



Full wwPDB EM Validation Report ⓘ

Jul 14, 2026 – 02:22 PM JST

PDB ID : 9XAI / pdb_00009xai
EMDB ID : EMD-66688
Title : Cryo-EM structure of the pre-40S ribosome (Enp1-Rrp12 Mut) from *Chaetomium thermophilum*, state Tsr1-1*
Authors : Lau, B.; Li, Y.; Zhu, J.; Fischer, P.; Hong, X.; Yuan, R.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2025-10-22
Resolution : 4.10 Å (reported)
Based on initial model : 6G18

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.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

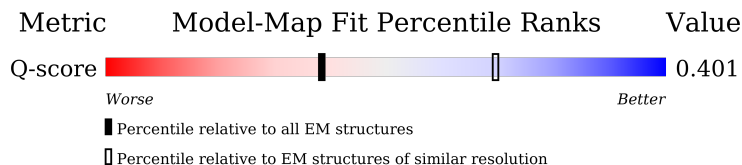
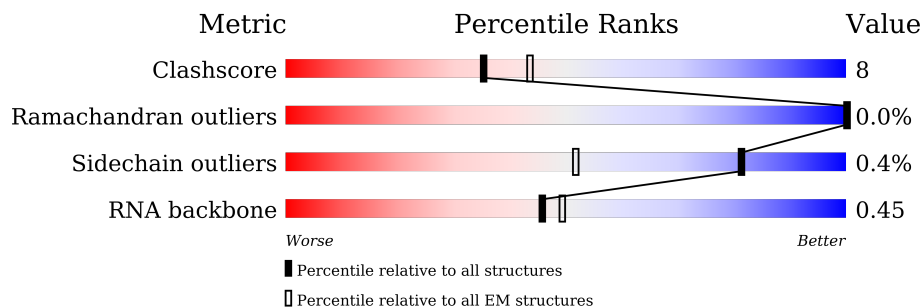
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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.



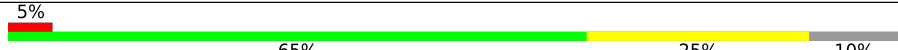
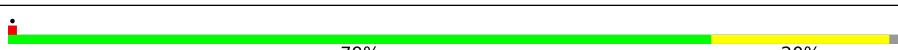
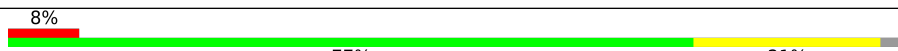
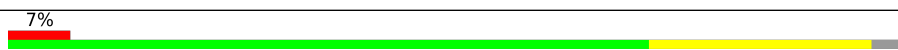
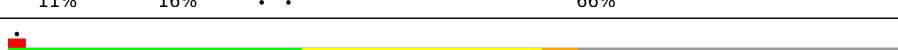
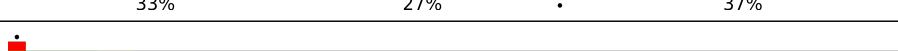
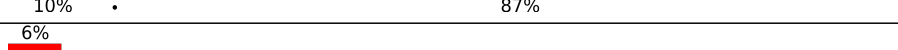
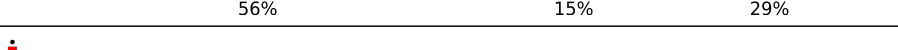
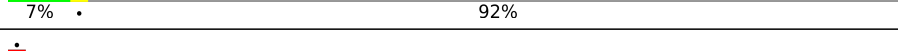
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	E	255	
2	H	264	
3	J	239	

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Mol	Chain	Length	Quality of chain
4	K	203	
5	L	202	
6	M	190	
7	O	161	
8	Q	151	
9	R	150	
10	Z	130	
11	a	145	
12	b	136	
13	e	82	
14	h	62	
15	A	1797	
16	1	282	
17	3	259	
18	6	519	
19	8	938	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 44705 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 protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	213	Total	C	N	O	S	0	0
			1723	1096	319	303	5		

- Molecule 2 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	261	Total	C	N	O	S	0	0
			2072	1314	389	362	7		

- Molecule 3 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	232	Total	C	N	O	S	0	0
			1875	1171	376	323	5		

- Molecule 4 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	195	Total	C	N	O	0	0
			1562	983	300	279		

- Molecule 5 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	201	Total	C	N	O	S	0	0
			1621	1009	330	281	1		

- Molecule 6 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	179	Total	C	N	O	S	0	0
			1466	933	290	241	2		

- Molecule 7 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	150	Total	C	N	O	S	0	0
			1222	780	236	201	5		

- Molecule 8 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	150	Total	C	N	O	S	0	0
			1182	756	220	205	1		

- Molecule 9 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	135	Total	C	N	O	S	0	0
			1002	614	199	184	5		

- Molecule 10 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	129	Total	C	N	O	S	0	0
			1037	659	195	178	5		

- Molecule 11 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	142	Total	C	N	O	S	0	0
			1099	694	215	188	2		

- Molecule 12 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	132	Total	C	N	O	S	0	0
			1061	668	209	182	2		

- Molecule 13 is a protein called Ribosomal protein s27-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	81	Total	C	N	O	S	0	0
			611	386	111	107	7		

- Molecule 14 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	h	21	Total	C	N	O	0	0
			181	117	38	26		

- Molecule 15 is a RNA chain called pre-18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A	1141	Total	C	N	O	P	0	0
			24337	10880	4340	7976	1141		

- Molecule 16 is a protein called Methyltransferase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1	37	Total	C	N	O	S	0	0
			307	195	62	49	1		

- Molecule 17 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	184	Total	C	N	O	S	0	0
			1451	921	267	256	7		

- Molecule 18 is a protein called Serine/threonine-protein kinase RIO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	43	Total	C	N	O	S	0	0
			352	222	74	54	2		

- Molecule 19 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	8	62	Total	C	N	O	S	0	0
			537	335	112	89	1		

- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
20	a	1	Total	Mg	0
			1	1	
20	A	1	Total	Mg	0
			1	1	

- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
21	e	1	Total 1	Zn 1	0

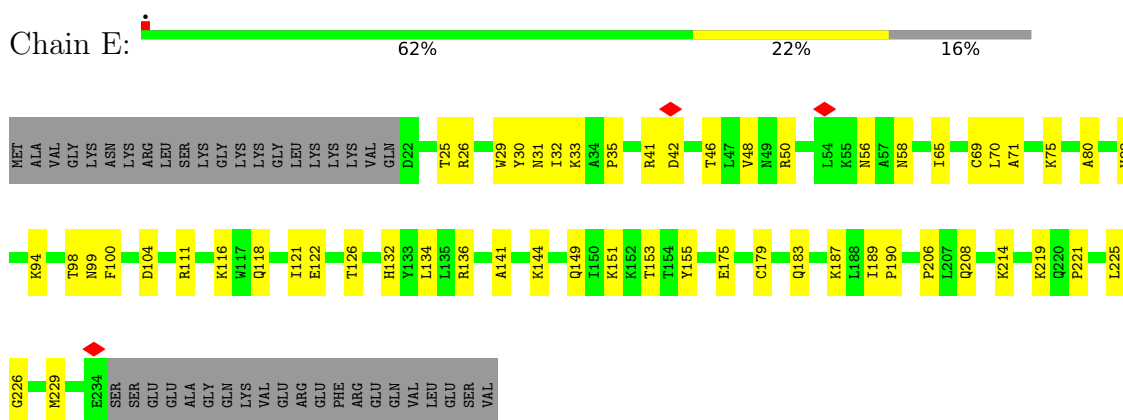
- Molecule 22 is water.

Mol	Chain	Residues	Atoms		AltConf
22	A	4	Total 4	O 4	0

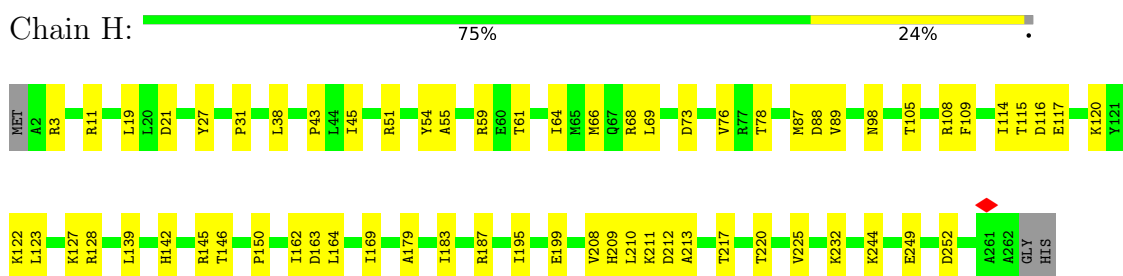
3 Residue-property plots

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.

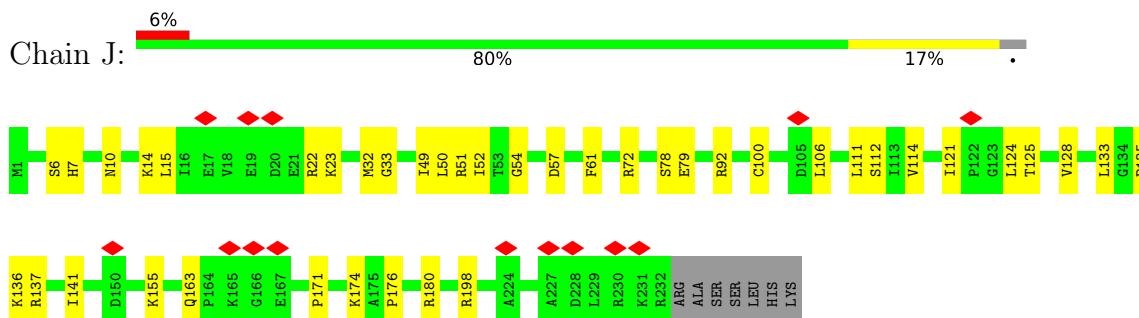
- Molecule 1: Small ribosomal subunit protein eS1



- Molecule 2: 40S ribosomal protein S4

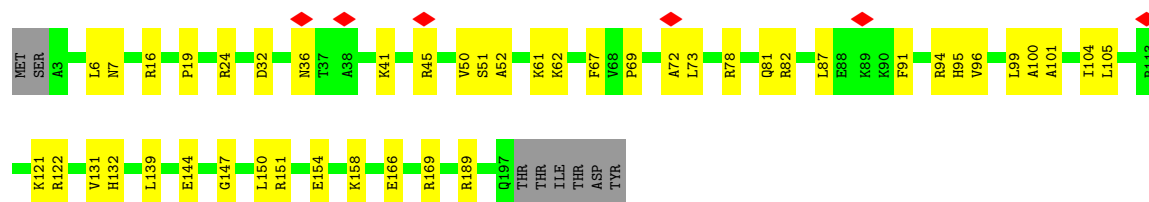


- Molecule 3: 40S ribosomal protein S6



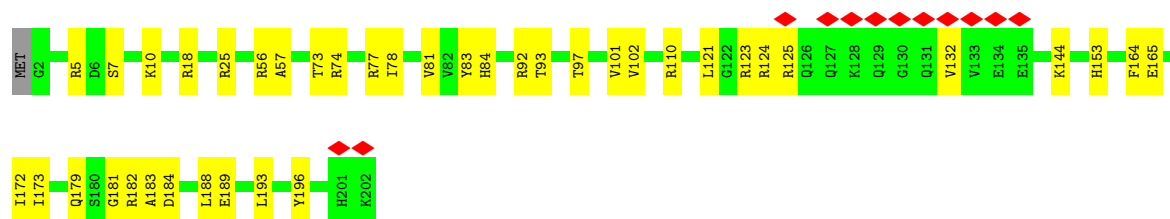
- Molecule 4: 40S ribosomal protein S7

Chain K:  74% 22%



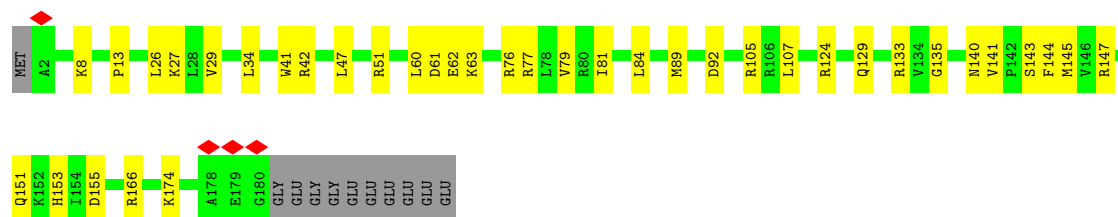
- Molecule 5: 40S ribosomal protein S8

Chain L:  6% 80% 20%



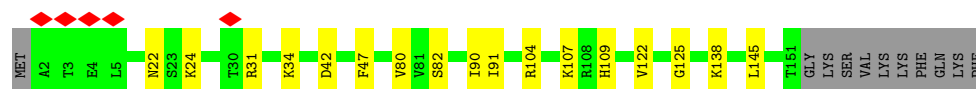
- Molecule 6: 40S ribosomal protein s9-like protein

Chain M:  74% 20% 6%



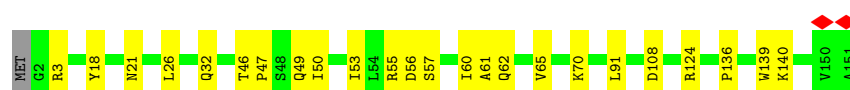
- Molecule 7: 40S ribosomal protein S11-like protein

Chain O:  83% 11% 7%



- Molecule 8: 40S ribosomal protein S13-like protein

Chain Q:  83% 16%

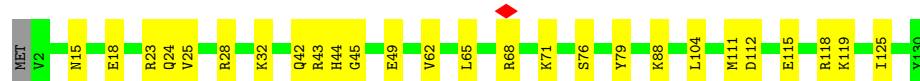
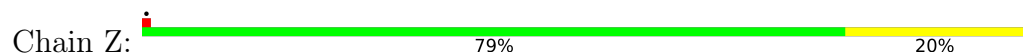


- Molecule 9: 40S ribosomal protein S14-like protein

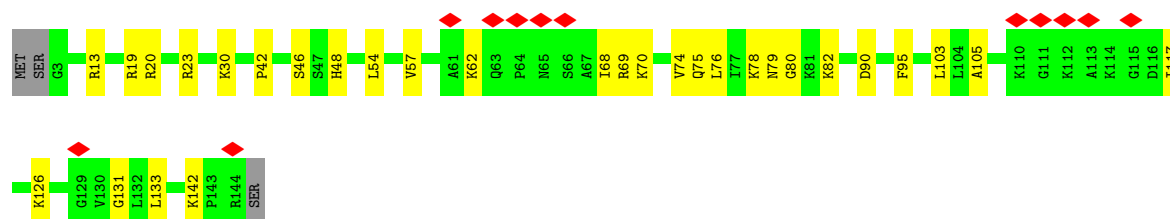
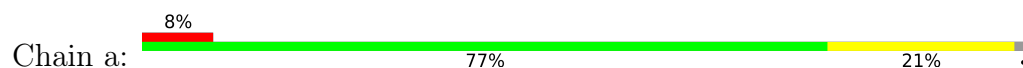
Chain R:  5% 65% 25% 10%



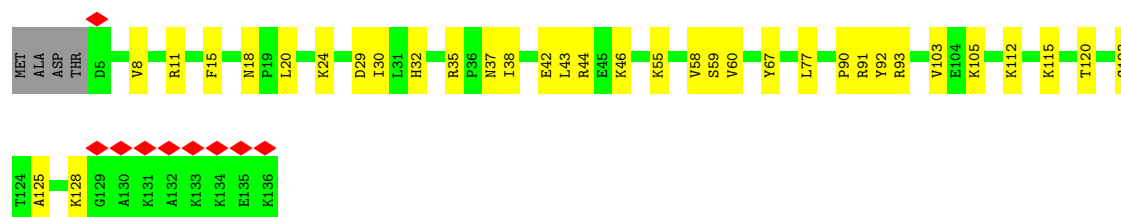
- Molecule 10: 40S ribosomal protein S22-like protein



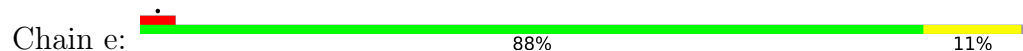
- Molecule 11: 40S ribosomal protein s23-like protein



- Molecule 12: Small ribosomal subunit protein eS24

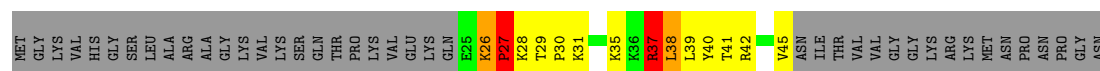


- Molecule 13: Ribosomal protein s27-like protein

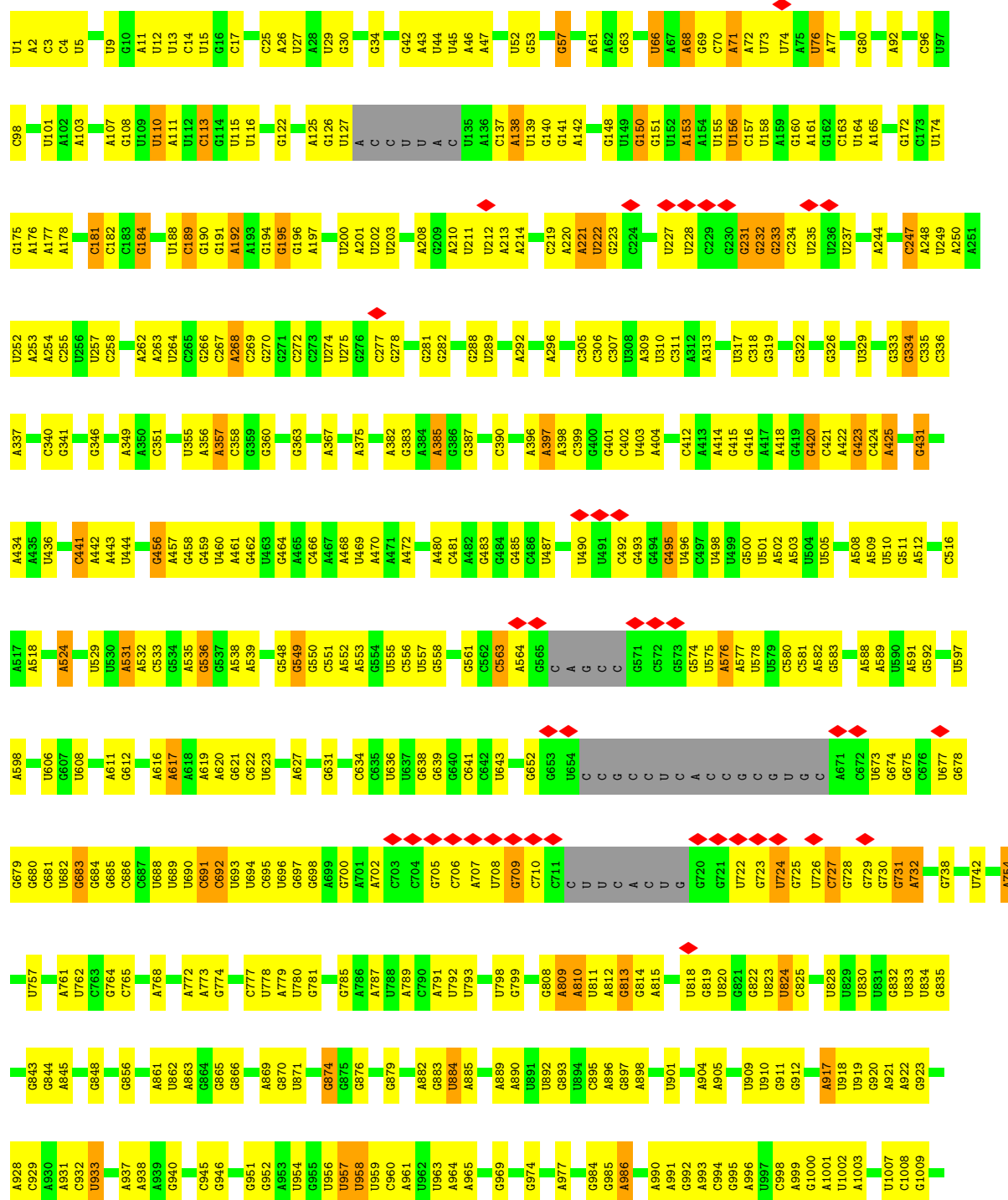
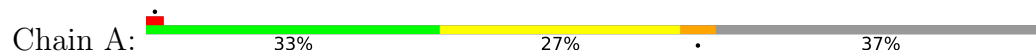


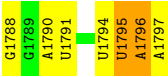
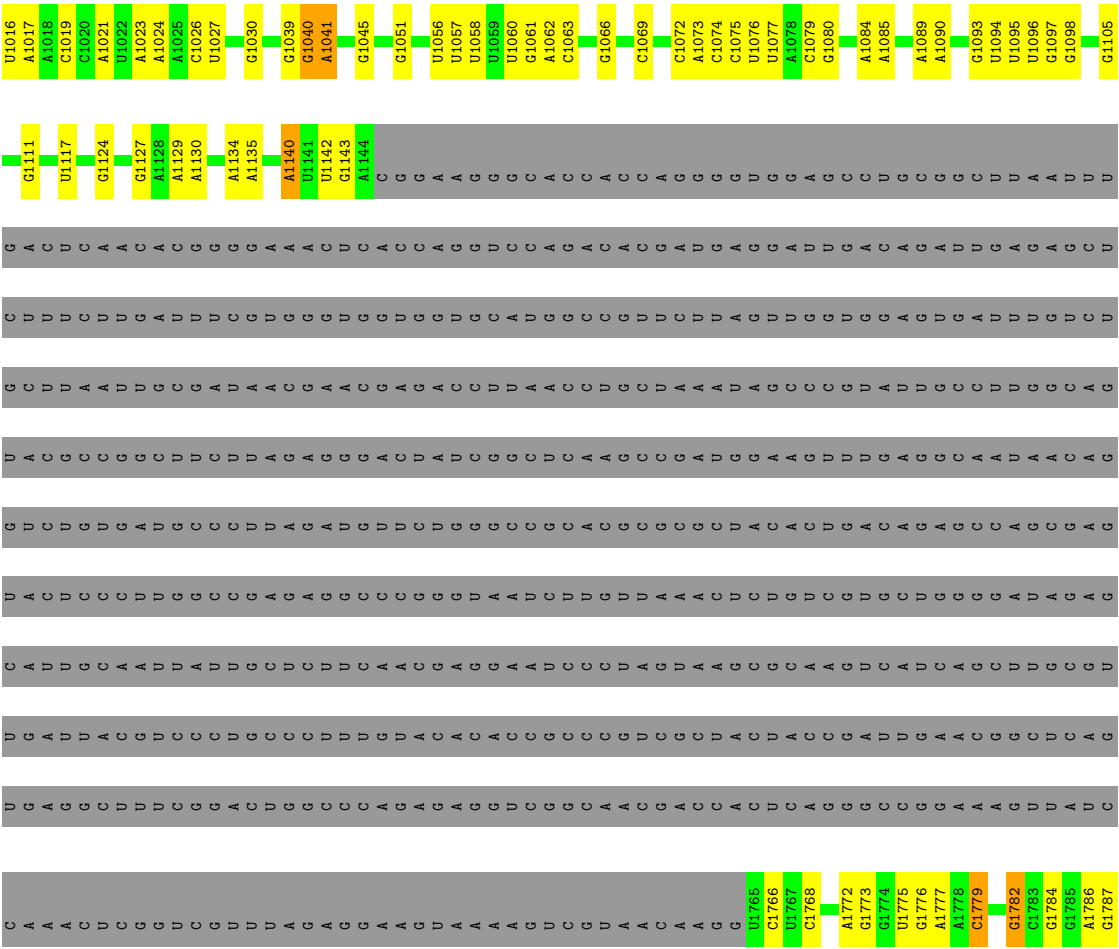
- Molecule 14: 40S ribosomal protein S30



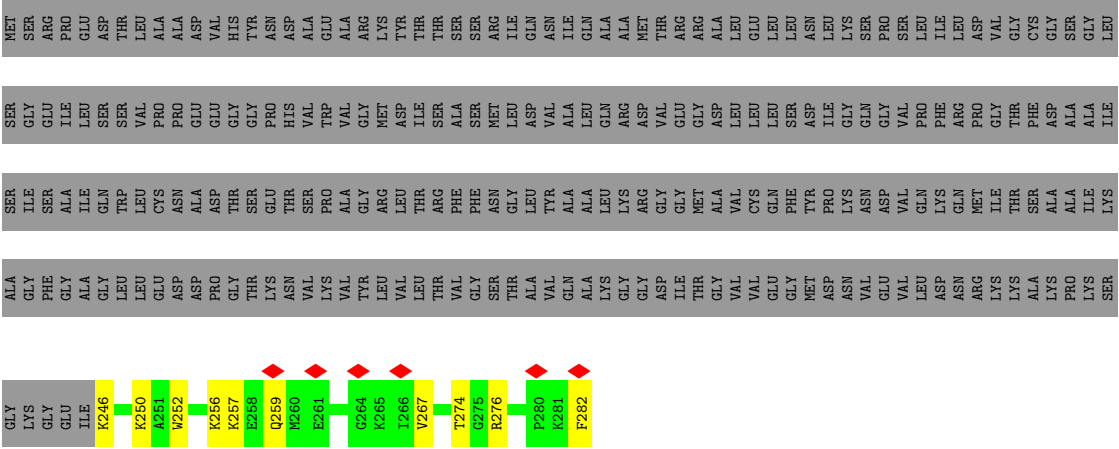


• Molecule 15: pre-18S





• Molecule 16: Methyltransferase-like protein



• Molecule 17: Pre-rRNA-processing protein PNO1



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6707	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.268	Depositor
Minimum map value	-0.146	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	376.19998, 376.19998, 376.19998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	E	0.21	0/1752	0.54	0/2361
2	H	0.29	0/2112	0.56	1/2842 (0.0%)
3	J	0.17	0/1906	0.49	0/2547
4	K	0.21	0/1587	0.57	0/2140
5	L	0.24	0/1654	0.53	0/2213
6	M	0.22	0/1489	0.50	0/1993
7	O	0.26	0/1249	0.46	0/1678
8	Q	0.22	0/1205	0.45	0/1627
9	R	0.25	0/1014	0.66	3/1361 (0.2%)
10	Z	0.27	0/1055	0.55	0/1416
11	a	0.21	0/1116	0.49	0/1489
12	b	0.23	0/1075	0.54	0/1431
13	e	0.21	0/623	0.53	0/843
14	h	0.61	0/184	1.17	1/242 (0.4%)
15	A	0.23	0/27224	0.38	0/42415
16	1	0.17	0/311	0.52	0/403
17	3	0.25	0/1475	0.66	1/1982 (0.1%)
18	6	0.20	0/356	0.47	0/462
19	8	0.29	0/544	0.80	0/717
All	All	0.24	0/47931	0.46	6/70162 (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
14	h	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	102	TYR	N-CA-C	5.68	122.37	109.81
9	R	85	LYS	CA-C-N	-5.41	111.67	121.14
9	R	85	LYS	C-N-CA	-5.41	111.67	121.14
14	h	37	ARG	N-CA-C	-5.17	105.33	110.97
2	H	232	LYS	CA-CB-CG	5.17	124.45	114.10
9	R	86	GLU	N-CA-CB	5.08	118.67	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	h	37	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1723	0	1804	38	0
2	H	2072	0	2155	42	0
3	J	1875	0	1983	32	0
4	K	1562	0	1641	32	0
5	L	1621	0	1645	29	0
6	M	1466	0	1582	27	0
7	O	1222	0	1289	17	0
8	Q	1182	0	1264	18	0
9	R	1002	0	1034	24	0
10	Z	1037	0	1076	20	0
11	a	1099	0	1169	22	0
12	b	1061	0	1150	27	0
13	e	611	0	633	8	0
14	h	181	0	207	10	0
15	A	24337	0	12252	312	0
16	1	307	0	346	8	0
17	3	1451	0	1524	32	0
18	6	352	0	402	7	0
19	8	537	0	573	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	e	1	0	0	0	0
22	A	4	0	0	0	0
All	All	44705	0	33729	603	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 8.

All (603) 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)
15:A:1041:A:H61	15:A:1072:C:N4	1.49	1.09
15:A:1041:A:N6	15:A:1072:C:H42	1.51	1.08
15:A:443:A:N6	15:A:458:G:H21	1.59	1.00
15:A:1117:U:H3	15:A:1124:G:H1	1.11	0.99
15:A:700:G:N2	15:A:732:A:C2	2.32	0.97
15:A:483:G:H1	15:A:498:U:H3	1.01	0.96
15:A:700:G:H21	15:A:732:A:H2	1.09	0.93
15:A:652:G:H1	15:A:673:U:H3	0.89	0.88
15:A:700:G:N2	15:A:732:A:H2	1.69	0.87
15:A:820:U:H3	15:A:848:G:H1	1.24	0.81
15:A:267:C:N4	15:A:268:A:H62	1.79	0.80
15:A:267:C:N4	15:A:268:A:N6	2.30	0.80
15:A:443:A:N6	15:A:458:G:N2	2.30	0.79
15:A:71:A:N1	15:A:80:G:C2	2.52	0.77
15:A:1794:U:H4'	17:3:91:ARG:HH22	1.48	0.77
15:A:220:A:N6	15:A:221:A:N6	2.34	0.76
15:A:709:G:H1	15:A:722:U:H3	1.34	0.76
15:A:874:G:O6	15:A:933:U:C4	2.39	0.75
15:A:309:A:N6	15:A:351:C:N4	2.35	0.74
17:3:243:LYS:O	17:3:247:ASN:ND2	2.22	0.73
15:A:561:G:H1	15:A:576:A:HO2'	1.34	0.73
15:A:71:A:C6	15:A:80:G:N1	2.59	0.71
15:A:220:A:N1	15:A:835:G:C6	2.58	0.70
15:A:71:A:N6	15:A:80:G:C6	2.59	0.70
15:A:71:A:N6	15:A:80:G:N1	2.39	0.70
15:A:70:C:N3	15:A:71:A:N6	2.39	0.70
3:J:32:MET:HB2	3:J:100:CYS:HB2	1.73	0.69
4:K:50:VAL:HG23	4:K:69:PRO:HD3	1.75	0.69
15:A:702:A:H62	15:A:731:G:N2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:146:ARG:NH2	15:A:1782:G:OP2	2.28	0.67
6:M:8:LYS:NZ	15:A:468:A:OP1	2.28	0.67
12:b:92:TYR:OH	12:b:93:ARG:NH2	2.29	0.66
15:A:267:C:H42	15:A:268:A:N6	1.94	0.66
10:Z:71:LYS:NZ	15:A:1096:U:OP1	2.27	0.65
15:A:200:U:H2'	15:A:201:A:H8	1.61	0.65
15:A:1:U:C4	15:A:367:A:C5	2.85	0.65
9:R:49:ARG:NH2	15:A:917:A:N3	2.45	0.65
4:K:67:PHE:HB3	4:K:101:ALA:HB2	1.79	0.65
9:R:26:VAL:HG13	9:R:89:ILE:HD12	1.79	0.64
15:A:184:G:C6	15:A:192:A:N6	2.66	0.64
17:3:87:ILE:HG21	17:3:95:LEU:HD22	1.78	0.64
4:K:73:LEU:HD22	4:K:100:ALA:HB2	1.79	0.64
10:Z:23:ARG:HA	10:Z:65:LEU:HB2	1.80	0.64
14:h:31:LYS:HA	14:h:35:LYS:HB2	1.79	0.64
2:H:139:LEU:HD22	2:H:150:PRO:HB3	1.79	0.64
3:J:50:LEU:HB3	3:J:111:LEU:HD12	1.80	0.63
2:H:19:LEU:HD11	2:H:108:ARG:HD2	1.81	0.62
15:A:688:U:C2	15:A:690:U:O4	2.53	0.62
15:A:874:G:O6	15:A:933:U:O4	2.17	0.62
10:Z:43:ARG:NH2	10:Z:115:GLU:OE2	2.33	0.62
2:H:66:MET:SD	2:H:78:THR:OG1	2.57	0.62
6:M:77:ARG:NH2	15:A:761:A:OP1	2.32	0.62
15:A:707:A:N1	15:A:724:U:O2'	2.33	0.62
15:A:71:A:N1	15:A:80:G:N1	2.48	0.61
12:b:35:ARG:NH1	12:b:37:ASN:O	2.33	0.61
15:A:1787:G:OP2	17:3:185:ARG:NH2	2.33	0.61
5:L:56:ARG:NH2	15:A:329:U:OP1	2.33	0.61
2:H:187:ARG:NH2	15:A:789:A:OP1	2.34	0.61
19:8:416:ARG:NH1	19:8:419:GLU:OE2	2.34	0.61
4:K:91:PHE:HB3	4:K:94:ARG:HG3	1.82	0.61
6:M:29:VAL:HG23	6:M:34:LEU:HB2	1.83	0.60
15:A:172:G:C2	15:A:263:A:C5	2.89	0.60
15:A:443:A:H61	15:A:458:G:N2	1.94	0.60
1:E:189:ILE:HG13	1:E:190:PRO:HD3	1.84	0.60
4:K:87:LEU:HB3	4:K:96:VAL:HG21	1.84	0.60
9:R:142:LYS:HD2	9:R:148:ARG:HH21	1.65	0.60
15:A:844:G:H2'	15:A:845:A:H8	1.65	0.60
15:A:1041:A:N1	15:A:1072:C:N3	2.50	0.60
11:a:46:SER:OG	11:a:78:LYS:NZ	2.35	0.60
15:A:549:G:H4'	16:1:257:LYS:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:79:VAL:HG11	6:M:89:MET:HE1	1.83	0.59
9:R:98:ALA:H	9:R:132:THR:HG22	1.67	0.59
2:H:73:ASP:OD2	2:H:145:ARG:NH2	2.35	0.59
12:b:125:ALA:HA	12:b:128:LYS:HE2	1.84	0.59
6:M:81:ILE:HA	6:M:147:ARG:HA	1.85	0.59
15:A:172:G:N2	15:A:263:A:C5	2.70	0.59
7:O:107:LYS:O	11:a:13:ARG:NH2	2.35	0.59
15:A:172:G:C2	15:A:263:A:N7	2.71	0.59
15:A:1775:U:O2	15:A:1779:C:N3	2.36	0.59
11:a:75:GLN:HE21	11:a:80:GLY:HA2	1.68	0.59
2:H:31:PRO:HG3	2:H:43:PRO:HG3	1.85	0.58
2:H:211:LYS:HE2	2:H:217:THR:HG22	1.85	0.58
12:b:123:GLY:O	12:b:128:LYS:NZ	2.34	0.58
15:A:574:G:H2'	15:A:576:A:H4'	1.85	0.58
15:A:1:U:O4	15:A:367:A:C6	2.56	0.58
15:A:11:A:OP1	16:1:259:GLN:NE2	2.36	0.58
5:L:92:ARG:HH21	5:L:93:THR:HG22	1.69	0.58
15:A:984:G:O6	18:6:488:LYS:NZ	2.36	0.58
1:E:144:LYS:HB3	1:E:206:PRO:HB2	1.85	0.58
1:E:149:GLN:NE2	1:E:151:LYS:O	2.37	0.58
12:b:15:PHE:HZ	12:b:24:LYS:HD2	1.68	0.58
17:3:80:ILE:HG23	17:3:125:ARG:HD3	1.86	0.58
3:J:10:ASN:HB2	3:J:128:VAL:HA	1.86	0.57
10:Z:24:GLN:NE2	13:e:6:ASP:OD1	2.36	0.57
15:A:172:G:N2	15:A:263:A:C4	2.71	0.57
5:L:84:HIS:NE2	5:L:97:THR:OG1	2.36	0.57
5:L:125:ARG:HE	5:L:132:VAL:HA	1.69	0.57
15:A:140:G:H2'	15:A:141:G:C8	2.40	0.57
15:A:431:G:N1	15:A:434:A:OP2	2.36	0.57
4:K:61:LYS:NZ	4:K:62:LYS:O	2.37	0.57
4:K:154:GLU:HA	10:Z:42:GLN:HE21	1.70	0.57
15:A:1:U:N3	15:A:367:A:N7	2.53	0.57
17:3:89:PRO:HB3	17:3:120:LYS:HE2	1.85	0.56
2:H:87:MET:O	2:H:122:LYS:NZ	2.31	0.56
12:b:11:ARG:HD2	15:A:778:U:H2'	1.87	0.56
3:J:50:LEU:HD12	3:J:111:LEU:HB3	1.87	0.56
3:J:92:ARG:NH2	15:A:390:C:O2'	2.38	0.56
4:K:69:PRO:O	4:K:73:LEU:N	2.37	0.56
8:Q:53:ILE:O	8:Q:57:SER:OG	2.23	0.56
15:A:869:A:H2'	15:A:870:G:C8	2.41	0.56
10:Z:119:LYS:NZ	15:A:683:G:OP2	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:222:U:H3	15:A:833:U:H3	1.54	0.56
13:e:22:LYS:NZ	15:A:1069:C:OP1	2.33	0.56
15:A:340:C:H2'	15:A:341:G:H8	1.71	0.56
14:h:39:LEU:O	14:h:40:TYR:C	2.49	0.56
15:A:834:U:H2'	15:A:835:G:H8	1.71	0.56
15:A:922:A:H2'	15:A:923:G:C8	2.41	0.56
1:E:32:ILE:HD11	1:E:46:THR:HB	1.87	0.56
6:M:133:ARG:NH2	6:M:155:ASP:OD2	2.39	0.56
12:b:37:ASN:ND2	15:A:518:A:N3	2.49	0.56
4:K:105:LEU:O	4:K:122:ARG:NH1	2.40	0.55
4:K:19:PRO:HD2	4:K:24:ARG:HE	1.71	0.55
15:A:870:G:N2	15:A:1045:G:O2'	2.38	0.55
1:E:144:LYS:HD2	1:E:208:GLN:HB3	1.88	0.55
14:h:41:THR:HA	14:h:45:VAL:HG22	1.89	0.55
15:A:53:G:C6	15:A:425:A:N1	2.75	0.55
11:a:57:VAL:O	11:a:70:LYS:HA	2.07	0.55
15:A:309:A:H61	15:A:351:C:N4	2.05	0.55
3:J:174:LYS:NZ	15:A:68:A:OP2	2.33	0.55
8:Q:3:ARG:NH2	15:A:865:G:OP2	2.39	0.55
9:R:140:ARG:NH1	15:A:1784:G:OP1	2.39	0.55
15:A:897:G:C2	15:A:909:U:O2	2.59	0.55
15:A:1111:G:O2'	15:A:1127:G:O6	2.24	0.55
11:a:42:PRO:O	11:a:79:ASN:ND2	2.37	0.55
15:A:125:A:H62	15:A:288:G:N2	2.04	0.55
1:E:132:HIS:HB2	1:E:221:PRO:HB3	1.89	0.55
12:b:44:ARG:HG3	12:b:58:VAL:HB	1.89	0.55
5:L:110:ARG:NH1	5:L:121:LEU:O	2.40	0.55
15:A:866:G:H1	15:A:958:U:H3	1.53	0.54
15:A:897:G:N1	15:A:909:U:C2	2.75	0.54
3:J:163:GLN:HB2	3:J:171:PRO:HB3	1.88	0.54
14:h:26:LYS:O	14:h:27:PRO:C	2.49	0.54
3:J:49:ILE:HG13	3:J:114:VAL:HB	1.89	0.54
15:A:991:A:OP1	15:A:1773:G:N2	2.39	0.54
15:A:1795:U:H1'	17:3:90:HIS:HB3	1.88	0.54
3:J:135:PRO:HG2	3:J:141:ILE:HG13	1.88	0.54
7:O:42:ASP:O	15:A:244:A:O2'	2.24	0.54
15:A:460:U:O2'	15:A:524:A:N6	2.41	0.54
15:A:483:G:N2	15:A:498:U:O2	2.31	0.54
15:A:1140:A:OP2	19:8:441:ARG:NH2	2.39	0.54
11:a:30:LYS:NZ	15:A:1129:A:OP1	2.37	0.54
17:3:235:LEU:HD13	17:3:244:VAL:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:61:PHE:HD2	3:J:72:ARG:HD2	1.73	0.54
7:O:104:ARG:NH2	10:Z:79:TYR:OH	2.41	0.54
15:A:247:C:H2'	15:A:248:A:H8	1.72	0.54
15:A:798:U:H2'	15:A:799:G:H8	1.73	0.54
17:3:116:ASN:O	17:3:120:LYS:HA	2.08	0.54
10:Z:76:SER:HB2	15:A:1098:G:H5''	1.90	0.54
13:e:51:GLN:NE2	15:A:956:U:O2	2.41	0.54
3:J:14:LYS:HG2	3:J:124:LEU:HD12	1.90	0.54
6:M:62:GLU:HG3	6:M:63:LYS:HG3	1.89	0.54
15:A:557:U:O4	16:1:276:ARG:NH2	2.41	0.54
18:6:513:ALA:HA	18:6:516:LYS:HG2	1.91	0.53
10:Z:18:GLU:HG2	10:Z:65:LEU:HD13	1.90	0.53
15:A:549:G:H3'	15:A:550:G:H21	1.72	0.53
15:A:986:A:OP1	18:6:477:LYS:NZ	2.39	0.53
5:L:182:ARG:NH1	15:A:202:U:O2	2.41	0.53
11:a:20:ARG:NH1	15:A:307:C:OP1	2.41	0.53
15:A:458:G:H2'	15:A:459:G:H8	1.73	0.53
17:3:111:LEU:HD11	17:3:136:LEU:HA	1.89	0.53
2:H:68:ARG:HG3	2:H:76:VAL:HG11	1.90	0.53
2:H:27:TYR:O	15:A:444:U:O2'	2.21	0.53
15:A:897:G:C2	15:A:909:U:C2	2.97	0.53
15:A:834:U:H2'	15:A:835:G:C8	2.44	0.53
4:K:7:ASN:HA	4:K:16:ARG:HH12	1.73	0.53
3:J:72:ARG:NH2	15:A:416:G:O5'	2.42	0.53
15:A:70:C:C4	15:A:71:A:N6	2.75	0.53
17:3:202:GLU:O	17:3:208:ARG:NH2	2.41	0.53
1:E:134:LEU:HB2	1:E:219:LYS:HB3	1.89	0.53
7:O:80:VAL:O	7:O:125:GLY:N	2.42	0.53
1:E:104:ASP:OD2	1:E:214:LYS:NZ	2.43	0.52
5:L:7:SER:O	5:L:18:ARG:NH1	2.41	0.52
9:R:26:VAL:HG12	9:R:90:THR:HG22	1.91	0.52
15:A:469:U:O2'	15:A:768:A:N3	2.38	0.52
6:M:107:LEU:HB2	6:M:144:PHE:HB3	1.91	0.52
12:b:30:ILE:HG22	12:b:32:HIS:HD2	1.75	0.52
7:O:80:VAL:HG21	7:O:122:VAL:HG11	1.92	0.52
15:A:385:A:OP2	15:A:420:G:O2'	2.25	0.52
3:J:14:LYS:HE2	3:J:124:LEU:HB2	1.92	0.52
3:J:92:ARG:O	15:A:402:C:O2'	2.23	0.52
4:K:104:ILE:HG13	4:K:131:VAL:HG21	1.92	0.52
6:M:27:LYS:HA	14:h:40:TYR:CE1	2.44	0.52
15:A:708:U:O2	15:A:723:G:O6	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:1129:A:H2'	15:A:1130:A:H8	1.75	0.52
17:3:135:ALA:O	17:3:139:GLY:N	2.32	0.52
1:E:175:GLU:HB2	1:E:187:LYS:HZ3	1.74	0.52
3:J:137:ARG:HD3	3:J:180:ARG:HE	1.74	0.52
2:H:11:ARG:NH1	2:H:21:ASP:O	2.37	0.52
6:M:42:ARG:NH1	15:A:470:A:OP1	2.37	0.52
15:A:107:A:H2'	15:A:108:G:C8	2.45	0.51
15:A:1796:A:N3	17:3:92:MET:HE1	2.25	0.51
15:A:336:C:H2'	15:A:337:A:H8	1.75	0.51
1:E:30:TYR:HE1	1:E:48:VAL:HG12	1.75	0.51
15:A:487:U:N3	15:A:495:G:N1	2.58	0.51
12:b:120:THR:HG23	15:A:156:U:H5'	1.91	0.51
15:A:1794:U:H4'	17:3:91:ARG:NH2	2.23	0.51
2:H:54:TYR:O	12:b:18:ASN:ND2	2.42	0.51
15:A:885:A:N1	15:A:923:G:O6	2.44	0.51
11:a:103:LEU:HD23	11:a:126:LYS:HD3	1.92	0.51
15:A:52:U:H2'	15:A:53:G:C8	2.45	0.51
17:3:115:MET:SD	17:3:115:MET:N	2.83	0.51
15:A:29:U:H2'	15:A:30:G:H8	1.74	0.51
15:A:639:G:N1	15:A:688:U:C2	2.79	0.51
15:A:1002:U:H5'	15:A:1003:A:H5''	1.91	0.51
15:A:44:U:OP2	15:A:434:A:N6	2.36	0.51
15:A:697:G:H2'	15:A:698:G:H8	1.76	0.51
15:A:882:A:H2'	15:A:883:G:C8	2.46	0.51
5:L:172:ILE:HD11	5:L:196:TYR:HE2	1.76	0.51
1:E:31:ASN:ND2	1:E:94:LYS:O	2.41	0.50
1:E:69:CYS:SG	1:E:70:LEU:N	2.84	0.50
3:J:198:ARG:NH2	15:A:281:G:OP1	2.40	0.50
2:H:98:ASN:HB2	2:H:114:ILE:HG13	1.93	0.50
7:O:80:VAL:O	7:O:125:GLY:HA2	2.11	0.50
8:Q:47:PRO:HA	8:Q:50:ILE:HD12	1.94	0.50
7:O:80:VAL:O	7:O:125:GLY:CA	2.59	0.50
15:A:694:U:H2'	15:A:695:C:C6	2.47	0.50
1:E:126:THR:HA	1:E:136:ARG:HA	1.93	0.50
15:A:638:G:O6	15:A:690:U:O4	2.29	0.50
15:A:684:G:H2'	15:A:685:G:H8	1.76	0.50
15:A:824:U:O4	15:A:844:G:O6	2.29	0.50
15:A:1061:G:H2'	15:A:1062:A:H8	1.75	0.50
7:O:34:LYS:NZ	15:A:208:A:O5'	2.44	0.50
11:a:90:ASP:OD1	11:a:90:ASP:N	2.45	0.50
7:O:138:LYS:HB2	15:A:334:G:H3'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:182:ARG:NH1	15:A:255:C:O2	2.44	0.50
6:M:13:PRO:HD3	6:M:41:TRP:NE1	2.26	0.50
6:M:166:ARG:NH2	15:A:532:A:OP1	2.45	0.50
15:A:220:A:C6	15:A:835:G:C6	3.00	0.50
15:A:267:C:C4	15:A:268:A:N6	2.80	0.50
5:L:5:ARG:NH1	15:A:333:G:O6	2.39	0.50
5:L:123:ARG:HB3	5:L:125:ARG:HG2	1.93	0.49
8:Q:70:LYS:NZ	15:A:961:A:N7	2.59	0.49
15:A:268:A:N1	15:A:282:G:C6	2.80	0.49
3:J:133:LEU:O	15:A:163:C:O2'	2.30	0.49
15:A:810:A:C6	15:A:856:G:C2	3.00	0.49
1:E:88:VAL:HA	1:E:98:THR:HA	1.93	0.49
6:M:129:GLN:OE1	15:A:509:A:O2'	2.27	0.49
9:R:74:MET:HE2	9:R:78:GLN:HE22	1.77	0.49
15:A:71:A:N6	15:A:80:G:H1	2.10	0.49
15:A:403:U:H2'	15:A:404:A:C8	2.47	0.49
15:A:137:C:H4'	15:A:138:A:C8	2.48	0.49
1:E:29:TRP:HA	1:E:46:THR:O	2.13	0.49
6:M:92:ASP:N	6:M:92:ASP:OD1	2.44	0.49
4:K:104:ILE:HD11	4:K:131:VAL:HG11	1.94	0.49
15:A:231:G:H2'	15:A:232:G:C8	2.48	0.49
15:A:457:A:H3'	15:A:458:G:H8	1.77	0.49
1:E:122:GLU:OE2	15:A:928:A:N6	2.41	0.49
3:J:33:GLY:O	3:J:51:ARG:NH1	2.43	0.49
3:J:133:LEU:HD23	15:A:164:U:H1'	1.93	0.49
5:L:25:ARG:HA	15:A:397:A:H5''	1.94	0.49
15:A:639:G:C2	15:A:688:U:O2	2.65	0.49
17:3:90:HIS:CD2	17:3:91:ARG:HE	2.30	0.49
2:H:31:PRO:HD2	2:H:38:LEU:HD11	1.95	0.49
4:K:62:LYS:HG2	4:K:94:ARG:HH21	1.77	0.49
15:A:772:A:O2'	15:A:785:G:N2	2.45	0.49
15:A:945:C:H2'	15:A:946:G:H8	1.76	0.49
15:A:1772:A:H2'	15:A:1773:G:C8	2.47	0.49
17:3:111:LEU:HD13	17:3:124:LEU:HD13	1.94	0.49
6:M:105:ARG:HH12	6:M:151:GLN:HG3	1.77	0.48
15:A:897:G:N1	15:A:909:U:N3	2.61	0.48
3:J:22:ARG:NH1	3:J:23:LYS:HG3	2.28	0.48
4:K:99:LEU:HD21	4:K:139:LEU:HD23	1.95	0.48
5:L:144:LYS:NZ	15:A:189:C:O2'	2.46	0.48
15:A:125:A:H62	15:A:288:G:H21	1.61	0.48
15:A:360:G:H21	15:A:754:A:H61	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:424:C:O2'	15:A:456:G:N3	2.42	0.48
12:b:112:LYS:NZ	15:A:456:G:OP1	2.37	0.48
15:A:536:G:OP2	15:A:536:G:N2	2.40	0.48
18:6:479:LEU:HD11	18:6:484:LYS:HD3	1.96	0.48
5:L:189:GLU:HA	5:L:193:LEU:HG	1.94	0.48
9:R:106:THR:HG21	17:3:168:SER:HB3	1.95	0.48
14:h:37:ARG:O	14:h:38:LEU:C	2.56	0.48
2:H:3:ARG:HG2	15:A:92:A:H1'	1.95	0.48
4:K:41:LYS:O	4:K:45:ARG:NH1	2.47	0.48
4:K:151:ARG:NH1	10:Z:49:GLU:OE1	2.42	0.48
15:A:252:U:H2'	15:A:253:A:H8	1.78	0.48
3:J:136:LYS:NZ	15:A:66:U:OP2	2.42	0.48
9:R:139:THR:O	17:3:176:GLN:NE2	2.36	0.48
15:A:141:G:H2'	15:A:142:A:H8	1.79	0.48
15:A:991:A:H62	15:A:1009:G:H21	1.62	0.48
14:h:29:THR:O	14:h:30:PRO:C	2.56	0.48
1:E:56:ASN:OD1	1:E:58:ASN:ND2	2.47	0.48
1:E:65:ILE:HD12	15:A:918:U:H5''	1.94	0.48
4:K:81:GLN:HG2	4:K:82:ARG:HD3	1.96	0.48
6:M:135:GLY:H	6:M:153:HIS:HB3	1.79	0.48
15:A:510:U:H2'	15:A:511:G:C8	2.48	0.48
15:A:1074:C:H2'	15:A:1075:C:C6	2.49	0.48
1:E:26:ARG:O	1:E:50:ARG:N	2.47	0.48
2:H:122:LYS:HD3	2:H:162:ILE:HD11	1.96	0.48
15:A:563:C:H2'	15:A:564:A:H8	1.79	0.48
15:A:1058:U:OP2	15:A:1060:U:N3	2.47	0.48
2:H:163:ASP:OD1	2:H:164:LEU:N	2.44	0.47
8:Q:136:PRO:HG2	8:Q:139:TRP:HB2	1.96	0.47
14:h:26:LYS:HD3	14:h:26:LYS:HA	1.72	0.47
8:Q:124:ARG:NH2	15:A:965:A:OP2	2.46	0.47
9:R:32:ILE:HD12	9:R:94:ILE:HG23	1.95	0.47
2:H:87:MET:HG2	2:H:123:LEU:HB2	1.95	0.47
6:M:76:ARG:NH2	15:A:762:U:OP1	2.41	0.47
13:e:36:LYS:HE2	13:e:43:ILE:HD11	1.96	0.47
14:h:41:THR:O	14:h:42:ARG:C	2.53	0.47
15:A:141:G:H2'	15:A:142:A:C8	2.50	0.47
18:6:513:ALA:HA	18:6:516:LYS:HE3	1.96	0.47
6:M:79:VAL:HG12	6:M:84:LEU:HB3	1.96	0.47
12:b:112:LYS:HA	12:b:115:LYS:HG2	1.97	0.47
15:A:70:C:N4	15:A:71:A:H62	2.12	0.47
15:A:1084:A:H2'	15:A:1085:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:144:GLU:OE2	8:Q:21:ASN:ND2	2.39	0.47
8:Q:46:THR:OG1	8:Q:49:GLN:OE1	2.28	0.47
15:A:1772:A:H2'	15:A:1773:G:H8	1.79	0.47
2:H:21:ASP:N	2:H:21:ASP:OD1	2.48	0.47
5:L:77:ARG:NH1	5:L:78:ILE:O	2.48	0.47
15:A:889:A:H2'	15:A:890:A:H8	1.79	0.47
19:8:442:ILE:HA	19:8:445:LYS:HG2	1.95	0.47
1:E:225:LEU:HG	1:E:229:MET:HE1	1.96	0.47
5:L:73:THR:O	5:L:74:ARG:NH1	2.38	0.47
11:a:19:ARG:O	11:a:23:ARG:HB2	2.15	0.47
15:A:814:G:H2'	15:A:815:A:H8	1.80	0.47
9:R:30:ALA:HB2	9:R:92:LEU:HD13	1.97	0.47
15:A:798:U:H2'	15:A:799:G:C8	2.49	0.47
17:3:196:LYS:O	17:3:200:ALA:N	2.41	0.47
8:Q:62:GLN:HB2	8:Q:65:VAL:HG22	1.95	0.47
9:R:113:SER:HB2	17:3:165:TYR:HE2	1.80	0.47
17:3:116:ASN:O	17:3:120:LYS:N	2.48	0.47
9:R:50:GLU:HA	15:A:893:G:H1'	1.95	0.46
15:A:113:C:C4	15:A:244:A:C6	3.04	0.46
15:A:424:C:N4	15:A:425:A:N6	2.64	0.46
15:A:844:G:H2'	15:A:845:A:C8	2.48	0.46
15:A:98:C:H2'	15:A:375:A:H4'	1.97	0.46
15:A:643:U:C2	15:A:684:G:N1	2.84	0.46
15:A:15:U:O2'	15:A:617:A:N6	2.48	0.46
15:A:531:A:H3'	15:A:532:A:H8	1.81	0.46
5:L:57:ALA:HB2	5:L:181:GLY:HA2	1.97	0.46
7:O:31:ARG:HB2	7:O:34:LYS:HB3	1.97	0.46
15:A:148:G:N1	15:A:161:A:C6	2.84	0.46
2:H:69:LEU:HD22	12:b:20:LEU:HD13	1.97	0.46
11:a:48:HIS:HB3	11:a:103:LEU:HD11	1.97	0.46
15:A:101:U:H3'	15:A:357:A:H61	1.80	0.46
15:A:219:C:N4	15:A:220:A:N6	2.64	0.46
15:A:403:U:H2'	15:A:404:A:H8	1.80	0.46
5:L:173:ILE:HD12	5:L:183:ALA:HB1	1.98	0.46
10:Z:88:LYS:HB3	10:Z:88:LYS:HE3	1.72	0.46
15:A:196:G:H2'	15:A:197:A:C8	2.49	0.46
15:A:631:G:N1	15:A:963:U:OP2	2.36	0.46
17:3:116:ASN:O	17:3:120:LYS:CA	2.64	0.46
15:A:702:A:H62	15:A:731:G:H21	1.64	0.46
15:A:937:A:H2'	15:A:938:A:C8	2.50	0.46
2:H:115:THR:OG1	2:H:116:ASP:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:78:SER:OG	3:J:79:GLU:N	2.48	0.46
12:b:105:LYS:NZ	15:A:441:C:OP1	2.41	0.46
15:A:727:C:H2'	15:A:728:G:C8	2.51	0.46
17:3:110:LYS:O	17:3:130:THR:OG1	2.31	0.46
1:E:151:LYS:NZ	1:E:153:THR:O	2.40	0.46
2:H:162:ILE:HG22	2:H:169:ILE:HG12	1.97	0.46
2:H:195:ILE:HA	2:H:210:LEU:HD23	1.98	0.46
5:L:153:HIS:HB3	7:O:24:LYS:NZ	2.31	0.46
5:L:188:LEU:HD12	5:L:193:LEU:HD23	1.98	0.46
12:b:29:ASP:OD1	12:b:29:ASP:N	2.48	0.46
15:A:70:C:N4	15:A:71:A:N6	2.64	0.46
9:R:21:ARG:HE	9:R:24:GLU:HG3	1.82	0.45
11:a:68:ILE:HD12	11:a:70:LYS:HE3	1.98	0.45
15:A:458:G:H2'	15:A:459:G:C8	2.51	0.45
11:a:54:LEU:HD12	11:a:75:GLN:HB2	1.98	0.45
15:A:1105:G:OP2	15:A:1105:G:N2	2.39	0.45
3:J:155:LYS:HA	3:J:155:LYS:HD3	1.76	0.45
5:L:83:TYR:HB3	5:L:101:VAL:HB	1.98	0.45
15:A:96:C:H1'	15:A:423:G:H5'	1.98	0.45
15:A:706:C:H2'	15:A:707:A:C8	2.51	0.45
15:A:897:G:C6	15:A:909:U:N3	2.85	0.45
19:8:427:ARG:O	19:8:431:ILE:HG12	2.16	0.45
1:E:75:LYS:HB3	1:E:75:LYS:HE3	1.74	0.45
4:K:6:LEU:O	4:K:16:ARG:NH1	2.49	0.45
5:L:10:LYS:NZ	15:A:334:G:O3'	2.50	0.45
6:M:141:VAL:HG12	6:M:143:SER:H	1.81	0.45
7:O:109:HIS:NE2	15:A:346:G:OP1	2.47	0.45
10:Z:28:ARG:NH1	15:A:863:A:OP1	2.39	0.45
15:A:61:A:N3	15:A:266:G:O2'	2.47	0.45
15:A:52:U:H2'	15:A:53:G:H8	1.81	0.45
15:A:176:A:H2'	15:A:177:A:C8	2.52	0.45
15:A:697:G:H2'	15:A:698:G:C8	2.51	0.45
5:L:110:ARG:NH2	5:L:164:PHE:O	2.48	0.45
6:M:81:ILE:HD12	6:M:145:MET:HE2	1.99	0.45
8:Q:61:ALA:HB1	15:A:957:U:H1'	1.99	0.45
8:Q:108:ASP:OD1	15:A:876:G:O2'	2.32	0.45
15:A:138:A:O2'	15:A:263:A:N3	2.48	0.45
15:A:985:G:H2'	18:6:476:LYS:HE3	1.99	0.45
16:1:257:LYS:HD2	16:1:267:VAL:HB	1.97	0.45
17:3:193:LYS:O	17:3:196:LYS:HB2	2.16	0.45
6:M:140:ASN:ND2	12:b:67:TYR:OH	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:62:GLN:NE2	15:A:957:U:O3'	2.45	0.45
9:R:93:HIS:ND1	9:R:126:GLY:O	2.37	0.45
11:a:95:PHE:O	11:a:142:LYS:NZ	2.36	0.45
15:A:443:A:H61	15:A:458:G:H21	1.44	0.45
15:A:581:C:H2'	15:A:582:A:H8	1.81	0.45
15:A:1016:U:H2'	15:A:1017:A:C8	2.52	0.45
16:1:246:LYS:HB3	16:1:252:TRP:CD1	2.51	0.45
15:A:882:A:H2'	15:A:883:G:H8	1.82	0.45
18:6:509:LYS:HE2	18:6:509:LYS:HB2	1.79	0.45
3:J:57:ASP:HA	3:J:106:LEU:HA	1.99	0.45
7:O:82:SER:HB3	7:O:90:ILE:HB	1.98	0.45
9:R:117:ALA:HA	9:R:120:ARG:HB2	1.98	0.45
3:J:6:SER:O	3:J:112:SER:HA	2.17	0.45
5:L:189:GLU:O	7:O:22:ASN:ND2	2.50	0.45
8:Q:56:ASP:HA	13:e:47:PHE:HB2	1.99	0.45
15:A:252:U:H2'	15:A:253:A:C8	2.52	0.45
15:A:892:U:H2'	15:A:893:G:C8	2.51	0.45
15:A:951:G:H2'	15:A:952:G:C8	2.52	0.45
3:J:32:MET:HE1	3:J:54:GLY:HA2	1.99	0.44
10:Z:25:VAL:O	10:Z:62:VAL:HA	2.16	0.44
15:A:113:C:C4	15:A:244:A:N6	2.85	0.44
15:A:639:G:C2	15:A:688:U:C2	3.05	0.44
15:A:464:G:O2'	15:A:466:C:OP2	2.27	0.44
15:A:485:G:O6	15:A:496:U:O4	2.35	0.44
15:A:487:U:N3	15:A:495:G:C6	2.86	0.44
15:A:696:U:H2'	15:A:697:G:H8	1.82	0.44
15:A:843:G:H2'	15:A:844:G:C8	2.52	0.44
15:A:905:A:H2	15:A:995:G:H21	1.65	0.44
1:E:111:ARG:HH12	15:A:928:A:H1'	1.82	0.44
1:E:226:GLY:HA2	1:E:229:MET:HE2	2.00	0.44
15:A:652:G:O6	15:A:673:U:O4	2.35	0.44
5:L:124:ARG:HG2	5:L:165:GLU:HG3	1.99	0.44
15:A:98:C:OP2	15:A:375:A:O2'	2.25	0.44
1:E:33:LYS:HE3	1:E:42:ASP:HB2	1.99	0.44
15:A:195:G:H2'	15:A:196:G:C8	2.51	0.44
15:A:897:G:H2'	15:A:898:A:H8	1.82	0.44
5:L:123:ARG:HH11	5:L:125:ARG:HD3	1.83	0.44
15:A:29:U:H2'	15:A:30:G:C8	2.52	0.44
15:A:1796:A:C4	17:3:92:MET:HE1	2.53	0.44
1:E:71:ALA:HB2	1:E:80:ALA:HA	2.00	0.44
9:R:44:THR:HA	9:R:52:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:150:G:H2'	15:A:151:G:C8	2.53	0.44
15:A:189:C:O3'	15:A:190:G:N2	2.51	0.44
15:A:820:U:O2	15:A:848:G:N2	2.39	0.44
1:E:116:LYS:HG2	15:A:929:C:H5''	2.00	0.44
1:E:71:ALA:HB3	9:R:127:ARG:HH12	1.82	0.44
9:R:100:GLY:HA3	9:R:133:PRO:HG2	2.00	0.44
15:A:597:U:H2'	15:A:598:A:C8	2.53	0.44
15:A:643:U:O2	15:A:684:G:C2	2.71	0.44
19:8:429:LYS:HA	19:8:432:LYS:HD2	1.99	0.44
19:8:444:ARG:HA	19:8:447:LEU:HG	2.00	0.44
15:A:597:U:H2'	15:A:598:A:H8	1.83	0.43
15:A:811:U:O2'	15:A:813:G:OP1	2.35	0.43
17:3:247:ASN:HA	17:3:250:ILE:HG12	2.00	0.43
1:E:25:THR:O	1:E:50:ARG:NH2	2.48	0.43
7:O:145:LEU:HD23	7:O:145:LEU:HA	1.78	0.43
3:J:176:PRO:HA	15:A:66:U:H5'	1.99	0.43
6:M:60:LEU:HD12	6:M:61:ASP:H	1.84	0.43
19:8:831:SER:OG	19:8:832:TRP:N	2.51	0.43
8:Q:140:LYS:HA	8:Q:140:LYS:HD2	1.81	0.43
15:A:184:G:N1	15:A:192:A:C5	2.86	0.43
15:A:363:G:OP1	15:A:757:U:O2'	2.28	0.43
15:A:673:U:H2'	15:A:674:G:C8	2.54	0.43
2:H:45:ILE:HG13	2:H:61:THR:HG21	1.99	0.43
4:K:32:ASP:O	4:K:36:ASN:ND2	2.52	0.43
4:K:61:LYS:HA	4:K:61:LYS:HD2	1.81	0.43
10:Z:32:LYS:N	15:A:634:C:OP1	2.51	0.43
15:A:110:U:O4	15:A:111:A:N6	2.52	0.43
15:A:177:A:H2'	15:A:178:A:C8	2.53	0.43
2:H:199:GLU:OE2	2:H:209:HIS:NE2	2.47	0.43
4:K:147:GLY:HA2	8:Q:18:TYR:HE2	1.84	0.43
15:A:17:C:O2'	15:A:1134:A:N1	2.52	0.43
15:A:232:G:H2'	15:A:233:G:C8	2.54	0.43
15:A:9:U:N3	15:A:12:U:OP2	2.48	0.43
15:A:674:G:H2'	15:A:675:G:C8	2.54	0.43
15:A:700:G:N3	15:A:732:A:N1	2.67	0.43
15:A:643:U:C2	15:A:684:G:C2	3.06	0.43
17:3:193:LYS:HG3	17:3:196:LYS:HD3	2.01	0.43
3:J:52:ILE:HA	3:J:111:LEU:HD13	2.01	0.43
4:K:61:LYS:HZ1	4:K:95:HIS:N	2.15	0.43
4:K:69:PRO:HG2	4:K:72:ALA:HB3	2.01	0.43
15:A:921:A:H2'	15:A:922:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:ILE:HB	1:E:141:ALA:HB3	2.01	0.42
2:H:211:LYS:HE3	2:H:211:LYS:HB2	1.88	0.42
7:O:47:PHE:CD2	7:O:145:LEU:HD13	2.54	0.42
12:b:115:LYS:NZ	15:A:57:G:OP1	2.49	0.42
4:K:51:SER:OG	4:K:52:ALA:N	2.52	0.42
15:A:561:G:N1	15:A:576:A:O2'	2.30	0.42
10:Z:111:MET:HE2	10:Z:111:MET:HB3	1.90	0.42
15:A:1:U:N3	15:A:367:A:C5	2.87	0.42
15:A:177:A:H2'	15:A:178:A:H8	1.84	0.42
15:A:249:U:H2'	15:A:250:A:H8	1.84	0.42
3:J:121:ILE:HB	3:J:125:THR:H	1.84	0.42
4:K:121:LYS:HE2	15:A:808:G:C5	2.54	0.42
15:A:194:G:O2'	15:A:195:G:O5'	2.37	0.42
15:A:355:U:O2'	15:A:357:A:OP1	2.34	0.42
2:H:212:ASP:OD1	2:H:213:ALA:N	2.51	0.42
5:L:81:VAL:HA	5:L:102:VAL:HA	2.01	0.42
9:R:43:VAL:HG13	9:R:52:ILE:HB	2.02	0.42
11:a:75:GLN:NE2	11:a:76:LEU:O	2.52	0.42
11:a:126:LYS:HG2	11:a:131:GLY:HA2	2.01	0.42
15:A:824:U:H2'	15:A:825:C:C6	2.54	0.42
15:A:977:A:H4'	15:A:1782:G:H22	1.84	0.42
9:R:59:MET:HB2	9:R:60:LYS:HZ3	1.84	0.42
15:A:181:C:H2'	15:A:182:C:C6	2.55	0.42
15:A:1117:U:O4	15:A:1124:G:O6	2.38	0.42
2:H:55:ALA:HB2	2:H:64:ILE:HD12	2.01	0.42
2:H:59:ARG:NH2	12:b:90:PRO:HG3	2.34	0.42
2:H:128:ARG:NH1	15:A:292:A:O3'	2.53	0.42
2:H:208:VAL:HG11	2:H:225:VAL:HG21	2.02	0.42
11:a:133:LEU:HD12	16:1:282:PHE:CG	2.55	0.42
17:3:133:ASN:N	17:3:133:ASN:OD1	2.52	0.42
2:H:249:GLU:HA	2:H:252:ASP:HB2	2.02	0.42
8:Q:55:ARG:HH22	13:e:51:GLN:NE2	2.18	0.42
10:Z:44:HIS:NE2	10:Z:112:ASP:OD2	2.34	0.42
15:A:992:G:H2'	15:A:993:A:C8	2.55	0.42
9:R:134:THR:O	15:A:884:U:O2'	2.36	0.42
10:Z:45:GLY:O	10:Z:68:ARG:NH2	2.52	0.42
12:b:43:LEU:HD23	12:b:60:VAL:HG11	2.02	0.42
12:b:91:ARG:HH21	12:b:103:VAL:HG23	1.84	0.42
15:A:125:A:N6	15:A:289:U:C5	2.87	0.42
5:L:179:GLN:HE22	15:A:329:U:H5	1.67	0.42
13:e:67:THR:HG21	13:e:72:ARG:HH22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:71:A:N1	15:A:80:G:C6	2.88	0.42
15:A:809:A:C4	15:A:856:G:H1'	2.54	0.42
1:E:35:PRO:O	1:E:41:ARG:NH1	2.53	0.41
1:E:118:GLN:O	15:A:929:C:O2'	2.37	0.41
2:H:179:ALA:HB3	2:H:195:ILE:HD12	2.02	0.41
11:a:62:LYS:NZ	15:A:1134:A:OP1	2.53	0.41
2:H:183:ILE:HD12	2:H:220:THR:HG21	2.01	0.41
14:h:39:LEU:HA	14:h:39:LEU:HD23	1.68	0.41
2:H:64:ILE:HG23	12:b:20:LEU:HD12	2.03	0.41
4:K:132:HIS:HB3	4:K:189:ARG:HH21	1.85	0.41
15:A:227:U:O2	15:A:231:G:C6	2.74	0.41
2:H:88:ASP:OD1	2:H:89:VAL:N	2.53	0.41
2:H:105:THR:HG22	2:H:244:LYS:HE3	2.02	0.41
6:M:26:LEU:HA	6:M:29:VAL:HG12	2.02	0.41
7:O:80:VAL:HG22	7:O:91:ILE:HG22	2.03	0.41
15:A:862:U:H6	15:A:862:U:H2'	1.72	0.41
15:A:959:U:H2'	15:A:960:C:H6	1.85	0.41
15:A:1007:U:H2'	15:A:1008:C:C6	2.55	0.41
15:A:1041:A:H61	15:A:1072:C:H42	0.68	0.41
4:K:150:LEU:HD21	4:K:158:LYS:HD3	2.03	0.41
6:M:47:LEU:HD21	6:M:51:ARG:NH2	2.35	0.41
15:A:268:A:C6	15:A:282:G:N1	2.88	0.41
15:A:1040:G:N2	19:8:418:ARG:HE	2.19	0.41
4:K:121:LYS:HG3	15:A:808:G:C2	2.56	0.41
11:a:103:LEU:HB3	11:a:126:LYS:HB2	2.03	0.41
12:b:42:GLU:OE2	12:b:46:LYS:NZ	2.47	0.41
15:A:622:C:H2'	15:A:623:U:C6	2.55	0.41
17:3:168:SER:HA	17:3:216:VAL:O	2.20	0.41
2:H:146:THR:HG21	15:A:122:G:H21	1.85	0.41
5:L:184:ASP:OD2	15:A:203:U:O2'	2.35	0.41
10:Z:118:ARG:NH1	15:A:681:C:O2'	2.46	0.41
15:A:382:A:H2'	15:A:383:G:C8	2.55	0.41
15:A:588:A:H2'	15:A:589:A:C8	2.55	0.41
15:A:709:G:O6	15:A:722:U:O4	2.38	0.41
13:e:57:GLN:CD	13:e:57:GLN:H	2.28	0.41
15:A:469:U:H2'	15:A:470:A:H8	1.86	0.41
1:E:31:ASN:ND2	1:E:94:LYS:HD3	2.35	0.41
1:E:31:ASN:HD21	1:E:94:LYS:HD3	1.86	0.41
1:E:153:THR:HB	1:E:155:TYR:CE2	2.56	0.41
3:J:7:HIS:HB2	3:J:124:LEU:HD21	2.03	0.41
3:J:15:LEU:HD11	15:A:150:G:H4'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:26:LEU:HD11	8:Q:60:ILE:HG22	2.02	0.41
8:Q:91:LEU:HD23	8:Q:91:LEU:HA	1.96	0.41
9:R:31:ARG:NH1	15:A:917:A:OP1	2.54	0.41
10:Z:104:LEU:HD23	10:Z:125:ILE:HA	2.02	0.41
11:a:48:HIS:CD2	11:a:105:ALA:HB2	2.56	0.41
11:a:74:VAL:O	11:a:82:LYS:HA	2.21	0.41
15:A:113:C:N3	15:A:244:A:C6	2.89	0.41
15:A:125:A:N6	15:A:289:U:C4	2.89	0.41
15:A:500:G:H2'	15:A:501:U:C6	2.55	0.41
15:A:954:U:OP1	15:A:1069:C:O2'	2.35	0.41
15:A:974:G:N1	15:A:1021:A:O2'	2.49	0.41
16:1:250:LYS:NZ	16:1:274:THR:OG1	2.42	0.41
16:1:256:LYS:HD3	16:1:256:LYS:HA	1.86	0.41
17:3:99:TRP:CG	19:8:829:TRP:HE1	2.39	0.41
2:H:117:GLU:O	2:H:120:LYS:HG2	2.21	0.41
4:K:166:GLU:OE2	4:K:169:ARG:NH1	2.54	0.41
6:M:124:ARG:NH1	15:A:472:A:OP1	2.54	0.41
6:M:174:LYS:HE3	6:M:174:LYS:HB3	1.89	0.41
2:H:51:ARG:HD2	2:H:51:ARG:HA	1.81	0.40
12:b:8:VAL:HG23	12:b:32:HIS:HB3	2.02	0.40
15:A:160:G:OP2	15:A:160:G:N2	2.39	0.40
6:M:107:LEU:HD12	6:M:107:LEU:HA	1.96	0.40
11:a:69:ARG:HD3	11:a:117:ILE:HD12	2.03	0.40
12:b:38:ILE:HD11	12:b:42:GLU:OE1	2.21	0.40
15:A:461:A:H2'	15:A:462:G:H8	1.87	0.40
1:E:149:GLN:HB2	15:A:1063:C:H4'	2.04	0.40
2:H:51:ARG:NH2	2:H:109:PHE:O	2.51	0.40
12:b:59:SER:HB3	12:b:77:LEU:HB2	2.02	0.40
15:A:1142:U:H2'	15:A:1143:G:H8	1.87	0.40
17:3:121:ARG:NH1	17:3:123:GLU:HG2	2.36	0.40
1:E:99:ASN:OD1	1:E:100:PHE:N	2.54	0.40
1:E:179:CYS:HB2	1:E:183:GLN:HB3	2.03	0.40
2:H:127:LYS:HG3	2:H:142:HIS:HA	2.04	0.40
3:J:155:LYS:NZ	15:A:76:U:O2'	2.51	0.40
4:K:78:ARG:HA	4:K:78:ARG:HD3	1.78	0.40
10:Z:118:ARG:HH22	15:A:682:U:P	2.44	0.40
12:b:44:ARG:HD2	12:b:55:LYS:HG2	2.03	0.40
15:A:153:A:C2	15:A:412:C:H1'	2.57	0.40
15:A:691:C:H1'	15:A:692:C:H2'	2.03	0.40
15:A:904:A:H2'	15:A:905:A:C8	2.56	0.40
15:A:1075:C:H2'	15:A:1076:U:C6	2.57	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	
1	E	211/255 (83%)	190 (90%)	21 (10%)	0	100	100
2	H	259/264 (98%)	241 (93%)	18 (7%)	0	100	100
3	J	230/239 (96%)	218 (95%)	12 (5%)	0	100	100
4	K	193/203 (95%)	182 (94%)	11 (6%)	0	100	100
5	L	199/202 (98%)	185 (93%)	14 (7%)	0	100	100
6	M	177/190 (93%)	172 (97%)	5 (3%)	0	100	100
7	O	148/161 (92%)	145 (98%)	3 (2%)	0	100	100
8	Q	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
9	R	133/150 (89%)	119 (90%)	14 (10%)	0	100	100
10	Z	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
11	a	140/145 (97%)	133 (95%)	7 (5%)	0	100	100
12	b	130/136 (96%)	124 (95%)	6 (5%)	0	100	100
13	e	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
14	h	19/62 (31%)	13 (68%)	5 (26%)	1 (5%)	1	17
16	1	35/282 (12%)	33 (94%)	2 (6%)	0	100	100
17	3	182/259 (70%)	176 (97%)	6 (3%)	0	100	100
18	6	41/519 (8%)	41 (100%)	0	0	100	100
19	8	58/938 (6%)	57 (98%)	1 (2%)	0	100	100
All	All	2509/4368 (57%)	2362 (94%)	146 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	h	27	PRO

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	
1	E	187/223 (84%)	187 (100%)	0	100	100
2	H	219/221 (99%)	219 (100%)	0	100	100
3	J	198/204 (97%)	198 (100%)	0	100	100
4	K	169/177 (96%)	169 (100%)	0	100	100
5	L	163/164 (99%)	163 (100%)	0	100	100
6	M	154/162 (95%)	154 (100%)	0	100	100
7	O	133/143 (93%)	133 (100%)	0	100	100
8	Q	129/130 (99%)	128 (99%)	1 (1%)	73	77
9	R	102/117 (87%)	102 (100%)	0	100	100
10	Z	112/113 (99%)	111 (99%)	1 (1%)	70	76
11	a	113/116 (97%)	113 (100%)	0	100	100
12	b	112/115 (97%)	112 (100%)	0	100	100
13	e	70/71 (99%)	70 (100%)	0	100	100
14	h	19/52 (36%)	15 (79%)	4 (21%)	1	7
16	1	32/227 (14%)	32 (100%)	0	100	100
17	3	155/215 (72%)	154 (99%)	1 (1%)	78	80
18	6	36/447 (8%)	35 (97%)	1 (3%)	38	59
19	8	57/765 (8%)	57 (100%)	0	100	100
All	All	2160/3662 (59%)	2152 (100%)	8 (0%)	81	83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	Q	32	GLN
10	Z	15	ASN
14	h	26	LYS
14	h	27	PRO
14	h	28	LYS
14	h	38	LEU

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Mol	Chain	Res	Type
17	3	98	ASN
18	6	515	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	182	HIS
2	H	9	GLN
3	J	116	GLN
4	K	7	ASN
5	L	94	ASN
7	O	22	ASN
7	O	86	HIS
7	O	103	ASN
8	Q	32	GLN
11	a	75	GLN
12	b	109	GLN
13	e	9	ASN
16	1	259	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	A	1135/1797 (63%)	277 (24%)	13 (1%)

All (277) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	A	2	A
15	A	3	C
15	A	4	C
15	A	5	U
15	A	13	U
15	A	14	C
15	A	25	C
15	A	26	A
15	A	27	U
15	A	34	G
15	A	42	G
15	A	43	A

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Mol	Chain	Res	Type
15	A	45	U
15	A	46	A
15	A	47	A
15	A	57	G
15	A	63	G
15	A	66	U
15	A	68	A
15	A	69	G
15	A	71	A
15	A	72	A
15	A	73	U
15	A	74	U
15	A	76	U
15	A	77	A
15	A	103	A
15	A	110	U
15	A	113	C
15	A	115	U
15	A	116	U
15	A	126	G
15	A	127	U
15	A	138	A
15	A	139	U
15	A	150	G
15	A	153	A
15	A	155	U
15	A	156	U
15	A	157	C
15	A	158	U
15	A	165	A
15	A	174	U
15	A	175	G
15	A	181	C
15	A	184	G
15	A	188	U
15	A	189	C
15	A	191	G
15	A	192	A
15	A	195	G
15	A	210	A
15	A	212	U
15	A	213	A

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Mol	Chain	Res	Type
15	A	214	A
15	A	221	A
15	A	222	U
15	A	223	G
15	A	228	U
15	A	231	G
15	A	232	G
15	A	234	C
15	A	235	U
15	A	237	U
15	A	247	C
15	A	254	A
15	A	257	U
15	A	258	C
15	A	262	A
15	A	264	U
15	A	268	A
15	A	269	C
15	A	270	G
15	A	272	C
15	A	274	U
15	A	275	U
15	A	277	C
15	A	278	G
15	A	296	A
15	A	305	C
15	A	306	C
15	A	310	U
15	A	311	C
15	A	313	A
15	A	317	U
15	A	318	C
15	A	319	G
15	A	322	G
15	A	326	G
15	A	334	G
15	A	335	C
15	A	349	A
15	A	356	A
15	A	357	A
15	A	358	C
15	A	385	A

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Mol	Chain	Res	Type
15	A	387	G
15	A	396	A
15	A	397	A
15	A	398	A
15	A	399	C
15	A	401	G
15	A	415	G
15	A	418	A
15	A	420	G
15	A	421	C
15	A	422	A
15	A	423	G
15	A	425	A
15	A	431	G
15	A	436	U
15	A	441	C
15	A	442	A
15	A	456	G
15	A	480	A
15	A	481	C
15	A	490	U
15	A	492	C
15	A	493	G
15	A	495	G
15	A	502	A
15	A	503	A
15	A	505	U
15	A	508	A
15	A	512	A
15	A	516	C
15	A	524	A
15	A	529	U
15	A	531	A
15	A	533	C
15	A	535	A
15	A	536	G
15	A	538	A
15	A	539	A
15	A	548	G
15	A	549	G
15	A	551	C
15	A	552	A

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Mol	Chain	Res	Type
15	A	553	A
15	A	555	U
15	A	556	C
15	A	558	G
15	A	563	C
15	A	575	U
15	A	576	A
15	A	577	A
15	A	578	U
15	A	580	C
15	A	583	G
15	A	591	A
15	A	592	G
15	A	606	U
15	A	608	U
15	A	612	G
15	A	616	A
15	A	617	A
15	A	619	A
15	A	620	A
15	A	621	G
15	A	627	A
15	A	636	U
15	A	641	C
15	A	677	U
15	A	678	G
15	A	679	G
15	A	680	G
15	A	683	G
15	A	686	C
15	A	689	U
15	A	691	C
15	A	692	C
15	A	693	U
15	A	705	G
15	A	709	G
15	A	710	C
15	A	724	U
15	A	725	G
15	A	726	U
15	A	727	C
15	A	729	G

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Mol	Chain	Res	Type
15	A	730	G
15	A	731	G
15	A	732	A
15	A	738	G
15	A	742	U
15	A	754	A
15	A	764	G
15	A	765	C
15	A	773	A
15	A	774	G
15	A	777	C
15	A	779	A
15	A	780	U
15	A	781	G
15	A	787	A
15	A	791	A
15	A	792	U
15	A	793	U
15	A	809	A
15	A	810	A
15	A	812	A
15	A	813	G
15	A	818	U
15	A	819	G
15	A	822	G
15	A	823	U
15	A	824	U
15	A	828	U
15	A	830	U
15	A	832	G
15	A	861	A
15	A	871	U
15	A	874	G
15	A	879	G
15	A	884	U
15	A	895	C
15	A	896	A
15	A	901	U
15	A	910	U
15	A	911	G
15	A	912	G
15	A	917	A

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Mol	Chain	Res	Type
15	A	919	U
15	A	920	G
15	A	931	A
15	A	932	C
15	A	933	U
15	A	940	G
15	A	957	U
15	A	958	U
15	A	964	A
15	A	969	G
15	A	986	A
15	A	990	A
15	A	994	C
15	A	996	A
15	A	998	C
15	A	999	A
15	A	1000	G
15	A	1001	A
15	A	1019	C
15	A	1023	A
15	A	1024	A
15	A	1026	C
15	A	1027	U
15	A	1030	G
15	A	1039	G
15	A	1040	G
15	A	1041	A
15	A	1051	G
15	A	1056	U
15	A	1057	U
15	A	1066	G
15	A	1073	A
15	A	1077	U
15	A	1079	C
15	A	1080	G
15	A	1089	A
15	A	1090	A
15	A	1093	G
15	A	1095	U
15	A	1097	G
15	A	1135	A
15	A	1140	A

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Mol	Chain	Res	Type
15	A	1766	C
15	A	1768	C
15	A	1776	G
15	A	1777	A
15	A	1779	C
15	A	1782	G
15	A	1786	A
15	A	1788	G
15	A	1790	A
15	A	1791	U
15	A	1795	U
15	A	1796	A
15	A	1797	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	A	211	U
15	A	231	G
15	A	233	G
15	A	269	C
15	A	414	A
15	A	421	C
15	A	552	A
15	A	611	A
15	A	678	G
15	A	792	U
15	A	1040	G
15	A	1094	U
15	A	1795	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

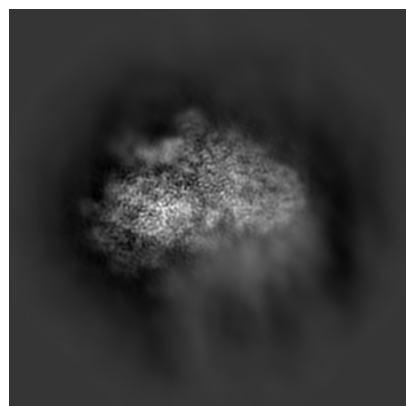
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66688. These allow visual inspection of the internal detail of the map and identification of artifacts.

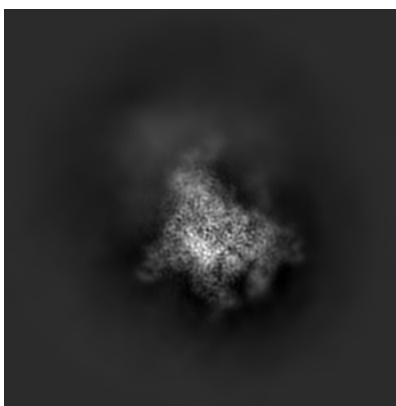
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

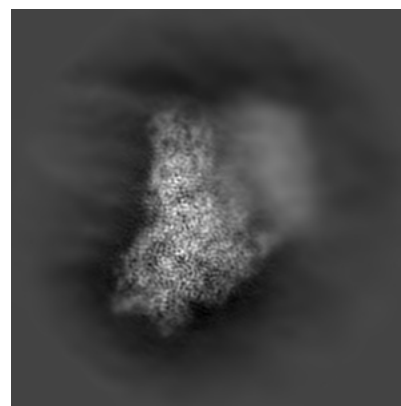
6.1.1 Primary map



X

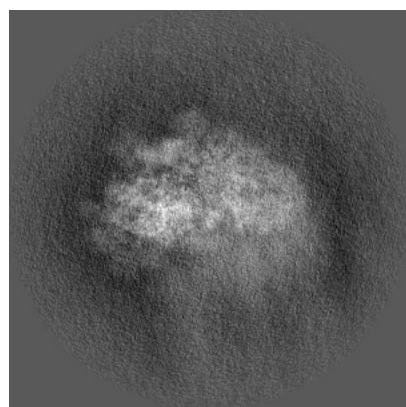


Y

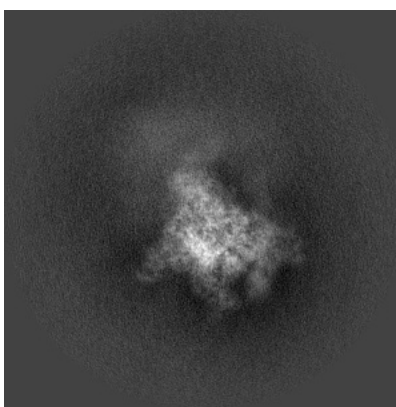


Z

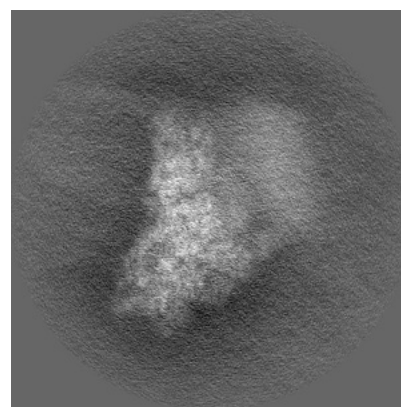
6.1.2 Raw map



X



Y

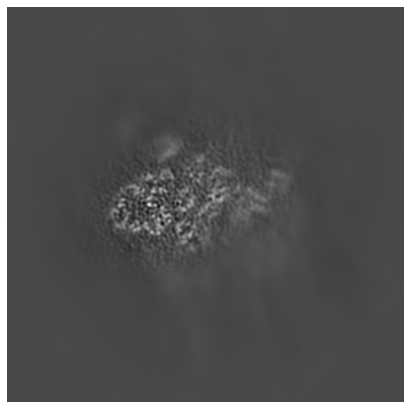


Z

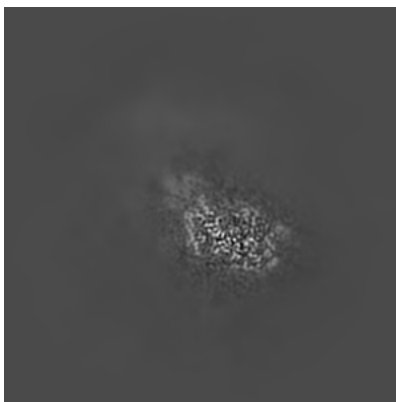
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

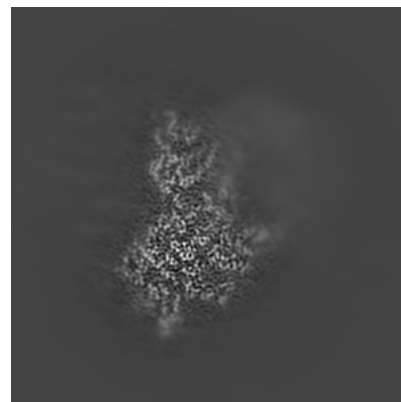
6.2.1 Primary map



X Index: 180

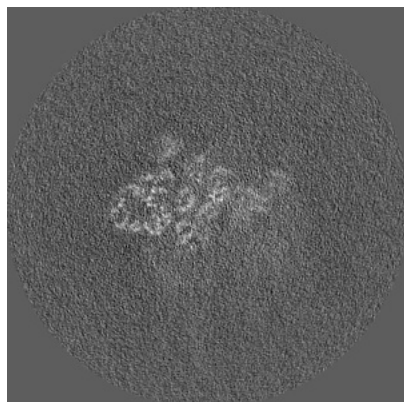


Y Index: 180

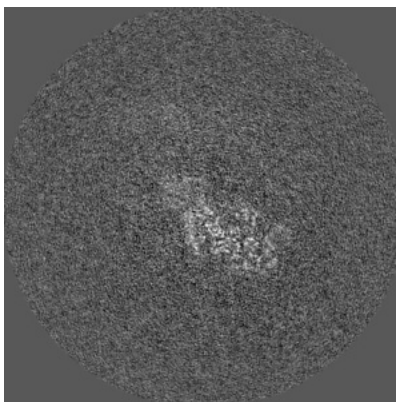


Z Index: 180

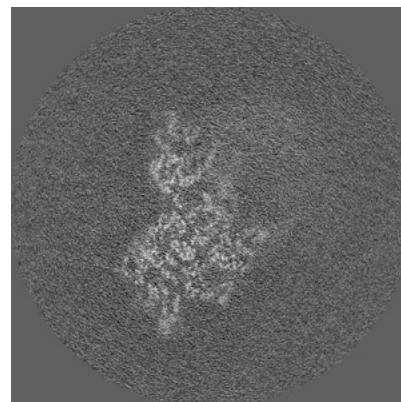
6.2.2 Raw map



X Index: 180



Y Index: 180

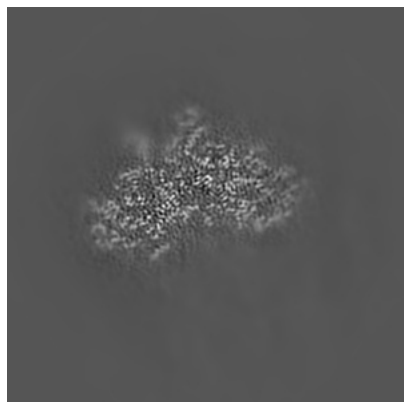


Z Index: 180

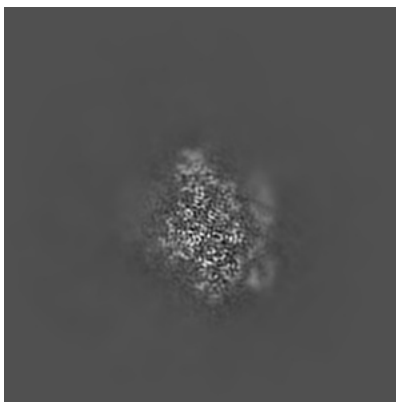
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

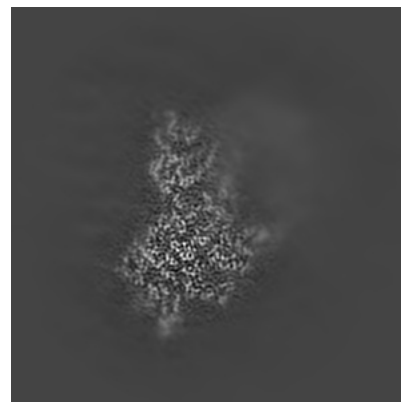
6.3.1 Primary map



X Index: 150

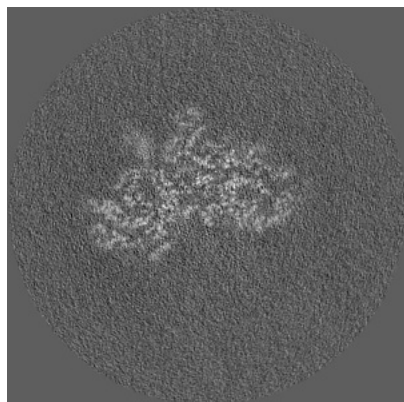


Y Index: 139

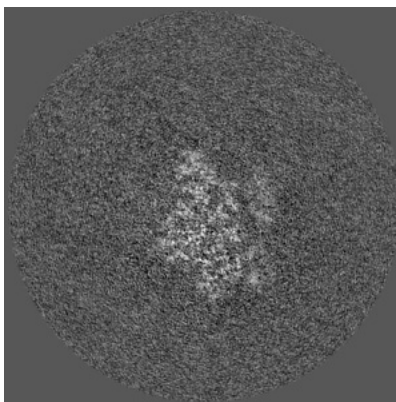


Z Index: 180

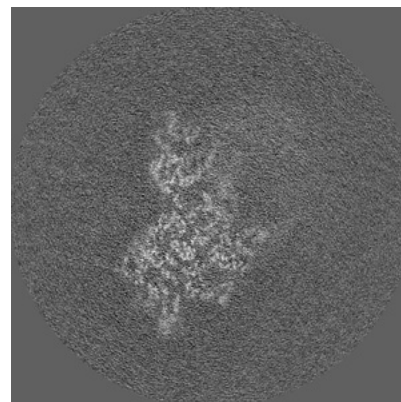
6.3.2 Raw map



X Index: 149



Y Index: 138

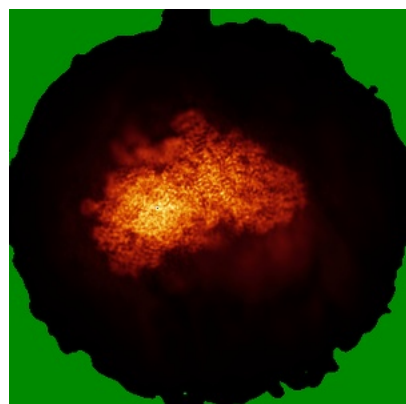


Z Index: 180

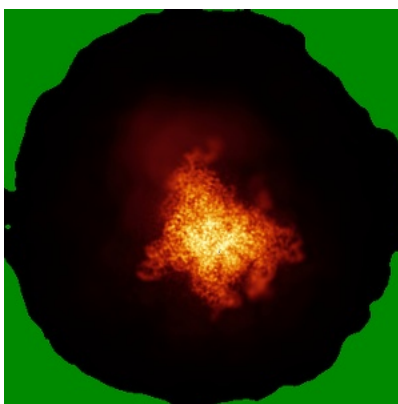
The images above show the largest variance slices of the map in three orthogonal directions.

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

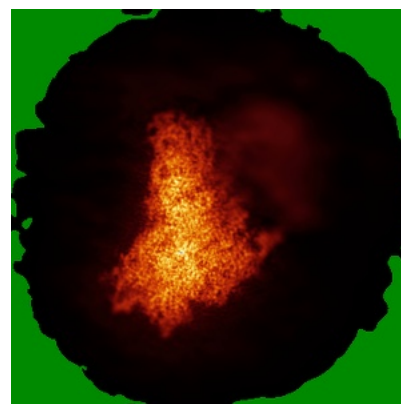
6.4.1 Primary map



X

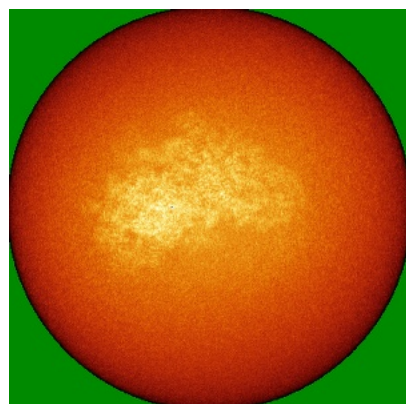


Y

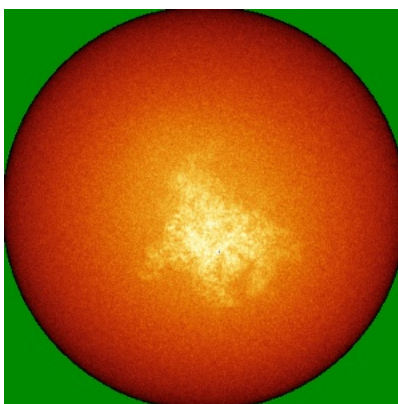


Z

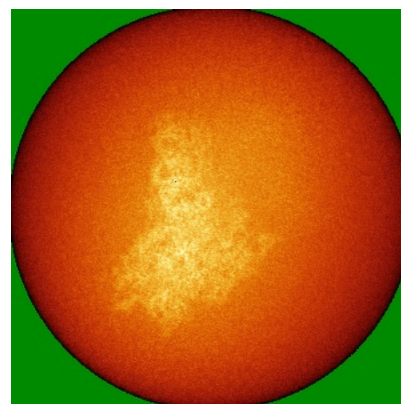
6.4.2 Raw map



X



Y

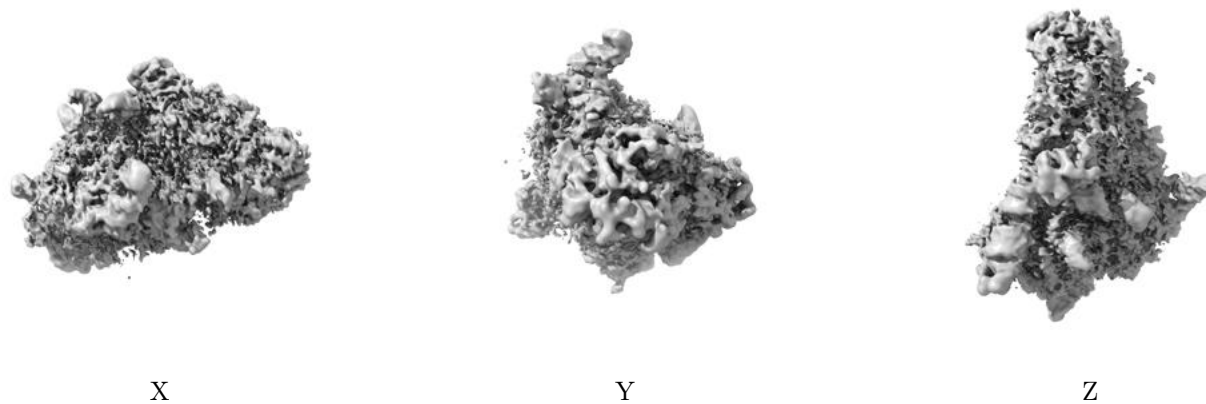


Z

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.

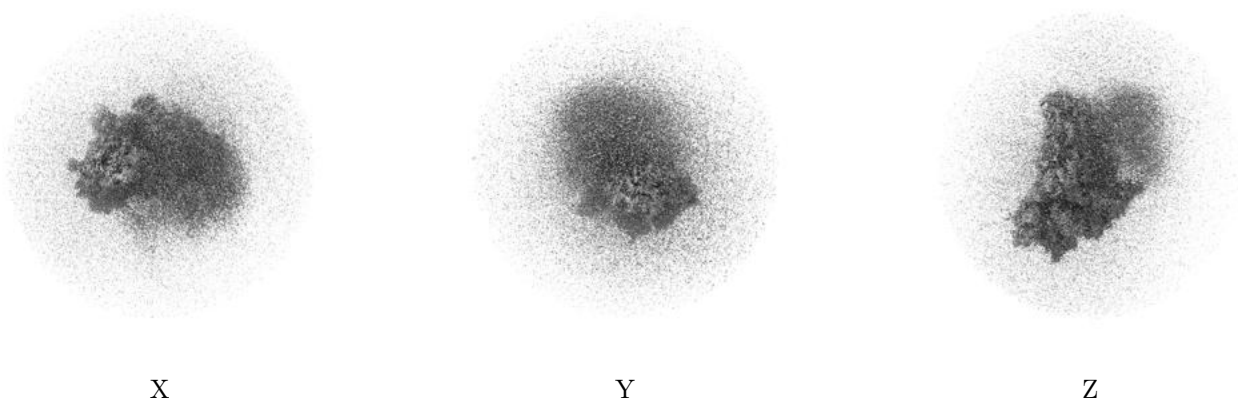
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

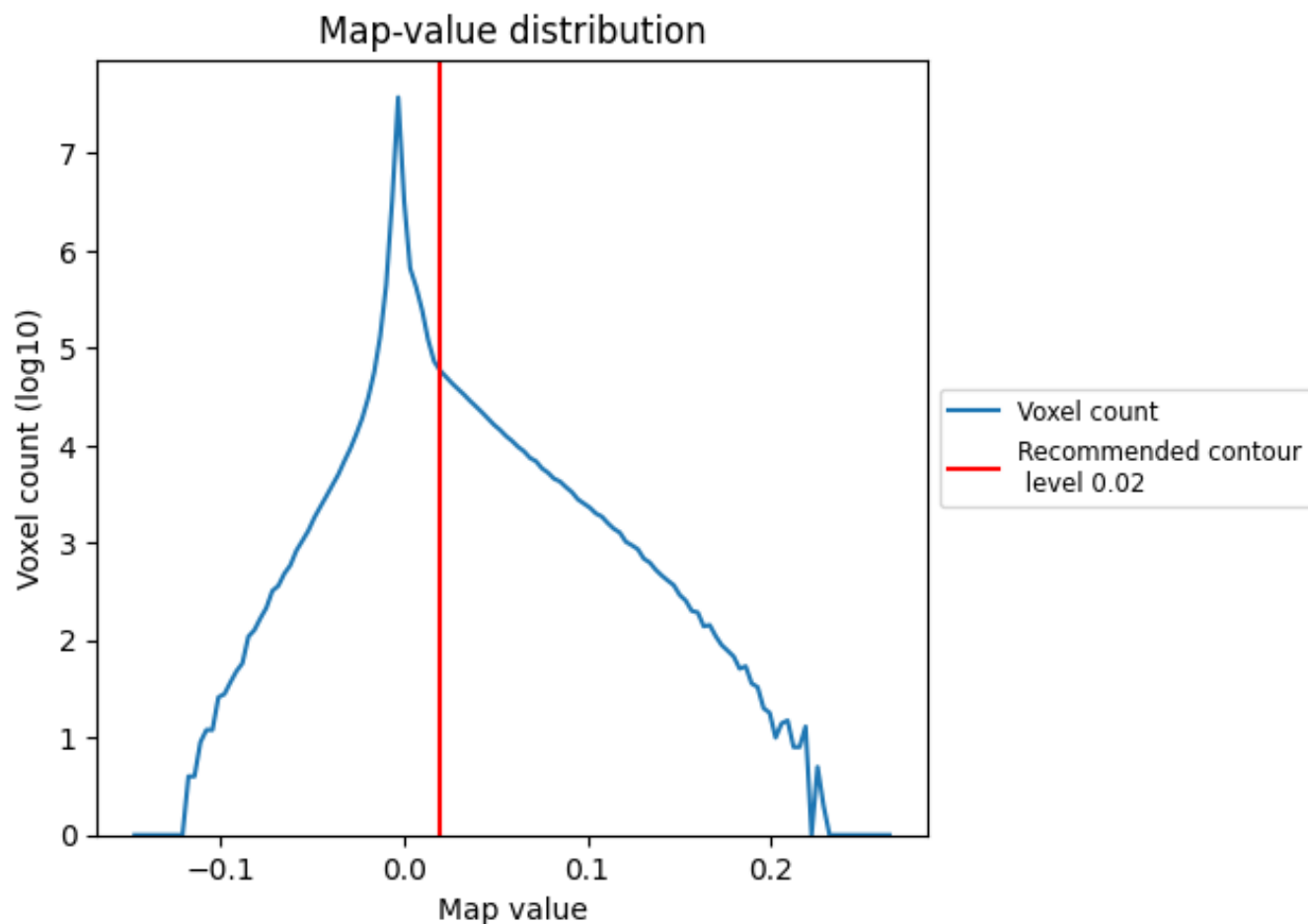
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

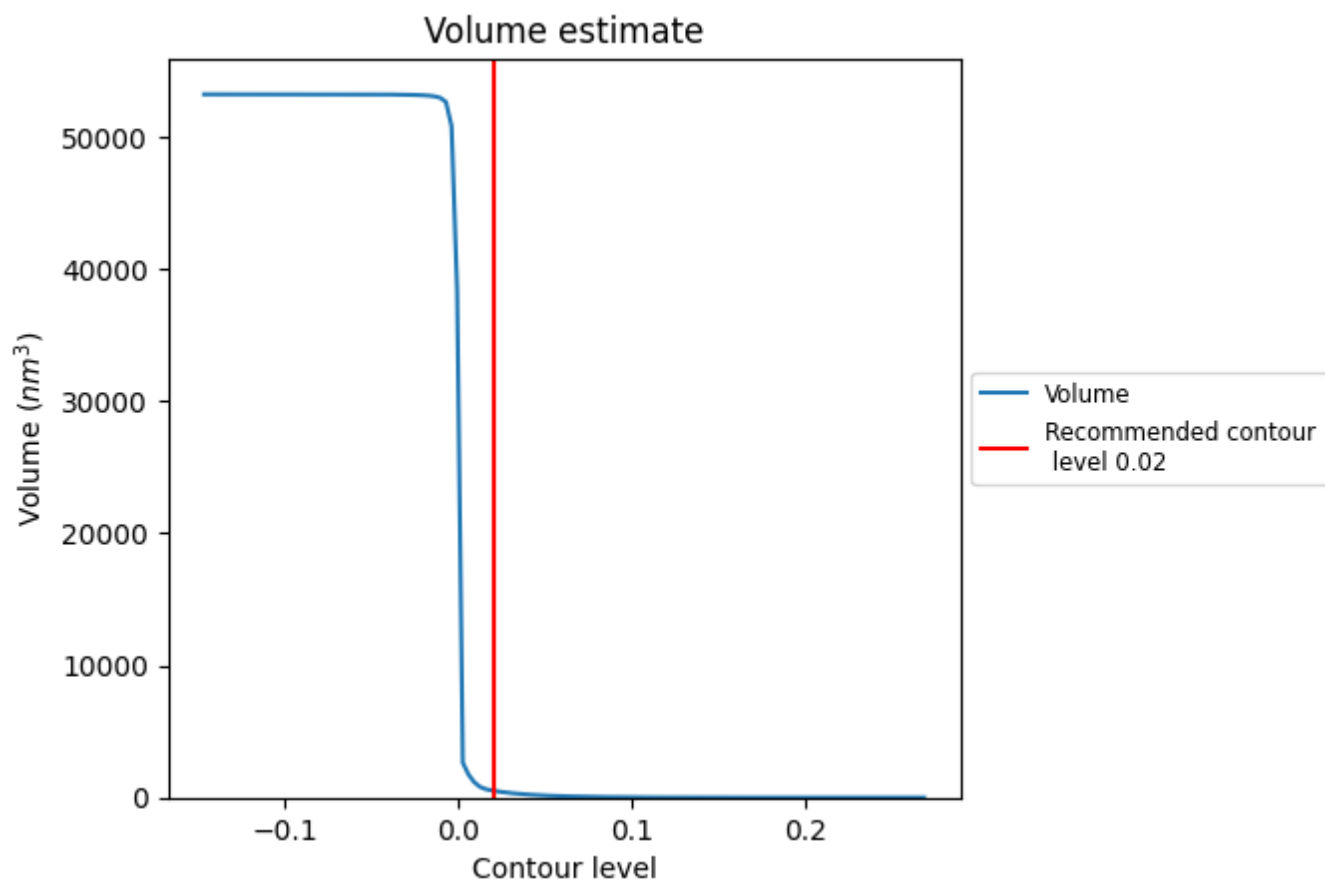
This section contains the results of statistical analysis of the map.

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.

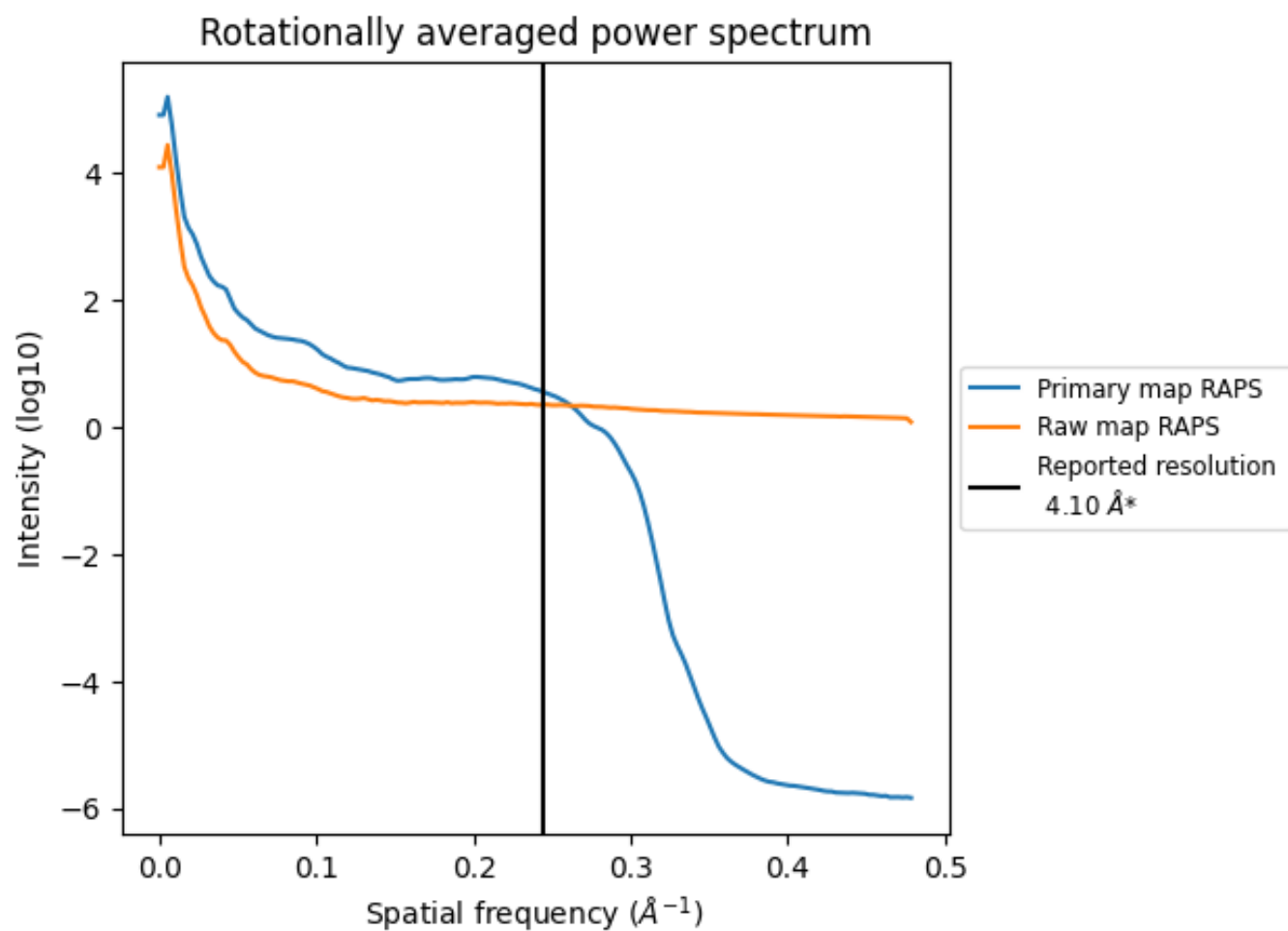
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 518 nm^3 ; this corresponds to an approximate mass of 468 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 ⓘ

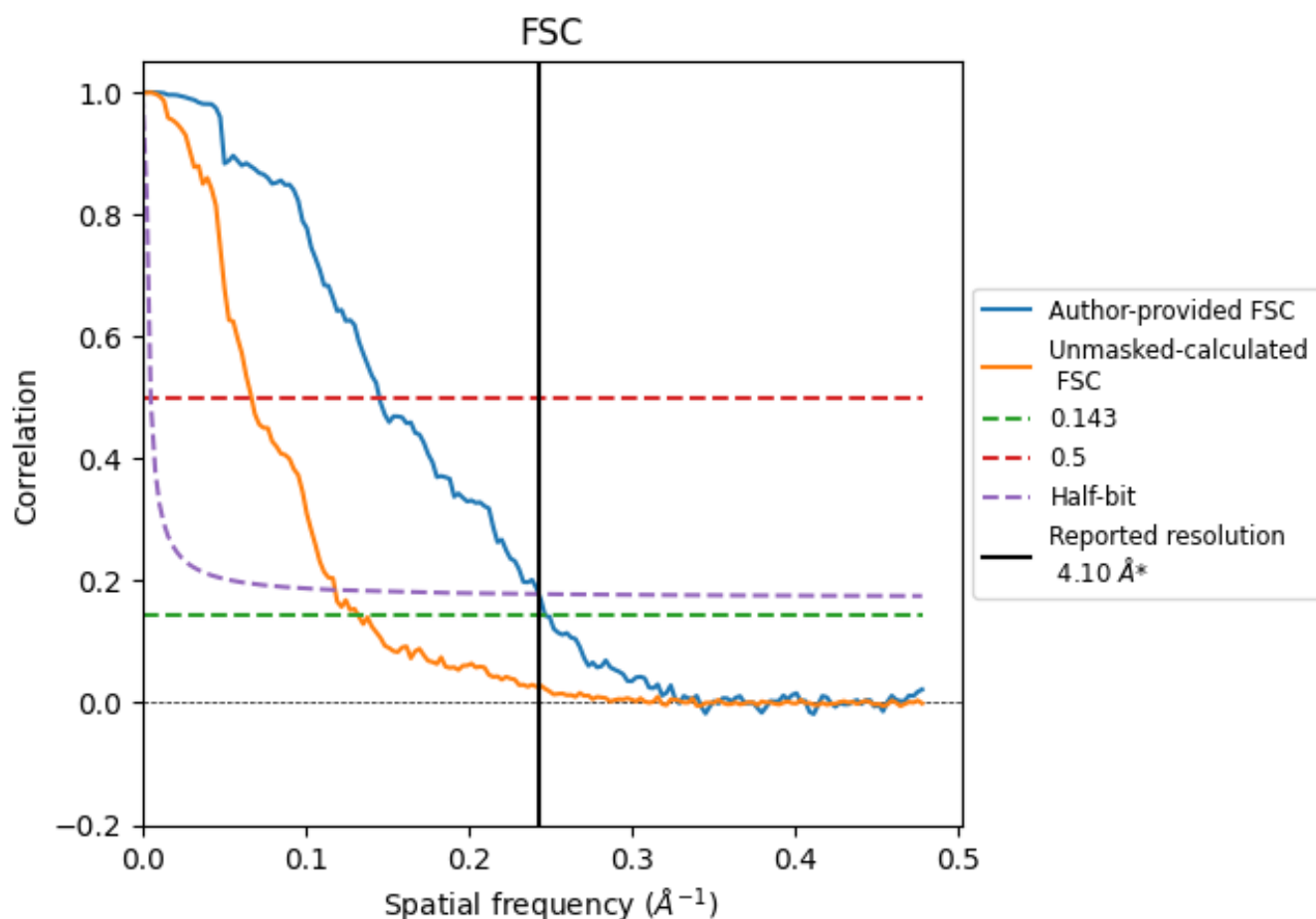


*Reported resolution corresponds to spatial frequency of 0.244 $\text{\AA}^{-1}$

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 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

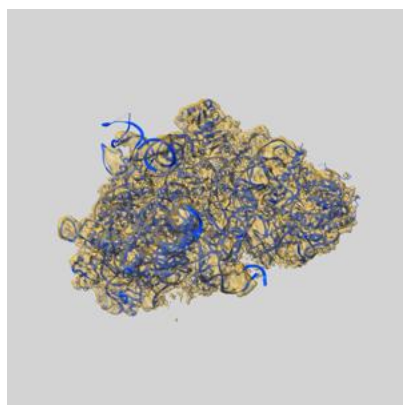
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.05	6.87	4.11
Unmasked-calculated*	7.55	14.95	8.45

*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 7.55 differs from the reported value 4.1 by more than 10 %

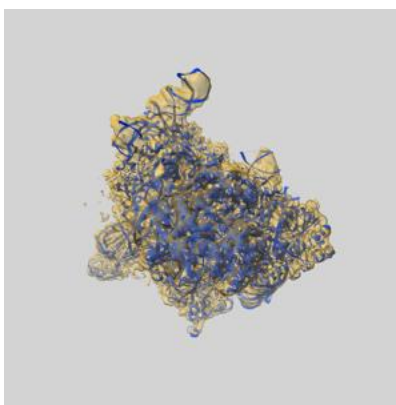
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66688 and PDB model 9XAI. Per-residue inclusion information can be found in section [3](#) on page [8](#).

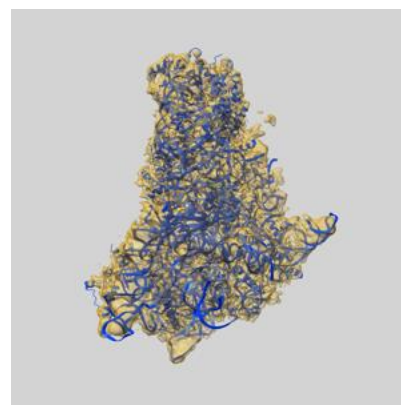
9.1 Map-model overlay [i](#)



X



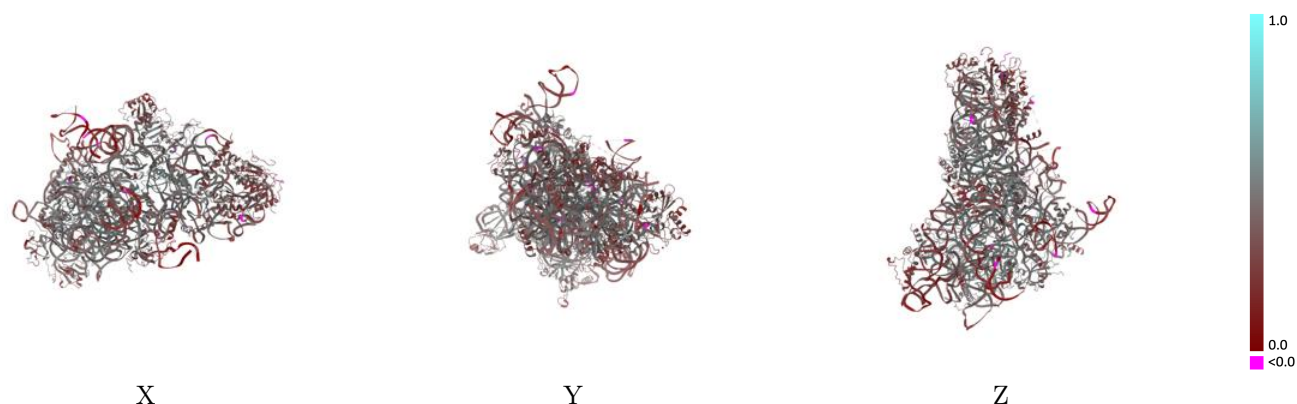
Y



Z

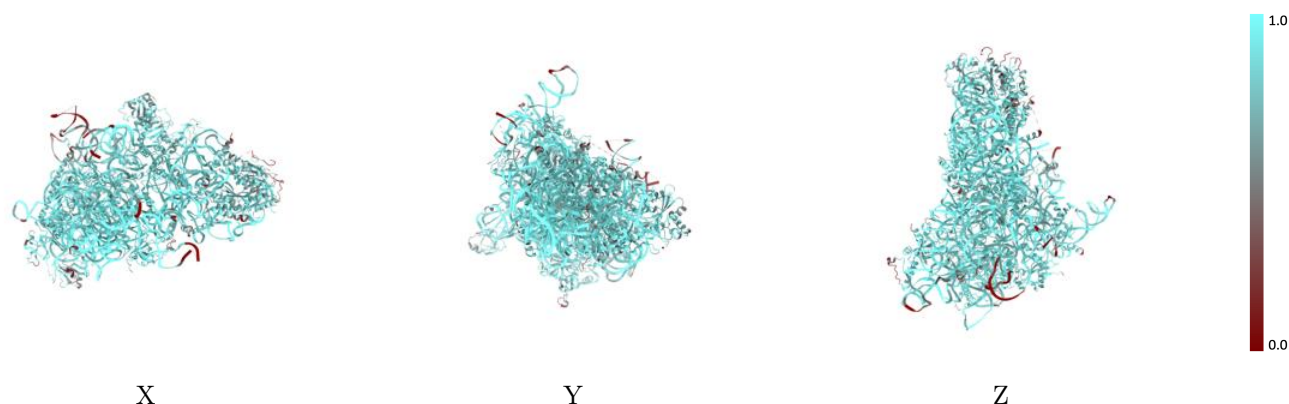
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



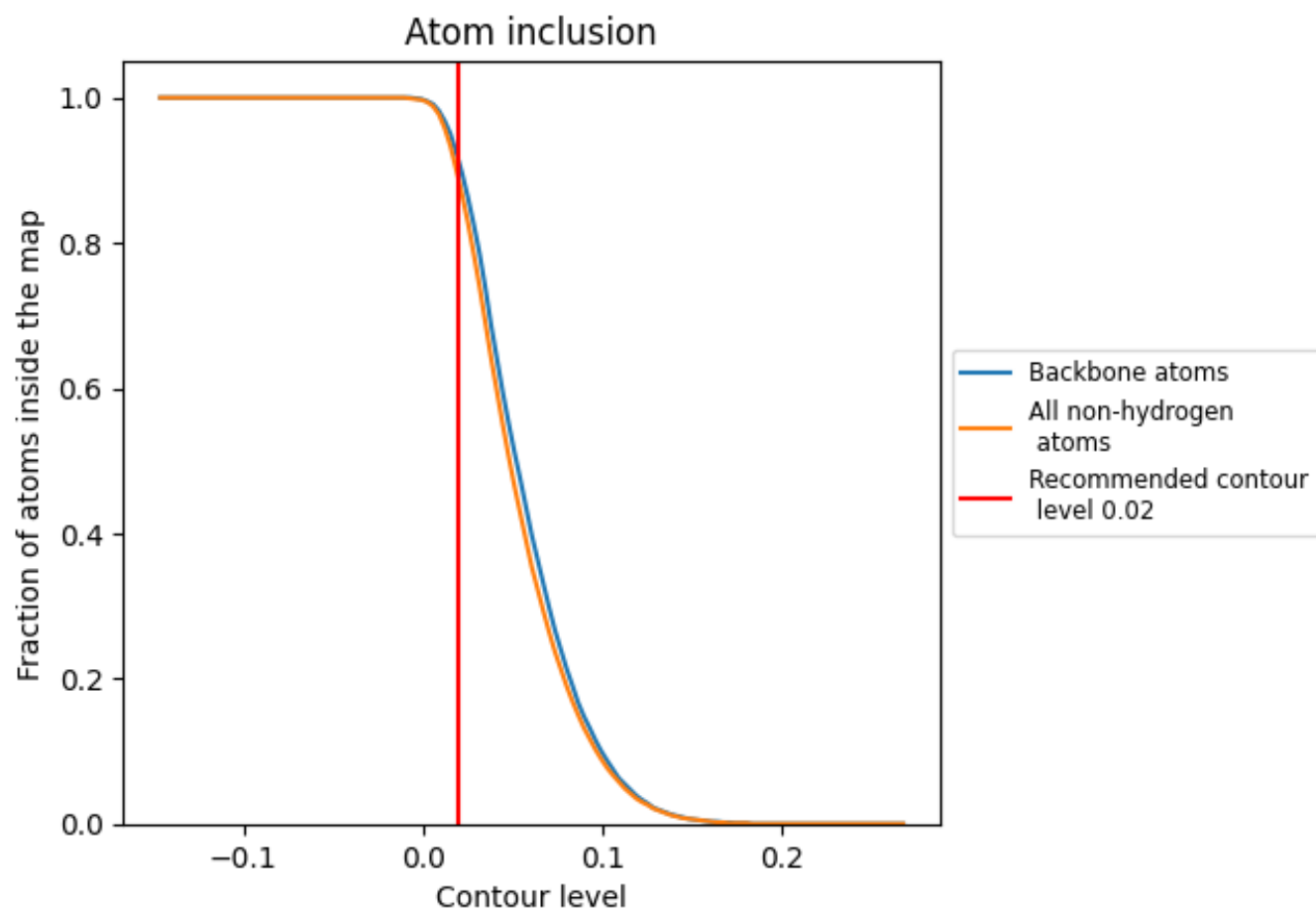
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8860	 0.4010
1	 0.7000	 0.2530
3	 0.7360	 0.3040
6	 0.6980	 0.3460
8	 0.6590	 0.3120
A	 0.9230	 0.3990
E	 0.8190	 0.3760
H	 0.9170	 0.4900
J	 0.8040	 0.3680
K	 0.8250	 0.3510
L	 0.8520	 0.4180
M	 0.8900	 0.4280
O	 0.9090	 0.4900
Q	 0.9120	 0.4490
R	 0.7960	 0.3450
Z	 0.9100	 0.4590
a	 0.8480	 0.4130
b	 0.8480	 0.4270
e	 0.8890	 0.4370
h	 0.8780	 0.4210

