



Full wwPDB EM Validation Report ⓘ

Jul 31, 2025 – 10:31 am BST

PDB ID : 9H9K / pdb_00009h9k
EMDB ID : EMD-51967
Title : Complex 3 (HEAD) 30S-tRNA-GE81112
Authors : Schedlbauer, A.; Han, X.; van Bakel, W.; Kaminishi, T.; Ochoa-Lizarralde, B.; Iturrioz, I.; Capuni, R.; Parry, R.; Zegarra, R.; Gil-Carton, D.; Lopez-Alonso, J.P.; Barragan Sanz, K.; Brandi, L.; Gualerzi, C.O.; Fucini, P.; Connell, S.R.
Deposited on : 2024-10-31
Resolution : 3.80 Å(reported)
Based on initial model : 4ybb

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev126
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

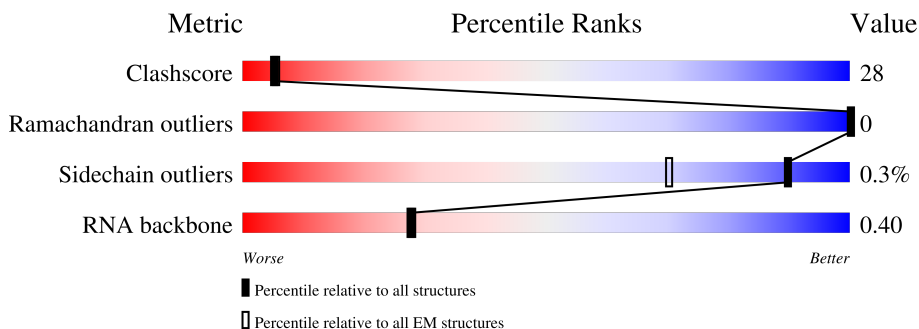
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	1541	
2	2	5	
3	3	77	
4	B	241	
5	C	233	
6	G	179	
7	I	130	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	J	103	<div><div></div><div>37%</div><div>58%</div><div></div><div>.</div><div>.</div></div>
9	M	118	<div><div></div><div>50%</div><div>47%</div><div></div><div>.</div><div>.</div></div>
10	N	101	<div><div></div><div>53%</div><div>46%</div><div></div><div>.</div></div>
11	S	92	<div><div></div><div>5%</div><div>62%</div><div>28%</div><div>10%</div></div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18869 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 16S RNA (456-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	456	Total	C	N	O	P	0	0
			9758	4357	1772	3173	456		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	5	Total	C	N	O	P	0	0
			107	48	19	35	5		

- Molecule 3 is a RNA chain called t-RNA (5'-R(P*UP*CP*GP*GP*GP*CP*UP*CP*AP*UP*AP*AP*CP*CP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	17	Total	C	N	O	P	0	0
			361	161	65	118	17		

- Molecule 4 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 5 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	211	Total	C	N	O	S	0	0
			1653	1046	310	293	4		

- Molecule 6 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	131	Total	C	N	O	S	0	0
			1023	638	195	187	3		

- Molecule 7 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	127	Total	C	N	O	S	0	0
			1021	634	206	178	3		

- Molecule 8 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	100	Total	C	N	O	S	0	0
			803	502	154	146	1		

- Molecule 9 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 11 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
12	1	28	Total	Mg	0
			28	28	
12	I	1	Total	Mg	0
			1	1	
12	N	1	Total	Mg	0
			1	1	

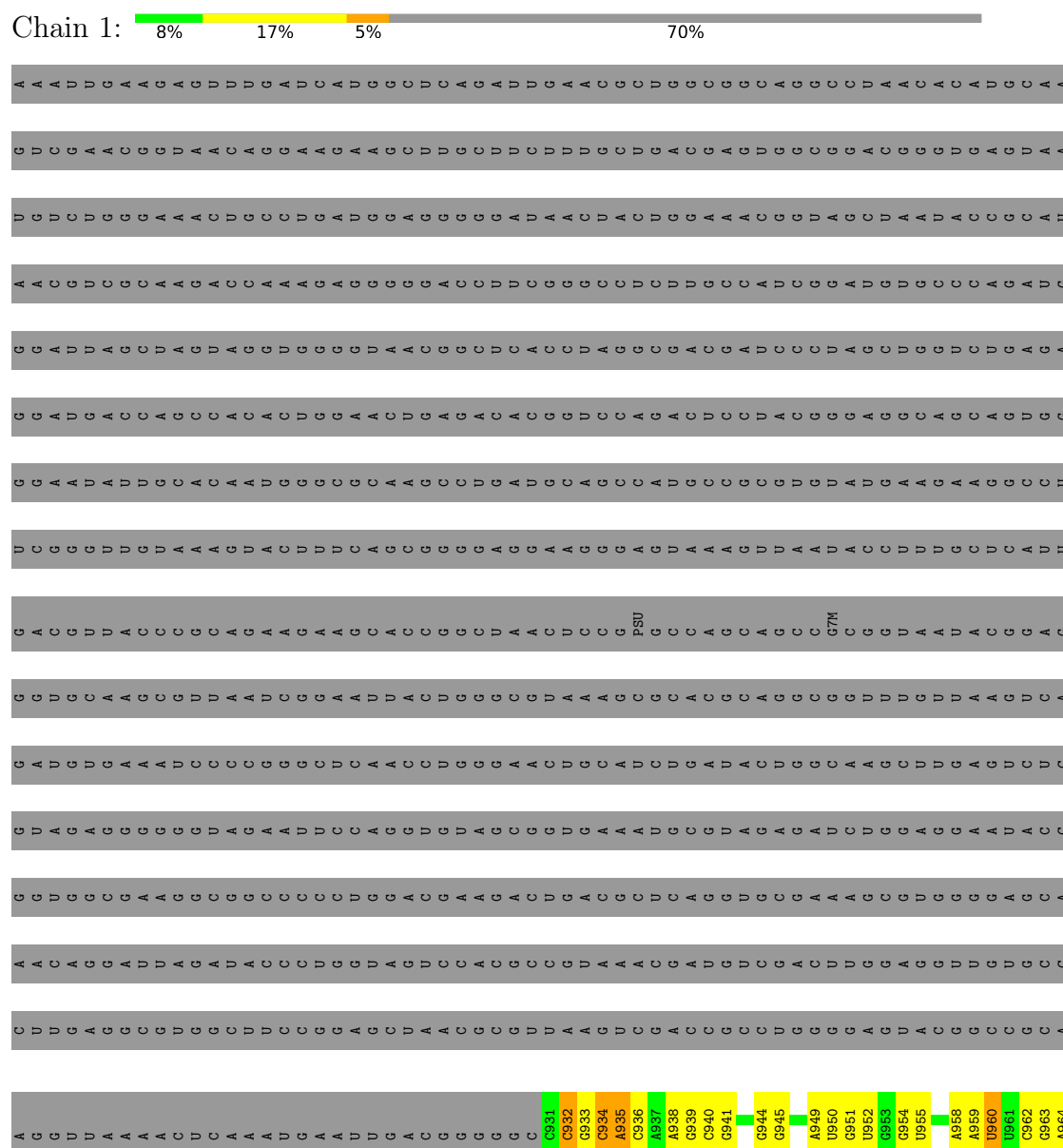
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

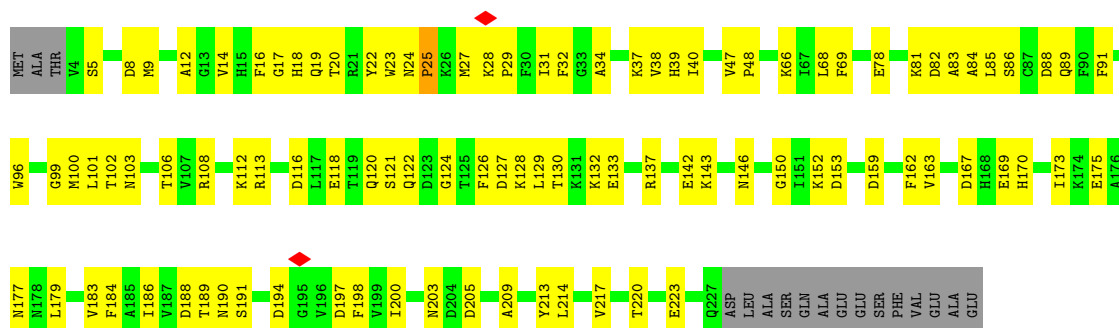
Mol	Chain	Residues	Atoms		AltConf
13	B	1	Total 1	Zn 1	0

3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

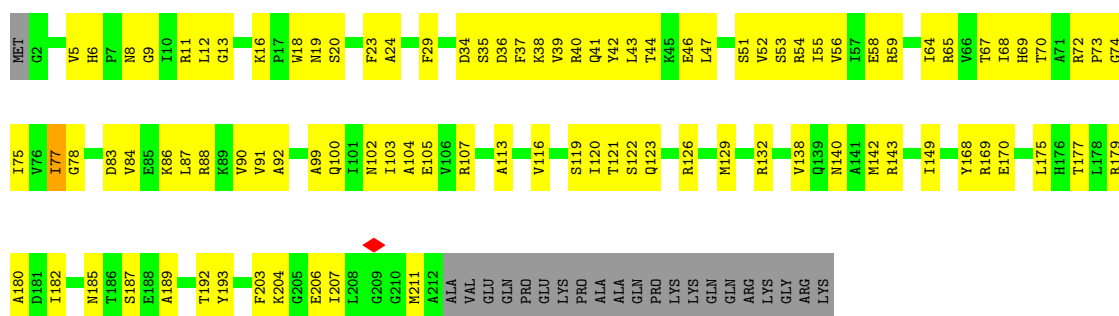
• Molecule 1: 16S RNA (456-MER)





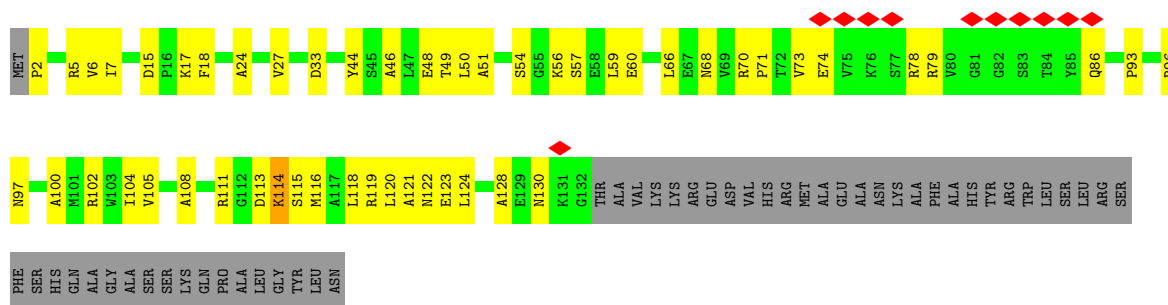
• Molecule 5: Small ribosomal subunit protein uS3

Chain C: 50% 40% 9%



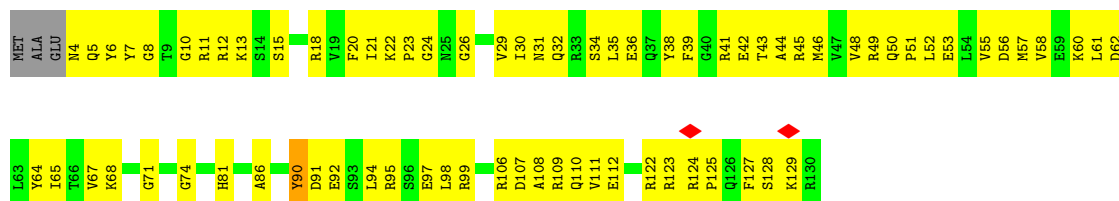
• Molecule 6: Small ribosomal subunit protein uS7

Chain G: 6% 44% 28% 27%

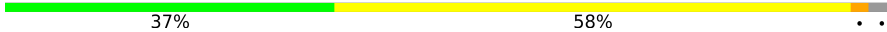


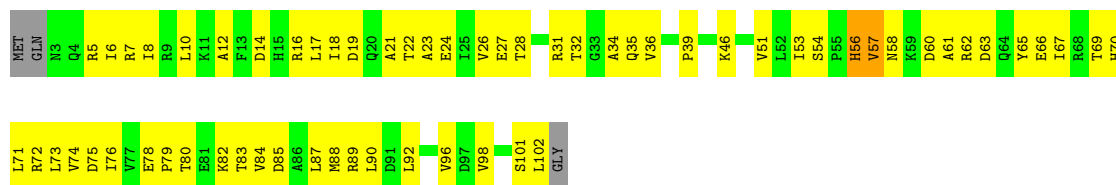
• Molecule 7: Small ribosomal subunit protein uS9

Chain I: 40% 57%



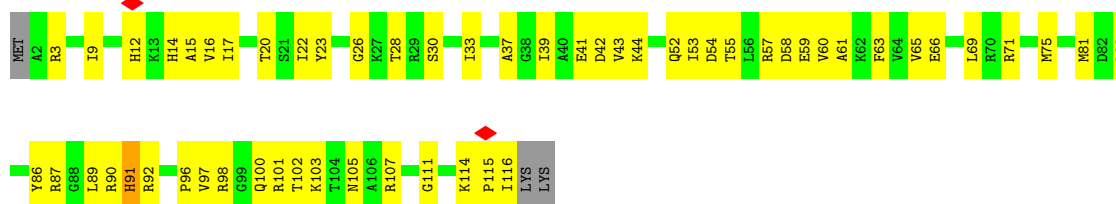
• Molecule 8: Small ribosomal subunit protein uS10

Chain J:  37% 58% ..



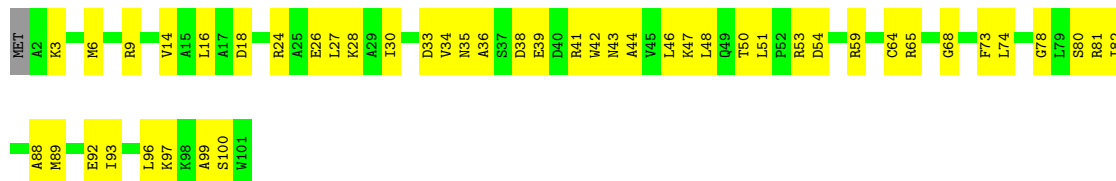
- Molecule 9: Small ribosomal subunit protein uS13

Chain M:  50% 47% ..



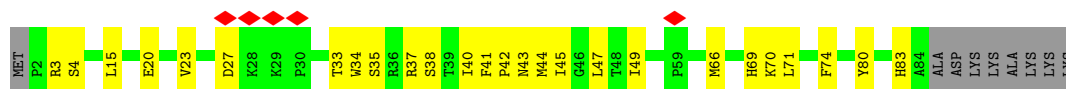
- Molecule 10: Small ribosomal subunit protein uS14

Chain N:  53% 46% .



- Molecule 11: Small ribosomal subunit protein uS19

Chain S:  5% 62% 28% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28111	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.08	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.032	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	427.39203, 427.39203, 427.39203	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113, 1.113, 1.113	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 2MG, 5MC

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	1	0.31	0/10842	0.41	2/16904 (0.0%)
2	2	0.42	0/119	0.86	0/183
3	3	0.46	0/402	0.85	3/624 (0.5%)
4	B	0.34	0/1784	0.52	1/2403 (0.0%)
5	C	0.39	0/1680	0.66	1/2263 (0.0%)
6	G	0.33	0/1035	0.62	2/1389 (0.1%)
7	I	0.40	0/1033	0.66	0/1375
8	J	0.56	0/813	0.94	3/1100 (0.3%)
9	M	0.32	0/900	0.51	0/1204
10	N	0.33	0/817	0.47	0/1088
11	S	0.29	0/680	0.46	0/915
All	All	0.35	0/20105	0.52	12/29448 (0.0%)

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
7	I	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	114	LYS	N-CA-C	11.94	123.85	111.07
8	J	57	VAL	N-CA-C	10.18	121.00	110.62
1	1	1101	A	P-O5'-C5'	7.14	131.60	120.90
8	J	56	HIS	N-CA-C	6.87	118.17	108.00
4	B	25	PRO	N-CA-C	-5.39	101.36	112.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	77	ILE	N-CA-C	5.35	115.61	110.74
3	3	38	A	C2'-C3'-O3'	-5.30	105.75	113.70
3	3	38	A	O4'-C1'-C2'	-5.22	102.38	107.60
8	J	56	HIS	CB-CA-C	-5.19	109.08	116.34
1	1	1382	C	C4'-C3'-O3'	-5.18	105.22	113.00
6	G	113	ASP	N-CA-C	5.12	119.56	112.45
3	3	28	C	C2'-C3'-O3'	-5.03	106.15	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	I	129	LYS	Mainchain

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	1	9758	0	4926	400	0
2	2	107	0	54	7	0
3	3	361	0	186	21	0
4	B	1753	0	1780	77	0
5	C	1653	0	1725	98	0
6	G	1023	0	1076	48	0
7	I	1021	0	1070	75	0
8	J	803	0	842	76	0
9	M	891	0	952	53	0
10	N	805	0	844	49	0
11	S	663	0	688	28	0
12	1	28	0	0	0	0
12	I	1	0	0	0	0
12	N	1	0	0	0	0
13	B	1	0	0	0	0
All	All	18869	0	14143	856	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 28.

All (856) 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)
1:1:1139:G:N2	1:1:1142:G:N7	2.16	0.94
1:1:1160:G:O6	1:1:1182:G:N1	2.02	0.93
1:1:1002:G:N2	1:1:1038:C:O2	2.03	0.92
1:1:1226:C:O2'	9:M:102:THR:O	1.89	0.91
1:1:1266:G:N2	1:1:1269:A:OP2	2.02	0.91
5:C:52:VAL:HG12	5:C:70:THR:HB	1.50	0.90
1:1:1013:G:N2	1:1:1016:A:OP2	2.05	0.90
1:1:1316:G:N1	1:1:1319:A:OP2	2.05	0.89
1:1:1026:G:O6	1:1:1035:A:N6	2.04	0.89
1:1:1004:A:O2'	1:1:1036:A:N1	2.04	0.88
4:B:78:GLU:O	4:B:81:LYS:HG2	1.71	0.88
1:1:1345:U:OP1	7:I:122:ARG:NH1	2.07	0.88
5:C:72:ARG:HE	5:C:75:ILE:CG1	1.85	0.88
1:1:1135:U:O2'	1:1:1138:G:O6	1.92	0.87
1:1:1237:C:O2'	1:1:1335:U:O4'	1.92	0.87
1:1:1077:G:N2	1:1:1080:A:OP2	2.07	0.87
6:G:115:SER:O	6:G:119:ARG:HD3	1.74	0.87
1:1:1046:A:N6	1:1:1211:U:O2	2.06	0.87
1:1:1028:C:N4	1:1:1033:G:O6	2.06	0.87
1:1:1101:A:O2'	1:1:1102:A:O5'	1.93	0.87
9:M:15:ALA:N	9:M:43:VAL:O	2.07	0.87
8:J:28:THR:HG22	8:J:31:ARG:NH2	1.90	0.86
1:1:1166:G:N2	1:1:1169:A:OP2	2.08	0.85
5:C:72:ARG:HE	5:C:75:ILE:HG13	1.38	0.85
5:C:36:ASP:OD1	5:C:59:ARG:NH2	2.10	0.85
1:1:1162:C:O2	1:1:1174:G:N2	2.08	0.85
1:1:1067:A:O2'	1:1:1093:A:O2'	1.89	0.85
1:1:1177:G:N1	1:1:1181:G:N7	2.25	0.85
1:1:1216:A:OP1	10:N:3:LYS:NZ	2.11	0.84
1:1:1177:G:N2	1:1:1181:G:O6	2.11	0.83
4:B:188:ASP:OD1	4:B:189:THR:N	2.12	0.83
1:1:1030:U:OP2	1:1:1031:C:N4	2.12	0.82
1:1:1301:U:OP2	1:1:1303:C:N4	2.11	0.82
1:1:1052:U:O4	1:1:1200:C:O2'	1.97	0.82
1:1:1314:C:OP2	11:S:4:SER:OG	1.97	0.82
8:J:8:ILE:N	8:J:74:VAL:O	2.11	0.82
1:1:1064:G:O6	1:1:1192:C:N4	2.12	0.82
1:1:1202:U:C2	10:N:82:ILE:HG21	2.15	0.81
9:M:90:ARG:NE	9:M:96:PRO:O	2.14	0.80
1:1:998:C:O2	1:1:1043:G:N2	2.12	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:86:GLN:N	6:G:86:GLN:OE1	2.15	0.79
5:C:100:GLN:OE1	5:C:102:ASN:ND2	2.15	0.79
1:1:977:A:O2'	1:1:979:C:OP2	2.01	0.79
5:C:168:TYR:OH	5:C:170:GLU:OE2	2.00	0.79
1:1:1384:C:H2'	1:1:1385:G:C8	2.16	0.79
6:G:60:GLU:N	6:G:60:GLU:OE1	2.16	0.78
4:B:78:GLU:HA	4:B:81:LYS:HE2	1.65	0.78
1:1:958:A:N3	1:1:985:C:O2'	2.15	0.78
8:J:28:THR:HG22	8:J:31:ARG:HH21	1.48	0.78
1:1:966:2MG:H2'	1:1:967:5MC:C6	2.18	0.78
4:B:19:GLN:HB2	4:B:37:LYS:HD2	1.65	0.78
2:2:15:A:H2	2:2:16:A:H62	1.32	0.78
1:1:1178:G:N2	1:1:1181:G:OP2	2.17	0.77
1:1:1379:G:N2	1:1:1381:U:O4	2.18	0.76
5:C:73:PRO:HG3	5:C:105:GLU:HB2	1.66	0.76
1:1:1358:U:OP2	1:1:1359:C:N4	2.16	0.75
6:G:93:PRO:O	6:G:97:ASN:ND2	2.19	0.75
1:1:962:C:N4	1:1:973:G:O6	2.20	0.74
8:J:85:ASP:O	8:J:89:ARG:HG2	1.88	0.73
1:1:1206:G:H3'	1:1:1207:2MG:H8	1.54	0.73
1:1:1260:G:OP1	1:1:1284:C:O2'	2.06	0.73
4:B:23:TRP:C	4:B:25:PRO:HD3	2.14	0.72
1:1:1307:U:OP1	9:M:100:GLN:NE2	2.23	0.72
8:J:56:HIS:CE1	8:J:57:VAL:HG13	2.24	0.72
1:1:1196:A:O2'	1:1:1197:A:OP2	2.08	0.71
1:1:1001:C:O2	1:1:1039:G:N2	2.20	0.71
1:1:1240:U:OP1	6:G:119:ARG:NH2	2.23	0.71
8:J:28:THR:HG21	8:J:90:LEU:HD21	1.73	0.71
1:1:1304:G:N1	1:1:1332:A:OP2	2.22	0.70
7:I:13:LYS:HG3	7:I:74:GLY:HA3	1.73	0.70
11:S:15:LEU:HD23	11:S:15:LEU:O	1.92	0.69
4:B:20:THR:HG23	4:B:37:LYS:HA	1.73	0.69
5:C:52:VAL:HA	5:C:70:THR:HA	1.75	0.69
7:I:39:PHE:O	7:I:45:ARG:NH2	2.25	0.69
1:1:1162:C:N3	1:1:1174:G:N1	2.40	0.69
5:C:58:GLU:O	5:C:65:ARG:N	2.26	0.69
8:J:12:ALA:HB3	8:J:18:ILE:HD11	1.74	0.68
1:1:1217:C:OP1	10:N:9:ARG:NE	2.27	0.68
1:1:1382:C:H2'	1:1:1383:C:O4'	1.94	0.67
10:N:54:ASP:OD1	10:N:59:ARG:NH2	2.26	0.67
5:C:72:ARG:NE	5:C:75:ILE:HG13	2.09	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:12:ARG:HH11	7:I:13:LYS:H	1.42	0.67
8:J:6:ILE:HG12	8:J:79:PRO:HG3	1.75	0.66
1:1:1309:G:OP2	9:M:98:ARG:NH2	2.25	0.66
1:1:1190:G:OP1	5:C:5:VAL:N	2.29	0.66
6:G:71:PRO:O	6:G:96:ARG:NE	2.24	0.66
1:1:1346:A:H61	1:1:1374:A:H3'	1.60	0.66
8:J:32:THR:HG21	8:J:83:THR:N	2.10	0.66
9:M:90:ARG:NH2	9:M:96:PRO:O	2.29	0.66
1:1:932:C:H6	1:1:932:C:OP2	1.79	0.65
6:G:50:LEU:C	6:G:50:LEU:HD23	2.21	0.65
6:G:70:ARG:NH2	6:G:97:ASN:OD1	2.29	0.65
11:S:49:ILE:HD13	11:S:71:LEU:CD1	2.27	0.65
2:2:15:A:N3	2:2:15:A:H2'	2.10	0.65
4:B:133:GLU:N	4:B:133:GLU:OE1	2.29	0.65
5:C:192:THR:HG23	5:C:193:TYR:CD2	2.31	0.65
1:1:1028:C:N3	1:1:1033:G:N1	2.44	0.65
5:C:37:PHE:O	5:C:41:GLN:HG2	1.96	0.65
1:1:1074:G:H2'	1:1:1075:U:O4'	1.96	0.65
1:1:1139:G:N1	1:1:1142:G:O6	2.29	0.65
1:1:1371:G:O3'	7:I:71:GLY:HA3	1.97	0.65
1:1:967:5MC:H2'	1:1:968:A:C8	2.32	0.65
1:1:1208:C:H2'	1:1:1209:C:C6	2.31	0.65
1:1:1239:A:H62	1:1:1299:A:H62	1.44	0.64
9:M:107:ARG:O	9:M:111:GLY:N	2.28	0.64
1:1:1144:G:O6	1:1:1145:A:N6	2.30	0.64
1:1:1257:A:O2'	1:1:1258:G:OP1	2.14	0.64
4:B:19:GLN:HA	4:B:37:LYS:O	1.98	0.64
1:1:1005:A:N7	1:1:1024:G:O2'	2.28	0.64
1:1:1317:C:OP2	10:N:28:LYS:NZ	2.26	0.64
5:C:42:TYR:O	5:C:46:GLU:HG2	1.97	0.64
5:C:83:ASP:OD1	5:C:86:LYS:NZ	2.30	0.64
7:I:26:GLY:N	7:I:61:LEU:O	2.28	0.64
1:1:1250:A:H2'	1:1:1251:A:C8	2.34	0.63
1:1:1105:A:OP1	4:B:113:ARG:NH1	2.23	0.63
8:J:26:VAL:HG23	8:J:36:VAL:HG11	1.79	0.62
7:I:110:GLN:HG3	7:I:111:VAL:H	1.64	0.62
4:B:28:LYS:N	4:B:29:PRO:HD2	2.14	0.62
4:B:24:ASN:N	4:B:25:PRO:HD3	2.14	0.62
5:C:47:LEU:HB3	5:C:52:VAL:HG13	1.81	0.62
6:G:59:LEU:H	6:G:59:LEU:HD12	1.65	0.62
1:1:1101:A:C2	4:B:99:GLY:N	2.68	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:99:GLY:N	4:B:175:GLU:OE2	2.34	0.61
5:C:58:GLU:N	5:C:65:ARG:O	2.31	0.61
9:M:90:ARG:CZ	9:M:96:PRO:O	2.49	0.61
1:1:935:A:O2'	1:1:1383:C:O2	2.18	0.61
7:I:106:ARG:NH1	7:I:107:ASP:O	2.34	0.61
7:I:124:ARG:HG3	7:I:125:PRO:HD2	1.83	0.60
8:J:56:HIS:CG	8:J:57:VAL:H	2.19	0.60
4:B:20:THR:HG22	4:B:39:HIS:NE2	2.16	0.60
11:S:49:ILE:HD13	11:S:71:LEU:HD12	1.82	0.60
1:1:1237:C:O2'	1:1:1300:G:N2	2.30	0.60
1:1:1163:A:H2'	1:1:1164:G:O4'	2.01	0.60
1:1:1112:C:O2	5:C:179:ARG:N	2.34	0.60
1:1:1226:C:O2	11:S:83:HIS:NE2	2.34	0.60
1:1:934:C:H5	1:1:1345:U:OP2	1.85	0.60
4:B:19:GLN:CB	4:B:37:LYS:HD2	2.31	0.60
6:G:115:SER:N	6:G:119:ARG:HH11	2.00	0.60
5:C:47:LEU:HD11	5:C:68:ILE:HD13	1.83	0.60
4:B:24:ASN:HD21	4:B:190:ASN:HA	1.66	0.59
4:B:17:GLY:HA3	4:B:39:HIS:O	2.01	0.59
1:1:1305:G:O2'	1:1:1332:A:N6	2.36	0.59
10:N:38:ASP:OD1	10:N:39:GLU:N	2.36	0.59
1:1:933:G:O5'	1:1:933:G:H8	1.86	0.59
1:1:1297:G:H1'	6:G:114:LYS:HE3	1.83	0.59
4:B:5:SER:N	4:B:8:ASP:OD2	2.31	0.59
2:2:15:A:C2	2:2:16:A:N6	2.64	0.59
3:3:33:C:N4	3:3:34:U:O4	2.35	0.58
5:C:192:THR:HG23	5:C:193:TYR:HD2	1.68	0.58
9:M:15:ALA:HB2	9:M:43:VAL:HG23	1.85	0.58
7:I:127:PHE:O	7:I:128:SER:OG	2.14	0.58
10:N:74:LEU:O	10:N:78:GLY:N	2.36	0.58
1:1:1196:A:HO2'	1:1:1197:A:P	2.26	0.58
7:I:5:GLN:OE1	7:I:6:TYR:N	2.34	0.58
8:J:28:THR:HA	8:J:31:ARG:HH21	1.67	0.58
6:G:15:ASP:OD2	6:G:17:LYS:HB3	2.04	0.58
5:C:19:ASN:HB2	10:N:92:GLU:CD	2.28	0.58
10:N:93:ILE:HG21	10:N:96:LEU:HD22	1.83	0.58
1:1:966:2MG:H2'	1:1:967:5MC:H6	1.64	0.58
10:N:42:TRP:NE1	10:N:46:LEU:HD11	2.19	0.58
1:1:944:G:N1	1:1:1338:G:OP2	2.37	0.58
8:J:14:ASP:OD1	8:J:16:ARG:N	2.37	0.58
1:1:1078:U:H2'	1:1:1079:G:O4'	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:934:C:C4	1:1:1344:C:C6	2.92	0.57
1:1:1148:U:H5'	7:I:7:TYR:OH	2.04	0.57
3:3:28:C:C6	3:3:28:C:OP2	2.58	0.57
5:C:121:THR:HG22	5:C:189:ALA:HB2	1.86	0.57
7:I:8:GLY:HA3	7:I:86:ALA:HB2	1.86	0.57
10:N:39:GLU:OE2	10:N:43:ASN:ND2	2.34	0.57
1:1:1205:U:H2'	1:1:1206:G:H8	1.69	0.57
11:S:40:ILE:HG23	11:S:44:MET:SD	2.45	0.57
4:B:220:THR:O	4:B:223:GLU:HG2	2.05	0.57
5:C:69:HIS:HA	5:C:104:ALA:O	2.03	0.57
1:1:1348:U:H4'	7:I:122:ARG:HG3	1.87	0.56
8:J:60:ASP:O	8:J:61:ALA:HB3	2.04	0.56
4:B:9:MET:HE1	4:B:47:VAL:HA	1.87	0.56
5:C:206:GLU:HA	5:C:206:GLU:OE1	2.06	0.56
8:J:56:HIS:CG	8:J:57:VAL:N	2.73	0.56
1:1:1181:G:O2'	1:1:1182:G:N7	2.37	0.56
1:1:1250:A:H2'	1:1:1251:A:H8	1.70	0.56
5:C:12:LEU:HA	5:C:16:LYS:HB2	1.87	0.56
8:J:5:ARG:O	8:J:102:LEU:HD12	2.06	0.56
9:M:16:VAL:HB	9:M:41:GLU:HB2	1.87	0.56
1:1:1384:C:N4	1:1:1385:G:O6	2.38	0.56
8:J:80:THR:HG22	8:J:82:LYS:H	1.70	0.56
9:M:58:ASP:O	9:M:61:ALA:HB3	2.06	0.56
1:1:1152:A:OP1	8:J:70:HIS:ND1	2.37	0.56
1:1:1168:U:O2'	1:1:1169:A:H5'	2.06	0.56
9:M:33:ILE:HD12	9:M:59:GLU:HB3	1.87	0.56
1:1:1160:G:C6	1:1:1161:C:C4	2.94	0.55
8:J:32:THR:HG22	8:J:32:THR:O	2.06	0.55
5:C:47:LEU:O	5:C:51:SER:N	2.37	0.55
11:S:40:ILE:HD12	11:S:69:HIS:HB2	1.88	0.55
1:1:1087:G:C6	1:1:1099:G:C6	2.94	0.55
11:S:27:ASP:OD1	11:S:27:ASP:N	2.39	0.55
10:N:89:MET:HE2	10:N:89:MET:HA	1.89	0.55
1:1:1206:G:H2'	1:1:1207:2MG:O4'	2.07	0.55
1:1:1132:C:N4	1:1:1133:G:O6	2.40	0.55
10:N:27:LEU:HD22	10:N:47:LYS:NZ	2.21	0.55
11:S:37:ARG:O	11:S:70:LYS:NZ	2.35	0.55
5:C:9:GLY:HA2	5:C:12:LEU:HD12	1.89	0.55
1:1:1005:A:N6	1:1:1024:G:O3'	2.40	0.55
1:1:1178:G:N7	7:I:99:ARG:NH1	2.56	0.54
1:1:1319:A:OP2	11:S:3:ARG:NH1	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1160:G:C5	1:1:1161:C:C5	2.95	0.54
1:1:1176:A:H2'	1:1:1177:G:O4'	2.07	0.54
1:1:1206:G:HO2'	5:C:193:TYR:HD1	1.54	0.54
1:1:1208:C:H2'	1:1:1209:C:H6	1.70	0.54
8:J:70:HIS:O	8:J:71:LEU:HD22	2.07	0.54
1:1:933:G:H8	1:1:933:G:P	2.30	0.54
10:N:27:LEU:HD23	10:N:48:LEU:HD13	1.89	0.54
7:I:94:LEU:O	7:I:98:LEU:HD23	2.08	0.54
1:1:934:C:C5	1:1:1345:U:OP2	2.60	0.54
1:1:1114:C:O2'	10:N:100:SER:O	2.12	0.54
5:C:142:MET:SD	5:C:149:ILE:HG22	2.47	0.54
7:I:11:ARG:HB2	7:I:106:ARG:NH2	2.23	0.54
8:J:8:ILE:O	8:J:74:VAL:N	2.38	0.54
1:1:1034:G:H2'	1:1:1035:A:O4'	2.08	0.54
9:M:86:TYR:CE1	9:M:90:ARG:HD2	2.42	0.54
1:1:1358:U:H3	1:1:1363:A:H62	1.56	0.53
3:3:28:C:H2'	3:3:29:C:O4'	2.08	0.53
11:S:33:THR:HG21	11:S:49:ILE:HD11	1.89	0.53
1:1:949:A:N7	9:M:105:ASN:ND2	2.56	0.53
1:1:1123:U:O2'	8:J:39:PRO:O	2.27	0.53
9:M:87:ARG:HG3	9:M:97:VAL:CG1	2.37	0.53
1:1:1343:G:H2'	1:1:1344:C:C6	2.43	0.53
1:1:1347:G:HO2'	1:1:1348:U:P	2.32	0.53
5:C:73:PRO:O	5:C:77:ILE:HG22	2.08	0.53
8:J:28:THR:CG2	8:J:31:ARG:HH21	2.19	0.53
1:1:979:C:N4	1:1:1360:A:H62	2.07	0.53
4:B:103:ASN:O	4:B:106:THR:N	2.42	0.53
5:C:40:ARG:O	5:C:44:THR:HG23	2.09	0.53
10:N:34:VAL:O	10:N:41:ARG:NH2	2.42	0.53
1:1:1077:G:N1	1:1:1080:A:OP2	2.42	0.53
1:1:1383:C:O2	1:1:1383:C:H2'	2.09	0.53
5:C:47:LEU:HD12	5:C:55:ILE:HD11	1.91	0.53
7:I:13:LYS:HG3	7:I:74:GLY:CA	2.39	0.53
5:C:77:ILE:HG23	5:C:78:GLY:N	2.24	0.53
8:J:6:ILE:O	8:J:76:ILE:N	2.36	0.53
1:1:1158:C:C4	1:1:1160:G:C4	2.97	0.52
1:1:1286:U:O2'	1:1:1287:A:OP1	2.20	0.52
7:I:36:GLU:OE1	7:I:36:GLU:N	2.30	0.52
6:G:46:ALA:HA	6:G:49:THR:HG22	1.92	0.52
1:1:1125:U:O2'	1:1:1126:U:O5'	2.23	0.52
1:1:1202:U:O2	10:N:82:ILE:HG21	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1101:A:H1'	1:1:1102:A:O4'	2.09	0.52
8:J:87:LEU:HA	8:J:90:LEU:HD12	1.90	0.52
10:N:93:ILE:HD12	10:N:96:LEU:HD23	1.92	0.52
1:1:1205:U:H2'	1:1:1206:G:C8	2.45	0.52
10:N:73:PHE:CZ	10:N:78:GLY:HA2	2.45	0.52
5:C:13:GLY:HA2	5:C:18:TRP:HH2	1.75	0.52
10:N:54:ASP:HA	10:N:59:ARG:NE	2.24	0.52
1:1:1298:U:H1'	1:1:1299:A:C2	2.45	0.52
7:I:22:LYS:HG2	7:I:23:PRO:HD2	1.92	0.52
1:1:1226:C:OP2	9:M:102:THR:HG21	2.10	0.52
7:I:29:VAL:CG1	7:I:32:GLN:HA	2.40	0.52
8:J:8:ILE:O	8:J:73:LEU:HA	2.10	0.52
8:J:53:ILE:HD11	8:J:61:ALA:HB1	1.92	0.52
4:B:78:GLU:O	4:B:81:LYS:CG	2.52	0.51
9:M:16:VAL:O	9:M:30:SER:OG	2.27	0.51
10:N:34:VAL:HG13	10:N:35:ASN:N	2.25	0.51
1:1:1158:C:N4	1:1:1160:G:C2	2.78	0.51
1:1:1298:U:H4'	1:1:1299:A:H5'	1.93	0.51
1:1:960:U:O2'	1:1:1223:C:H4'	2.10	0.51
8:J:19:ASP:O	8:J:22:THR:OG1	2.28	0.51
8:J:88:MET:HG3	8:J:89:ARG:NH2	2.25	0.51
1:1:1108:G:H2'	1:1:1109:C:H5'	1.93	0.51
4:B:88:ASP:OD1	4:B:88:ASP:O	2.28	0.51
8:J:7:ARG:N	8:J:101:SER:O	2.30	0.51
9:M:20:THR:HG22	9:M:30:SER:HB2	1.92	0.51
1:1:1207:2MG:H2'	1:1:1208:C:C6	2.45	0.51
4:B:83:ALA:O	4:B:86:SER:OG	2.28	0.51
7:I:22:LYS:CG	7:I:23:PRO:HD2	2.41	0.51
1:1:1332:A:H2'	1:1:1333:A:O4'	2.11	0.51
5:C:175:LEU:HD23	5:C:182:ILE:HG13	1.92	0.51
9:M:65:VAL:HG22	9:M:66:GLU:HG3	1.92	0.51
11:S:43:ASN:OD1	11:S:44:MET:N	2.44	0.51
1:1:996:A:H2'	1:1:997:U:C6	2.45	0.51
1:1:1237:C:HO2'	1:1:1335:U:C4'	2.14	0.51
1:1:1328:C:H2'	1:1:1329:A:O4'	2.11	0.51
9:M:12:HIS:O	9:M:44:LYS:NZ	2.33	0.51
1:1:1129:C:O4'	1:1:1146:A:N6	2.41	0.51
1:1:1163:A:C6	1:1:1164:G:C5	2.99	0.51
1:1:1209:C:O2'	1:1:1210:C:H5'	2.11	0.51
1:1:1293:C:H2'	1:1:1294:G:O4'	2.09	0.51
4:B:188:ASP:N	4:B:191:SER:OG	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:988:G:N1	1:1:989:U:C2	2.79	0.50
1:1:988:G:C2	1:1:989:U:H1'	2.46	0.50
1:1:1099:G:C5	1:1:1100:C:C2	2.99	0.50
1:1:1365:G:C6	1:1:1366:C:C4	3.00	0.50
7:I:10:GLY:HA2	7:I:81:HIS:ND1	2.26	0.50
10:N:47:LYS:O	10:N:50:THR:OG1	2.28	0.50
1:1:1029:U:H3'	1:1:1031:C:N4	2.26	0.50
1:1:1162:C:H2'	1:1:1163:A:O4'	2.12	0.50
7:I:12:ARG:HG3	7:I:13:LYS:HG2	1.92	0.50
4:B:99:GLY:HA2	4:B:102:THR:HG22	1.92	0.50
4:B:129:LEU:N	4:B:129:LEU:HD22	2.27	0.50
8:J:34:ALA:HB1	8:J:79:PRO:HA	1.94	0.50
1:1:1350:A:OP1	7:I:123:ARG:NE	2.40	0.50
5:C:13:GLY:HA2	5:C:18:TRP:CH2	2.47	0.50
9:M:33:ILE:HD11	9:M:63:PHE:CZ	2.45	0.50
1:1:964:A:C1'	8:J:57:VAL:HG11	2.42	0.50
1:1:1063:C:C4	1:1:1064:G:C5	3.00	0.50
1:1:1148:U:H2'	1:1:1149:C:O4'	2.11	0.50
2:2:15:A:H2'	2:2:16:A:N7	2.27	0.50
3:3:39:A:C4	3:3:40:C:C6	2.99	0.50
1:1:950:U:H1'	1:1:971:G:N7	2.26	0.50
1:1:1160:G:N1	1:1:1181:G:O6	2.45	0.50
1:1:1228:C:H1'	9:M:116:ILE:HD13	1.93	0.50
1:1:1379:G:N3	6:G:78:ARG:NH2	2.52	0.50
5:C:77:ILE:HG23	5:C:78:GLY:H	1.77	0.50
7:I:41:ARG:HB2	7:I:41:ARG:CZ	2.42	0.50
8:J:66:GLU:HB3	10:N:99:ALA:HB2	1.93	0.50
8:J:80:THR:HB	8:J:83:THR:OG1	2.12	0.50
4:B:99:GLY:HA2	4:B:102:THR:CG2	2.42	0.50
1:1:1077:G:C2	1:1:1080:A:OP2	2.65	0.50
4:B:108:ARG:O	4:B:112:LYS:HG2	2.11	0.50
4:B:162:PHE:CE2	4:B:214:LEU:HD21	2.46	0.50
7:I:107:ASP:OD1	7:I:108:ALA:N	2.44	0.50
8:J:69:THR:O	8:J:69:THR:HG23	2.11	0.49
1:1:1121:U:H2'	1:1:1122:U:O4'	2.11	0.49
1:1:1345:U:O2	1:1:1375:A:N6	2.45	0.49
7:I:11:ARG:HB2	7:I:106:ARG:HH21	1.77	0.49
8:J:76:ILE:CG2	8:J:79:PRO:HB3	2.42	0.49
7:I:30:ILE:HG22	7:I:38:TYR:CE2	2.47	0.49
8:J:39:PRO:HA	8:J:73:LEU:O	2.12	0.49
9:M:57:ARG:O	9:M:60:VAL:HG22	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:24:ARG:HG2	10:N:51:LEU:HD12	1.95	0.49
1:1:978:A:C6	1:1:1318:A:C6	3.01	0.49
5:C:35:SER:O	5:C:39:VAL:HG23	2.13	0.49
10:N:64:CYS:HB2	10:N:80:SER:N	2.27	0.49
4:B:133:GLU:O	4:B:137:ARG:HG2	2.12	0.49
5:C:52:VAL:HB	5:C:69:HIS:O	2.13	0.49
6:G:49:THR:HG23	6:G:121:ALA:CB	2.42	0.49
1:1:1160:G:C6	1:1:1181:G:C6	3.00	0.49
1:1:1347:G:O2'	1:1:1348:U:OP2	2.25	0.49
1:1:1130:A:H2'	1:1:1131:G:O4'	2.11	0.49
3:3:31:G:C2	3:3:32:G:C8	3.01	0.49
7:I:92:GLU:HA	7:I:92:GLU:OE1	2.12	0.49
8:J:82:LYS:HA	8:J:85:ASP:OD2	2.13	0.49
4:B:32:PHE:N	4:B:40:ILE:O	2.46	0.49
4:B:96:TRP:CD2	4:B:100:MET:SD	3.06	0.49
1:1:1338:G:N2	3:3:42:C:O2'	2.46	0.49
9:M:22:ILE:HG23	9:M:66:GLU:OE2	2.13	0.49
1:1:945:G:N1	1:1:1337:G:C2	2.80	0.49
1:1:1329:A:H5''	9:M:26:GLY:H	1.77	0.49
3:3:39:A:C5	3:3:40:C:C5	3.00	0.49
5:C:116:VAL:O	5:C:119:SER:OG	2.29	0.49
1:1:935:A:C6	1:1:936:C:C4	3.01	0.48
1:1:1244:G:H2'	1:1:1245:C:C6	2.48	0.48
1:1:1127:G:H1'	1:1:1280:A:N6	2.28	0.48
4:B:143:LYS:HA	4:B:146:ASN:ND2	2.27	0.48
5:C:47:LEU:HD13	5:C:52:VAL:HG21	1.95	0.48
1:1:1076:U:H2'	1:1:1077:G:H8	1.78	0.48
1:1:1346:A:O4'	1:1:1348:U:C6	2.65	0.48
4:B:203:ASN:ND2	4:B:205:ASP:OD1	2.46	0.48
8:J:23:ALA:O	8:J:27:GLU:HG2	2.13	0.48
1:1:934:C:N4	1:1:1344:C:H2'	2.27	0.48
1:1:1104:G:H2'	1:1:1105:A:H8	1.77	0.48
1:1:1216:A:P	10:N:3:LYS:HZ1	2.27	0.48
1:1:1227:A:H2'	9:M:116:ILE:HG22	1.95	0.48
1:1:1315:U:H2'	1:1:1316:G:O4'	2.14	0.48
1:1:1328:C:H5''	9:M:28:THR:HG21	1.95	0.48
3:3:40:C:N3	3:3:41:C:C5	2.81	0.48
5:C:87:LEU:O	5:C:91:VAL:HG22	2.14	0.48
6:G:68:ASN:HB3	6:G:130:ASN:OD1	2.13	0.48
1:1:1269:A:C2	1:1:1313:U:O4'	2.66	0.48
5:C:6:HIS:CE1	5:C:8:ASN:HB3	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1077:G:C6	1:1:1081:A:C6	3.02	0.48
1:1:1159:U:C5	1:1:1182:G:C4	3.02	0.48
4:B:142:GLU:O	4:B:146:ASN:OD1	2.32	0.48
1:1:1177:G:O6	1:1:1178:G:C2	2.67	0.48
5:C:88:ARG:HA	5:C:91:VAL:HG22	1.95	0.48
7:I:50:GLN:O	7:I:53:GLU:HB3	2.14	0.48
1:1:1237:C:O2	1:1:1334:G:O2'	2.31	0.48
1:1:1260:G:H4'	1:1:1283:U:O2'	2.13	0.48
1:1:1372:U:C4	1:1:1373:G:C5	3.02	0.48
8:J:6:ILE:CG1	8:J:79:PRO:HG3	2.42	0.48
8:J:18:ILE:HD12	8:J:70:HIS:HB2	1.96	0.48
11:S:44:MET:HA	11:S:47:LEU:CD1	2.44	0.48
2:2:15:A:H2'	2:2:16:A:C8	2.49	0.48
6:G:6:VAL:HG12	6:G:7:ILE:N	2.28	0.48
7:I:52:LEU:HB3	7:I:58:VAL:HG12	1.95	0.48
8:J:46:LYS:HA	8:J:67:ILE:O	2.14	0.48
1:1:938:A:N3	1:1:1376:U:O2'	2.29	0.48
1:1:939:G:C6	1:1:940:C:C4	3.02	0.48
1:1:993:G:H2'	1:1:995:C:H41	1.79	0.48
1:1:1137:C:O2	1:1:1138:G:N2	2.46	0.48
1:1:1141:C:O2'	1:1:1142:G:P	2.72	0.48
11:S:41:PHE:O	11:S:44:MET:HG2	2.13	0.47
1:1:933:G:N2	1:1:1385:G:C2	2.82	0.47
1:1:1210:C:N4	1:1:1211:U:O4	2.47	0.47
1:1:1346:A:C8	1:1:1348:U:C2	3.02	0.47
5:C:8:ASN:O	5:C:12:LEU:N	2.46	0.47
5:C:69:HIS:CD2	5:C:104:ALA:HB3	2.49	0.47
1:1:1305:G:H2'	1:1:1306:A:C8	2.49	0.47
1:1:1367:C:C2	1:1:1368:A:C8	3.03	0.47
7:I:107:ASP:OD1	7:I:109:ARG:N	2.45	0.47
9:M:16:VAL:HG13	9:M:17:ILE:N	2.30	0.47
1:1:998:C:N3	1:1:1043:G:N1	2.47	0.47
5:C:39:VAL:O	5:C:43:LEU:HG	2.14	0.47
7:I:55:VAL:HG23	7:I:57:MET:H	1.79	0.47
11:S:15:LEU:HD23	11:S:15:LEU:C	2.39	0.47
1:1:949:A:C4	1:1:1233:G:N2	2.81	0.47
1:1:1029:U:H2'	1:1:1032:G:O6	2.15	0.47
1:1:1050:G:C2	1:1:1209:C:C2	3.03	0.47
1:1:1177:G:O6	1:1:1178:G:N1	2.47	0.47
1:1:1205:U:C2'	1:1:1206:G:H8	2.27	0.47
1:1:1316:G:H22	1:1:1319:A:P	2.37	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:32:G:C2	3:3:41:C:C2	3.03	0.47
4:B:47:VAL:HB	4:B:48:PRO:HD3	1.97	0.47
4:B:213:TYR:O	4:B:217:VAL:HG23	2.15	0.47
8:J:22:THR:O	8:J:26:VAL:HG12	2.15	0.47
8:J:65:TYR:CE1	10:N:89:MET:HE3	2.49	0.47
10:N:6:MET:HE2	10:N:6:MET:N	2.30	0.47
11:S:66:MET:HB3	11:S:74:PHE:CZ	2.50	0.47
1:1:1292:G:C6	1:1:1293:C:C5	3.03	0.47
1:1:1351:U:O4'	6:G:33:ASP:OD1	2.32	0.47
4:B:112:LYS:O	4:B:116:ASP:CG	2.58	0.47
1:1:1304:G:N1	1:1:1305:G:N2	2.63	0.47
3:3:42:C:C2	3:3:43:G:C8	3.02	0.47
1:1:934:C:N3	1:1:1344:C:C5	2.84	0.47
1:1:1065:U:H5''	1:1:1190:G:N2	2.30	0.47
1:1:1382:C:H5'	6:G:79:ARG:HH21	1.79	0.47
5:C:11:ARG:HB3	5:C:16:LYS:HG2	1.96	0.47
7:I:55:VAL:O	7:I:56:ASP:CG	2.58	0.47
7:I:90:TYR:CE2	7:I:91:ASP:HB2	2.50	0.47
1:1:1272:G:H2'	1:1:1273:C:C6	2.49	0.46
8:J:8:ILE:HD12	8:J:74:VAL:O	2.15	0.46
10:N:24:ARG:NH1	10:N:51:LEU:HB2	2.30	0.46
1:1:949:A:C4	1:1:1233:G:C2	3.03	0.46
1:1:1064:G:H1'	1:1:1190:G:N2	2.30	0.46
1:1:1114:C:C4	1:1:1115:U:C4	3.04	0.46
1:1:1227:A:C2	11:S:83:HIS:HB3	2.50	0.46
1:1:1276:G:H2'	1:1:1277:C:O4'	2.16	0.46
1:1:1329:A:O2'	1:1:1330:U:H5'	2.15	0.46
1:1:1347:G:H5''	7:I:110:GLN:O	2.14	0.46
1:1:1383:C:O2	1:1:1383:C:C2'	2.64	0.46
5:C:88:ARG:HA	5:C:91:VAL:CG2	2.46	0.46
8:J:10:LEU:CD2	8:J:98:VAL:HG22	2.45	0.46
10:N:88:ALA:CB	10:N:96:LEU:HD23	2.45	0.46
11:S:42:PRO:O	11:S:45:ILE:HG12	2.15	0.46
1:1:1121:U:C4	1:1:1122:U:C4	3.03	0.46
1:1:1158:C:N4	1:1:1160:G:N3	2.63	0.46
1:1:1316:G:N2	1:1:1318:A:H3'	2.29	0.46
4:B:173:ILE:O	4:B:177:ASN:OD1	2.33	0.46
8:J:57:VAL:O	8:J:58:ASN:C	2.57	0.46
1:1:1060:U:H4'	8:J:54:SER:HB2	1.96	0.46
1:1:1108:G:H4'	1:1:1191:A:O4'	2.15	0.46
1:1:1225:A:OP2	9:M:103:LYS:NZ	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1226:C:O2	11:S:83:HIS:CE1	2.68	0.46
2:2:15:A:C6	3:3:38:A:N6	2.83	0.46
3:3:28:C:C4	3:3:29:C:C4	3.03	0.46
5:C:168:TYR:CZ	5:C:170:GLU:OE2	2.69	0.46
9:M:87:ARG:HG3	9:M:97:VAL:HG12	1.97	0.46
10:N:27:LEU:HD21	10:N:44:ALA:O	2.15	0.46
11:S:33:THR:OG1	11:S:34:TRP:N	2.49	0.46
5:C:36:ASP:OD1	5:C:36:ASP:N	2.48	0.46
7:I:13:LYS:CG	7:I:74:GLY:HA3	2.43	0.46
7:I:18:ARG:NH2	7:I:20:PHE:HE2	2.14	0.46
10:N:16:LEU:C	10:N:16:LEU:HD23	2.40	0.46
5:C:113:ALA:HB1	5:C:185:ASN:CG	2.40	0.46
6:G:115:SER:N	6:G:119:ARG:NH1	2.63	0.46
9:M:83:LEU:CG	11:S:74:PHE:HE1	2.28	0.46
1:1:1298:U:H4'	1:1:1299:A:O4'	2.15	0.46
7:I:45:ARG:HB3	7:I:49:ARG:NH1	2.31	0.46
7:I:111:VAL:HG22	7:I:112:GLU:N	2.31	0.46
1:1:1202:U:C4	1:1:1203:C:C2	3.04	0.46
4:B:66:LYS:O	4:B:159:ASP:N	2.41	0.46
1:1:1060:U:H4'	8:J:54:SER:CB	2.46	0.46
4:B:194:ASP:OD1	4:B:194:ASP:N	2.48	0.46
7:I:107:ASP:OD1	7:I:107:ASP:C	2.59	0.46
8:J:92:LEU:HD23	8:J:98:VAL:HG21	1.98	0.46
1:1:1089:G:O2'	1:1:1169:A:N6	2.35	0.46
1:1:1163:A:C6	1:1:1174:G:C6	3.03	0.46
1:1:1330:U:O4	1:1:1331:G:C6	2.70	0.46
4:B:28:LYS:N	4:B:29:PRO:CD	2.78	0.46
4:B:118:GLU:O	4:B:122:GLN:HG2	2.16	0.46
7:I:92:GLU:OE2	7:I:95:ARG:HD2	2.15	0.46
9:M:71:ARG:O	9:M:75:MET:HG2	2.16	0.46
1:1:1005:A:N6	1:1:1024:G:O2'	2.37	0.45
1:1:1164:G:C6	1:1:1165:U:C4	3.04	0.45
4:B:34:ALA:HA	4:B:38:VAL:O	2.15	0.45
5:C:18:TRP:HZ2	10:N:97:LYS:HB2	1.81	0.45
3:3:39:A:C5	3:3:40:C:C4	3.04	0.45
8:J:34:ALA:HB3	8:J:83:THR:HG21	1.98	0.45
3:3:28:C:H2'	3:3:29:C:O5'	2.17	0.45
4:B:188:ASP:O	4:B:191:SER:OG	2.26	0.45
7:I:44:ALA:O	7:I:48:VAL:HG22	2.16	0.45
8:J:7:ARG:HA	8:J:75:ASP:HA	1.98	0.45
8:J:89:ARG:NE	8:J:89:ARG:HA	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1146:A:C6	1:1:1147:C:C2	3.05	0.45
1:1:1277:C:O2'	1:1:1279:G:H8	1.99	0.45
5:C:11:ARG:CB	5:C:16:LYS:HG2	2.46	0.45
6:G:46:ALA:HB3	6:G:120:LEU:HD23	1.97	0.45
7:I:6:TYR:CE2	7:I:23:PRO:HD3	2.51	0.45
7:I:42:GLU:OE1	7:I:49:ARG:NH2	2.42	0.45
9:M:52:GLN:O	9:M:55:THR:HG22	2.16	0.45
1:1:932:C:C2	1:1:1386:G:N2	2.84	0.45
1:1:1102:A:O2'	1:1:1103:C:H5'	2.16	0.45
1:1:1226:C:H4'	1:1:1227:A:OP1	2.15	0.45
4:B:16:PHE:HB2	4:B:203:ASN:ND2	2.31	0.45
4:B:167:ASP:O	4:B:170:HIS:HB2	2.15	0.45
5:C:43:LEU:O	5:C:47:LEU:HG	2.17	0.45
5:C:179:ARG:HD3	5:C:207:ILE:O	2.16	0.45
8:J:35:GLN:O	8:J:76:ILE:HG23	2.17	0.45
8:J:80:THR:O	8:J:83:THR:HB	2.17	0.45
9:M:14:HIS:HA	9:M:42:ASP:O	2.16	0.45
1:1:1038:C:H2'	1:1:1039:G:C8	2.52	0.45
1:1:1099:G:H3'	1:1:1100:C:C5	2.51	0.45
1:1:1102:A:C6	1:1:1103:C:C4	3.05	0.45
1:1:1240:U:P	6:G:116:MET:HB2	2.56	0.45
1:1:1340:A:C2	1:1:1341:U:H1'	2.52	0.45
4:B:84:ALA:HB1	4:B:89:GLN:O	2.16	0.45
4:B:179:LEU:N	4:B:179:LEU:HD22	2.31	0.45
5:C:140:ASN:HA	5:C:143:ARG:NH2	2.32	0.45
6:G:104:ILE:HD12	6:G:124:LEU:HD11	1.99	0.45
1:1:978:A:C4	1:1:1319:A:C2	3.04	0.45
1:1:1043:G:C6	1:1:1044:A:C6	3.04	0.45
1:1:1090:U:O3'	1:1:1171:A:O2'	2.34	0.45
4:B:14:VAL:O	4:B:203:ASN:N	2.47	0.45
7:I:21:ILE:HG12	7:I:61:LEU:HD12	1.98	0.45
11:S:35:SER:O	11:S:38:SER:OG	2.20	0.45
1:1:1118:U:H1'	1:1:1179:A:C8	2.52	0.45
1:1:1232:U:C4	1:1:1233:G:N7	2.84	0.45
5:C:40:ARG:HH21	5:C:56:VAL:HA	1.81	0.45
5:C:56:VAL:CG2	5:C:67:THR:HB	2.46	0.45
7:I:38:TYR:HD1	7:I:39:PHE:CE2	2.35	0.45
9:M:23:TYR:CE1	9:M:69:LEU:HD23	2.52	0.45
10:N:14:VAL:O	10:N:18:ASP:CG	2.59	0.45
1:1:1332:A:N7	1:1:1333:A:C4	2.85	0.45
1:1:1350:A:OP1	7:I:123:ARG:NH2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:120:GLN:O	4:B:124:GLY:N	2.50	0.45
8:J:39:PRO:HA	8:J:74:VAL:HG22	1.99	0.45
1:1:935:A:C6	1:1:936:C:C5	3.05	0.45
1:1:1074:G:C2	1:1:1102:A:C5	3.04	0.45
1:1:1136:C:H3'	1:1:1137:C:H5''	1.99	0.45
5:C:68:ILE:HB	5:C:103:ILE:HD13	1.99	0.45
6:G:102:ARG:O	6:G:105:VAL:HG22	2.17	0.45
7:I:18:ARG:NH2	7:I:20:PHE:CE2	2.84	0.45
11:S:15:LEU:C	11:S:15:LEU:CD2	2.90	0.45
1:1:1215:G:C2	1:1:1216:A:C8	3.05	0.44
8:J:51:VAL:HB	10:N:81:ARG:HB2	1.97	0.44
1:1:1006:G:C6	1:1:1024:G:H1'	2.52	0.44
1:1:1151:A:O2'	1:1:1152:A:H5''	2.17	0.44
1:1:1198:G:H2'	1:1:1199:U:C6	2.53	0.44
1:1:1219:A:H5''	10:N:53:ARG:HH11	1.82	0.44
3:3:39:A:C6	3:3:40:C:N3	2.86	0.44
7:I:48:VAL:O	7:I:51:PRO:HD2	2.17	0.44
9:M:23:TYR:CD1	9:M:66:GLU:HA	2.52	0.44
11:S:44:MET:HA	11:S:47:LEU:HD12	1.98	0.44
1:1:1075:U:C4	1:1:1076:U:O4	2.71	0.44
1:1:1089:G:H1'	1:1:1167:A:N6	2.32	0.44
1:1:1323:G:H2'	1:1:1324:A:C8	2.52	0.44
4:B:22:TYR:O	4:B:23:TRP:CG	2.70	0.44
7:I:6:TYR:HB2	7:I:21:ILE:HG23	1.99	0.44
8:J:12:ALA:HB3	8:J:18:ILE:CD1	2.46	0.44
1:1:970:C:O5'	1:1:970:C:H6	2.01	0.44
1:1:1166:G:C2	1:1:1169:A:OP2	2.70	0.44
1:1:1170:A:H2'	1:1:1171:A:O4'	2.18	0.44
1:1:1236:A:C2	1:1:1237:C:N3	2.86	0.44
5:C:53:SER:N	5:C:69:HIS:O	2.49	0.44
1:1:1115:U:C4	1:1:1116:U:C4	3.06	0.44
1:1:1349:A:H2'	1:1:1350:A:O4'	2.17	0.44
1:1:1350:A:O2'	6:G:33:ASP:OD1	2.28	0.44
4:B:184:PHE:CD2	4:B:198:PHE:HB2	2.52	0.44
7:I:60:LYS:C	7:I:61:LEU:HD22	2.41	0.44
8:J:53:ILE:HG23	8:J:62:ARG:HA	2.00	0.44
11:S:20:GLU:O	11:S:23:VAL:HG12	2.18	0.44
1:1:988:G:C2	1:1:1218:C:C2	3.05	0.44
1:1:1033:G:C6	1:1:1034:G:C5	3.05	0.44
1:1:1054:C:C2	1:1:1196:A:C6	3.05	0.44
1:1:1099:G:C6	1:1:1100:C:C2	3.06	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1134:G:H2'	1:1:1135:U:C6	2.52	0.44
1:1:1213:A:O2'	1:1:1215:G:N7	2.34	0.44
1:1:1338:G:C6	1:1:1339:A:C5	3.05	0.44
3:3:31:G:H2'	3:3:31:G:N3	2.32	0.44
4:B:152:LYS:HG3	4:B:153:ASP:OD1	2.17	0.44
5:C:43:LEU:O	5:C:47:LEU:N	2.43	0.44
5:C:203:PHE:CD1	5:C:204:LYS:N	2.85	0.44
7:I:46:MET:SD	7:I:49:ARG:NH2	2.90	0.44
1:1:1179:A:H2'	1:1:1180:A:O4'	2.17	0.44
4:B:163:VAL:HG13	4:B:169:GLU:CG	2.48	0.44
10:N:64:CYS:O	10:N:68:GLY:HA2	2.18	0.44
1:1:935:A:N1	1:1:936:C:C4	2.86	0.44
1:1:1186:G:C4	1:1:1187:G:C8	3.06	0.44
1:1:1304:G:N2	1:1:1332:A:OP2	2.50	0.44
1:1:1373:G:O5'	1:1:1373:G:H8	2.01	0.44
4:B:101:LEU:HB2	4:B:175:GLU:OE1	2.18	0.44
5:C:168:TYR:CD1	5:C:169:ARG:N	2.86	0.44
6:G:111:ARG:HD3	6:G:119:ARG:HA	1.99	0.44
1:1:1090:U:H5'	1:1:1170:A:C2	2.53	0.44
1:1:1092:A:C4	1:1:1183:U:O4	2.70	0.44
1:1:1101:A:O2'	1:1:1102:A:P	2.75	0.44
1:1:1142:G:H2'	1:1:1143:G:O4'	2.18	0.44
1:1:1347:G:C5	7:I:109:ARG:NH1	2.86	0.44
1:1:1033:G:C2	1:1:1034:G:C4	3.06	0.43
1:1:1076:U:H2'	1:1:1077:G:C8	2.53	0.43
1:1:1099:G:C6	1:1:1100:C:O2	2.71	0.43
1:1:1183:U:H4'	1:1:1184:G:OP2	2.16	0.43
5:C:54:ARG:HG3	5:C:69:HIS:ND1	2.33	0.43
6:G:73:VAL:HG22	6:G:74:GLU:N	2.33	0.43
9:M:3:ARG:CZ	9:M:9:ILE:HB	2.48	0.43
9:M:107:ARG:NH2	9:M:111:GLY:O	2.48	0.43
1:1:1042:A:C6	1:1:1043:G:C6	3.06	0.43
1:1:1141:C:C2	1:1:1142:G:C8	3.06	0.43
5:C:6:HIS:ND1	5:C:8:ASN:HB3	2.33	0.43
5:C:23:PHE:CD1	8:J:12:ALA:HA	2.52	0.43
1:1:1138:G:N3	1:1:1138:G:H3'	2.33	0.43
1:1:1237:C:H3'	1:1:1238:A:H5'	2.00	0.43
1:1:1381:U:H1'	6:G:79:ARG:O	2.19	0.43
5:C:113:ALA:CB	5:C:185:ASN:CG	2.86	0.43
6:G:115:SER:HB3	6:G:118:LEU:CB	2.49	0.43
7:I:34:SER:HB2	7:I:36:GLU:OE2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1014:A:H2'	1:1:1015:G:O4'	2.18	0.43
1:1:1091:U:N3	1:1:1095:U:C4	2.87	0.43
1:1:1236:A:C2	1:1:1237:C:C2	3.06	0.43
1:1:1330:U:O4	1:1:1331:G:N1	2.51	0.43
5:C:58:GLU:HB2	5:C:65:ARG:HB3	2.00	0.43
5:C:105:GLU:OE2	5:C:107:ARG:HA	2.18	0.43
5:C:211:MET:SD	8:J:16:ARG:NH1	2.92	0.43
8:J:6:ILE:HB	8:J:76:ILE:HB	1.99	0.43
8:J:92:LEU:HD13	8:J:92:LEU:HA	1.86	0.43
10:N:65:ARG:HG3	10:N:78:GLY:O	2.18	0.43
1:1:1126:U:C2	1:1:1281:C:C4	3.07	0.43
1:1:1147:C:C4	1:1:1148:U:C5	3.06	0.43
4:B:82:ASP:O	4:B:85:LEU:HG	2.18	0.43
5:C:92:ALA:HB2	5:C:99:ALA:HB3	2.00	0.43
5:C:138:VAL:HG11	5:C:168:TYR:CE2	2.53	0.43
6:G:66:LEU:HD12	6:G:66:LEU:O	2.17	0.43
1:1:958:A:C6	1:1:959:A:C6	3.07	0.43
1:1:1288:A:C6	1:1:1289:A:C5	3.07	0.43
5:C:19:ASN:CB	10:N:92:GLU:CD	2.91	0.43
5:C:177:THR:HG22	5:C:179:ARG:N	2.33	0.43
9:M:53:ILE:HG22	9:M:57:ARG:CZ	2.48	0.43
5:C:83:ASP:O	5:C:84:VAL:C	2.62	0.43
7:I:24:GLY:HA3	7:I:62:ASP:CG	2.44	0.43
7:I:64:TYR:O	7:I:65:ILE:HD13	2.19	0.43
8:J:14:ASP:OD1	8:J:14:ASP:C	2.61	0.43
1:1:1052:U:C4	1:1:1200:C:C2	3.07	0.43
1:1:1081:A:C6	1:1:1082:A:C6	3.07	0.43
1:1:1150:A:N6	1:1:1151:A:N6	2.67	0.43
1:1:1277:C:H2'	1:1:1279:G:C8	2.53	0.43
6:G:48:GLU:OE1	6:G:49:THR:N	2.51	0.43
9:M:81:MET:SD	9:M:91:HIS:HB3	2.58	0.43
1:1:1226:C:H2'	9:M:102:THR:HB	2.00	0.43
1:1:1277:C:O2'	1:1:1279:G:H1'	2.19	0.43
1:1:1297:G:N2	6:G:114:LYS:O	2.51	0.43
4:B:28:LYS:O	4:B:31:ILE:HG12	2.19	0.43
1:1:949:A:C6	1:1:1233:G:C6	3.07	0.43
1:1:1370:G:C2	1:1:1371:G:C8	3.06	0.43
4:B:137:ARG:HA	4:B:137:ARG:NE	2.33	0.43
5:C:42:TYR:CZ	5:C:90:VAL:HG11	2.54	0.43
6:G:66:LEU:HD21	6:G:70:ARG:HH21	1.83	0.43
9:M:114:LYS:HB2	9:M:115:PRO:HD2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1029:U:H3'	1:1:1031:C:C4	2.54	0.42
1:1:1379:G:O2'	6:G:78:ARG:NH2	2.52	0.42
7:I:67:VAL:C	7:I:68:LYS:HG3	2.43	0.42
8:J:8:ILE:O	8:J:73:LEU:HG	2.19	0.42
8:J:17:LEU:HD11	8:J:96:VAL:CG2	2.49	0.42
10:N:27:LEU:HD22	10:N:47:LYS:HZ1	1.84	0.42
10:N:64:CYS:HB2	10:N:80:SER:HB3	2.01	0.42
1:1:1084:G:C5	1:1:1085:U:C4	3.07	0.42
1:1:1100:C:C6	1:1:1100:C:OP2	2.72	0.42
1:1:1102:A:C5	1:1:1103:C:C5	3.06	0.42
1:1:1112:C:H1'	5:C:179:ARG:CZ	2.49	0.42
1:1:983:A:H5'	1:1:984:C:OP2	2.19	0.42
1:1:1168:U:O2'	1:1:1168:U:O2	2.35	0.42
1:1:1277:C:H1'	1:1:1282:C:H1'	2.01	0.42
5:C:170:GLU:OE1	5:C:170:GLU:HA	2.20	0.42
8:J:10:LEU:HD21	8:J:98:VAL:HG13	2.01	0.42
8:J:80:THR:O	8:J:84:VAL:HG23	2.20	0.42
1:1:933:G:H1	1:1:1384:C:H42	1.67	0.42
1:1:1004:A:H4'	1:1:1004:A:OP2	2.18	0.42
1:1:1226:C:H4'	11:S:80:TYR:CZ	2.54	0.42
1:1:1356:G:C2	1:1:1357:A:C5	3.08	0.42
1:1:1382:C:O2	1:1:1383:C:H1'	2.20	0.42
3:3:28:C:C4	3:3:29:C:C5	3.07	0.42
4:B:91:PHE:CZ	4:B:150:GLY:HA2	2.53	0.42
4:B:130:THR:HG22	4:B:132:LYS:H	1.84	0.42
1:1:1186:G:C2	1:1:1187:G:C8	3.07	0.42
1:1:1330:U:C4	1:1:1331:G:C6	3.07	0.42
4:B:18:HIS:HB3	4:B:190:ASN:HD22	1.85	0.42
10:N:38:ASP:CG	10:N:39:GLU:N	2.77	0.42
1:1:1029:U:C2	1:1:1033:G:C6	3.07	0.42
1:1:1043:G:O6	1:1:1044:A:N6	2.52	0.42
1:1:1054:C:OP2	1:1:1197:A:P	2.78	0.42
1:1:1147:C:O3'	7:I:7:TYR:OH	2.38	0.42
1:1:1152:A:P	8:J:72:ARG:HH22	2.43	0.42
1:1:1187:G:N1	1:1:1188:A:C2	2.88	0.42
1:1:1299:A:N3	1:1:1299:A:H2'	2.34	0.42
6:G:111:ARG:CZ	6:G:122:ASN:HB3	2.49	0.42
10:N:93:ILE:HD12	10:N:96:LEU:CD2	2.49	0.42
1:1:976:G:N2	1:1:1362:A:H2'	2.34	0.42
1:1:1004:A:C8	1:1:1025:U:H5'	2.54	0.42
1:1:1098:C:H2'	1:1:1099:G:H8	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1108:G:O2'	1:1:1191:A:C1'	2.67	0.42
1:1:1118:U:O4	1:1:1156:G:N2	2.53	0.42
4:B:205:ASP:OD1	4:B:205:ASP:N	2.52	0.42
5:C:123:GLN:HG3	5:C:126:ARG:HH22	1.84	0.42
8:J:8:ILE:HB	8:J:74:VAL:HB	2.00	0.42
9:M:53:ILE:O	9:M:57:ARG:HG3	2.19	0.42
1:1:958:A:N6	1:1:1221:G:O2'	2.53	0.42
1:1:1061:G:C5	1:1:1062:U:C4	3.07	0.42
1:1:1213:A:C8	1:1:1215:G:C5	3.08	0.42
1:1:1304:G:C6	1:1:1305:G:C2	3.08	0.42
1:1:1386:G:H5''	1:1:1386:G:H8	1.83	0.42
7:I:127:PHE:O	7:I:127:PHE:CG	2.72	0.42
10:N:54:ASP:HA	10:N:59:ARG:HE	1.84	0.42
1:1:1005:A:N7	1:1:1025:U:OP1	2.53	0.42
1:1:1227:A:O2'	9:M:114:LYS:NZ	2.53	0.42
4:B:189:THR:O	4:B:190:ASN:HB2	2.19	0.42
4:B:209:ALA:HB1	4:B:213:TYR:CZ	2.55	0.42
5:C:42:TYR:CZ	5:C:46:GLU:HG3	2.55	0.42
6:G:115:SER:C	6:G:119:ARG:NH1	2.78	0.42
1:1:951:G:C6	1:1:952:U:C4	3.08	0.41
1:1:1138:G:H2'	1:1:1140:C:O4'	2.19	0.41
1:1:1142:G:C2	1:1:1143:G:H1'	2.55	0.41
1:1:1336:C:H4'	1:1:1337:G:O4'	2.19	0.41
3:3:39:A:C6	3:3:40:C:C4	3.08	0.41
4:B:142:GLU:HA	4:B:142:GLU:OE1	2.20	0.41
5:C:129:MET:HG3	5:C:132:ARG:H	1.85	0.41
6:G:2:PRO:HG2	6:G:5:ARG:O	2.19	0.41
7:I:15:SER:HA	7:I:68:LYS:O	2.20	0.41
1:1:990:C:N4	1:1:991:U:O4	2.53	0.41
1:1:1102:A:H2'	1:1:1103:C:H6	1.85	0.41
1:1:1165:U:O2	1:1:1171:A:N1	2.52	0.41
1:1:1206:G:C5	1:1:1207:2MG:C5	3.08	0.41
5:C:34:ASP:CG	5:C:38:LYS:HE2	2.45	0.41
5:C:74:GLY:HA2	5:C:77:ILE:HG22	2.02	0.41
7:I:94:LEU:HA	7:I:97:GLU:CD	2.45	0.41
1:1:1114:C:H2'	1:1:1115:U:C6	2.54	0.41
4:B:68:LEU:HD12	4:B:69:PHE:H	1.84	0.41
5:C:56:VAL:HG22	5:C:67:THR:HB	2.02	0.41
7:I:4:ASN:OD1	7:I:6:TYR:CE1	2.74	0.41
7:I:23:PRO:HA	7:I:61:LEU:HD13	2.02	0.41
8:J:21:ALA:HA	8:J:24:GLU:CD	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:940:C:N3	1:1:941:G:C5	2.88	0.41
1:1:976:G:OP2	1:1:1358:U:O2'	2.38	0.41
3:3:39:A:N1	3:3:40:C:C2	2.88	0.41
4:B:183:VAL:H	4:B:197:ASP:HB3	1.85	0.41
4:B:184:PHE:HA	4:B:198:PHE:O	2.20	0.41
5:C:68:ILE:HB	5:C:103:ILE:CD1	2.51	0.41
7:I:22:LYS:O	7:I:23:PRO:C	2.63	0.41
7:I:124:ARG:HG3	7:I:125:PRO:CD	2.49	0.41
1:1:988:G:N2	1:1:989:U:H1'	2.36	0.41
1:1:990:C:C4	1:1:991:U:O4	2.74	0.41
1:1:1148:U:H5'	7:I:7:TYR:HH	1.84	0.41
1:1:1207:2MG:C6	1:1:1208:C:C4	3.09	0.41
1:1:1338:G:O6	1:1:1339:A:N6	2.54	0.41
2:2:18:G:H5'	2:2:19:U:OP1	2.21	0.41
4:B:12:ALA:HB3	4:B:14:VAL:HG23	2.01	0.41
5:C:58:GLU:O	5:C:64:ILE:HA	2.20	0.41
5:C:168:TYR:CE1	5:C:170:GLU:OE2	2.74	0.41
5:C:179:ARG:HB3	5:C:206:GLU:OE2	2.20	0.41
7:I:11:ARG:O	7:I:106:ARG:CZ	2.68	0.41
8:J:17:LEU:HD21	8:J:96:VAL:HG23	2.02	0.41
8:J:53:ILE:CG2	8:J:63:ASP:CG	2.94	0.41
1:1:975:A:N3	1:1:975:A:H5'	2.35	0.41
1:1:1096:C:H2'	1:1:1097:C:C6	2.55	0.41
1:1:1222:G:H2'	1:1:1223:C:O4'	2.21	0.41
1:1:1227:A:H2'	9:M:116:ILE:CG2	2.50	0.41
1:1:1303:C:N4	1:1:1304:G:C6	2.89	0.41
6:G:111:ARG:NH1	6:G:123:GLU:OE2	2.47	0.41
7:I:35:LEU:HD21	7:I:45:ARG:HB3	2.01	0.41
9:M:37:ALA:HB1	9:M:39:ILE:CD1	2.50	0.41
9:M:54:ASP:HA	9:M:57:ARG:HD2	2.02	0.41
10:N:33:ASP:OD1	10:N:34:VAL:N	2.53	0.41
1:1:940:C:C4	1:1:941:G:N7	2.88	0.41
1:1:950:U:OP2	9:M:101:ARG:NH1	2.41	0.41
1:1:954:G:H2'	1:1:955:U:C6	2.56	0.41
1:1:1036:A:C6	1:1:1037:C:C2	3.08	0.41
1:1:1101:A:H4'	1:1:1102:A:C5'	2.51	0.41
1:1:1143:G:N2	1:1:1144:G:H1'	2.35	0.41
1:1:1237:C:C5	1:1:1336:C:N4	2.89	0.41
1:1:1269:A:N1	1:1:1312:G:O2'	2.35	0.41
1:1:1287:A:N1	1:1:1370:G:N2	2.60	0.41
1:1:932:C:OP2	1:1:932:C:C6	2.65	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:991:U:C2	1:1:1212:U:O4'	2.74	0.41
1:1:1143:G:C4	1:1:1144:G:C8	3.08	0.41
1:1:1185:G:C4	1:1:1186:G:C8	3.09	0.41
1:1:1192:C:H2'	1:1:1193:G:O4'	2.20	0.41
1:1:1222:G:OP2	1:1:1322:C:N4	2.47	0.41
1:1:1269:A:H2	1:1:1312:G:N3	2.19	0.41
4:B:127:ASP:OD1	4:B:128:LYS:N	2.53	0.41
5:C:18:TRP:C	5:C:20:SER:N	2.78	0.41
5:C:18:TRP:HB3	5:C:20:SER:O	2.20	0.41
6:G:48:GLU:CD	6:G:49:THR:N	2.79	0.41
6:G:56:LYS:HG3	6:G:57:SER:N	2.36	0.41
8:J:34:ALA:HB2	8:J:80:THR:H	1.85	0.41
1:1:935:A:O2'	1:1:1383:C:C2	2.65	0.41
1:1:935:A:C2	1:1:1383:C:N4	2.89	0.41
1:1:993:G:H2'	1:1:993:G:N3	2.36	0.41
1:1:1071:C:H2'	1:1:1072:G:C8	2.55	0.41
1:1:1183:U:O2'	1:1:1184:G:OP1	2.39	0.41
1:1:1279:G:H4'	1:1:1280:A:OP1	2.21	0.41
1:1:1316:G:C4	1:1:1318:A:OP2	2.74	0.41
3:3:40:C:C2	3:3:41:C:C6	3.09	0.41
4:B:19:GLN:O	4:B:190:ASN:ND2	2.49	0.41
5:C:116:VAL:HG12	5:C:120:ILE:CD1	2.51	0.41
5:C:119:SER:O	5:C:122:SER:OG	2.31	0.41
5:C:121:THR:HG21	5:C:187:SER:OG	2.21	0.41
6:G:18:PHE:HB3	6:G:59:LEU:HD21	2.03	0.41
6:G:44:TYR:N	6:G:44:TYR:CD1	2.88	0.41
6:G:51:ALA:HA	6:G:54:SER:O	2.20	0.41
6:G:68:ASN:OD1	6:G:128:ALA:HA	2.21	0.41
7:I:26:GLY:CA	7:I:61:LEU:O	2.68	0.41
7:I:31:ASN:OD1	7:I:31:ASN:N	2.54	0.41
7:I:42:GLU:O	7:I:43:THR:C	2.63	0.41
9:M:83:LEU:HD21	11:S:74:PHE:CE1	2.56	0.41
10:N:64:CYS:SG	10:N:80:SER:N	2.88	0.41
1:1:959:A:H2	1:1:1221:G:N3	2.19	0.41
1:1:1072:G:H2'	1:1:1073:U:O4'	2.21	0.41
1:1:1108:G:Cl'	1:1:1191:A:H1'	2.51	0.41
3:3:29:C:C4	3:3:30:G:N7	2.89	0.41
4:B:186:ILE:CD1	4:B:200:ILE:HB	2.51	0.41
5:C:18:TRP:O	5:C:19:ASN:C	2.64	0.41
5:C:23:PHE:CD2	5:C:24:ALA:N	2.89	0.41
6:G:66:LEU:HD12	6:G:66:LEU:C	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:100:ALA:O	6:G:104:ILE:HG12	2.21	0.41
6:G:108:ALA:N	6:G:123:GLU:HG3	2.36	0.41
1:1:1028:C:H3'	1:1:1029:U:H5''	2.03	0.40
1:1:1202:U:N3	10:N:82:ILE:HG21	2.35	0.40
1:1:1290:G:C2	1:1:1291:U:H1'	2.56	0.40
4:B:121:SER:HA	4:B:126:PHE:CE2	2.56	0.40
5:C:177:THR:HG22	5:C:180:ALA:H	1.86	0.40
9:M:41:GLU:OE1	9:M:41:GLU:N	2.49	0.40
1:1:1000:A:C6	1:1:1041:G:C6	3.08	0.40
1:1:1055:A:C2	1:1:1056:U:H1'	2.57	0.40
1:1:1076:U:H3	1:1:1081:A:H61	1.68	0.40
1:1:1078:U:C2	1:1:1079:G:C8	3.09	0.40
6:G:24:ALA:O	6:G:27:VAL:HG22	2.20	0.40
7:I:124:ARG:CG	7:I:125:PRO:HD2	2.51	0.40
8:J:61:ALA:O	8:J:62:ARG:C	2.59	0.40
8:J:78:GLU:N	8:J:79:PRO:CD	2.85	0.40
10:N:33:ASP:HB3	10:N:36:ALA:HB2	2.02	0.40
1:1:935:A:O2'	1:1:1383:C:N3	2.51	0.40
1:1:1076:U:C6	1:1:1076:U:OP2	2.73	0.40
1:1:1104:G:O2'	1:1:1105:A:H5'	2.21	0.40
1:1:1185:G:C2	1:1:1186:G:C4	3.09	0.40
1:1:1202:U:H2'	1:1:1203:C:O4'	2.20	0.40
1:1:1347:G:N7	7:I:109:ARG:CZ	2.85	0.40
1:1:1353:G:C6	1:1:1370:G:C6	3.09	0.40
9:M:89:LEU:HA	9:M:92:ARG:HG2	2.03	0.40
10:N:26:GLU:O	10:N:30:ILE:HG12	2.21	0.40
1:1:1004:A:C8	1:1:1026:G:C8	3.10	0.40
1:1:1004:A:H2'	1:1:1005:A:C5'	2.51	0.40
1:1:1151:A:C2	1:1:1152:A:C5	3.10	0.40
1:1:1367:C:C2'	1:1:1368:A:O5'	2.69	0.40
5:C:123:GLN:HG3	5:C:126:ARG:NH2	2.36	0.40
1:1:1168:U:OP2	1:1:1168:U:C6	2.75	0.40
1:1:1225:A:H3'	9:M:102:THR:OG1	2.22	0.40
4:B:27:MET:HE3	4:B:27:MET:HB2	1.98	0.40
4:B:81:LYS:HG3	4:B:82:ASP:OD1	2.21	0.40
9:M:33:ILE:CD1	9:M:59:GLU:HB3	2.51	0.40
11:S:41:PHE:O	11:S:44:MET:CG	2.70	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 PDB entries followed by that with respect to all EM entries.

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	
4	B	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
5	C	209/233 (90%)	200 (96%)	9 (4%)	0	100	100
6	G	129/179 (72%)	126 (98%)	3 (2%)	0	100	100
7	I	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
8	J	98/103 (95%)	95 (97%)	3 (3%)	0	100	100
9	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
10	N	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
11	S	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
All	All	1075/1197 (90%)	1032 (96%)	43 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	
4	B	186/199 (94%)	186 (100%)	0	100	100
5	C	172/190 (90%)	171 (99%)	1 (1%)	84	88
6	G	109/147 (74%)	109 (100%)	0	100	100
7	I	105/107 (98%)	104 (99%)	1 (1%)	73	80
8	J	88/90 (98%)	88 (100%)	0	100	100
9	M	93/96 (97%)	92 (99%)	1 (1%)	70	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	N	83/84 (99%)	83 (100%)	0	100	100
11	S	72/79 (91%)	72 (100%)	0	100	100
All	All	908/992 (92%)	905 (100%)	3 (0%)	90	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	29	PHE
7	I	90	TYR
9	M	91	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	24	ASN
4	B	103	ASN
4	B	168	HIS
4	B	178	ASN
4	B	190	ASN
5	C	25	ASN
6	G	9	GLN
8	J	58	ASN
9	M	12	HIS
10	N	66	GLN
11	S	14	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	455/1541 (29%)	87 (19%)	6 (1%)
2	2	4/5 (80%)	3 (75%)	0
3	3	16/77 (20%)	10 (62%)	1 (6%)
All	All	475/1623 (29%)	100 (21%)	7 (1%)

All (100) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	932	C
1	1	934	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	935	A
1	1	960	U
1	1	963	G
1	1	966	2MG
1	1	969	A
1	1	973	G
1	1	975	A
1	1	976	G
1	1	977	A
1	1	978	A
1	1	993	G
1	1	1003	G
1	1	1004	A
1	1	1020	G
1	1	1022	A
1	1	1024	G
1	1	1025	U
1	1	1026	G
1	1	1028	C
1	1	1029	U
1	1	1030	U
1	1	1031	C
1	1	1032	G
1	1	1033	G
1	1	1037	C
1	1	1043	G
1	1	1056	U
1	1	1065	U
1	1	1066	C
1	1	1076	U
1	1	1081	A
1	1	1085	U
1	1	1088	G
1	1	1094	G
1	1	1095	U
1	1	1100	C
1	1	1101	A
1	1	1102	A
1	1	1104	G
1	1	1124	G
1	1	1135	U
1	1	1137	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1139	G
1	1	1142	G
1	1	1168	U
1	1	1169	A
1	1	1184	G
1	1	1185	G
1	1	1190	G
1	1	1196	A
1	1	1197	A
1	1	1213	A
1	1	1214	C
1	1	1226	C
1	1	1227	A
1	1	1228	C
1	1	1240	U
1	1	1241	G
1	1	1250	A
1	1	1257	A
1	1	1258	G
1	1	1279	G
1	1	1280	A
1	1	1281	C
1	1	1285	A
1	1	1286	U
1	1	1287	A
1	1	1292	G
1	1	1297	G
1	1	1299	A
1	1	1300	G
1	1	1302	C
1	1	1305	G
1	1	1317	C
1	1	1319	A
1	1	1331	G
1	1	1336	C
1	1	1338	G
1	1	1346	A
1	1	1363	A
1	1	1364	U
1	1	1379	G
1	1	1382	C
1	1	1383	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1384	C
2	2	16	A
2	2	18	G
2	2	19	U
3	3	29	C
3	3	31	G
3	3	32	G
3	3	35	C
3	3	36	A
3	3	37	U
3	3	38	A
3	3	39	A
3	3	43	G
3	3	45	G

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1031	C
1	1	1101	A
1	1	1183	U
1	1	1196	A
1	1	1279	G
1	1	1286	U
3	3	36	A

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1	967	1	18,22,23	0.98	2 (11%)	26,32,35	1.29	3 (11%)
1	2MG	1	1207	1	18,26,27	0.99	1 (5%)	16,38,41	1.43	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	1	966	1	18,26,27	1.00	1 (5%)	16,38,41	1.42	3 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1	967	1	-	0/7/25/26	0/2/2/2
1	2MG	1	1207	1	-	0/5/27/28	0/3/3/3
1	2MG	1	966	1	-	0/5/27/28	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	967	5MC	C6-C5	2.62	1.38	1.34
1	1	966	2MG	C6-N1	-2.43	1.34	1.37
1	1	967	5MC	C6-N1	-2.40	1.33	1.38
1	1	1207	2MG	C6-N1	-2.29	1.34	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	967	5MC	C5-C6-N1	-3.45	119.79	123.34
1	1	966	2MG	C3'-C2'-C1'	3.22	105.83	100.98
1	1	1207	2MG	C3'-C2'-C1'	3.17	105.75	100.98
1	1	967	5MC	C5-C4-N3	-2.41	119.08	121.67
1	1	1207	2MG	C8-N7-C5	2.39	107.54	102.99
1	1	1207	2MG	CM2-N2-C2	-2.36	118.65	123.86
1	1	1207	2MG	C5-C6-N1	2.36	118.11	113.95
1	1	966	2MG	C8-N7-C5	2.32	107.41	102.99
1	1	967	5MC	C3'-C2'-C1'	2.30	105.80	101.43
1	1	966	2MG	C5-C6-N1	2.30	118.01	113.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	967	5MC	3	0
1	1	1207	2MG	5	0
1	1	966	2MG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 31 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.

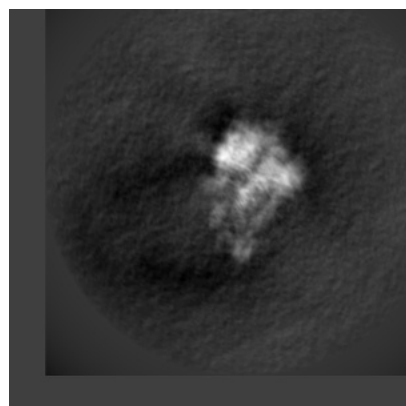
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51967. These allow visual inspection of the internal detail of the map and identification of artifacts.

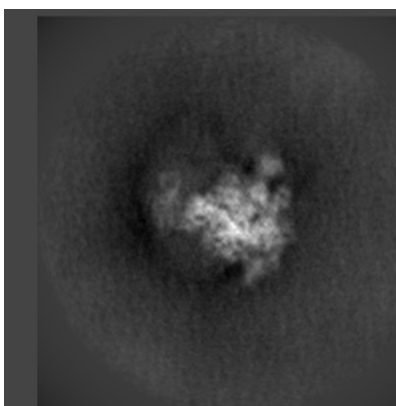
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

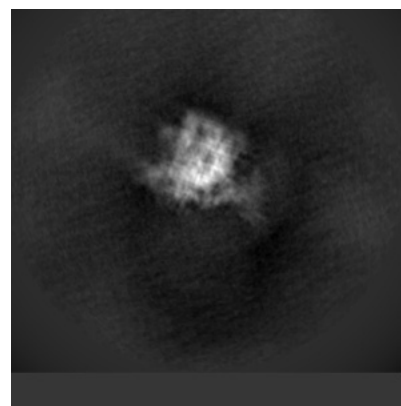
6.1.1 Primary map



X

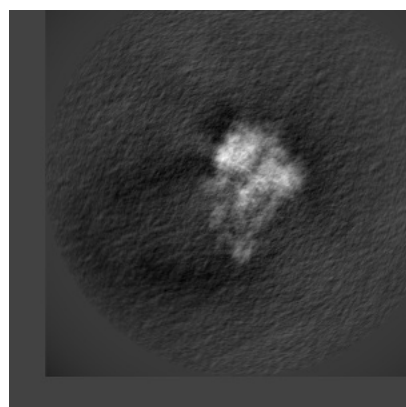


Y

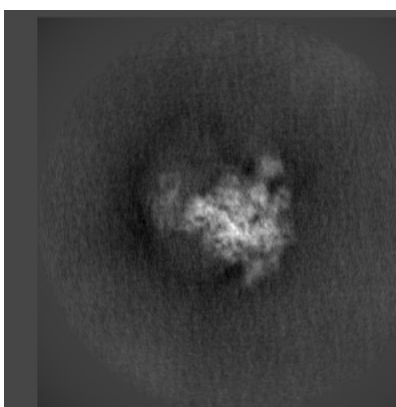


Z

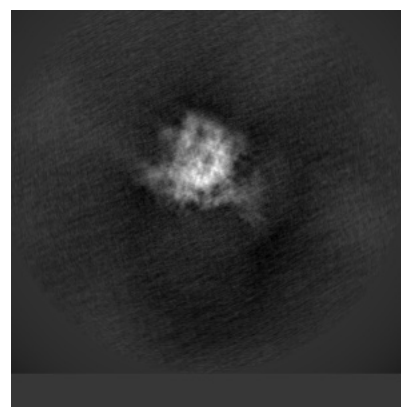
6.1.2 Raw map



X



Y

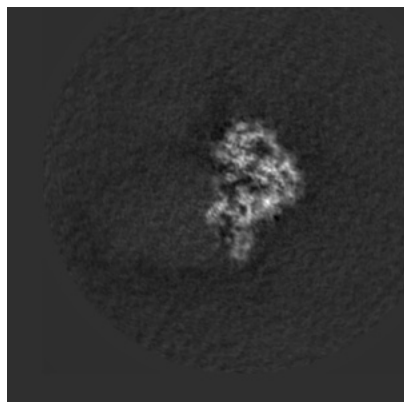


Z

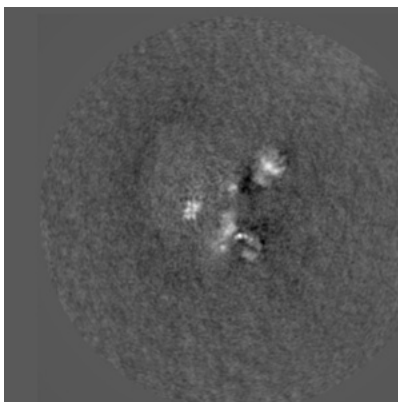
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

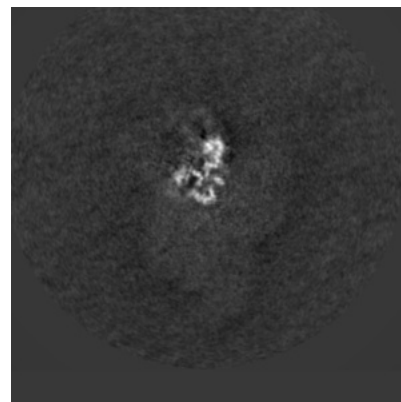
6.2.1 Primary map



X Index: 192

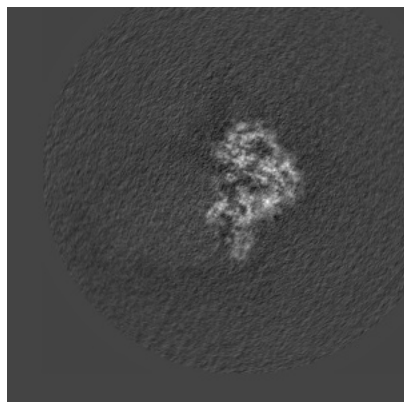


Y Index: 192

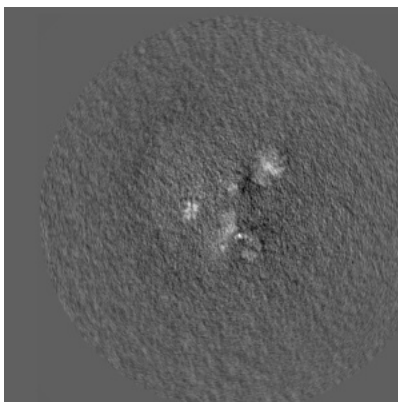


Z Index: 192

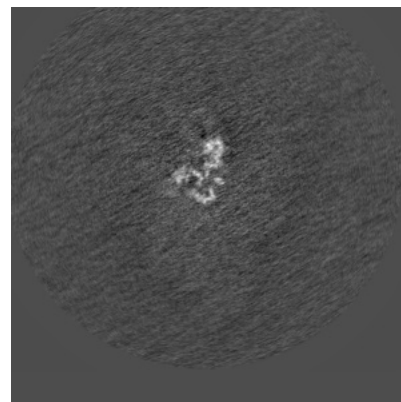
6.2.2 Raw map



X Index: 192



Y Index: 192

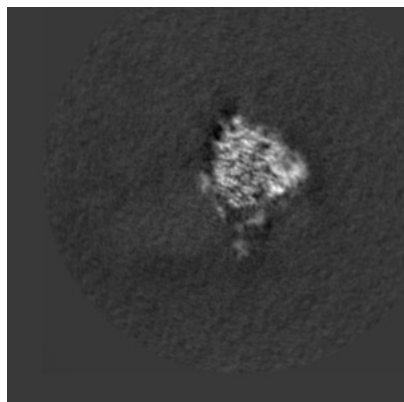


Z Index: 192

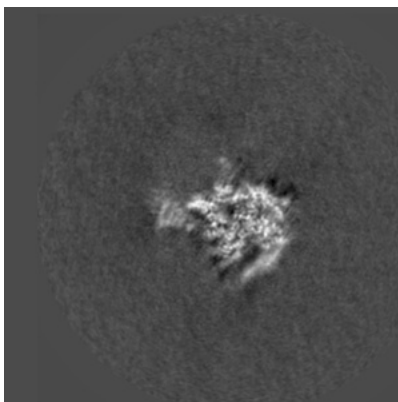
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

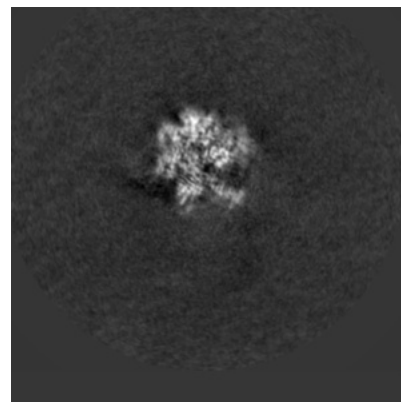
6.3.1 Primary map



X Index: 169

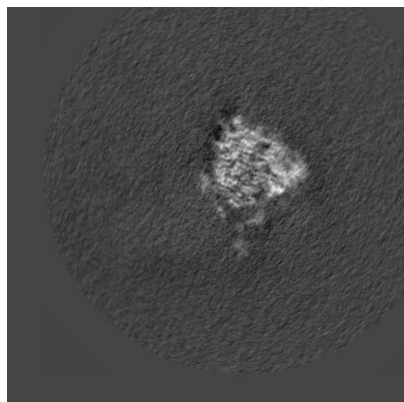


Y Index: 231

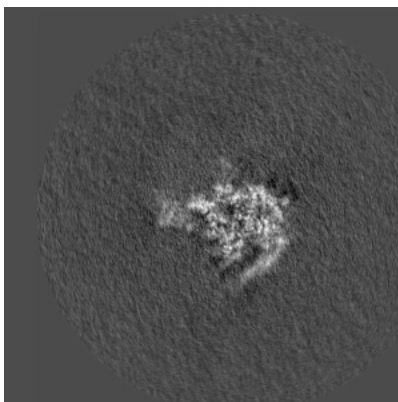


Z Index: 220

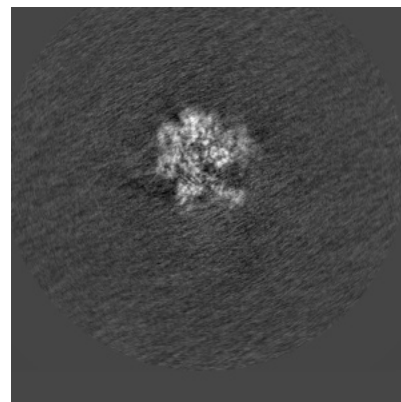
6.3.2 Raw map



X Index: 169



Y Index: 232

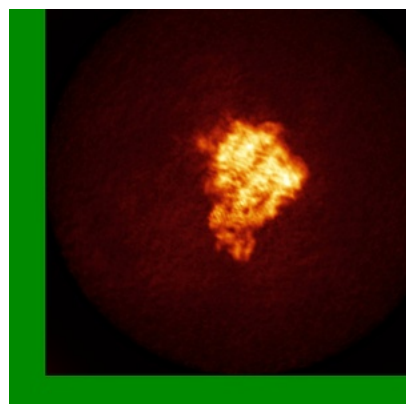


Z Index: 220

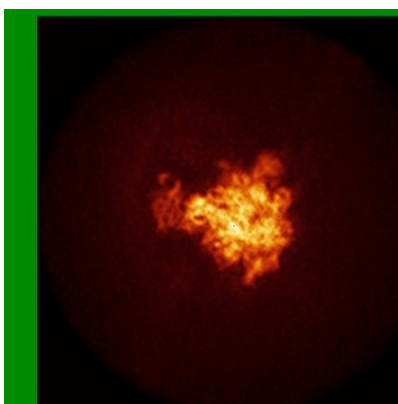
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

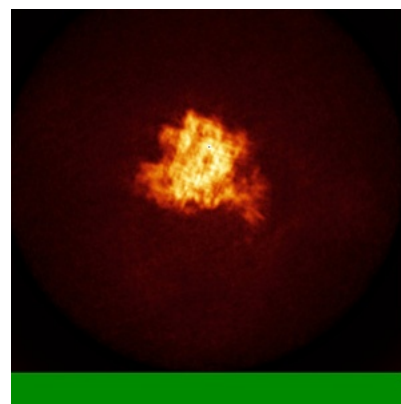
6.4.1 Primary map



X

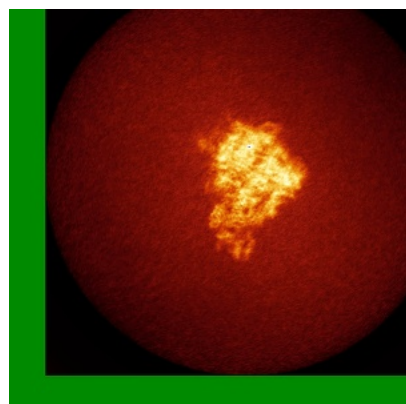


Y

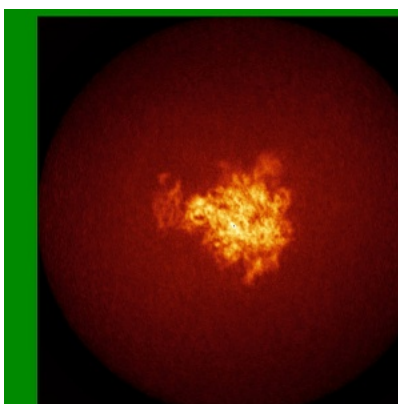


Z

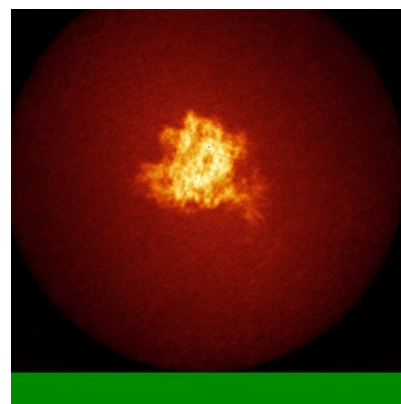
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

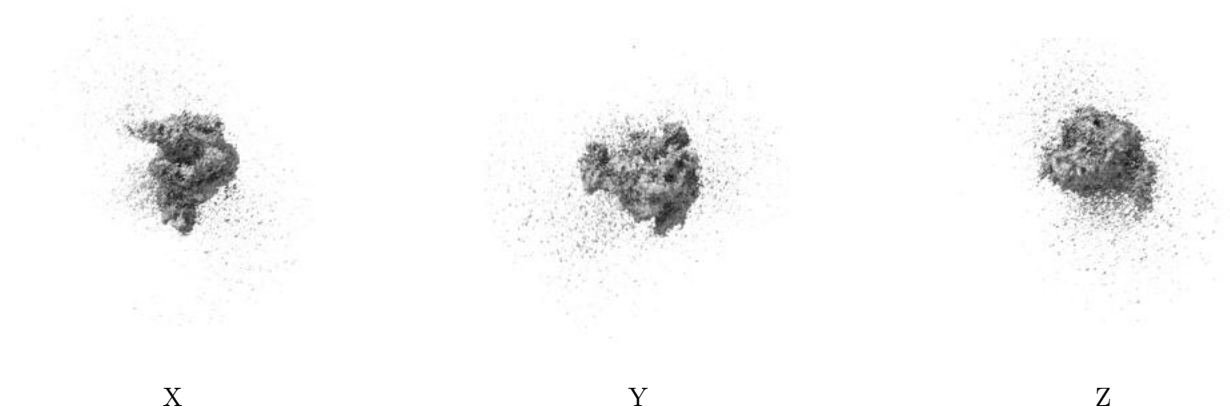
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

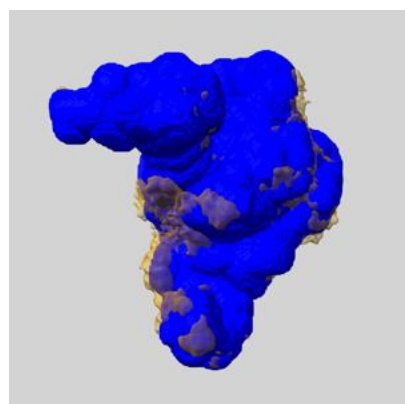
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

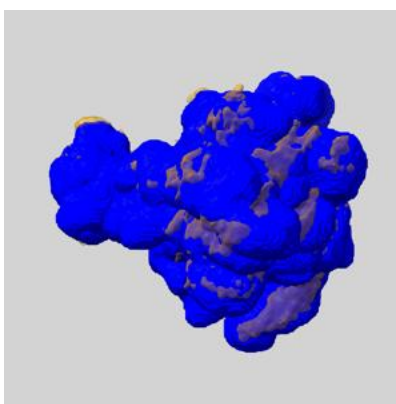
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

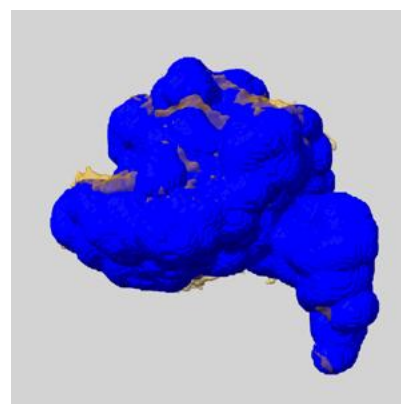
6.6.1 emd_51967_msk_1.map [i](#)



X



Y

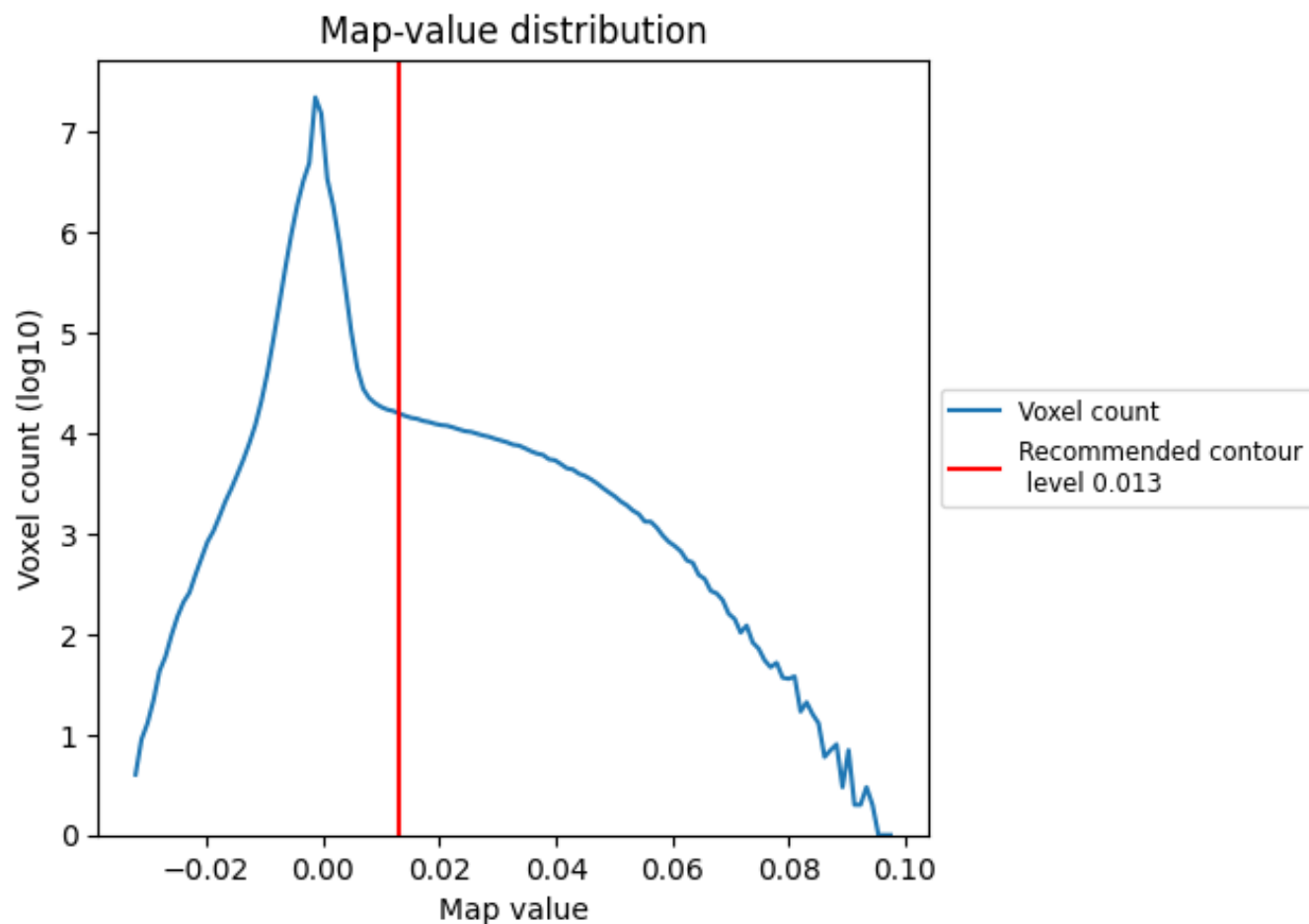


Z

7 Map analysis [i](#)

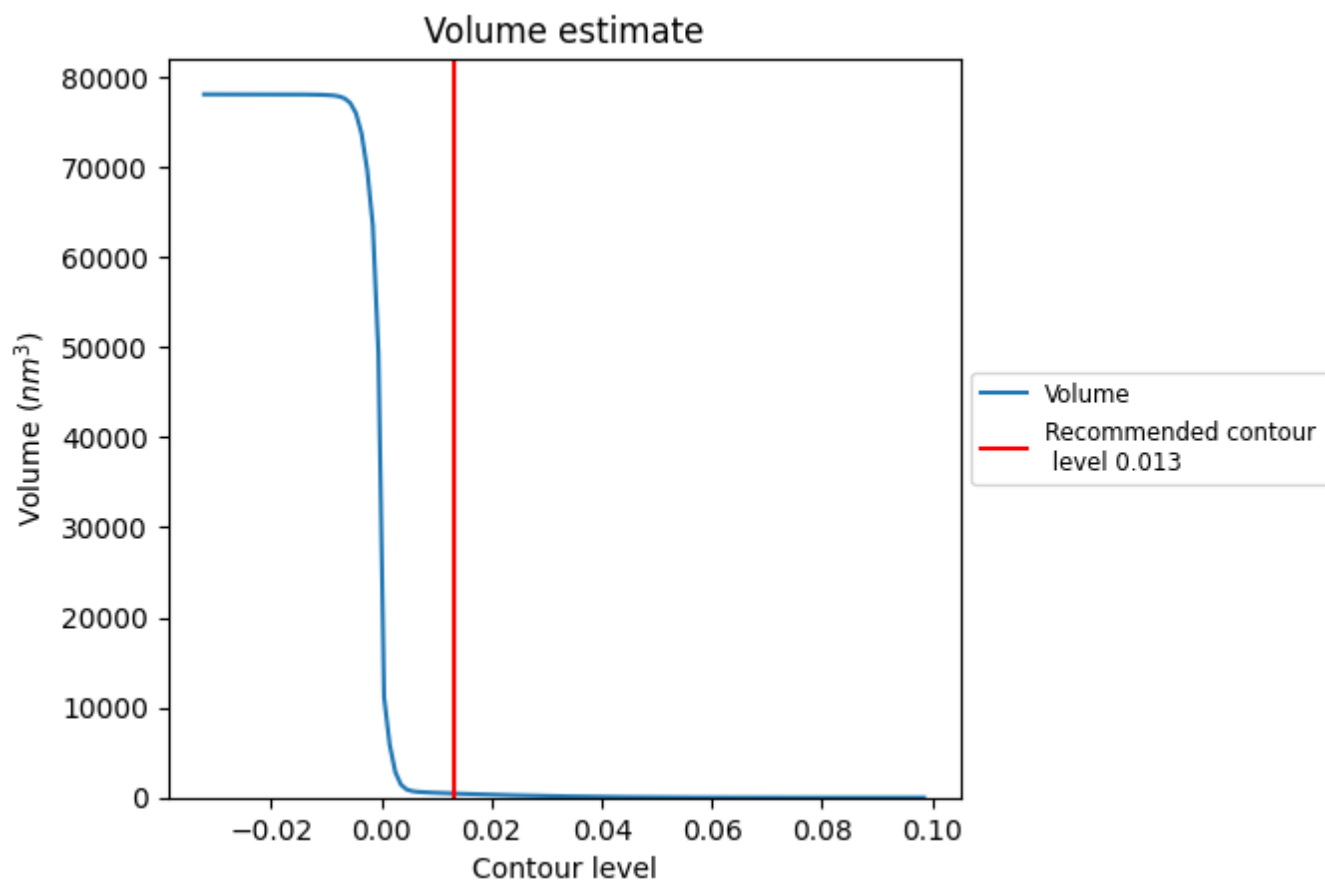
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

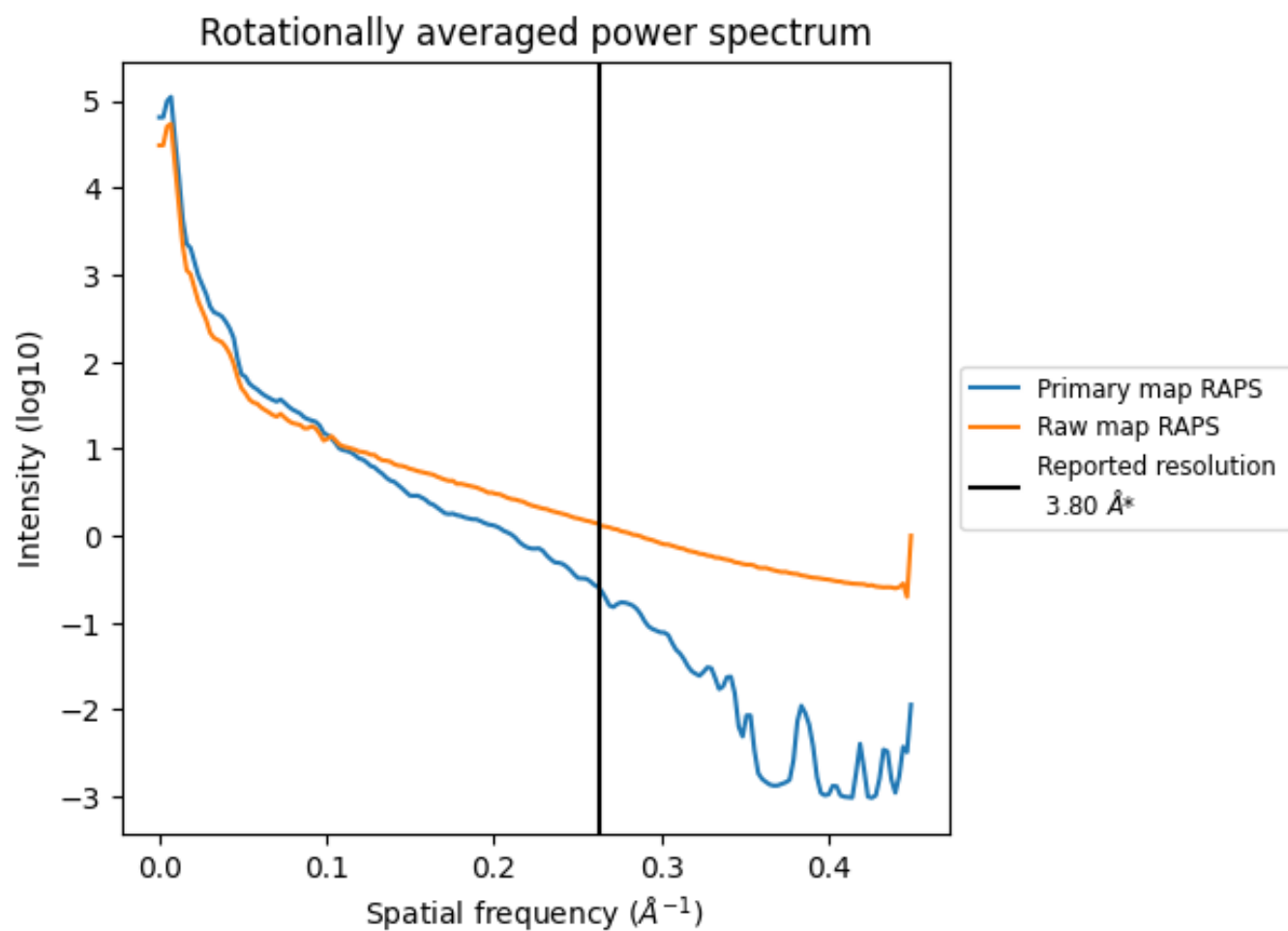
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 452 nm³; this corresponds to an approximate mass of 408 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

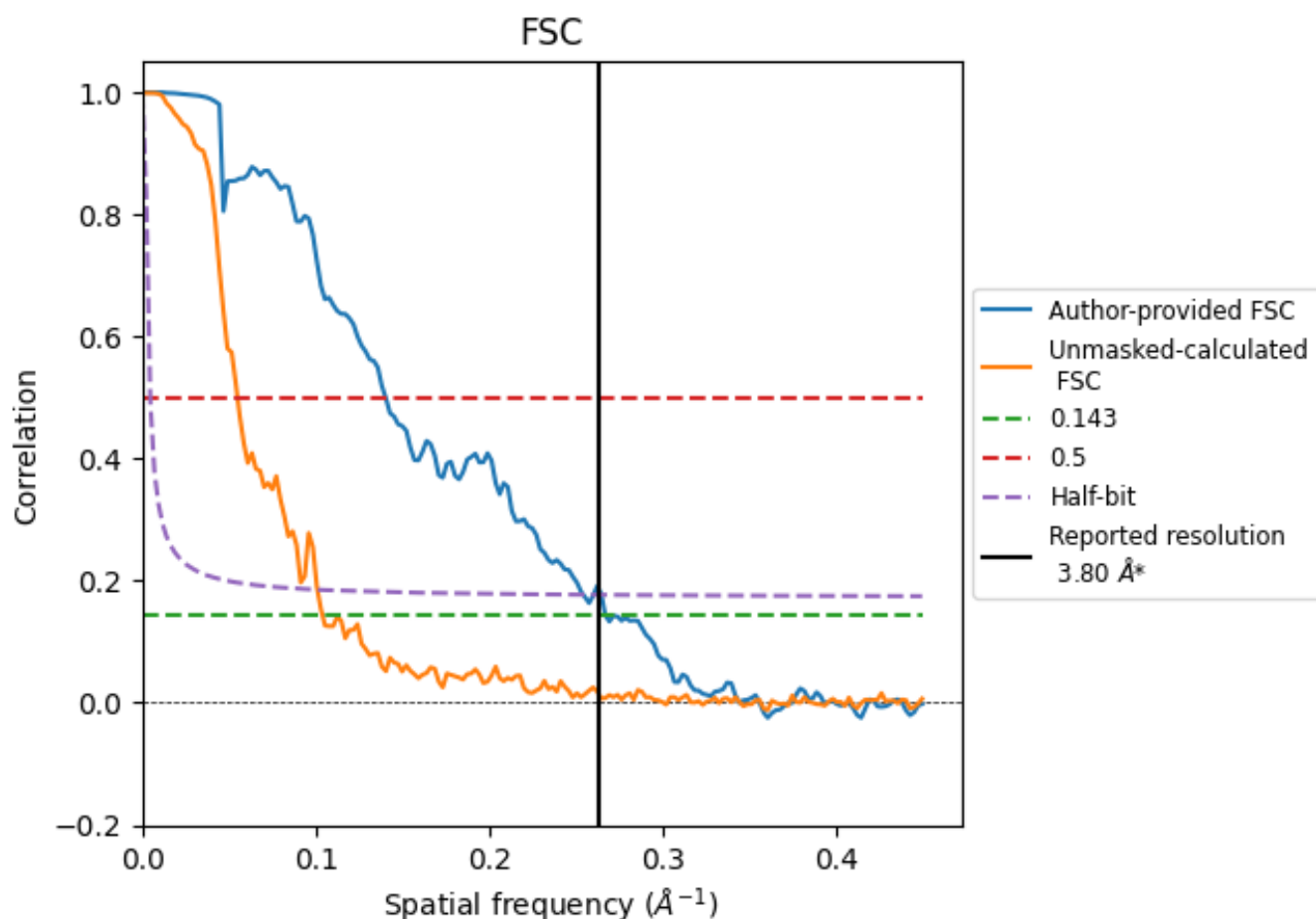


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

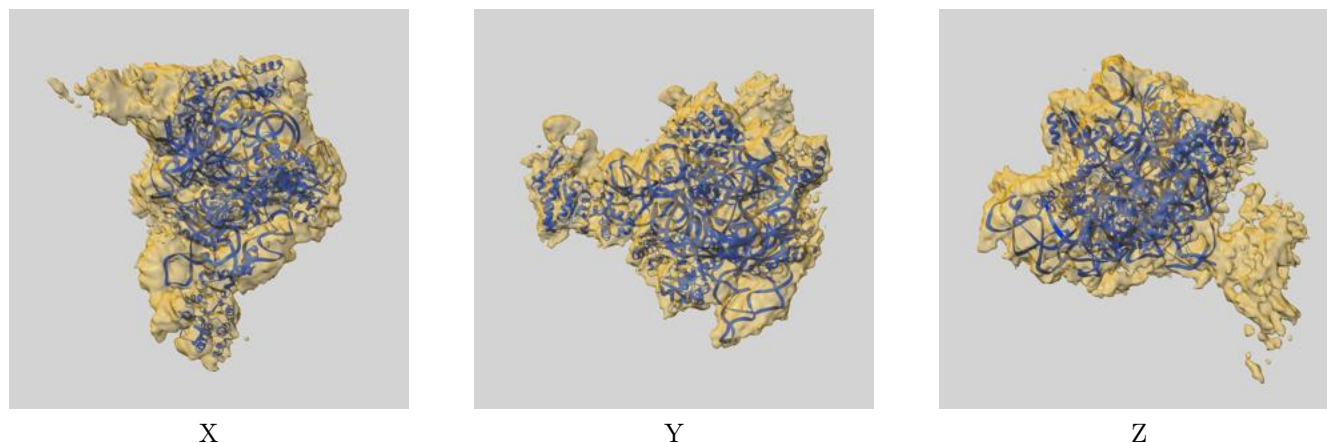
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.75	7.13	3.94
Unmasked-calculated*	9.62	18.21	9.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.62 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

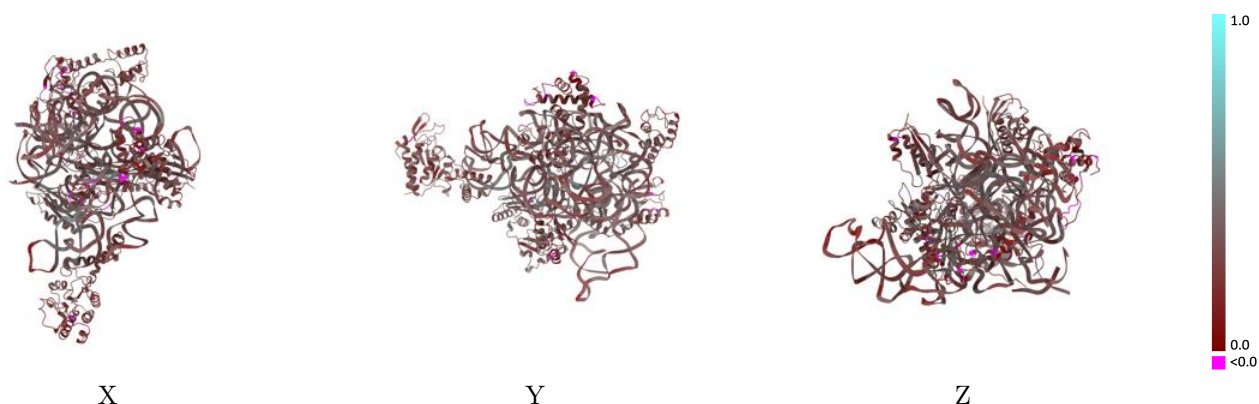
This section contains information regarding the fit between EMDB map EMD-51967 and PDB model 9H9K. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



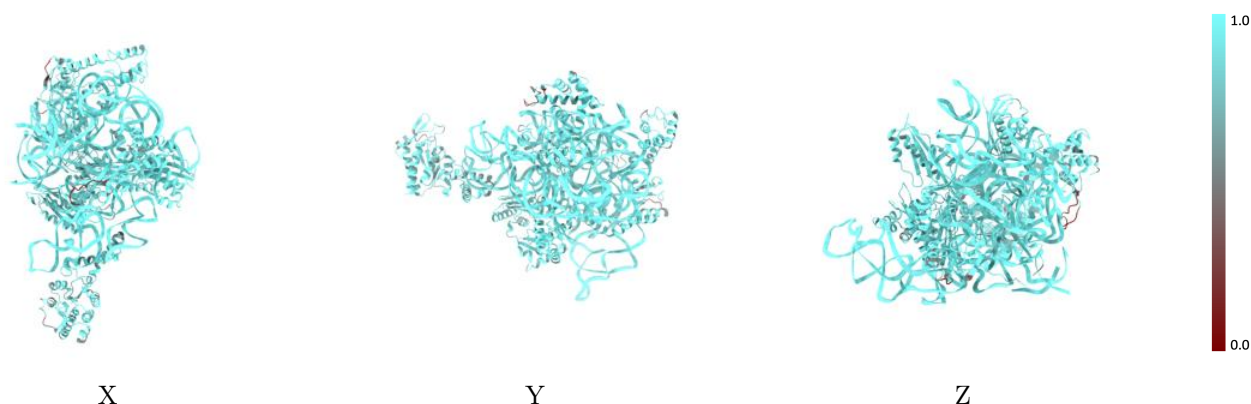
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



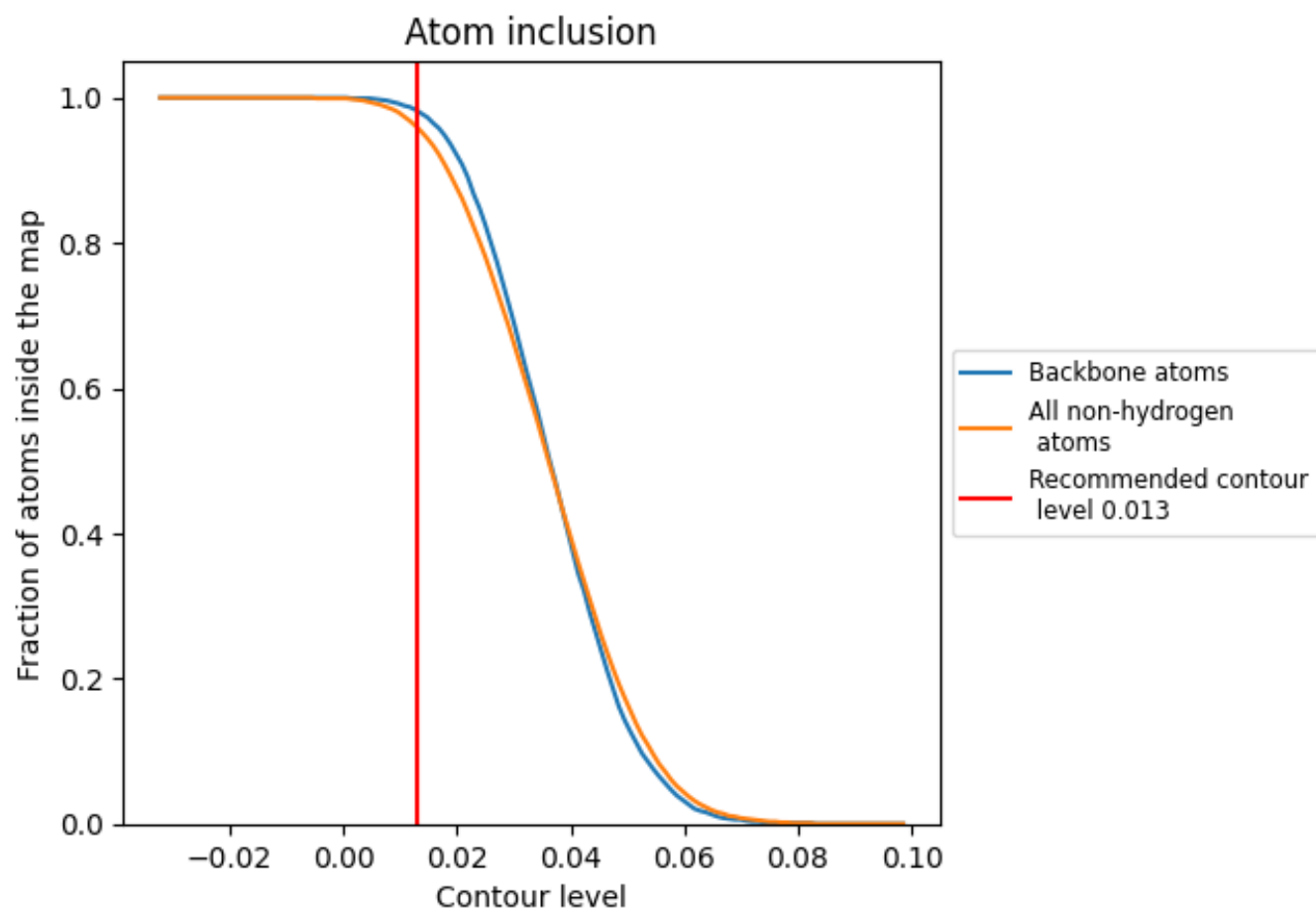
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).

























9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9590	 0.3090
1	 0.9910	 0.3370
2	 0.9720	 0.3020
3	 0.9950	 0.3300
B	 0.8680	 0.2490
C	 0.9390	 0.3290
G	 0.8660	 0.1960
I	 0.9650	 0.3070
J	 0.9740	 0.2810
M	 0.9280	 0.2590
N	 0.9790	 0.3190
S	 0.8920	 0.2590

