WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 1, 2016 – 11:05 PM EDT

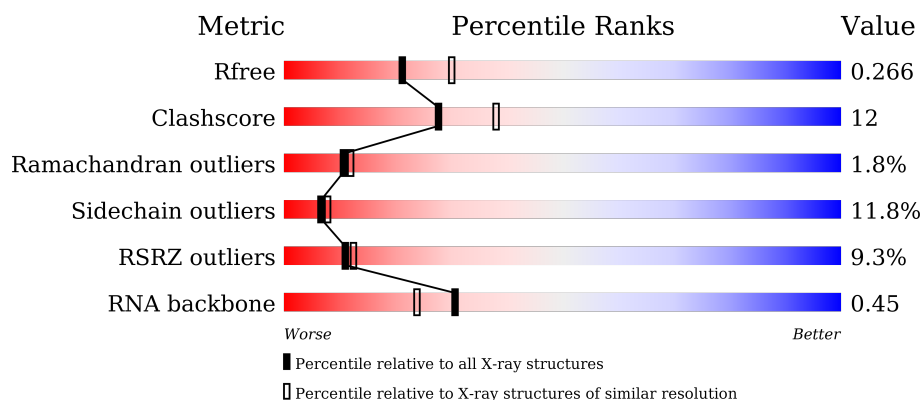|		
PDB ID	:	5ID6
Title	:	Structure of Cpf1/RNA Complex
Authors	:	Dong, D.; Ren, K.; Qiu, X.; Wang, J.; Huang, Z.
Deposited on	:	2016-02-24
Resolution	:	2.38 Å(reported)

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 2.38 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	Percentile Ranks	Value
Rfree		0.266
Clashscore		12
Ramachandran outliers		1.8%
Sidechain outliers		11.8%
RSRZ outliers		9.3%
RNA backbone		0.45

Worse ... *Better*

■ 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)
RNA backbone	2183	1092 (2.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1228	9% / 68% / 25% / 6% ·
2	G	21	48% / 38% / 5% / 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	1301	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10400 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 Cpf1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1209	Total	C	N	O	S	Se	0	0	0
			9949	6407	1632	1882	9	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	21	Total	C	N	O	P	0	0	0
			443	199	75	148	21			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	6	Total	O	0	0
			6	6		

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: Cpf1

Y1106 Q1107 Q1108 G1109 D1110 I1111 L1114 L1115 C1116 S1125 L1130 M1131 S1132 L1133 R1138 T1142 G1143 R1144 T1145 D1146 V1147 D1148 F1149 L1150 I1151 S1152 P1153 V1154 K1155 N1156 S1157 F1161 Y1162 D1163 S1164 R1165 N1166 Y1167 E1168 E1171 N1172 A1173 A1184 Y1185 N1186 R1189 L1192 W1193 A1194

F1198 D1203 L1206 D1207 K1208 I1211 A1212 V1226 K1227
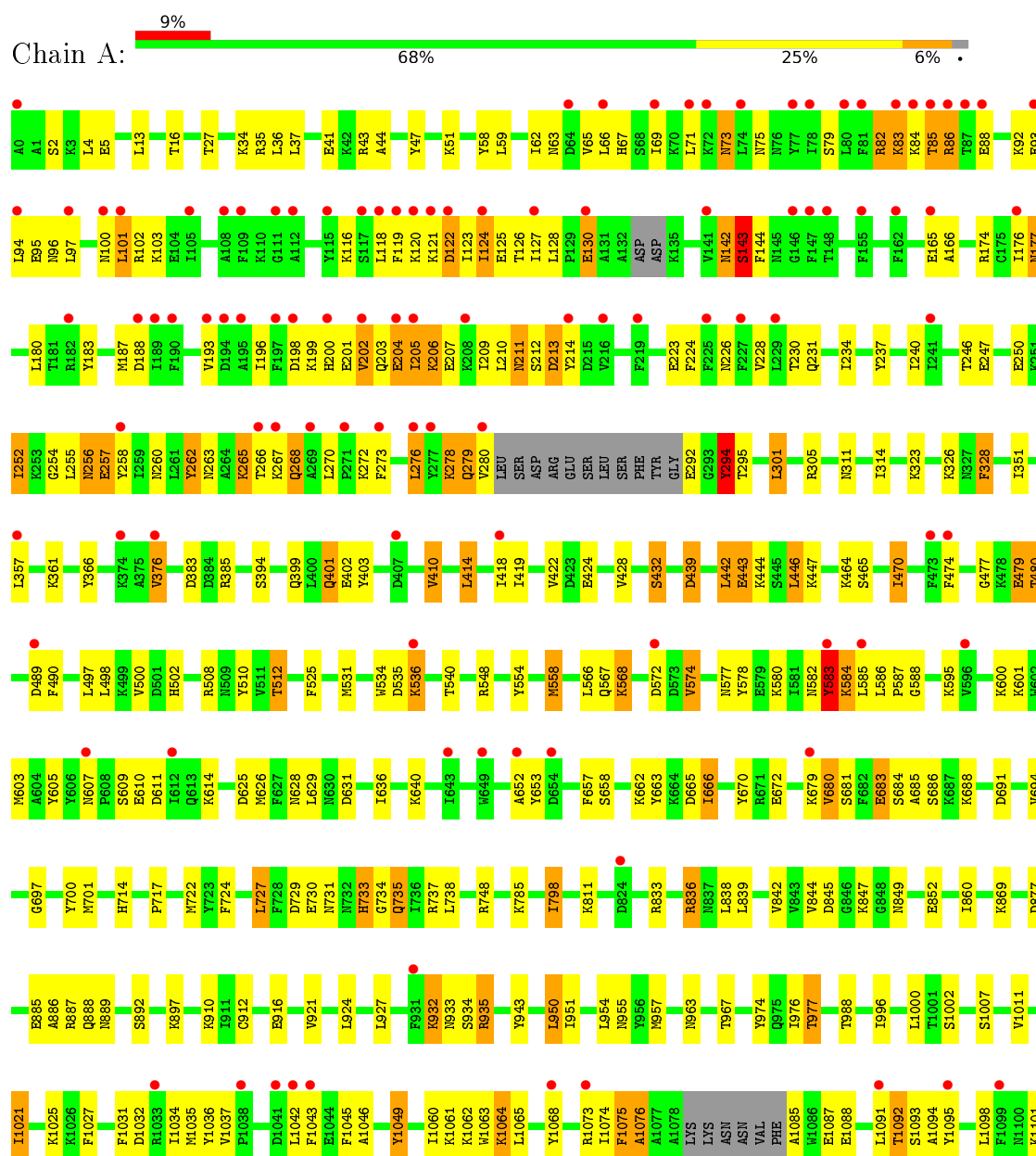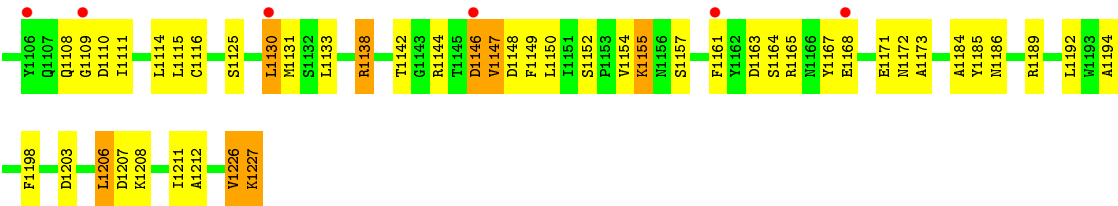
• Molecule 2: RNA (5'-R(P*AP*AP*UP*UP*UP*CP*UP*AP*CP*UP*AP*AP*GP*UP*GP*U P*AP*GP*AP*UP*C)-3')

Chain G:

48%   38%   5%   10%

A3 U9 A10 C11 U12 A13 A14 G15 U16 G17 G20 A21 U22 C23

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.35Å 83.01Å 124.09Å 90.00° 106.72° 90.00°	Depositor
Resolution (Å)	41.51 – 2.38 49.58 – 2.38	Depositor EDS
% Data completeness (in resolution range)	97.8 (41.51-2.38) 97.7 (49.58-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.32 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.202 , 0.261 0.207 , 0.266	Depositor DCC
R_{free} test set	3266 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	58.3	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.8	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10400	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.49	1/10136 (0.0%)	0.66	5/13584 (0.0%)
2	G	1.01	1/494 (0.2%)	1.76	13/766 (1.7%)
All	All	0.53	2/10630 (0.0%)	0.76	18/14350 (0.1%)

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	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	14	A	N9-C4	-5.82	1.34	1.37
1	A	583	TYR	CD1-CE1	-5.71	1.30	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	734	GLY	N-CA-C	9.98	138.05	113.10
2	G	14	A	C2-N3-C4	-8.11	106.55	110.60
2	G	20	G	C8-N9-C4	-7.14	103.55	106.40
2	G	15	G	N1-C6-O6	-7.08	115.65	119.90
2	G	14	A	N1-C6-N6	7.01	122.81	118.60
2	G	23	C	O5'-P-OP2	-6.83	99.55	105.70
2	G	20	G	O5'-P-OP1	-6.21	100.11	105.70
2	G	14	A	C5-N7-C8	-6.16	100.82	103.90
2	G	11	C	O5'-P-OP2	-5.96	100.33	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	9	U	C5-C6-N1	-5.94	119.73	122.70
1	A	583	TYR	N-CA-C	5.92	126.98	111.00
2	G	14	A	C4-C5-N7	5.75	113.58	110.70
2	G	9	U	N1-C2-N3	5.74	118.34	114.90
1	A	142	ASN	C-N-CA	5.48	135.41	121.70
1	A	143	SER	N-CA-CB	5.35	118.53	110.50
2	G	20	G	N7-C8-N9	5.20	115.70	113.10
2	G	20	G	C5'-C4'-C3'	-5.14	107.77	116.00
1	A	294	TYR	CA-CB-CG	5.03	122.95	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	583	TYR	Peptide
1	A	733	HIS	Peptide

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	9949	0	9908	237	1
2	G	443	0	224	7	0
3	A	1	0	0	0	0
3	G	1	0	0	0	0
4	G	6	0	0	0	0
All	All	10400	0	10132	242	1

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 (242) 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:A:536:LYS:NZ	1:A:653:TYR:OH	1.97	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:GLN:HG2	1:A:280:VAL:HG13	1.48	0.95
1:A:658:SER:HB3	1:A:662:LYS:HE2	1.52	0.88
1:A:933:ASN:O	1:A:935:ARG:N	2.07	0.86
1:A:1073:ARG:HD3	1:A:1133:LEU:HD21	1.58	0.85
1:A:583:TYR:HA	1:A:584:LYS:HD3	1.61	0.82
2:G:20:G:H5"	2:G:20:G:H8	1.43	0.82
1:A:735:GLN:OE1	1:A:737:ARG:NE	2.12	0.80
1:A:531:MSE:HE3	1:A:534:TRP:CH2	2.16	0.80
1:A:207:GLU:O	1:A:212:SER:N	2.12	0.79
1:A:263:ASN:HA	1:A:268:GLN:HG2	1.64	0.79
1:A:442:LEU:HD11	1:A:446:LEU:HD13	1.65	0.79
1:A:558:MSE:HE2	1:A:566:LEU:HD12	1.64	0.78
1:A:231:GLN:HB2	1:A:278:LYS:HZ2	1.51	0.75
1:A:439:ASP:N	1:A:439:ASP:OD1	2.17	0.75
1:A:531:MSE:HE3	1:A:534:TRP:HH2	1.52	0.74
1:A:566:LEU:O	1:A:580:LYS:NZ	2.15	0.73
1:A:142:ASN:N	1:A:143:SER:HB3	2.04	0.72
1:A:1163:ASP:OD2	1:A:1165:ARG:NH2	2.22	0.71
1:A:833:ARG:HH12	1:A:932:LYS:HD3	1.56	0.70
1:A:27:THR:HG21	1:A:701:MSE:H	1.58	0.69
1:A:272:LYS:NZ	1:A:489:ASP:OD1	2.26	0.69
1:A:833:ARG:HH22	1:A:932:LYS:HE3	1.57	0.69
1:A:314:ILE:HD13	1:A:500:VAL:HG12	1.75	0.68
1:A:361:LYS:NZ	1:A:403:TYR:O	2.21	0.68
1:A:63:ASN:ND2	1:A:231:GLN:OE1	2.27	0.68
1:A:205:ILE:HB	1:A:252:ILE:HD13	1.75	0.67
1:A:1155:LYS:HA	1:A:1161:PHE:HB3	1.77	0.67
1:A:1021:ILE:HD11	1:A:1025:LYS:HE3	1.76	0.67
1:A:73:ASN:HD21	1:A:97:LEU:HG	1.60	0.67
1:A:203:GLN:O	1:A:207:GLU:HB3	1.95	0.66
1:A:912:CYS:HA	1:A:957:MSE:HE2	1.78	0.66
1:A:1036:TYR:HB2	1:A:1043:PHE:CE1	2.31	0.65
1:A:206:LYS:O	1:A:210:LEU:HB2	1.97	0.65
1:A:326:LYS:HD3	1:A:419:ILE:HD11	1.79	0.63
1:A:785:LYS:HB2	2:G:3:A:H5"	1.81	0.63
1:A:1165:ARG:HA	1:A:1168:GLU:HB2	1.82	0.62
2:G:20:G:H5"	2:G:20:G:C8	2.30	0.62
1:A:1186:ASN:OD1	1:A:1189:ARG:NH1	2.31	0.62
1:A:27:THR:CG2	1:A:701:MSE:H	2.14	0.61
1:A:733:HIS:O	1:A:735:GLN:HB2	1.99	0.61
1:A:582:ASN:ND2	1:A:583:TYR:H	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLU:HB3	1:A:258:TYR:CE2	2.36	0.61
1:A:583:TYR:HE1	1:A:681:SER:O	1.84	0.61
1:A:200:HIS:HA	1:A:204:GLU:HG3	1.82	0.61
1:A:584:LYS:HB3	1:A:653:TYR:CE1	2.35	0.61
1:A:535:ASP:O	1:A:584:LYS:N	2.30	0.60
1:A:79:SER:O	1:A:83:LYS:HD3	2.02	0.60
1:A:1226:VAL:O	1:A:1227:LYS:NZ	2.35	0.60
1:A:572:ASP:OD2	1:A:574:VAL:N	2.33	0.59
1:A:1138:ARG:NH1	1:A:1148:ASP:OD2	2.36	0.59
1:A:209:ILE:HG21	1:A:246:THR:HG22	1.84	0.59
1:A:477:GLY:HA3	1:A:479:GLU:HB2	1.83	0.59
1:A:301:LEU:HD23	1:A:305:ARG:HD2	1.83	0.59
1:A:1000:LEU:HD22	1:A:1011:VAL:HG21	1.86	0.58
1:A:1076:ALA:HA	1:A:1085:ALA:HB1	1.85	0.58
1:A:211:ASN:OD1	1:A:211:ASN:N	2.37	0.58
1:A:955:ASN:OD1	1:A:977:THR:HG22	2.03	0.57
1:A:79:SER:HB3	1:A:83:LYS:NZ	2.19	0.57
2:G:20:G:H2'	2:G:21:A:O4'	2.03	0.57
1:A:34:LYS:NZ	1:A:697:GLY:O	2.37	0.57
1:A:628:ASN:HB3	1:A:631:ASP:HB2	1.86	0.57
1:A:256:ASN:HD21	1:A:273:PHE:H	1.50	0.57
1:A:418:ILE:HG12	1:A:470:ILE:HD11	1.86	0.57
1:A:237:TYR:HA	1:A:240:ILE:HD12	1.87	0.56
1:A:63:ASN:OD1	1:A:231:GLN:NE2	2.37	0.56
1:A:724:PHE:O	1:A:727:LEU:HB2	2.06	0.56
1:A:75:ASN:ND2	1:A:223:GLU:OE2	2.38	0.56
1:A:1091:LEU:O	1:A:1094:ALA:N	2.35	0.56
1:A:73:ASN:HB3	1:A:101:LEU:HD13	1.88	0.56
2:G:14:A:H8	2:G:14:A:H5"	1.71	0.56
1:A:1198:PHE:CE1	1:A:1211:ILE:HD11	2.41	0.56
1:A:1150:LEU:H	1:A:1164:SER:HB2	1.71	0.56
1:A:120:LYS:O	1:A:123:ILE:HG22	2.06	0.56
1:A:572:ASP:HB2	1:A:577:ASN:HD21	1.70	0.56
1:A:1144:ARG:HG2	1:A:1146:ASP:HB2	1.89	0.55
1:A:954:LEU:HD11	1:A:957:MSE:HE3	1.87	0.55
1:A:1185:TYR:CZ	1:A:1189:ARG:HD2	2.41	0.55
1:A:1068:TYR:OH	1:A:1161:PHE:N	2.40	0.55
1:A:658:SER:CB	1:A:662:LYS:HE2	2.32	0.54
1:A:860:ILE:HG12	1:A:869:LYS:HB3	1.88	0.54
1:A:394:SER:OG	1:A:479:GLU:OE1	2.19	0.54
1:A:1167:TYR:HD1	1:A:1173:ALA:HB1	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:NH2	1:A:188:ASP:OD1	2.32	0.54
2:G:14:A:H5"	2:G:14:A:C8	2.43	0.54
1:A:231:GLN:HB2	1:A:278:LYS:NZ	2.21	0.53
1:A:366:TYR:CE2	1:A:385:ARG:HB2	2.43	0.53
1:A:508:ARG:O	1:A:512:THR:HB	2.07	0.53
1:A:361:LYS:HZ3	1:A:403:TYR:HB3	1.74	0.53
1:A:1147:VAL:HG11	1:A:1165:ARG:HG2	1.91	0.53
1:A:717:PRO:HG2	1:A:722:MSE:HE3	1.91	0.53
1:A:100:ASN:HA	1:A:103:LYS:HB2	1.90	0.52
1:A:177:ASN:N	1:A:177:ASN:OD1	2.42	0.52
1:A:202:VAL:HG13	1:A:203:GLN:H	1.73	0.52
1:A:174:ARG:HG2	1:A:279:GLN:HB3	1.91	0.52
1:A:292:GLU:HB3	1:A:502:HIS:NE2	2.24	0.52
1:A:600:LYS:HA	1:A:603:MSE:HB2	1.90	0.52
1:A:1147:VAL:HG12	1:A:1149:PHE:HB3	1.92	0.52
1:A:102:ARG:NH2	1:A:166:ALA:HB2	2.25	0.52
1:A:912:CYS:SG	1:A:957:MSE:HE2	2.50	0.52
1:A:954:LEU:CD1	1:A:957:MSE:HE3	2.40	0.51
1:A:729:ASP:OD2	1:A:731:ASN:N	2.37	0.51
1:A:193:VAL:O	1:A:196:ILE:HG12	2.11	0.50
1:A:127:ILE:HA	1:A:130:GLU:OE1	2.11	0.50
1:A:536:LYS:HZ3	1:A:585:LEU:C	2.14	0.50
1:A:665:ASP:OD1	1:A:665:ASP:N	2.44	0.50
1:A:73:ASN:OD1	1:A:100:ASN:HB2	2.12	0.50
1:A:1111:ILE:HD12	1:A:1115:LEU:HD21	1.92	0.50
1:A:626:MSE:HA	1:A:626:MSE:HE2	1.94	0.50
1:A:1007:SER:O	1:A:1226:VAL:HG21	2.12	0.50
1:A:852:GLU:HG2	1:A:1172:ASN:ND2	2.26	0.49
1:A:1138:ARG:HD3	1:A:1148:ASP:OD1	2.12	0.49
1:A:211:ASN:HB2	1:A:213:ASP:H	1.76	0.49
1:A:578:TYR:CE1	1:A:701:MSE:HE1	2.47	0.49
1:A:96:ASN:O	1:A:100:ASN:ND2	2.45	0.49
1:A:202:VAL:HG13	1:A:203:GLN:OE1	2.12	0.49
1:A:206:LYS:HE2	1:A:252:ILE:HD11	1.93	0.49
1:A:1063:TRP:CE3	1:A:1154:VAL:HG11	2.48	0.49
1:A:663:TYR:OH	1:A:672:GLU:OE1	2.16	0.49
1:A:67:HIS:ND1	1:A:230:THR:HG21	2.28	0.48
1:A:474:PHE:CE1	1:A:490:PHE:HE2	2.31	0.48
1:A:79:SER:HB3	1:A:83:LYS:HZ2	1.77	0.48
1:A:246:THR:HG21	1:A:250:GLU:HB3	1.94	0.48
1:A:401:GLN:HG2	1:A:410:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:VAL:O	1:A:69:ILE:HG12	2.14	0.48
1:A:103:LYS:HE2	1:A:103:LYS:HB3	1.57	0.48
1:A:1025:LYS:HE2	1:A:1116:CYS:O	2.13	0.48
1:A:836:ARG:HH12	1:A:1142:THR:HA	1.76	0.48
1:A:1075:PHE:CD2	1:A:1087:GLU:HB2	2.48	0.48
1:A:43:ARG:HG2	1:A:144:PHE:CE1	2.49	0.48
1:A:92:LYS:HA	1:A:95:GLU:OE1	2.14	0.48
1:A:1046:ALA:HB2	1:A:1064:LYS:HE2	1.95	0.47
1:A:294:TYR:HA	1:A:510:TYR:CD1	2.50	0.47
1:A:1111:ILE:O	1:A:1115:LEU:HG	2.15	0.47
1:A:666:ILE:HD12	1:A:670:TYR:CE2	2.49	0.47
1:A:47:TYR:CZ	1:A:51:LYS:HD2	2.48	0.47
1:A:230:THR:O	1:A:234:ILE:HG13	2.14	0.47
1:A:842:VAL:HG23	1:A:1184:ALA:HB3	1.96	0.47
1:A:196:ILE:HD12	1:A:262:TYR:CE1	2.50	0.47
1:A:536:LYS:HG3	1:A:584:LYS:HD2	1.97	0.47
1:A:951:ILE:O	1:A:977:THR:HG21	2.15	0.47
1:A:1194:ALA:HB1	1:A:1211:ILE:HD12	1.96	0.47
1:A:262:TYR:C	1:A:268:GLN:HE21	2.17	0.47
1:A:536:LYS:NZ	1:A:653:TYR:HH	2.10	0.47
1:A:798:ILE:HG13	1:A:798:ILE:O	2.14	0.46
1:A:574:VAL:HG11	1:A:688:LYS:NZ	2.31	0.46
1:A:566:LEU:HA	1:A:566:LEU:HD23	1.77	0.46
1:A:582:ASN:CG	1:A:583:TYR:H	2.19	0.46
1:A:652:ALA:O	1:A:679:LYS:HD3	2.15	0.45
1:A:927:LEU:HD21	1:A:943:TYR:HD2	1.82	0.45
1:A:102:ARG:CZ	1:A:166:ALA:HB2	2.46	0.45
1:A:176:ILE:O	1:A:180:LEU:HB3	2.17	0.45
1:A:446:LEU:HD12	1:A:446:LEU:HA	1.78	0.45
1:A:567:GLN:HB3	1:A:568:LYS:HD3	1.98	0.45
1:A:610:GLU:OE1	1:A:614:LYS:NZ	2.43	0.45
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.87	0.45
1:A:924:LEU:HA	1:A:924:LEU:HD23	1.77	0.45
1:A:554:TYR:CD1	1:A:701:MSE:HE3	2.52	0.45
1:A:686:SER:OG	1:A:688:LYS:HG3	2.17	0.45
1:A:142:ASN:CA	1:A:143:SER:HB3	2.46	0.45
1:A:36:LEU:HD13	1:A:525:PHE:HD1	1.82	0.45
1:A:1037:VAL:HG22	1:A:1042:LEU:O	2.17	0.45
1:A:123:ILE:HG23	1:A:124:ILE:HG23	1.99	0.45
1:A:536:LYS:HD2	1:A:584:LYS:HA	1.99	0.44
1:A:636:ILE:HD11	1:A:666:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:HG23	1:A:694:VAL:HG13	1.98	0.44
1:A:572:ASP:CG	1:A:574:VAL:HG23	2.38	0.44
1:A:399:GLN:O	1:A:402:GLU:HB2	2.18	0.43
1:A:1095:TYR:CZ	1:A:1130:LEU:HD22	2.53	0.43
1:A:27:THR:HG22	1:A:700:TYR:HA	2.00	0.43
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.83	0.43
1:A:845:ASP:OD2	1:A:849:ASN:HB2	2.18	0.43
1:A:1060:ILE:O	1:A:1062:LYS:N	2.44	0.43
1:A:1068:TYR:CE2	1:A:1161:PHE:CE2	3.07	0.43
1:A:328:PHE:HD1	1:A:328:PHE:HA	1.73	0.43
1:A:85:THR:HG23	1:A:86:ARG:H	1.83	0.43
1:A:1147:VAL:CG1	1:A:1149:PHE:HB3	2.49	0.43
1:A:118:LEU:HD23	1:A:119:PHE:CE2	2.54	0.43
1:A:183:TYR:O	1:A:187:MSE:HG3	2.19	0.43
1:A:4:LEU:HD23	1:A:976:ILE:HG21	1.99	0.43
1:A:58:TYR:O	1:A:62:ILE:HG13	2.19	0.43
1:A:658:SER:OG	1:A:672:GLU:OE2	2.35	0.43
1:A:1144:ARG:CD	1:A:1146:ASP:HB2	2.49	0.42
1:A:1203:ASP:HA	1:A:1206:LEU:HD22	2.01	0.42
1:A:428:VAL:O	1:A:432:SER:OG	2.34	0.42
1:A:102:ARG:HH11	1:A:177:ASN:HD21	1.66	0.42
1:A:1109:GLY:HA2	1:A:1110:ASP:C	2.38	0.42
1:A:714:HIS:NE2	2:G:14:A:OP2	2.50	0.42
1:A:128:LEU:HD12	1:A:128:LEU:HA	1.95	0.42
1:A:497:LEU:O	1:A:500:VAL:HG13	2.19	0.42
1:A:996:ILE:HA	1:A:996:ILE:HD13	1.71	0.42
1:A:1207:ASP:OD2	1:A:1208:LYS:NZ	2.53	0.42
1:A:554:TYR:CG	1:A:701:MSE:HE3	2.54	0.42
1:A:1108:GLN:OE1	1:A:1108:GLN:N	2.53	0.42
1:A:123:ILE:HD12	1:A:127:ILE:HB	2.01	0.42
1:A:237:TYR:CD2	1:A:276:LEU:HD22	2.54	0.42
1:A:351:ILE:HD13	1:A:410:VAL:HG22	2.01	0.42
1:A:86:ARG:CZ	1:A:86:ARG:HB2	2.48	0.42
1:A:586:LEU:HD12	1:A:587:PRO:HD2	2.02	0.42
1:A:279:GLN:O	1:A:280:VAL:HG22	2.20	0.42
1:A:666:ILE:HD12	1:A:670:TYR:CZ	2.55	0.42
1:A:4:LEU:HB3	1:A:974:TYR:CE1	2.55	0.42
1:A:1032:ASP:HB2	1:A:1046:ALA:O	2.20	0.41
1:A:1192:LEU:HA	1:A:1192:LEU:HD23	1.78	0.41
1:A:323:LYS:HB3	1:A:323:LYS:HE2	1.83	0.41
1:A:582:ASN:C	1:A:583:TYR:CD1	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:LEU:HD21	1:A:1068:TYR:HB3	2.01	0.41
1:A:265:LYS:O	1:A:267:LYS:N	2.47	0.41
1:A:246:THR:O	1:A:247:GLU:HB3	2.21	0.41
1:A:640:LYS:HE2	1:A:657:PHE:HB3	2.01	0.41
1:A:82:ARG:H	1:A:82:ARG:HG2	1.71	0.41
1:A:447:LYS:HB3	1:A:447:LYS:HE2	1.70	0.41
1:A:1034:ILE:HG12	1:A:1045:PHE:HD1	1.85	0.41
1:A:121:LYS:HD3	1:A:125:GLU:OE2	2.20	0.41
1:A:174:ARG:HG2	1:A:279:GLN:CB	2.50	0.41
1:A:595:LYS:HE3	1:A:595:LYS:HB2	1.89	0.41
1:A:886:ALA:HB1	1:A:889:ASN:ND2	2.35	0.41
1:A:950:LEU:HA	1:A:950:LEU:HD23	1.85	0.41
1:A:1035:MSE:SE	1:A:1109:GLY:HA3	2.71	0.41
1:A:574:VAL:HG11	1:A:688:LYS:HZ2	1.86	0.41
1:A:254:GLY:N	1:A:257:GLU:OE1	2.40	0.41
1:A:2:SER:H	1:A:5:GLU:HG3	1.85	0.41
1:A:580:LYS:HB3	1:A:683:GLU:HB3	2.03	0.41
1:A:116:LYS:HE2	1:A:116:LYS:HB3	1.90	0.41
1:A:1206:LEU:HA	1:A:1206:LEU:HD12	1.78	0.41
1:A:210:LEU:HA	1:A:210:LEU:HD13	1.82	0.41
1:A:424:GLU:O	1:A:428:VAL:HG23	2.21	0.41
1:A:572:ASP:HB3	1:A:577:ASN:OD1	2.21	0.41
1:A:41:GLU:O	1:A:44:ALA:HB3	2.21	0.40
1:A:66:LEU:HB3	1:A:230:THR:HG22	2.03	0.40
1:A:1027:PHE:CE2	1:A:1031:PHE:HE2	2.40	0.40
1:A:122:ASP:HA	1:A:125:GLU:HB2	2.03	0.40
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.91	0.40
1:A:443:GLU:HG3	1:A:444:LYS:H	1.85	0.40
1:A:577:ASN:HD22	1:A:685:ALA:C	2.25	0.40
1:A:82:ARG:C	1:A:84:LYS:H	2.25	0.40
1:A:1208:LYS:HA	1:A:1208:LYS:HD3	1.87	0.40
1:A:811:LYS:HE2	1:A:811:LYS:HB3	1.78	0.40
1:A:1098:LEU:HD12	1:A:1098:LEU:HA	1.82	0.40
1:A:910:LYS:HA	1:A:910:LYS:HD3	1.82	0.40
1:A:1095:TYR:CE1	1:A:1130:LEU:HD22	2.56	0.40
1:A:845:ASP:C	1:A:847:LYS:H	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLU:OE1	1:A:607:ASN:ND2[2_646]	2.11	0.09

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	1201/1228 (98%)	1106 (92%)	73 (6%)	22 (2%)	11 12

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	THR
1	A	202	VAL
1	A	934	SER
1	A	143	SER
1	A	376	VAL
1	A	480	THR
1	A	83	LYS
1	A	214	TYR
1	A	294	TYR
1	A	1049	TYR
1	A	1092	THR
1	A	1212	ALA
1	A	204	GLU
1	A	266	THR
1	A	588	GLY
1	A	625	ASP
1	A	988	THR
1	A	1061	LYS
1	A	1076	ALA
1	A	1146	ASP
1	A	680	VAL
1	A	584	LYS

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	1085/1084 (100%)	957 (88%)	128 (12%)	6　8

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	16	THR
1	A	35	ARG
1	A	37	LEU
1	A	59	LEU
1	A	71	LEU
1	A	73	ASN
1	A	82	ARG
1	A	86	ARG
1	A	88	GLU
1	A	93	GLU
1	A	94	LEU
1	A	101	LEU
1	A	122	ASP
1	A	124	ILE
1	A	126	THR
1	A	130	GLU
1	A	165	GLU
1	A	177	ASN
1	A	198	ASP
1	A	199	LYS
1	A	205	ILE
1	A	206	LYS
1	A	211	ASN
1	A	213	ASP
1	A	224	PHE
1	A	226	ASN
1	A	228	VAL
1	A	252	ILE
1	A	255	LEU

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Mol	Chain	Res	Type
1	A	256	ASN
1	A	257	GLU
1	A	260	ASN
1	A	262	TYR
1	A	265	LYS
1	A	268	GLN
1	A	276	LEU
1	A	278	LYS
1	A	279	GLN
1	A	294	TYR
1	A	295	THR
1	A	301	LEU
1	A	311	ASN
1	A	328	PHE
1	A	357	LEU
1	A	376	VAL
1	A	383	ASP
1	A	401	GLN
1	A	410	VAL
1	A	414	LEU
1	A	422	VAL
1	A	432	SER
1	A	439	ASP
1	A	442	LEU
1	A	443	GLU
1	A	446	LEU
1	A	464	LYS
1	A	465	SER
1	A	470	ILE
1	A	479	GLU
1	A	480	THR
1	A	498	LEU
1	A	512	THR
1	A	536	LYS
1	A	540	THR
1	A	548	ARG
1	A	558	MSE
1	A	568	LYS
1	A	574	VAL
1	A	583	TYR
1	A	601	LYS
1	A	605	TYR

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Mol	Chain	Res	Type
1	A	609	SER
1	A	611	ASP
1	A	629	LEU
1	A	666	ILE
1	A	680	VAL
1	A	683	GLU
1	A	684	SER
1	A	691	ASP
1	A	727	LEU
1	A	730	GLU
1	A	735	GLN
1	A	738	LEU
1	A	748	ARG
1	A	798	ILE
1	A	836	ARG
1	A	838	LEU
1	A	839	LEU
1	A	844	VAL
1	A	877	ASP
1	A	885	GLU
1	A	887	ARG
1	A	888	GLN
1	A	892	SER
1	A	897	LYS
1	A	916	GLU
1	A	921	VAL
1	A	932	LYS
1	A	935	ARG
1	A	950	LEU
1	A	963	ASN
1	A	967	THR
1	A	977	THR
1	A	1002	SER
1	A	1021	ILE
1	A	1049	TYR
1	A	1064	LYS
1	A	1065	LEU
1	A	1074	ILE
1	A	1075	PHE
1	A	1088	GLU
1	A	1092	THR
1	A	1093	SER

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Mol	Chain	Res	Type
1	A	1101	LYS
1	A	1114	LEU
1	A	1125	SER
1	A	1130	LEU
1	A	1131	MSE
1	A	1138	ARG
1	A	1147	VAL
1	A	1152	SER
1	A	1155	LYS
1	A	1157	SER
1	A	1171	GLU
1	A	1206	LEU
1	A	1226	VAL
1	A	1227	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	256	ASN
1	A	401	GLN
1	A	577	ASN
1	A	582	ASN
1	A	861	ASN
1	A	906	GLN
1	A	1172	ASN

5.3.3   RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	20/21 (95%)	6 (30%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	13	A
2	G	14	A
2	G	16	U
2	G	17	G
2	G	20	G

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Mol	Chain	Res	Type
2	G	23	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (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(Å^2)	Q<0.9
1	A	1190/1228 (96%)	0.78	113 (9%)	10	12	33, 83, 131, 159	0
2	G	21/21 (100%)	0.70	0	100	100	39, 43, 59, 108	0
All	All	1211/1249 (96%)	0.78	113 (9%)	11	12	33, 82, 131, 159	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	LEU	7.9
1	A	197	PHE	7.9
1	A	101	LEU	7.0
1	A	1091	LEU	7.0
1	A	583	TYR	6.5
1	A	1068	TYR	6.5
1	A	195	ALA	6.5
1	A	202	VAL	6.4
1	A	1161	PHE	6.1
1	A	193	VAL	6.0
1	A	88	GLU	5.5
1	A	1095	TYR	5.5
1	A	85	THR	5.5
1	A	105	ILE	5.0
1	A	124	ILE	5.0
1	A	69	ILE	4.8
1	A	83	LYS	4.8
1	A	87	THR	4.6
1	A	208	LYS	4.5
1	A	189	ILE	4.4
1	A	216	VAL	4.4
1	A	74	LEU	4.2
1	A	97	LEU	4.1
1	A	205	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	120	LYS	4.0
1	A	81	PHE	4.0
1	A	227	PHE	4.0
1	A	117	SER	3.9
1	A	1042	LEU	3.9
1	A	214	TYR	3.8
1	A	111	GLY	3.7
1	A	115	TYR	3.7
1	A	194	ASP	3.6
1	A	204	GLU	3.6
1	A	269	ALA	3.5
1	A	100	ASN	3.5
1	A	80	LEU	3.4
1	A	162	PHE	3.4
1	A	679	LYS	3.4
1	A	119	PHE	3.3
1	A	1099	PHE	3.3
1	A	376	VAL	3.3
1	A	127	ILE	3.3
1	A	219	PHE	3.2
1	A	198	ASP	3.2
1	A	273	PHE	3.2
1	A	931	PHE	3.1
1	A	652	ALA	3.0
1	A	266	THR	3.0
1	A	280	VAL	3.0
1	A	109	PHE	2.9
1	A	121	LYS	2.9
1	A	357	LEU	2.9
1	A	141	VAL	2.8
1	A	130	GLU	2.8
1	A	190	PHE	2.8
1	A	277	TYR	2.8
1	A	612	ILE	2.8
1	A	1041	ASP	2.7
1	A	200	HIS	2.7
1	A	84	LYS	2.7
1	A	271	PRO	2.7
1	A	148	THR	2.7
1	A	1106	TYR	2.6
1	A	71	LEU	2.5
1	A	229	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1043	PHE	2.5
1	A	112	ALA	2.5
1	A	649	TRP	2.5
1	A	94	LEU	2.5
1	A	267	LYS	2.5
1	A	276	LEU	2.5
1	A	489	ASP	2.5
1	A	182	ARG	2.4
1	A	1038	PRO	2.4
1	A	572	ASP	2.4
1	A	108	ALA	2.4
1	A	155	PHE	2.4
1	A	122	ASP	2.4
1	A	176	ILE	2.3
1	A	77	TYR	2.3
1	A	146	GLY	2.3
1	A	473	PHE	2.3
1	A	78	ILE	2.3
1	A	258	TYR	2.2
1	A	241	ILE	2.2
1	A	1168	GLU	2.2
1	A	1033	ARG	2.2
1	A	86	ARG	2.2
1	A	824	ASP	2.2
1	A	1130	LEU	2.2
1	A	474	PHE	2.2
1	A	536	LYS	2.2
1	A	1073	ARG	2.1
1	A	596	VAL	2.1
1	A	225	PHE	2.1
1	A	66	LEU	2.1
1	A	1109	GLY	2.1
1	A	0	ALA	2.1
1	A	654	ASP	2.1
1	A	64	ASP	2.1
1	A	407	ASP	2.1
1	A	1146	ASP	2.1
1	A	72	LYS	2.1
1	A	643	ILE	2.1
1	A	165	GLU	2.1
1	A	147	PHE	2.1
1	A	188	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	418	ILE	2.0
1	A	585	LEU	2.0
1	A	93	GLU	2.0
1	A	374	LYS	2.0
1	A	607	ASN	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	A	1301	1/1	0.65	0.37	9.16	53,53,53,53	0
3	MG	G	101	1/1	0.97	0.15	-	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.