH1	2:A:1161:LEU:HD21	2.11	0.66
2:B:979:GLU:HB3	2:B:1016:HIS:CD2	2.29	0.66
2:A:1113:TYR:CE1	2:A:1150:THR:HG21	2.30	0.66
2:A:828:GLY:HA2	3:A:230:HOH:O	1.95	0.66
2:B:949:GLN:N	2:B:949:GLN:NE2	2.43	0.66
2:B:883:ASN:HD22	2:B:884:GLU:N	1.94	0.65
2:A:1066:ARG:HH11	2:A:1066:ARG:HG3	1.61	0.65
2:A:978:ILE:HD13	2:A:1013:ILE:HG13	1.79	0.65
2:B:860:GLN:HE22	2:B:864:ARG:NH1	1.94	0.65
2:B:1145:ARG:N	2:B:1146:PRO:HD2	2.12	0.65
2:B:1018:LEU:H	2:B:1021:GLN:HE21	1.45	0.65
2:A:952:GLU:HA	2:A:955:ARG:NH1	2.12	0.64
2:B:950:GLN:HB3	2:B:981:VAL:HG22	1.80	0.64
2:A:910:SER:H	2:A:913:GLN:NE2	1.96	0.63
2:B:919:GLU:HG2	2:B:922:ARG:HH22	1.62	0.63
2:B:896:VAL:HB	2:B:933:TYR:CZ	2.34	0.63
2:A:1086:VAL:HG12	2:A:1131:VAL:HG21	1.80	0.62
2:B:1118:ASP:HB3	2:B:1121:ALA:HB3	1.80	0.62
2:A:921:ILE:HG23	2:A:928:LEU:CD1	2.30	0.61
2:B:978:ILE:HD11	2:B:1009:VAL:HG13	1.81	0.61
2:B:907:GLU:HG2	2:B:944:PHE:CE1	2.35	0.61
2:B:1062:VAL:HG12	2:B:1085:CYS:SG	2.40	0.61
2:B:889:ALA:O	2:B:893:MET:HG3	1.99	0.61
2:A:1033:THR:HG21	2:A:1064:GLU:HG3	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1141:MET:O	2:B:1145:ARG:HG3	2.01	0.61
2:A:1051:GLU:OE1	2:A:1084:LYS:HE2	1.99	0.61
2:B:1018:LEU:O	2:B:1021:GLN:HB2	2.00	0.61
1:D:11:A:H5"	1:D:12:U:O5'	2.00	0.61
1:C:11:A:H5"	1:C:12:U:H6	1.66	0.60
1:C:20:A:H2'	2:A:860:GLN:OE1	2.01	0.60
2:B:888:ALA:HB1	2:B:891:GLN:NE2	2.16	0.60
2:A:1086:VAL:CG1	2:A:1131:VAL:HG21	2.31	0.60
2:B:941:ALA:O	2:B:945:ILE:HG12	2.02	0.60
2:A:1109:HIS:CD2	2:A:1110:SER:H	2.19	0.59
2:A:838:ASN:HB3	2:B:1019:PRO:HG2	1.85	0.59
2:A:1127:LYS:HE3	2:A:1127:LYS:HA	1.85	0.59
2:B:946:PRO:O	2:B:950:GLN:HG3	2.02	0.59
2:A:1136:GLN:O	2:A:1140:VAL:HG23	2.03	0.58
2:B:838:ASN:O	2:B:840:ARG:N	2.35	0.58
2:A:1126:GLN:HG3	2:A:1160:ILE:HD13	1.85	0.58
2:B:1004:PRO:HB3	2:B:1041:TYR:CZ	2.39	0.58
2:B:951:ASN:HA	2:B:954:VAL:HG22	1.84	0.58
2:B:999:ALA:O	2:B:1002:THR:HG22	2.03	0.57
2:A:1125:VAL:O	2:A:1129:ILE:HG13	2.04	0.57
2:B:1094:ARG:HD3	2:B:1131:VAL:CG2	2.35	0.57
2:B:829:ARG:HH11	2:B:829:ARG:HG3	1.69	0.57
2:A:854:MET:O	2:A:858:GLN:HG3	2.05	0.57
2:A:882:PHE:HA	2:A:885:ILE:HG13	1.87	0.57
2:B:967:ASP:O	2:B:971:ASN:HB3	2.04	0.57
2:B:916:ALA:O	2:B:919:GLU:HB3	2.04	0.56
2:A:951:ASN:O	2:A:955:ARG:HG3	2.04	0.56
2:B:1047:GLN:HG2	2:B:1084:LYS:HG3	1.87	0.56
2:B:1040:GLN:HG2	3:B:103:HOH:O	2.05	0.56
2:B:849:ILE:O	2:B:852:HIS:HB2	2.06	0.56
2:B:912:GLU:HG3	3:B:112:HOH:O	2.06	0.56
1:D:17:C:C6	2:B:1008:ARG:NH2	2.74	0.56
2:A:1033:THR:HG21	2:A:1064:GLU:CG	2.35	0.56
2:B:874:THR:HB	2:B:875:PRO:CD	2.36	0.55
2:A:1113:TYR:HE1	2:A:1150:THR:HG21	1.71	0.55
2:B:971:ASN:HD21	2:B:972:HIS:CE1	2.25	0.55
1:C:12:U:O2'	1:C:13:U:P	2.65	0.55
2:B:1124:VAL:O	2:B:1128:MET:HG3	2.07	0.55
2:B:1138:LYS:HZ2	2:B:1138:LYS:HB3	1.70	0.55
2:A:1033:THR:HG23	2:A:1034:GLU:H	1.72	0.55
2:A:882:PHE:HA	2:A:885:ILE:CG1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1091:ARG:HH11	2:B:1091:ARG:HA	1.72	0.55
1:D:12:U:O2'	1:D:13:U:OP1	2.17	0.55
2:A:975:GLN:O	2:A:979:GLU:HG3	2.06	0.55
2:B:1018:LEU:N	2:B:1021:GLN:HE21	2.06	0.55
2:A:966:LYS:HG2	2:A:1003:HIS:NE2	2.21	0.54
2:A:1138:LYS:HE3	3:A:217:HOH:O	2.06	0.54
2:B:1155:THR:HA	2:B:1158:LYS:HG3	1.88	0.54
2:B:885:ILE:C	2:B:885:ILE:HD12	2.27	0.54
2:B:987:GLN:HG3	2:B:991:ASP:OD2	2.07	0.54
2:B:997:VAL:HB	2:B:1028:GLU:HG2	1.89	0.54
2:A:1152:ARG:HH11	2:A:1161:LEU:HD21	1.72	0.54
2:A:950:GLN:HB3	2:A:981:VAL:HG22	1.88	0.54
2:B:1108:PRO:O	2:B:1109:HIS:HB2	2.08	0.54
2:B:1098:ILE:HD13	2:B:1132:ALA:HB2	1.89	0.54
2:A:1109:HIS:CE1	2:A:1147:HIS:NE2	2.76	0.54
2:A:831:ARG:HD2	2:A:831:ARG:C	2.28	0.54
2:A:1033:THR:HG23	2:A:1034:GLU:N	2.22	0.54
2:B:984:GLN:H	2:B:984:GLN:NE2	2.05	0.54
2:B:1052:HIS:O	2:B:1053:GLY:O	2.26	0.53
2:B:1162:ALA:O	2:B:1166:LYS:HG2	2.08	0.53
2:B:1074:GLN:HG2	2:B:1118:ASP:CG	2.28	0.53
2:B:1124:VAL:HG12	2:B:1128:MET:CE	2.38	0.53
2:B:1075:HIS:O	2:B:1079:SER:HB2	2.07	0.53
2:B:831:ARG:HH11	2:B:832:LEU:H	1.55	0.53
2:B:981:VAL:CG1	2:B:982:GLN:N	2.71	0.53
2:A:1050:LEU:O	2:A:1058:LYS:NZ	2.38	0.53
2:A:854:MET:SD	2:A:888:ALA:HB3	2.49	0.53
2:B:1013:ILE:HG23	2:B:1017:CYS:SG	2.49	0.53
2:B:907:GLU:CG	2:B:940:LYS:HD2	2.38	0.53
2:A:906:PHE:O	2:A:914:LYS:HD3	2.09	0.53
2:B:975:GLN:HG3	2:B:1012:ARG:CG	2.30	0.52
2:A:854:MET:CE	2:A:888:ALA:HB3	2.39	0.52
2:B:935:CYS:O	2:B:939:GLN:HG3	2.09	0.52
2:B:951:ASN:C	2:B:953:MET:H	2.12	0.52
2:A:941:ALA:O	2:A:945:ILE:HG12	2.10	0.52
2:B:1139:ILE:O	2:B:1142:HIS:HB3	2.09	0.52
2:B:1122:ASN:HA	2:B:1160:ILE:HD11	1.92	0.52
2:A:910:SER:H	2:A:913:GLN:HE21	1.58	0.52
2:A:966:LYS:HG2	2:A:1003:HIS:CD2	2.45	0.51
2:B:1113:TYR:HA	2:B:1116:MET:CE	2.41	0.51
2:B:874:THR:HB	2:B:875:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:PHE:CE1	2:B:886:LEU:HD22	2.46	0.51
2:B:972:HIS:HE1	3:B:41:HOH:O	1.93	0.51
2:A:879:GLN:HE21	2:A:883:ASN:ND2	2.08	0.51
2:B:1070:LEU:HD13	2:B:1111:ALA:HB1	1.93	0.51
2:A:885:ILE:C	2:A:885:ILE:HD12	2.31	0.51
2:A:1116:MET:HB3	2:A:1151:LEU:HD21	1.93	0.51
2:B:1019:PRO:C	2:B:1021:GLN:H	2.13	0.50
1:C:11:A:H5'	1:C:14:G:OP2	2.11	0.50
2:B:1076:LYS:HD3	2:B:1077:PHE:CE2	2.47	0.50
2:B:1076:LYS:HA	2:B:1120:TYR:CD1	2.47	0.50
2:B:984:GLN:H	2:B:984:GLN:CD	2.13	0.50
2:B:1141:MET:O	2:B:1145:ARG:NH1	2.44	0.50
2:B:950:GLN:HB3	2:B:981:VAL:CG2	2.40	0.50
2:B:961:VAL:O	2:B:965:VAL:HG23	2.11	0.50
2:A:854:MET:HE3	2:A:892:LEU:HD21	1.93	0.50
2:B:1144:ILE:HD11	2:B:1151:LEU:HD11	1.94	0.50
2:B:886:LEU:HA	2:B:889:ALA:HB2	1.94	0.50
2:A:948:ASP:O	2:A:952:GLU:HG3	2.12	0.49
2:B:829:ARG:NH1	2:B:829:ARG:HG3	2.27	0.49
2:B:954:VAL:HG12	2:B:977:CYS:SG	2.52	0.49
1:C:15:U:H1'	2:A:1077:PHE:HE2	1.77	0.49
2:B:1048:HIS:CE1	2:B:1052:HIS:HD2	2.30	0.49
2:B:1084:LYS:HA	2:B:1087:THR:CG2	2.41	0.49
2:A:862:GLY:O	2:A:865:PHE:HB3	2.12	0.49
2:A:838:ASN:CG	2:B:1019:PRO:HG3	2.32	0.49
2:A:951:ASN:HA	2:A:954:VAL:HG12	1.93	0.49
2:B:1005:TYR:O	2:B:1008:ARG:HB2	2.13	0.49
2:B:1148:ILE:HG23	2:B:1149:ALA:N	2.28	0.49
2:A:1113:TYR:HA	2:A:1116:MET:CE	2.38	0.49
2:B:1117:LYS:HD2	2:B:1154:TYR:CZ	2.48	0.49
1:C:11:A:P	1:C:14:G:N7	2.86	0.49
2:B:873:ALA:HA	2:B:877:GLU:OE1	2.13	0.49
2:B:882:PHE:HE1	2:B:886:LEU:HD22	1.77	0.49
2:B:846:LEU:HA	2:B:846:LEU:HD12	1.70	0.48
2:A:1137:ARG:HH11	2:A:1137:ARG:CB	2.25	0.48
2:B:907:GLU:HG2	2:B:944:PHE:CZ	2.47	0.48
2:A:854:MET:CE	2:A:892:LEU:HG	2.43	0.48
2:B:1121:ALA:O	2:B:1125:VAL:HG23	2.13	0.48
2:B:906:PHE:O	2:B:914:LYS:HD3	2.13	0.48
2:B:982:GLN:HB3	2:B:984:GLN:HE21	1.78	0.48
1:C:11:A:C5'	1:C:14:G:OP2	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1122:ASN:CA	2:B:1160:ILE:HD11	2.44	0.48
2:B:1119:GLN:HG3	2:B:1120:TYR:CD2	2.49	0.47
2:B:860:GLN:HE22	2:B:864:ARG:HH12	1.62	0.47
2:B:1028:GLU:O	2:B:1032:HIS:HD2	1.97	0.47
2:B:978:ILE:HD13	2:B:1013:ILE:HG13	1.95	0.47
2:A:1132:ALA:O	2:A:1137:ARG:NH1	2.47	0.47
2:B:1050:LEU:O	2:B:1058:LYS:HE2	2.14	0.47
2:A:838:ASN:HB3	2:B:1019:PRO:CG	2.44	0.47
2:A:1141:MET:CE	2:A:1164:LEU:HA	2.29	0.47
2:A:880:LEU:C	2:A:880:LEU:HD23	2.36	0.47
2:B:1059:SER:HA	2:B:1062:VAL:HG22	1.97	0.47
2:B:1067:GLY:N	2:B:1100:GLU:OE2	2.39	0.47
2:A:1066:ARG:HG3	2:A:1066:ARG:NH1	2.29	0.46
2:A:928:LEU:HD13	2:A:938:ILE:HD11	1.97	0.46
2:A:949:GLN:NE2	2:A:949:GLN:H	2.14	0.46
2:B:1086:VAL:HG11	2:B:1128:MET:HG2	1.97	0.46
2:B:1113:TYR:HA	2:B:1116:MET:HE2	1.98	0.46
2:A:1153:LYS:NZ	2:A:1153:LYS:HB3	2.31	0.46
2:B:972:HIS:CD2	3:B:56:HOH:O	2.68	0.46
2:B:1087:THR:HB	2:B:1127:LYS:HE2	1.97	0.46
2:A:854:MET:HE1	2:A:892:LEU:HG	1.98	0.46
2:A:983:PRO:HG2	2:A:984:GLN:NE2	2.31	0.46
2:A:946:PRO:HD2	2:A:949:GLN:NE2	2.31	0.46
2:B:1003:HIS:CG	2:B:1004:PRO:HD2	2.51	0.46
2:B:1145:ARG:N	2:B:1146:PRO:CD	2.79	0.46
2:A:879:GLN:HE21	2:A:883:ASN:HD21	1.63	0.46
2:B:1023:LEU:HB3	2:B:1024:PRO:CD	2.46	0.46
1:C:20:A:H1'	2:A:897:PHE:CE2	2.45	0.45
2:B:971:ASN:ND2	2:B:972:HIS:CE1	2.84	0.45
2:A:1029:LEU:HA	2:A:1029:LEU:HD23	1.79	0.45
2:A:863:SER:O	2:A:867:GLN:HG3	2.16	0.45
2:B:907:GLU:HG3	2:B:940:LYS:HD2	1.98	0.45
2:A:1141:MET:CE	2:A:1164:LEU:HD12	2.46	0.45
2:A:887:GLN:HA	2:A:887:GLN:NE2	2.32	0.45
2:A:981:VAL:HG12	2:A:982:GLN:N	2.32	0.45
2:B:1026:LEU:HD13	2:B:1057:ASP:OD1	2.17	0.45
2:B:838:ASN:O	2:B:840:ARG:HG3	2.17	0.45
2:A:1075:HIS:HB3	2:A:1078:ALA:HB3	1.99	0.44
2:A:1061:ILE:O	2:A:1065:ILE:HD13	2.17	0.44
2:B:1116:MET:SD	2:B:1151:LEU:HG	2.58	0.44
2:A:1027:GLU:OE1	2:A:1027:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1098:ILE:HD13	2:A:1132:ALA:HB2	2.00	0.44
2:A:1098:ILE:HG12	2:A:1128:MET:HG2	1.99	0.44
2:B:1003:HIS:HB3	2:B:1006:GLY:HA3	1.98	0.44
2:B:1089:ALA:HB3	2:B:1094:ARG:CB	2.39	0.44
2:B:1089:ALA:CB	2:B:1094:ARG:HB2	2.40	0.44
2:B:978:ILE:HG21	2:B:1012:ARG:C	2.38	0.44
2:B:1094:ARG:O	2:B:1094:ARG:HG2	2.18	0.44
2:B:1155:THR:HA	2:B:1158:LYS:HE3	2.00	0.44
2:B:978:ILE:CD1	2:B:1012:ARG:HB2	2.48	0.44
2:A:978:ILE:HD13	2:A:1013:ILE:CG1	2.45	0.43
2:B:1164:LEU:O	2:B:1167:TYR:HB3	2.18	0.43
2:B:832:LEU:HD21	2:B:849:ILE:HG22	2.00	0.43
2:B:981:VAL:HG13	2:B:982:GLN:N	2.34	0.43
2:B:1104:MET:HG2	2:B:1104:MET:O	2.18	0.43
2:B:1086:VAL:HG12	2:B:1131:VAL:HG21	2.00	0.43
2:B:906:PHE:CE1	2:B:941:ALA:HB2	2.52	0.43
2:B:935:CYS:SG	2:B:969:ASN:HB3	2.58	0.43
2:A:1137:ARG:HB2	2:A:1137:ARG:NH1	2.32	0.43
2:A:1141:MET:HE1	2:A:1164:LEU:HD12	1.99	0.43
2:B:1109:HIS:ND1	2:B:1110:SER:HB2	2.32	0.43
2:B:957:LEU:HB3	2:B:988:PHE:HE1	1.83	0.43
2:B:972:HIS:HD2	3:B:56:HOH:O	2.00	0.43
2:A:1126:GLN:HG3	2:A:1160:ILE:CD1	2.49	0.43
1:C:18:A:H2	2:A:935:CYS:SG	2.42	0.43
2:A:1070:LEU:HD21	2:A:1106:ASP:HB2	2.01	0.43
2:A:870:LEU:HD23	2:A:878:ARG:HG2	2.00	0.43
1:C:14:G:C6	2:A:1123:TYR:CD2	3.06	0.43
2:A:860:GLN:HB2	2:A:897:PHE:CZ	2.54	0.43
2:B:879:GLN:O	2:B:880:LEU:C	2.56	0.43
2:B:951:ASN:HB3	2:B:955:ARG:NH2	2.20	0.43
2:B:1043:ASN:OD1	2:B:1047:GLN:NE2	2.52	0.43
2:B:882:PHE:O	2:B:885:ILE:HG13	2.19	0.43
2:A:1098:ILE:O	2:A:1101:VAL:HG22	2.18	0.42
2:A:971:ASN:O	2:A:975:GLN:HG3	2.19	0.42
2:A:1092:THR:O	2:A:1096:VAL:HG23	2.18	0.42
2:B:1021:GLN:O	2:B:1024:PRO:HD2	2.18	0.42
2:B:1111:ALA:O	2:B:1115:MET:HG3	2.19	0.42
2:B:1138:LYS:HZ3	2:B:1138:LYS:HB3	1.79	0.42
2:A:1109:HIS:CD2	2:A:1110:SER:N	2.86	0.42
2:A:1161:LEU:O	2:A:1165:GLU:HB2	2.20	0.42
2:B:1055:PRO:HA	2:B:1058:LYS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1087:THR:HG23	2:B:1088:HIS:CD2	2.54	0.42
2:B:1110:SER:O	2:B:1113:TYR:HB3	2.19	0.42
2:B:978:ILE:HD12	2:B:1012:ARG:HB2	2.01	0.42
1:D:20:A:O2'	2:B:860:GLN:NE2	2.52	0.42
2:B:951:ASN:ND2	2:B:951:ASN:N	2.68	0.42
2:A:924:HIS:O	2:A:928:LEU:HD12	2.19	0.42
2:A:978:ILE:HA	2:A:986:LEU:HD21	2.02	0.42
2:B:1061:ILE:O	2:B:1065:ILE:HG12	2.20	0.42
1:D:18:A:C5	2:B:972:HIS:CD2	3.08	0.42
2:A:924:HIS:HA	3:A:5:HOH:O	2.20	0.42
2:B:1010:ILE:HG22	2:B:1011:GLN:N	2.35	0.42
2:B:1119:GLN:HA	2:B:1156:TYR:CG	2.55	0.42
2:A:981:VAL:CG1	2:A:982:GLN:N	2.83	0.41
2:B:1050:LEU:HD21	2:B:1061:ILE:HB	2.03	0.41
2:A:1027:GLU:O	2:A:1031:GLN:HG3	2.20	0.41
2:B:1050:LEU:HD21	2:B:1061:ILE:HG21	2.01	0.41
2:B:951:ASN:C	2:B:953:MET:N	2.73	0.41
2:B:1145:ARG:HH22	2:B:1167:TYR:HD2	1.69	0.41
2:B:945:ILE:HD12	2:B:949:GLN:HB3	2.02	0.41
2:A:1086:VAL:O	2:A:1094:ARG:HD3	2.20	0.41
2:B:886:LEU:O	2:B:920:ARG:NH1	2.54	0.41
2:A:1062:VAL:HG23	2:A:1097:LEU:HD11	2.03	0.41
2:B:1117:LYS:HD2	2:B:1154:TYR:CE2	2.55	0.41
2:B:971:ASN:O	2:B:975:GLN:HB2	2.20	0.41
2:A:1129:ILE:HG22	2:A:1129:ILE:O	2.20	0.41
2:A:1112:LEU:O	2:A:1116:MET:HG3	2.21	0.41
2:B:951:ASN:HD22	2:B:951:ASN:N	2.17	0.41
2:B:986:LEU:HA	2:B:988:PHE:CE2	2.56	0.41
2:B:958:ASP:HA	2:B:988:PHE:HD1	1.86	0.41
2:B:1007:CYS:O	2:B:1011:GLN:HG3	2.21	0.41
2:B:1141:MET:SD	2:B:1164:LEU:HD23	2.60	0.41
2:B:982:GLN:HG2	3:B:195:HOH:O	2.21	0.41
2:A:882:PHE:HA	2:A:885:ILE:HD11	2.02	0.41
2:B:1124:VAL:HG12	2:B:1128:MET:HE1	2.02	0.41
2:B:1013:ILE:C	2:B:1015:GLU:H	2.24	0.40
2:A:1126:GLN:CG	2:A:1160:ILE:HD13	2.50	0.40
2:A:829:ARG:HD3	2:A:833:LEU:CD2	2.45	0.40
2:B:1050:LEU:HD21	2:B:1061:ILE:CG2	2.51	0.40
2:B:988:PHE:HD2	2:B:988:PHE:H	1.69	0.40
2:A:835:ASP:HB2	2:A:841:TYR:HE2	1.86	0.40
2:B:1089:ALA:O	2:B:1090:SER:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1059:SER:HA	2:A:1062:VAL:HG12	2.03	0.40
2:A:896:VAL:HG13	2:A:897:PHE:CD1	2.56	0.40
2:B:1076:LYS:HA	2:B:1120:TYR:CE1	2.57	0.40
2:B:845:GLN:HE22	2:B:869:LYS:NZ	2.19	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	339/349 (97%)	325 (96%)	10 (3%)	4 (1%)	13 27
2	B	340/349 (97%)	306 (90%)	28 (8%)	6 (2%)	8 16
All	All	679/698 (97%)	631 (93%)	38 (6%)	10 (2%)	10 21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1110	SER
2	A	1166	LYS
2	B	839	ASN
2	B	1090	SER
2	B	1105	ASN
2	B	1109	HIS
2	B	909	GLY
2	B	1053	GLY
2	A	1104	MET
2	A	961	VAL

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
2	A	303/310 (98%)	294 (97%)	9 (3%)	41 67
2	B	303/310 (98%)	287 (95%)	16 (5%)	22 45
All	All	606/620 (98%)	581 (96%)	25 (4%)	30 56

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	904	LYS
2	A	935	CYS
2	A	957	LEU
2	A	962	LEU
2	A	986	LEU
2	A	1019	PRO
2	A	1127	LYS
2	A	1153	LYS
2	A	1165	GLU
2	B	831	ARG
2	B	847	ARG
2	B	860	GLN
2	B	880	LEU
2	B	883	ASN
2	B	896	VAL
2	B	906	PHE
2	B	949	GLN
2	B	955	ARG
2	B	971	ASN
2	B	984	GLN
2	B	988	PHE
2	B	1002	THR
2	B	1018	LEU
2	B	1105	ASN
2	B	1138	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such

sidechains are listed below:

Mol	Chain	Res	Type
2	A	839	ASN
2	A	858	GLN
2	A	883	ASN
2	A	887	GLN
2	A	891	GLN
2	A	913	GLN
2	A	949	GLN
2	A	968	GLN
2	A	972	HIS
2	A	984	GLN
2	A	1031	GLN
2	A	1032	HIS
2	A	1105	ASN
2	A	1109	HIS
2	A	1159	HIS
2	B	843	ASN
2	B	858	GLN
2	B	860	GLN
2	B	879	GLN
2	B	883	ASN
2	B	891	GLN
2	B	949	GLN
2	B	951	ASN
2	B	971	ASN
2	B	972	HIS
2	B	984	GLN
2	B	1021	GLN
2	B	1032	HIS
2	B	1052	HIS
2	B	1088	HIS
2	B	1136	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	9/10 (90%)	2 (22%)	1 (11%)
1	D	9/10 (90%)	2 (22%)	1 (11%)
All	All	18/20 (90%)	4 (22%)	2 (11%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	12	U
1	C	13	U
1	D	12	U
1	D	13	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	12	U
1	D	12	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 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	C	10/10 (100%)	-0.68	0	100	100	15, 34, 53, 57	0
1	D	10/10 (100%)	-0.44	0	100	100	29, 45, 87, 98	0
2	A	341/349 (97%)	-0.71	2 (0%)	89	88	6, 20, 56, 94	0
2	B	342/349 (97%)	-0.24	6 (1%)	68	64	14, 38, 73, 90	0
All	All	703/718 (97%)	-0.48	8 (1%)	80	78	6, 31, 70, 98	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1104	MET	3.9
2	B	1106	ASP	3.3
2	B	1139	ILE	3.1
2	B	872	ARG	2.7
2	A	1167	TYR	2.6
2	B	1089	ALA	2.5
2	B	888	ALA	2.1
2	A	1104	MET	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.