



Full wwPDB EM Validation Report ⓘ

Jul 14, 2026 – 10:54 AM JST

PDB ID : 9XA9 / pdb_00009xa9
EMDB ID : EMD-66679
Title : Cryo-EM structure of the pre-40S ribosome (Enp1-Rrp12 WT) 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 : 3.30 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

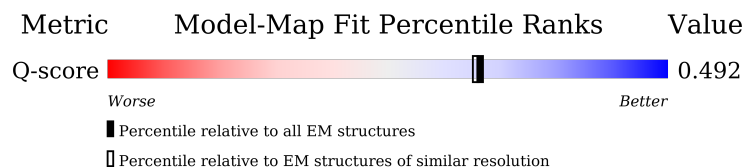
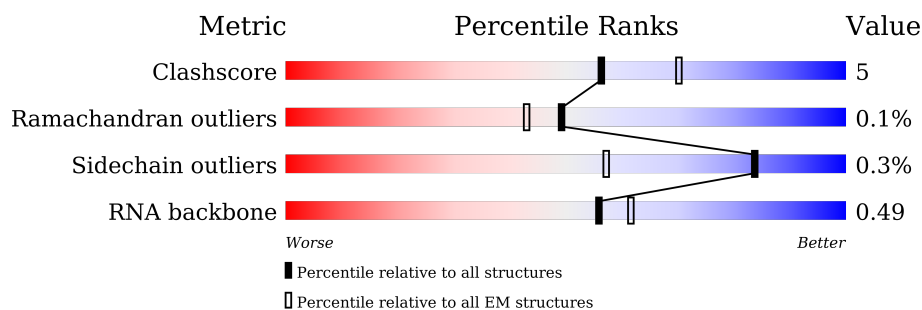
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



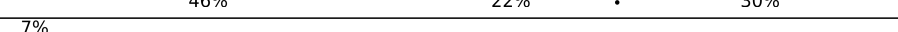
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	D	285	
2	E	255	
3	F	263	

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Mol	Chain	Length	Quality of chain
4	H	264	 85% 14%
5	J	239	 78% 18%
6	K	203	 81% 15%
7	L	202	 79% 20%
8	M	190	 81% 13% 6%
9	O	161	 84% 9% 7%
10	Q	151	 89% 11%
11	R	150	 69% 21% 10%
12	U	143	 5% 22% 77%
13	Y	98	 77% 11% 12%
14	Z	130	 88% 11%
15	a	145	 83% 14%
16	b	136	 74% 23%
17	e	82	 88% 11%
18	h	62	 53% 8% 35%
19	A	1796	 46% 22% 30%
20	3	259	 7% 63% 8% 29%

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 50364 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 uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	208	Total	C	N	O	S	0	0
			1641	1051	289	295	6		

- Molecule 2 is a protein called Small ribosomal subunit protein eS1.

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

- Molecule 3 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	216	Total	C	N	O	S	0	0
			1672	1074	294	301	3		

- Molecule 4 is a protein called 40S ribosomal protein S4.

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

- Molecule 5 is a protein called 40S ribosomal protein S6.

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

- Molecule 6 is a protein called 40S ribosomal protein S7.

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

- Molecule 7 is a protein called 40S ribosomal protein S8.

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

- Molecule 8 is a protein called 40S ribosomal protein s9-like protein.

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

- Molecule 9 is a protein called 40S ribosomal protein S11-like protein.

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

- Molecule 10 is a protein called 40S ribosomal protein S13-like protein.

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

- Molecule 11 is a protein called 40S ribosomal protein S14-like protein.

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

- Molecule 12 is a protein called 40S ribosomal protein S17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	33	Total	C	N	O	S	0	0
			255	161	40	53	1		

- Molecule 13 is a protein called 40S ribosomal protein S21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	86	Total	C	N	O	S	0	0
			664	408	124	128	4		

- Molecule 14 is a protein called 40S ribosomal protein S22-like protein.

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

- Molecule 15 is a protein called 40S ribosomal protein s23-like protein.

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

- Molecule 16 is a protein called Small ribosomal subunit protein eS24.

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

- Molecule 17 is a protein called Ribosomal protein s27-like protein.

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

- Molecule 18 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	h	40	Total	C	N	O	0	0
			321	203	66	52		

- Molecule 19 is a RNA chain called 18S pre-rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	1257	Total	C	N	O	P	0	0
			26820	11988	4795	8780	1257		

- Molecule 20 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3	184	Total	C	N	O	S	0	0
			1451	921	267	256	7		

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

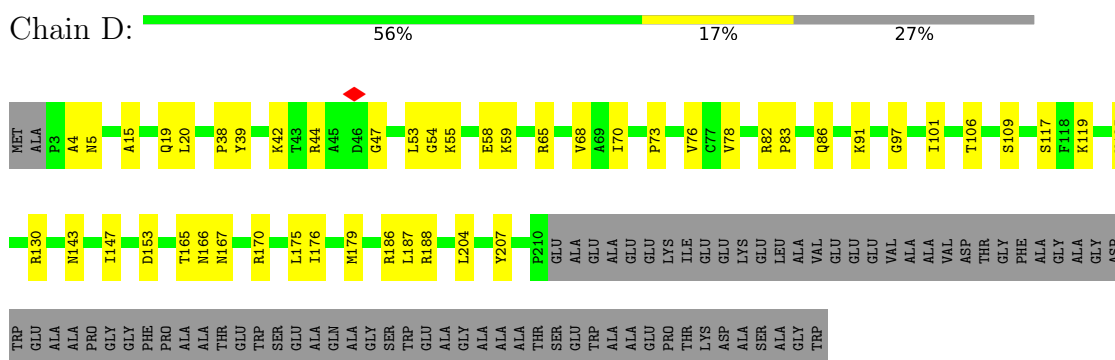
- Molecule 23 is water.

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

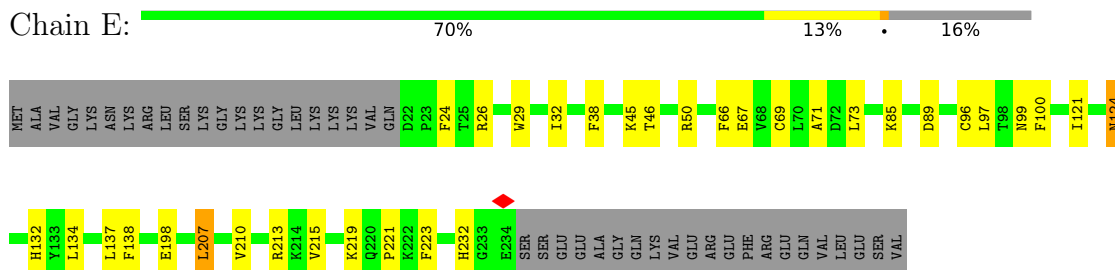
3 Residue-property plots

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.

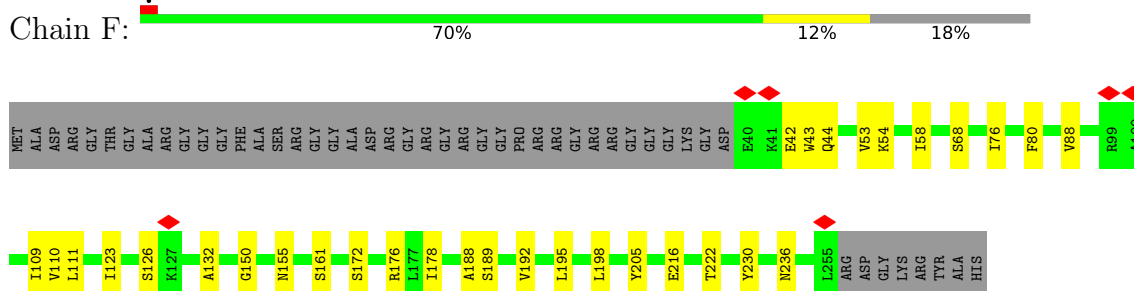
- Molecule 1: Small ribosomal subunit protein uS2



- Molecule 2: Small ribosomal subunit protein eS1

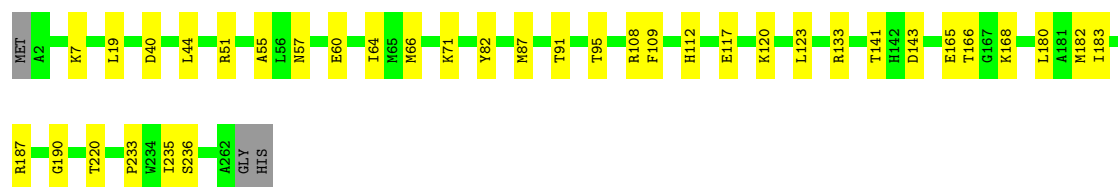


- Molecule 3: Small ribosomal subunit protein uS5



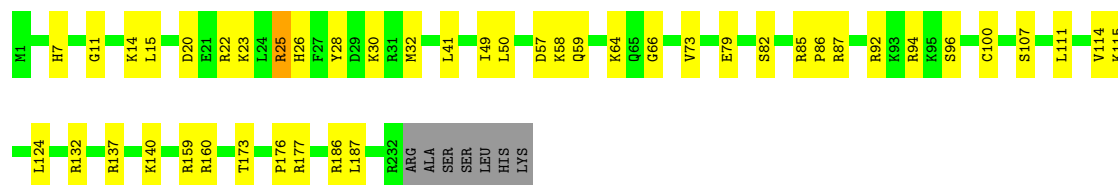
- Molecule 4: 40S ribosomal protein S4

Chain H:  85% 14% .



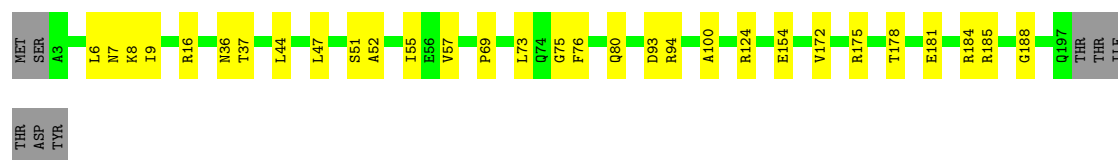
- Molecule 5: 40S ribosomal protein S6

Chain J:  78% 18% .



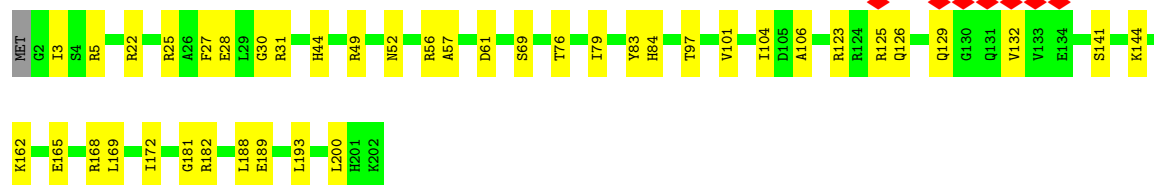
- Molecule 6: 40S ribosomal protein S7

Chain K:  81% 15% .



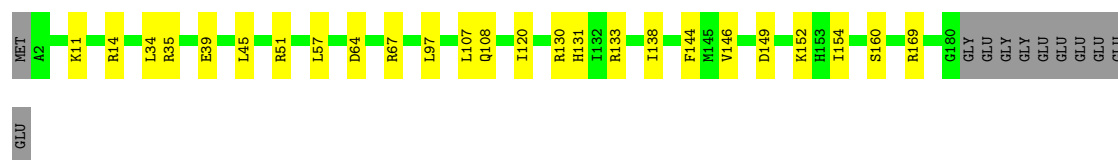
- Molecule 7: 40S ribosomal protein S8

Chain L:  79% 20% .



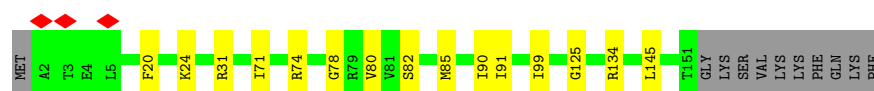
- Molecule 8: 40S ribosomal protein s9-like protein

Chain M:  81% 13% 6%



- Molecule 9: 40S ribosomal protein S11-like protein

Chain O:  84% 9% 7%



- Molecule 10: 40S ribosomal protein S13-like protein

Chain Q:  89% 11%



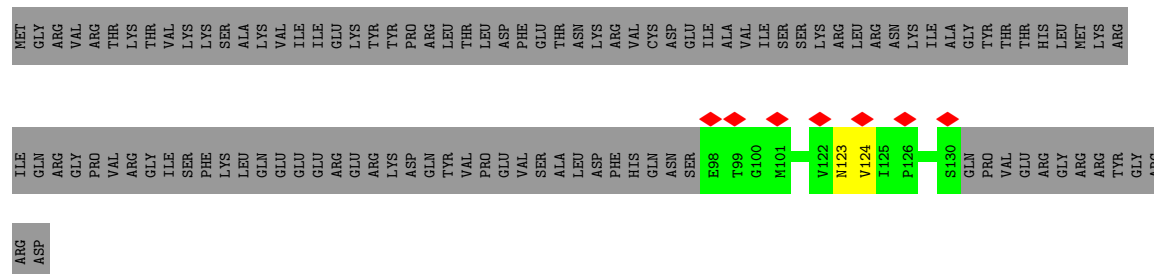
- Molecule 11: 40S ribosomal protein S14-like protein

Chain R:  69% 21% 10%



- Molecule 12: 40S ribosomal protein S17-like protein

Chain U:  5% 22% 77%



- Molecule 13: 40S ribosomal protein S21-like protein

Chain Y:  77% 11% 12%



- Molecule 14: 40S ribosomal protein S22-like protein

Chain Z:  88% 11%



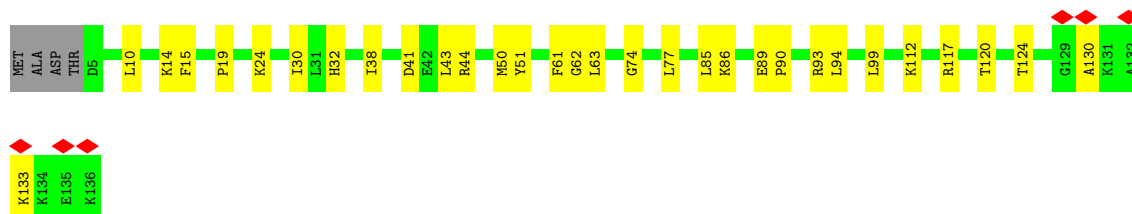
- Molecule 15: 40S ribosomal protein s23-like protein

Chain a: 



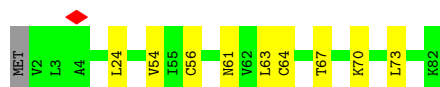
- Molecule 16: Small ribosomal subunit protein eS24

Chain b: 



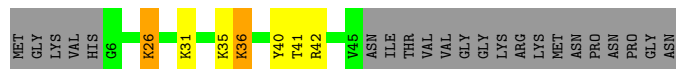
- Molecule 17: Ribosomal protein s27-like protein

Chain e: 



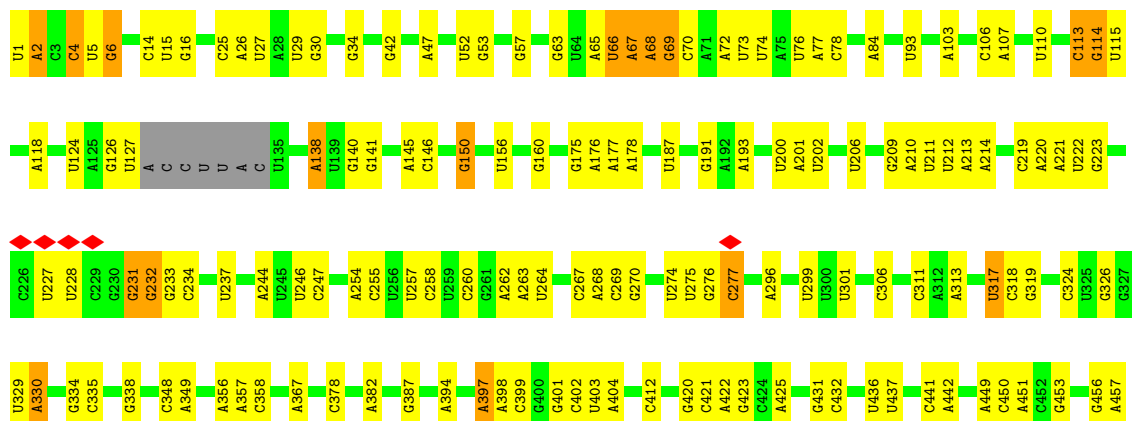
- Molecule 18: 40S ribosomal protein S30

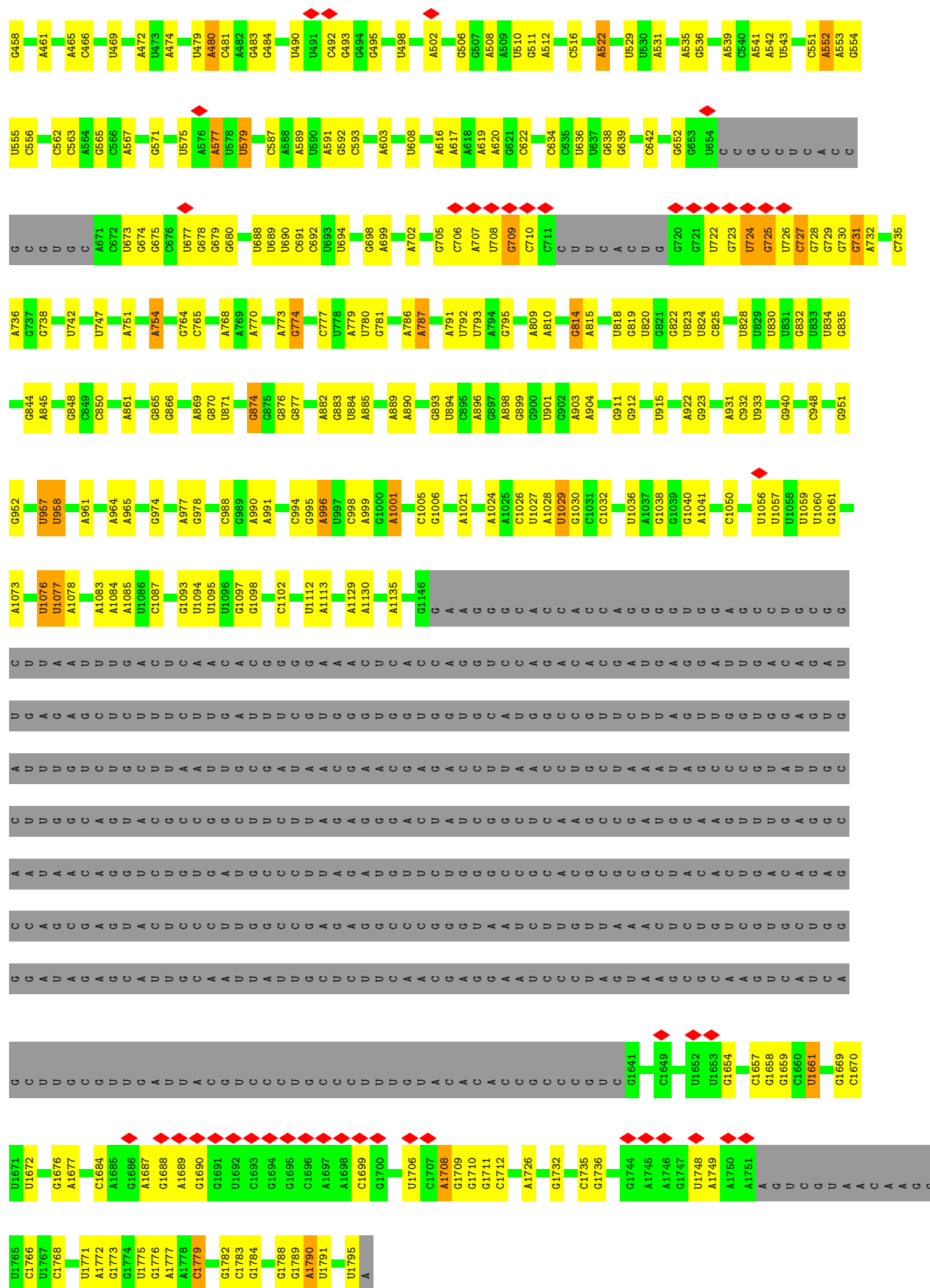
Chain h: 



- Molecule 19: 18S pre-rRNA

Chain A: 





- Molecule 20: Pre-rRNA-processing protein PNO1



MET	PRO	ALA	PRO	THR	ALA	LEU	LYS	GLN	PRO	PRO	ALA	PRO	GLN	GLN	ALA	ALA	PRO	ALA	ALA	THR	ILE	ASP	ILE	GLN	ALA	ALA	THR	LEU	THR	ASP	PRO	ASN	ALA	GLU	PRO	GLU	GLU	THR	MET	ASN	GLU	MET	ALA	VAL
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ASP	GLU	GLY	ARG	PRO	ARG	PHE	ALA	PRO	GLY	LYS	ASN	ILE	ASP	P76	I77	R78	T87	R91	M92	D107	H108	C109	K110	L111	K118	V122	S127	K128	Y129	T130	V131	S132	N133	E134	A135	L136	Q137	M138	F146	Q167	S168	D173	R189	E202	T218
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I225	G226	M227	A228	R229	E230	R249	M255	K256	E257	R258	W259
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12066	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.474	Depositor
Minimum map value	-0.280	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	412.56, 412.56, 412.56	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.146, 1.146, 1.146	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

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	D	0.20	0/1683	0.48	0/2299
2	E	0.21	0/1752	0.51	0/2361
3	F	0.22	0/1703	0.53	0/2303
4	H	0.23	0/2112	0.49	0/2842
5	J	0.20	0/1906	0.52	2/2547 (0.1%)
6	K	0.21	0/1587	0.51	0/2140
7	L	0.23	0/1654	0.46	0/2213
8	M	0.22	0/1489	0.52	0/1993
9	O	0.27	0/1249	0.44	0/1678
10	Q	0.21	0/1205	0.42	0/1627
11	R	0.25	0/1014	0.62	0/1361
12	U	0.24	0/258	0.58	0/350
13	Y	0.21	0/671	0.49	0/900
14	Z	0.24	0/1055	0.49	0/1416
15	a	0.23	0/1116	0.49	0/1489
16	b	0.23	0/1075	0.49	0/1431
17	e	0.22	0/623	0.49	0/843
18	h	0.65	0/325	0.98	0/429
19	A	0.22	0/30003	0.35	0/46749
20	3	0.19	0/1475	0.45	0/1982
All	All	0.22	0/53955	0.42	2/78953 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	25	ARG	CA-C-N	-5.67	111.21	121.14
5	J	25	ARG	C-N-CA	-5.67	111.21	121.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1641	0	1650	28	0
2	E	1723	0	1804	20	0
3	F	1672	0	1777	22	0
4	H	2072	0	2155	25	0
5	J	1875	0	1983	33	0
6	K	1562	0	1641	23	0
7	L	1621	0	1645	30	0
8	M	1466	0	1582	16	0
9	O	1222	0	1289	14	0
10	Q	1182	0	1264	11	0
11	R	1002	0	1034	28	0
12	U	255	0	255	1	0
13	Y	664	0	662	9	0
14	Z	1037	0	1076	11	0
15	a	1099	0	1169	14	0
16	b	1061	0	1150	21	0
17	e	611	0	635	5	0
18	h	321	0	363	5	0
19	A	26820	0	13507	177	0
20	3	1451	0	1524	18	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	e	1	0	0	0	0
23	A	4	0	0	0	0
All	All	50364	0	38165	426	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 5.

All (426) 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)
19:A:1661:U:H3	19:A:1732:G:H1	1.07	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:702:A:H62	19:A:731:G:N2	1.78	0.81
14:Z:2:VAL:N	19:A:1032:C:HO2'	1.77	0.81
19:A:652:G:H1	19:A:673:U:H3	1.29	0.80
19:A:219:C:N4	19:A:220:A:N6	2.31	0.78
19:A:709:G:H1	19:A:722:U:H3	1.28	0.78
19:A:220:A:N1	19:A:835:G:C6	2.56	0.74
19:A:866:G:H1	19:A:958:U:H3	1.36	0.73
19:A:893:G:H1	19:A:915:U:H3	1.36	0.72
9:O:74:ARG:NH1	19:A:301:U:O2	2.23	0.71
15:a:51:GLY:O	15:a:101:GLU:HA	1.90	0.71
19:A:694:U:H3	19:A:738:G:H1	1.38	0.70
6:K:73:LEU:HD22	6:K:100:ALA:HB2	1.72	0.69
11:R:116:ARG:NH1	20:3:138:MET:SD	2.65	0.69
5:J:49:ILE:HG12	5:J:115:LYS:HG2	1.73	0.69
9:O:82:SER:HB3	9:O:90:ILE:HB	1.76	0.68
19:A:702:A:N6	19:A:731:G:N2	2.43	0.67
19:A:483:G:H1	19:A:498:U:H3	1.44	0.66
9:O:85:MET:HE1	9:O:90:ILE:HG12	1.78	0.65
4:H:87:MET:HE1	4:H:235:ILE:HD13	1.79	0.65
2:E:132:HIS:HB2	2:E:221:PRO:HB3	1.79	0.64
8:M:14:ARG:NH2	19:A:1:U:O2'	2.31	0.63
11:R:148:ARG:HG3	11:R:149:ARG:HG3	1.79	0.63
7:L:141:SER:HA	7:L:144:LYS:HD2	1.81	0.63
2:E:198:GLU:HG3	2:E:210:VAL:HB	1.80	0.62
2:E:69:CYS:SG	11:R:127:ARG:NH1	2.73	0.62
11:R:149:ARG:HH12	20:3:229:ARG:HH22	1.48	0.62
7:L:84:HIS:HE2	7:L:97:THR:HG1	1.42	0.62
18:h:31:LYS:NZ	19:A:541:A:O3'	2.34	0.61
4:H:51:ARG:NH2	4:H:109:PHE:O	2.33	0.61
7:L:182:ARG:NH1	19:A:255:C:O2	2.34	0.61
19:A:820:U:H3	19:A:848:G:H1	1.48	0.60
19:A:844:G:H2'	19:A:845:A:H8	1.67	0.60
7:L:83:TYR:HB2	7:L:200:LEU:HD21	1.83	0.60
8:M:149:ASP:OD1	8:M:152:LYS:NZ	2.35	0.59
1:D:78:VAL:HG12	1:D:125:VAL:HB	1.85	0.59
5:J:57:ASP:OD1	5:J:58:LYS:N	2.36	0.59
6:K:93:ASP:OD2	6:K:94:ARG:NH2	2.36	0.59
9:O:80:VAL:O	9:O:125:GLY:N	2.35	0.59
19:A:1688:G:N1	19:A:1706:U:N3	2.51	0.59
11:R:102:ASN:O	11:R:141:ARG:NH1	2.36	0.58
9:O:71:ILE:HG21	9:O:145:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:125:ILE:HD12	11:R:128:ILE:HD11	1.86	0.58
1:D:91:LYS:NZ	1:D:204:LEU:O	2.36	0.58
19:A:552:A:N3	19:A:587:C:O2'	2.32	0.58
7:L:31:ARG:NH1	19:A:329:U:OP1	2.36	0.57
19:A:378:C:O2'	19:A:754:A:N1	2.37	0.57
4:H:19:LEU:HD11	4:H:108:ARG:HD2	1.86	0.57
1:D:117:SER:OG	1:D:119:LYS:NZ	2.38	0.57
19:A:1735:C:H2'	19:A:1736:G:H8	1.69	0.57
7:L:83:TYR:HB3	7:L:101:VAL:HB	1.85	0.57
9:O:99:ILE:HD13	15:a:16:ARG:HD2	1.86	0.57
5:J:160:ARG:NH2	19:A:68:A:OP1	2.37	0.57
6:K:188:GLY:HA3	19:A:638:G:H21	1.68	0.57
2:E:38:PHE:HB3	2:E:73:LEU:HB3	1.87	0.56
19:A:442:A:H1'	19:A:522:A:H5''	1.85	0.56
16:b:30:ILE:HD11	16:b:43:LEU:HD13	1.87	0.56
3:F:42:GLU:OE1	3:F:54:LYS:NZ	2.37	0.56
10:Q:104:ARG:NH2	19:A:948:C:O2'	2.39	0.56
9:O:71:ILE:HG13	9:O:145:LEU:HD21	1.86	0.56
7:L:44:HIS:ND1	19:A:1672:U:OP1	2.39	0.56
4:H:57:ASN:HB2	4:H:60:GLU:H	1.71	0.56
15:a:17:ASN:OD1	15:a:20:ARG:NH2	2.39	0.56
16:b:15:PHE:HZ	16:b:24:LYS:HD2	1.70	0.56
18:h:31:LYS:HD3	19:A:542:A:H2'	1.88	0.56
1:D:170:ARG:NH1	1:D:207:TYR:O	2.39	0.55
8:M:169:ARG:NH2	19:A:511:G:N7	2.54	0.55
19:A:702:A:N6	19:A:731:G:C2	2.74	0.55
3:F:150:GLY:N	3:F:161:SER:O	2.37	0.55
4:H:7:LYS:HE3	19:A:93:U:H1'	1.86	0.55
4:H:141:THR:OG1	4:H:143:ASP:OD1	2.25	0.55
6:K:6:LEU:O	6:K:16:ARG:NH1	2.40	0.55
10:Q:48:SER:OG	19:A:866:G:N2	2.40	0.55
20:3:111:LEU:HD11	20:3:136:LEU:HA	1.88	0.55
5:J:49:ILE:HG13	5:J:114:VAL:HB	1.89	0.55
1:D:83:PRO:HA	1:D:86:GLN:HG3	1.89	0.55
19:A:67:A:O2'	19:A:69:G:OP1	2.22	0.55
8:M:131:HIS:ND1	8:M:160:SER:OG	2.33	0.55
13:Y:17:CYS:HB2	13:Y:56:SER:HB3	1.89	0.55
5:J:186:ARG:NH1	19:A:264:U:OP1	2.40	0.54
19:A:893:G:O6	19:A:915:U:O4	2.25	0.54
2:E:29:TRP:HB3	2:E:45:LYS:HD3	1.89	0.54
7:L:79:ILE:HG21	7:L:168:ARG:HH12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:51:ARG:NH2	8:M:97:LEU:O	2.41	0.54
1:D:188:ARG:O	13:Y:44:ARG:NH1	2.40	0.54
5:J:22:ARG:HE	5:J:25:ARG:CZ	2.20	0.54
4:H:187:ARG:NH1	19:A:751:A:OP2	2.41	0.54
5:J:79:GLU:HG2	5:J:86:PRO:HG3	1.90	0.54
9:O:78:GLY:HA3	9:O:91:ILE:HD12	1.88	0.54
4:H:95:THR:HG22	16:b:19:PRO:HD2	1.89	0.54
20:3:87:ILE:HD11	20:3:122:VAL:HG23	1.90	0.54
10:Q:124:ARG:NH2	19:A:965:A:OP2	2.37	0.53
10:Q:108:ASP:OD1	19:A:876:G:O2'	2.26	0.53
11:R:32:ILE:HG23	11:R:96:ILE:HA	1.89	0.53
2:E:89:ASP:HB3	2:E:223:PHE:HE1	1.72	0.53
7:L:182:ARG:NH1	19:A:202:U:O2	2.41	0.53
19:A:220:A:N1	19:A:835:G:O6	2.41	0.53
19:A:707:A:N1	19:A:724:U:O2'	2.41	0.53
4:H:182:MET:HE3	4:H:190:GLY:HA2	1.91	0.53
3:F:230:TYR:OH	13:Y:12:TYR:O	2.25	0.53
10:Q:47:PRO:HG3	10:Q:75:LEU:HD12	1.90	0.53
1:D:82:ARG:NH2	1:D:167:ASN:O	2.42	0.53
19:A:484:G:N1	19:A:498:U:C2	2.77	0.53
3:F:111:LEU:HD12	3:F:198:LEU:HD12	1.90	0.53
5:J:177:ARG:HG3	19:A:77:A:H2	1.73	0.53
13:Y:35:THR:HB	13:Y:50:ASN:HD22	1.74	0.53
19:A:200:U:H2'	19:A:201:A:H8	1.73	0.53
19:A:589:A:O2'	19:A:593:C:OP1	2.27	0.53
19:A:1060:U:H2'	19:A:1061:G:H8	1.74	0.53
4:H:108:ARG:NH1	19:A:787:A:OP1	2.42	0.52
8:M:11:LYS:HD2	8:M:45:LEU:HD13	1.90	0.52
6:K:55:ILE:HD12	6:K:185:ARG:HD2	1.90	0.52
19:A:874:G:O6	19:A:933:U:O4	2.28	0.52
19:A:1709:G:H2'	19:A:1710:G:H8	1.74	0.52
1:D:130:ARG:NH1	1:D:153:ASP:O	2.30	0.52
5:J:25:ARG:HA	5:J:28:TYR:HD2	1.73	0.52
19:A:708:U:O2	19:A:723:G:O6	2.28	0.52
1:D:143:ASN:ND2	3:F:68:SER:O	2.42	0.52
16:b:86:LYS:HG2	16:b:99:LEU:HD21	1.92	0.52
3:F:123:ILE:HD13	3:F:216:GLU:HG3	1.90	0.52
7:L:76:THR:HG21	7:L:104:ILE:HD12	1.92	0.52
8:M:107:LEU:HB2	8:M:144:PHE:HB3	1.90	0.52
2:E:138:PHE:O	2:E:213:ARG:N	2.43	0.52
5:J:20:ASP:HB3	5:J:23:LYS:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:469:U:O2'	19:A:768:A:N3	2.39	0.52
2:E:97:LEU:HB3	2:E:232:HIS:CD2	2.44	0.52
7:L:22:ARG:HB3	19:A:382:A:H5''	1.91	0.52
8:M:130:ARG:NH1	19:A:529:U:OP1	2.39	0.52
19:A:869:A:H2'	19:A:870:G:C8	2.45	0.52
1:D:73:PRO:HB2	1:D:97:GLY:HA3	1.93	0.51
5:J:137:ARG:HB3	5:J:140:LYS:HG3	1.92	0.51
8:M:64:ASP:HB3	8:M:67:ARG:HB3	1.92	0.51
6:K:57:VAL:HG11	6:K:178:THR:HG22	1.92	0.51
3:F:188:ALA:HB1	3:F:192:VAL:HG23	1.92	0.51
2:E:124:ASN:C	2:E:124:ASN:HD22	2.15	0.51
19:A:267:C:H2'	19:A:268:A:H8	1.75	0.51
19:A:1658:G:H2'	19:A:1659:G:H8	1.74	0.51
3:F:195:LEU:HD22	3:F:222:THR:HG22	1.93	0.51
19:A:1661:U:O4	19:A:1732:G:O6	2.28	0.51
8:M:35:ARG:NH1	19:A:472:A:OP2	2.41	0.51
19:A:84:A:N3	19:A:145:A:O2'	2.40	0.51
19:A:219:C:C4	19:A:220:A:N6	2.79	0.51
4:H:183:ILE:HD12	4:H:220:THR:HG21	1.93	0.51
5:J:85:ARG:O	5:J:87:ARG:NH1	2.44	0.51
7:L:57:ALA:HB2	7:L:181:GLY:HA2	1.92	0.51
5:J:25:ARG:HA	5:J:28:TYR:CD2	2.46	0.50
4:H:112:HIS:NE2	4:H:236:SER:O	2.45	0.50
19:A:140:G:H2'	19:A:141:G:C8	2.47	0.50
16:b:62:GLY:O	16:b:74:GLY:CA	2.60	0.50
19:A:450:C:H2'	19:A:451:A:H5''	1.94	0.50
3:F:155:ASN:ND2	13:Y:3:ASN:O	2.45	0.50
11:R:106:THR:HG21	20:3:168:SER:HB2	1.92	0.50
11:R:142:LYS:HB2	19:A:988:C:H5'	1.94	0.50
5:J:66:GLY:HA2	19:A:1677:A:H1'	1.93	0.50
5:J:92:ARG:O	19:A:402:C:O2'	2.26	0.50
11:R:103:GLY:HA2	11:R:141:ARG:HH12	1.77	0.50
3:F:172:SER:HB2	19:A:1083:A:H5'	1.94	0.50
5:J:7:HIS:O	5:J:11:GLY:N	2.45	0.49
4:H:55:ALA:HB2	4:H:64:ILE:HD12	1.94	0.49
15:a:74:VAL:HG11	15:a:104:LEU:HD11	1.93	0.49
1:D:101:ILE:HD11	1:D:119:LYS:HE2	1.94	0.49
5:J:94:ARG:NH2	19:A:1669:G:OP1	2.38	0.49
6:K:154:GLU:HA	14:Z:42:GLN:HE21	1.78	0.49
3:F:109:ILE:HG23	3:F:123:ILE:HG12	1.95	0.49
6:K:36:ASN:OD1	6:K:37:THR:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:e:64:CYS:HB3	17:e:73:LEU:HD23	1.94	0.49
19:A:29:U:H2'	19:A:30:G:H8	1.77	0.49
1:D:186:ARG:O	13:Y:44:ARG:NH2	2.46	0.48
2:E:137:LEU:HD13	2:E:215:VAL:HG22	1.95	0.48
19:A:844:G:H2'	19:A:845:A:C8	2.46	0.48
17:e:67:THR:OG1	17:e:70:LYS:O	2.30	0.48
5:J:15:LEU:HD13	19:A:150:G:H4'	1.94	0.48
17:e:56:CYS:HB3	17:e:63:LEU:HD11	1.93	0.48
20:3:218:ILE:HG22	20:3:225:ILE:HG12	1.95	0.48
10:Q:26:LEU:HD21	10:Q:60:ILE:HG22	1.94	0.48
15:a:19:ARG:O	15:a:23:ARG:HB2	2.13	0.48
4:H:71:LYS:HB2	4:H:91:THR:HB	1.94	0.48
7:L:189:GLU:HA	7:L:193:LEU:HB2	1.95	0.48
19:A:834:U:H2'	19:A:835:G:C8	2.48	0.48
1:D:125:VAL:HA	1:D:147:ILE:O	2.14	0.48
3:F:88:VAL:HA	3:F:110:VAL:HG12	1.95	0.48
15:a:3:GLY:O	19:A:1102:C:N4	2.46	0.48
18:h:40:TYR:O	18:h:41:THR:C	2.57	0.48
19:A:160:G:OP2	19:A:160:G:N2	2.35	0.48
16:b:62:GLY:O	16:b:74:GLY:HA2	2.13	0.47
19:A:484:G:C2	19:A:498:U:O2	2.67	0.47
1:D:39:TYR:OH	1:D:59:LYS:NZ	2.44	0.47
6:K:44:LEU:HA	6:K:47:LEU:HD12	1.95	0.47
11:R:33:PHE:HD1	11:R:97:ARG:HG3	1.80	0.47
19:A:1005:C:H2'	19:A:1006:G:H8	1.79	0.47
9:O:134:ARG:HD3	19:A:114:G:H5'	1.96	0.47
19:A:974:G:N1	19:A:1021:A:O2'	2.43	0.47
16:b:90:PRO:HD2	16:b:93:ARG:HD2	1.97	0.47
19:A:1027:U:O2'	19:A:1029:U:OP2	2.30	0.47
19:A:1084:A:H2'	19:A:1085:A:C8	2.48	0.47
3:F:53:VAL:HG21	3:F:76:ILE:HG23	1.97	0.47
4:H:19:LEU:HD22	19:A:786:A:H2'	1.97	0.47
4:H:87:MET:HE3	4:H:123:LEU:HB2	1.97	0.47
7:L:25:ARG:HA	19:A:397:A:H5''	1.96	0.47
6:K:51:SER:OG	6:K:52:ALA:N	2.48	0.47
19:A:220:A:C2	19:A:835:G:C6	3.03	0.47
2:E:134:LEU:HB3	2:E:219:LYS:HB3	1.96	0.47
6:K:69:PRO:O	6:K:73:LEU:N	2.44	0.47
19:A:577:A:O2'	19:A:579:U:OP1	2.33	0.47
6:K:8:LYS:NZ	6:K:44:LEU:O	2.36	0.47
14:Z:88:LYS:O	14:Z:92:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:56:ARG:HH12	19:A:328:G:H5''	1.80	0.46
16:b:10:LEU:HD22	16:b:50:MET:SD	2.56	0.46
19:A:814:G:H2'	19:A:815:A:H8	1.80	0.46
19:A:889:A:H2'	19:A:890:A:H8	1.81	0.46
20:3:167:GLN:OE1	20:3:229:ARG:NE	2.47	0.46
19:A:1783:C:H2'	19:A:1784:G:C8	2.50	0.46
8:M:108:GLN:HE21	8:M:120:ILE:HG13	1.81	0.46
15:a:69:ARG:HA	15:a:69:ARG:HD3	1.69	0.46
7:L:5:ARG:HH21	7:L:28:GLU:HA	1.80	0.46
5:J:32:MET:HB2	5:J:100:CYS:HB2	1.98	0.46
6:K:7:ASN:HA	6:K:16:ARG:HH12	1.80	0.46
11:R:33:PHE:HB3	11:R:40:PHE:HB2	1.97	0.46
19:A:317:U:H5'	19:A:318:C:H2'	1.97	0.46
14:Z:87:GLU:HA	14:Z:90:VAL:HG22	1.97	0.46
16:b:14:LYS:NZ	19:A:774:G:N7	2.62	0.46
19:A:484:G:C2	19:A:498:U:C2	3.03	0.46
5:J:187:LEU:HD23	19:A:138:A:H62	1.80	0.46
15:a:69:ARG:HG3	15:a:117:ILE:HG12	1.98	0.46
5:J:159:ARG:HH21	5:J:173:THR:HG23	1.81	0.46
19:A:457:A:H3'	19:A:458:G:H8	1.81	0.46
20:3:258:ARG:HE	20:3:259:TRP:HD1	1.63	0.46
5:J:23:LYS:HA	5:J:26:HIS:CE1	2.51	0.46
4:H:40:ASP:OD1	4:H:40:ASP:N	2.45	0.45
5:J:73:VAL:O	5:J:96:SER:HA	2.16	0.45
10:Q:136:PRO:HG2	10:Q:139:TRP:HB2	1.97	0.45
11:R:66:ASP:OD1	11:R:66:ASP:N	2.50	0.45
19:A:231:G:H2'	19:A:232:G:C8	2.51	0.45
19:A:1658:G:H2'	19:A:1659:G:C8	2.51	0.45
4:H:51:ARG:HA	4:H:51:ARG:HD2	1.88	0.45
4:H:133:ARG:NH2	19:A:124:U:O2'	2.49	0.45
4:H:166:THR:O	4:H:168:LYS:NZ	2.48	0.45
3:F:178:ILE:HB	3:F:205:TYR:HB2	1.98	0.45
4:H:180:LEU:HD22	4:H:233:PRO:HB3	1.99	0.45
6:K:6:LEU:HD12	6:K:9:ILE:HD12	1.99	0.45
16:b:61:PHE:HE1	16:b:77:LEU:HD13	1.81	0.45
7:L:126:GLN:O	7:L:129:GLN:NE2	2.41	0.45
9:O:74:ARG:NH2	19:A:795:G:O2'	2.39	0.45
6:K:57:VAL:HG21	6:K:178:THR:HA	1.97	0.45
14:Z:76:SER:HB2	19:A:1098:G:H5''	1.99	0.45
19:A:1735:C:H2'	19:A:1736:G:C8	2.51	0.45
19:A:1789:G:C2	20:3:189:ARG:HD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ARG:HD2	1:D:47:GLY:HA3	1.99	0.45
3:F:236:ASN:O	13:Y:1:MET:N	2.49	0.45
9:O:80:VAL:O	9:O:125:GLY:CA	2.65	0.45
11:R:74:MET:HE3	11:R:74:MET:HB3	1.88	0.45
14:Z:53:VAL:HG21	17:e:24:LEU:HD21	1.97	0.45
20:3:109:CYS:HB3	20:3:135:ALA:HB1	1.98	0.45
19:A:1708:A:H4'	19:A:1708:A:OP1	2.17	0.45
11:R:77:ALA:HB1	11:R:118:LEU:HD22	1.97	0.45
14:Z:76:SER:OG	19:A:1098:G:O3'	2.31	0.45
19:A:922:A:H2'	19:A:923:G:C8	2.52	0.45
19:A:1129:A:H2'	19:A:1130:A:H8	1.82	0.45
19:A:1689:A:H2'	19:A:1690:G:H8	1.80	0.45
5:J:14:LYS:HB3	5:J:124:LEU:HD12	1.99	0.45
19:A:673:U:H2'	19:A:674:G:C8	2.51	0.45
19:A:698:G:H2'	19:A:699:A:C8	2.52	0.45
6:K:124:ARG:NH1	19:A:634:C:O2	2.35	0.44
19:A:735:C:H2'	19:A:736:A:H8	1.82	0.44
19:A:1748:U:H2'	19:A:1749:A:C8	2.53	0.44
1:D:20:LEU:HD13	1:D:53:LEU:HD12	1.98	0.44
5:J:176:PRO:HA	19:A:66:U:H5''	1.99	0.44
11:R:133:PRO:HB3	19:A:885:A:H5''	1.99	0.44
1:D:165:THR:HG21	1:D:176:ILE:HG21	1.98	0.44
19:A:52:U:H2'	19:A:53:G:C8	2.53	0.44
19:A:1775:U:O2	19:A:1779:C:N3	2.51	0.44
1:D:68:VAL:HG21	1:D:187:LEU:HB2	1.99	0.44
7:L:69:SER:HB2	9:O:24:LYS:HG3	1.99	0.44
7:L:125:ARG:HE	7:L:132:VAL:HA	1.83	0.44
19:A:219:C:N4	19:A:220:A:H62	2.15	0.44
19:A:276:G:H8	19:A:277:C:H4'	1.81	0.44
19:A:1790:A:H5''	20:3:189:ARG:HH21	1.83	0.44
8:M:34:LEU:HD13	8:M:39:GLU:HB2	1.99	0.44
8:M:57:LEU:HD22	8:M:67:ARG:HA	2.00	0.44
19:A:1076:U:H3'	19:A:1077:U:H4'	1.99	0.44
4:H:117:GLU:HA	4:H:120:LYS:HE2	2.00	0.44
11:R:44:THR:HG22	11:R:51:THR:HA	2.00	0.44
19:A:403:U:H2'	19:A:404:A:C8	2.53	0.44
19:A:479:U:H2'	19:A:480:A:H8	1.82	0.44
16:b:94:LEU:HD22	16:b:99:LEU:HD22	1.99	0.44
1:D:42:LYS:HE3	1:D:42:LYS:HB2	1.83	0.43
19:A:824:U:O4	19:A:844:G:O6	2.36	0.43
19:A:1001:A:H62	20:3:227:MET:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:99:ASN:OD1	2:E:100:PHE:N	2.50	0.43
5:J:132:ARG:NH1	19:A:146:C:O2'	2.51	0.43
6:K:8:LYS:HA	6:K:8:LYS:HD3	1.79	0.43
11:R:31:ARG:N	11:R:42:HIS:O	2.49	0.43
19:A:727:C:H2'	19:A:728:G:C8	2.52	0.43
19:A:995:G:H2'	19:A:996:A:C8	2.53	0.43
7:L:27:PHE:HB2	19:A:330:A:H62	1.83	0.43
10:Q:83:ASP:OD1	10:Q:84:ILE:N	2.50	0.43
7:L:3:ILE:O	7:L:30:GLY:N	2.51	0.43
7:L:49:ARG:O	7:L:52:ASN:ND2	2.51	0.43
8:M:146:VAL:HG11	8:M:154:ILE:HD11	1.99	0.43
17:e:54:VAL:HG12	17:e:63:LEU:HD12	1.99	0.43
20:3:91:ARG:NH2	20:3:146:PHE:O	2.36	0.43
14:Z:23:ARG:NH1	14:Z:24:GLN:OE1	2.51	0.43
16:b:41:ASP:OD1	16:b:44:ARG:NH2	2.32	0.43
11:R:62:LYS:HA	11:R:62:LYS:HD2	1.80	0.43
14:Z:20:MET:HE1	19:A:1036:U:H4'	2.00	0.43
3:F:189:SER:HB3	19:A:4:C:H4'	2.00	0.43
2:E:66:PHE:CZ	11:R:47:SER:HB3	2.54	0.43
4:H:165:GLU:HG2	4:H:166:THR:HG23	2.00	0.43
5:J:28:TYR:O	5:J:30:LYS:NZ	2.45	0.43
7:L:172:ILE:HG13	7:L:188:LEU:HD23	1.99	0.43
12:U:123:ASN:OD1	12:U:124:VAL:N	2.52	0.43
19:A:706:C:H2'	19:A:707:A:C8	2.53	0.43
4:H:66:MET:HE2	19:A:451:A:H5'	2.01	0.43
6:K:55:ILE:HG23	6:K:185:ARG:HE	1.82	0.43
1:D:70:ILE:HD13	1:D:76:VAL:HG23	2.00	0.43
5:J:23:LYS:HG2	5:J:41:LEU:HA	2.01	0.43
5:J:177:ARG:HB2	19:A:78:C:H1'	2.00	0.43
19:A:29:U:H2'	19:A:30:G:C8	2.52	0.43
11:R:150:LEU:HD21	20:3:230:GLU:HG3	2.01	0.42
16:b:63:LEU:HD23	16:b:74:GLY:HA3	2.01	0.42
19:A:118:A:H1'	19:A:394:A:C5	2.54	0.42
19:A:882:A:H2'	19:A:883:G:H8	1.84	0.42
19:A:1077:U:O4	19:A:1087:C:N3	2.52	0.42
1:D:175:LEU:O	1:D:179:MET:HG3	2.19	0.42
3:F:176:ARG:HD3	3:F:178:ILE:HD11	2.01	0.42
11:R:120:ARG:NH2	20:3:134:GLU:OE1	2.50	0.42
14:Z:122:ALA:O	19:A:747:U:O2'	2.30	0.42
16:b:117:ARG:O	16:b:120:THR:OG1	2.38	0.42
3:F:111:LEU:HD22	3:F:195:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:89:ASN:HB3	15:a:136:TRP:CE2	2.55	0.42
1:D:15:ALA:O	1:D:19:GLN:HG2	2.19	0.42
15:a:55:GLU:OE2	15:a:73:ARG:NH1	2.50	0.42
15:a:116:ASP:OD1	15:a:116:ASP:N	2.49	0.42
19:A:220:A:C6	19:A:835:G:O6	2.72	0.42
2:E:32:ILE:HD13	2:E:96:CYS:SG	2.60	0.42
19:A:227:U:O2	19:A:231:G:C6	2.73	0.42
19:A:510:U:H2'	19:A:511:G:C8	2.54	0.42
10:Q:61:ALA:HB1	19:A:957:U:H1'	2.02	0.42
15:a:103:LEU:HB3	15:a:126:LYS:HB2	2.01	0.42
19:A:200:U:O2	19:A:260:C:N3	2.53	0.42
19:A:824:U:H2'	19:A:825:C:C6	2.55	0.42
19:A:874:G:O6	19:A:933:U:C4	2.72	0.42
3:F:58:ILE:HG13	3:F:80:PHE:HZ	1.84	0.42
19:A:5:U:H2'	19:A:6:G:H8	1.84	0.42
19:A:106:C:H2'	19:A:107:A:H8	1.85	0.42
19:A:177:A:H2'	19:A:178:A:C8	2.55	0.42
20:3:255:MET:HE3	20:3:255:MET:HB3	1.90	0.42
16:b:30:ILE:HD13	16:b:38:ILE:HG21	2.02	0.42
11:R:97:ARG:HB3	11:R:131:VAL:HG23	2.01	0.42
16:b:50:MET:HG3	16:b:51:TYR:HD1	1.84	0.42
19:A:138:A:H2	19:A:263:A:H4'	1.85	0.42
19:A:425:A:N3	19:A:437:U:O2'	2.41	0.42
19:A:876:G:H2'	19:A:877:G:H8	1.84	0.42
1:D:4:ALA:HB3	13:Y:77:GLY:HA3	2.02	0.41
1:D:54:GLY:O	1:D:58:GLU:HG2	2.20	0.41
6:K:124:ARG:HA	6:K:124:ARG:HD3	1.88	0.41
16:b:112:LYS:NZ	19:A:456:G:OP1	2.46	0.41
4:H:44:LEU:HD12	4:H:82:TYR:HB3	2.02	0.41
7:L:27:PHE:O	7:L:28:GLU:HG2	2.21	0.41
7:L:123:ARG:O	7:L:126:GLN:NE2	2.53	0.41
16:b:30:ILE:HG22	16:b:32:HIS:HD2	1.85	0.41
19:A:1112:U:H2'	19:A:1113:A:C8	2.55	0.41
19:A:1772:A:H2'	19:A:1773:G:H8	1.85	0.41
10:Q:41:ALA:HB3	10:Q:80:LEU:HD13	2.02	0.41
18:h:26:LYS:HB2	18:h:26:LYS:HE2	1.52	0.41
19:A:951:G:H2'	19:A:952:G:H8	1.86	0.41
1:D:170:ARG:HH11	1:D:207:TYR:H	1.68	0.41
2:E:26:ARG:HA	2:E:50:ARG:HH21	1.85	0.41
3:F:42:GLU:OE2	3:F:44:GLN:NE2	2.53	0.41
19:A:893:G:H2'	19:A:894:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:24:PHE:CE2	11:R:87:LEU:HD11	2.56	0.41
2:E:46:THR:OG1	11:R:45:ASP:OD2	2.31	0.41
3:F:43:TRP:O	3:F:54:LYS:NZ	2.40	0.41
7:L:44:HIS:HB2	7:L:56:ARG:HB2	2.02	0.41
2:E:121:ILE:HD12	2:E:207:LEU:HD21	2.02	0.41
3:F:126:SER:HB2	3:F:132:ALA:HB2	2.03	0.41
10:Q:70:LYS:NZ	19:A:961:A:N7	2.68	0.41
19:A:2:A:H5''	19:A:367:A:OP1	2.21	0.41
19:A:639:G:C2	19:A:688:U:O2	2.73	0.41
7:L:162:LYS:HA	7:L:165:GLU:HB2	2.02	0.41
19:A:889:A:H2'	19:A:890:A:C8	2.56	0.41
19:A:951:G:H2'	19:A:952:G:C8	2.56	0.41
1:D:38:PRO:O	1:D:55:LYS:NZ	2.42	0.41
2:E:67:GLU:HG2	2:E:85:LYS:HG2	2.03	0.41
5:J:58:LYS:HA	5:J:107:SER:HB3	2.02	0.41
19:A:15:U:H2'	19:A:16:G:O4'	2.21	0.41
19:A:542:A:H4'	19:A:543:U:H5'	2.03	0.41
19:A:1669:G:H2'	19:A:1670:C:C6	2.55	0.41
2:E:71:ALA:HB3	11:R:127:ARG:HH22	1.86	0.41
5:J:50:LEU:HD13	5:J:111:LEU:HD13	2.03	0.41
6:K:172:VAL:HG23	6:K:175:ARG:HD3	2.03	0.41
7:L:56:ARG:NH1	19:A:328:G:OP1	2.54	0.41
7:L:61:ASP:N	7:L:61:ASP:OD1	2.53	0.41
7:L:106:ALA:HB2	7:L:169:LEU:HG	2.03	0.41
8:M:130:ARG:H	8:M:130:ARG:HG2	1.58	0.41
8:M:133:ARG:HB3	8:M:138:ILE:HG22	2.03	0.41
15:a:61:ALA:HB1	15:a:116:ASP:HB2	2.03	0.41
16:b:85:LEU:HG	16:b:89:GLU:HG3	2.02	0.41
19:A:724:U:H3'	19:A:725:G:H5''	2.03	0.41
19:A:977:A:N3	19:A:1771:U:O2'	2.53	0.41
19:A:995:G:H2'	19:A:996:A:H8	1.85	0.41
18:h:36:LYS:HA	18:h:36:LYS:HD3	1.80	0.41
19:A:978:G:H4'	19:A:1772:A:H4'	2.02	0.41
19:A:1687:A:H2'	19:A:1688:G:C8	2.55	0.41
1:D:5:ASN:OD1	1:D:65:ARG:NH2	2.43	0.40
15:a:59:VAL:HG23	15:a:69:ARG:HB2	2.02	0.40
16:b:130:ALA:O	16:b:133:LYS:HG2	2.21	0.40
19:A:113:C:C4	19:A:244:A:C6	3.09	0.40
19:A:674:G:H2'	19:A:675:G:C8	2.56	0.40
9:O:20:PHE:CG	19:A:206:U:H5''	2.57	0.40
13:Y:38:LYS:HD3	13:Y:49:GLU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:118:A:H1'	19:A:394:A:C4	2.56	0.40
19:A:876:G:H2'	19:A:877:G:C8	2.56	0.40
5:J:22:ARG:HE	5:J:25:ARG:NH1	2.19	0.40
6:K:181:GLU:OE2	6:K:184:ARG:NH1	2.54	0.40
11:R:116:ARG:HH22	20:3:138:MET:HA	1.86	0.40
11:R:141:ARG:NE	20:3:173:ASP:O	2.55	0.40
14:Z:31:SER:HB2	14:Z:34:ILE:HG13	2.02	0.40
19:A:106:C:H2'	19:A:107:A:C8	2.57	0.40
5:J:64:LYS:HZ3	5:J:82:SER:HB3	1.86	0.40
6:K:47:LEU:HD21	6:K:75:GLY:HA3	2.03	0.40
6:K:76:PHE:O	6:K:80:GLN:HB2	2.21	0.40
19:A:1112:U:H2'	19:A:1113:A:H8	1.86	0.40
1:D:106:THR:O	1:D:109:SER:OG	2.39	0.40
9:O:31:ARG:NH1	19:A:209:G:OP2	2.52	0.40
16:b:124:THR:H	19:A:84:A:H4'	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	D	206/285 (72%)	198 (96%)	8 (4%)	0	100	100
2	E	211/255 (83%)	201 (95%)	9 (4%)	1 (0%)	24	55
3	F	214/263 (81%)	204 (95%)	10 (5%)	0	100	100
4	H	259/264 (98%)	248 (96%)	11 (4%)	0	100	100
5	J	230/239 (96%)	224 (97%)	6 (3%)	0	100	100
6	K	193/203 (95%)	183 (95%)	10 (5%)	0	100	100
7	L	199/202 (98%)	191 (96%)	8 (4%)	0	100	100
8	M	177/190 (93%)	168 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	O	148/161 (92%)	145 (98%)	3 (2%)	0	100	100
10	Q	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
11	R	133/150 (89%)	124 (93%)	9 (7%)	0	100	100
12	U	31/143 (22%)	28 (90%)	3 (10%)	0	100	100
13	Y	84/98 (86%)	82 (98%)	2 (2%)	0	100	100
14	Z	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
15	a	140/145 (97%)	130 (93%)	10 (7%)	0	100	100
16	b	130/136 (96%)	125 (96%)	5 (4%)	0	100	100
17	e	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
18	h	38/62 (61%)	33 (87%)	4 (10%)	1 (3%)	4	23
20	3	182/259 (70%)	171 (94%)	11 (6%)	0	100	100
All	All	2929/3418 (86%)	2794 (95%)	133 (4%)	2 (0%)	49	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	h	42	ARG
2	E	207	LEU

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	D	178/225 (79%)	177 (99%)	1 (1%)	78	81
2	E	187/223 (84%)	186 (100%)	1 (0%)	81	83
3	F	181/206 (88%)	181 (100%)	0	100	100
4	H	219/221 (99%)	219 (100%)	0	100	100
5	J	198/204 (97%)	197 (100%)	1 (0%)	81	83
6	K	169/177 (96%)	169 (100%)	0	100	100
7	L	163/164 (99%)	163 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	M	154/162 (95%)	154 (100%)	0	100	100
9	O	133/143 (93%)	133 (100%)	0	100	100
10	Q	129/130 (99%)	129 (100%)	0	100	100
11	R	102/117 (87%)	102 (100%)	0	100	100
12	U	31/131 (24%)	31 (100%)	0	100	100
13	Y	69/80 (86%)	69 (100%)	0	100	100
14	Z	112/113 (99%)	112 (100%)	0	100	100
15	a	113/116 (97%)	113 (100%)	0	100	100
16	b	112/115 (97%)	112 (100%)	0	100	100
17	e	70/71 (99%)	69 (99%)	1 (1%)	59	73
18	h	34/52 (65%)	31 (91%)	3 (9%)	9	32
20	3	155/215 (72%)	155 (100%)	0	100	100
All	All	2509/2865 (88%)	2502 (100%)	7 (0%)	84	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	166	ASN
2	E	124	ASN
5	J	59	GLN
17	e	61	ASN
18	h	26	LYS
18	h	35	LYS
18	h	36	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	166	ASN
2	E	183	GLN
3	F	166	GLN
3	F	197	GLN
4	H	9	GLN
4	H	67	GLN
4	H	130	GLN
4	H	157	ASN
4	H	253	GLN

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Mol	Chain	Res	Type
5	J	81	HIS
6	K	132	HIS
7	L	52	ASN
7	L	53	HIS
8	M	129	GLN
8	M	137	GLN
9	O	18	HIS
9	O	86	HIS
10	Q	32	GLN
10	Q	69	ASN
10	Q	78	ASN
10	Q	105	ASN
12	U	114	HIS
16	b	25	GLN
18	h	24	GLN
20	3	108	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	A	1251/1796 (69%)	251 (20%)	8 (0%)

All (251) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	A	2	A
19	A	4	C
19	A	6	G
19	A	14	C
19	A	25	C
19	A	26	A
19	A	27	U
19	A	34	G
19	A	42	G
19	A	47	A
19	A	57	G
19	A	63	G
19	A	65	A
19	A	66	U
19	A	67	A
19	A	68	A

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Mol	Chain	Res	Type
19	A	69	G
19	A	70	C
19	A	72	A
19	A	73	U
19	A	74	U
19	A	76	U
19	A	103	A
19	A	110	U
19	A	113	C
19	A	114	G
19	A	115	U
19	A	126	G
19	A	127	U
19	A	138	A
19	A	150	G
19	A	156	U
19	A	175	G
19	A	176	A
19	A	187	U
19	A	191	G
19	A	193	A
19	A	210	A
19	A	212	U
19	A	213	A
19	A	214	A
19	A	221	A
19	A	222	U
19	A	223	G
19	A	228	U
19	A	231	G
19	A	232	G
19	A	234	C
19	A	237	U
19	A	246	U
19	A	247	C
19	A	254	A
19	A	257	U
19	A	258	C
19	A	262	A
19	A	269	C
19	A	270	G
19	A	274	U

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Mol	Chain	Res	Type
19	A	275	U
19	A	277	C
19	A	296	A
19	A	299	U
19	A	306	C
19	A	311	C
19	A	313	A
19	A	317	U
19	A	319	G
19	A	324	C
19	A	326	G
19	A	330	A
19	A	334	G
19	A	335	C
19	A	338	G
19	A	348	C
19	A	349	A
19	A	356	A
19	A	357	A
19	A	358	C
19	A	387	G
19	A	397	A
19	A	398	A
19	A	399	C
19	A	401	G
19	A	412	C
19	A	420	G
19	A	421	C
19	A	422	A
19	A	423	G
19	A	431	G
19	A	432	C
19	A	436	U
19	A	441	C
19	A	449	A
19	A	453	G
19	A	461	A
19	A	465	A
19	A	466	C
19	A	474	A
19	A	480	A
19	A	481	C

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Mol	Chain	Res	Type
19	A	490	U
19	A	492	C
19	A	493	G
19	A	495	G
19	A	502	A
19	A	506	G
19	A	508	A
19	A	512	A
19	A	516	C
19	A	522	A
19	A	531	A
19	A	535	A
19	A	536	G
19	A	539	A
19	A	551	C
19	A	552	A
19	A	553	A
19	A	554	G
19	A	555	U
19	A	556	C
19	A	562	C
19	A	563	C
19	A	565	G
19	A	567	A
19	A	571	G
19	A	575	U
19	A	577	A
19	A	579	U
19	A	591	A
19	A	592	G
19	A	603	A
19	A	608	U
19	A	616	A
19	A	617	A
19	A	619	A
19	A	620	A
19	A	622	C
19	A	636	U
19	A	642	C
19	A	677	U
19	A	678	G
19	A	679	G

Continued on next page...

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Mol	Chain	Res	Type
19	A	680	G
19	A	689	U
19	A	690	U
19	A	691	C
19	A	692	C
19	A	705	G
19	A	709	G
19	A	710	C
19	A	724	U
19	A	725	G
19	A	726	U
19	A	727	C
19	A	729	G
19	A	730	G
19	A	731	G
19	A	732	A
19	A	742	U
19	A	754	A
19	A	764	G
19	A	765	C
19	A	770	A
19	A	773	A
19	A	774	G
19	A	777	C
19	A	779	A
19	A	780	U
19	A	781	G
19	A	787	A
19	A	791	A
19	A	792	U
19	A	793	U
19	A	809	A
19	A	810	A
19	A	814	G
19	A	818	U
19	A	819	G
19	A	822	G
19	A	823	U
19	A	828	U
19	A	830	U
19	A	832	G
19	A	850	C

Continued on next page...

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Mol	Chain	Res	Type
19	A	861	A
19	A	865	G
19	A	871	U
19	A	874	G
19	A	884	U
19	A	896	A
19	A	898	A
19	A	899	G
19	A	901	U
19	A	903	A
19	A	904	A
19	A	911	G
19	A	912	G
19	A	931	A
19	A	932	C
19	A	940	G
19	A	957	U
19	A	958	U
19	A	964	A
19	A	990	A
19	A	991	A
19	A	994	C
19	A	996	A
19	A	998	C
19	A	999	A
19	A	1001	A
19	A	1024	A
19	A	1026	C
19	A	1028	A
19	A	1029	U
19	A	1030	G
19	A	1038	G
19	A	1040	G
19	A	1041	A
19	A	1050	C
19	A	1056	U
19	A	1057	U
19	A	1059	U
19	A	1073	A
19	A	1076	U
19	A	1077	U
19	A	1078	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	A	1093	G
19	A	1094	U
19	A	1095	U
19	A	1097	G
19	A	1135	A
19	A	1654	G
19	A	1657	C
19	A	1661	U
19	A	1676	G
19	A	1684	C
19	A	1699	C
19	A	1708	A
19	A	1711	G
19	A	1712	C
19	A	1726	A
19	A	1766	C
19	A	1768	C
19	A	1776	G
19	A	1777	A
19	A	1779	C
19	A	1782	G
19	A	1788	G
19	A	1790	A
19	A	1791	U
19	A	1795	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
19	A	211	U
19	A	222	U
19	A	231	G
19	A	233	G
19	A	269	C
19	A	552	A
19	A	678	G
19	A	792	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

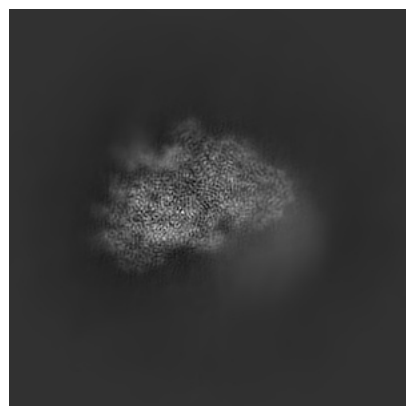
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66679. These allow visual inspection of the internal detail of the map and identification of artifacts.

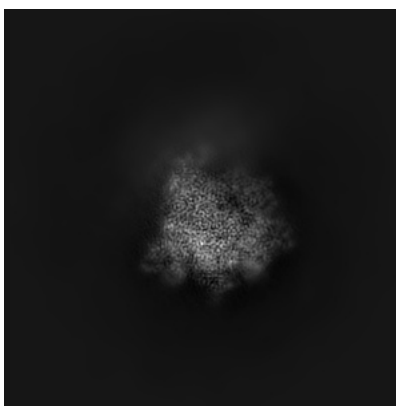
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

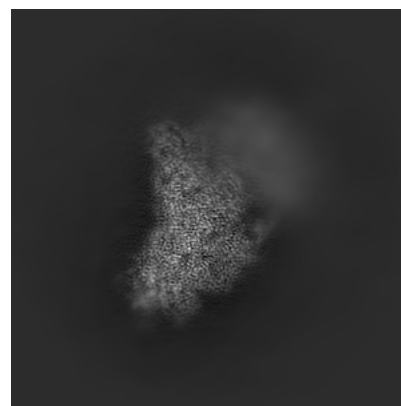
6.1.1 Primary map



X

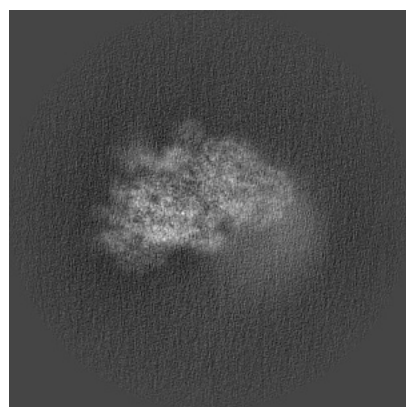


Y

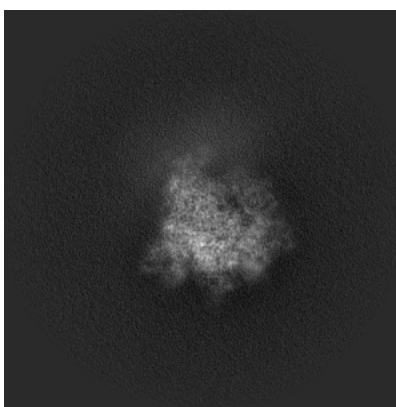


Z

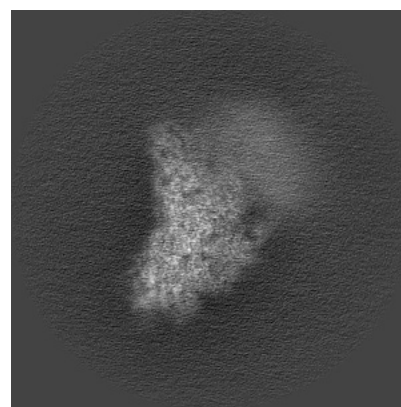
6.1.2 Raw map



X



Y

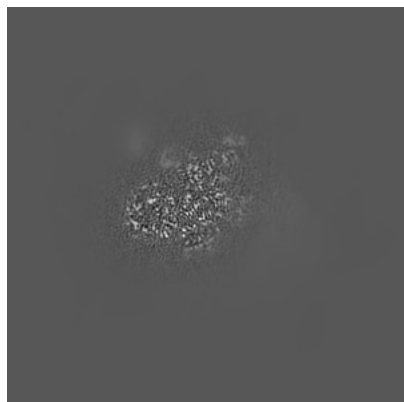


Z

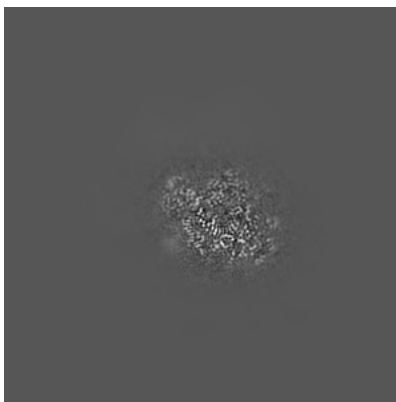
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

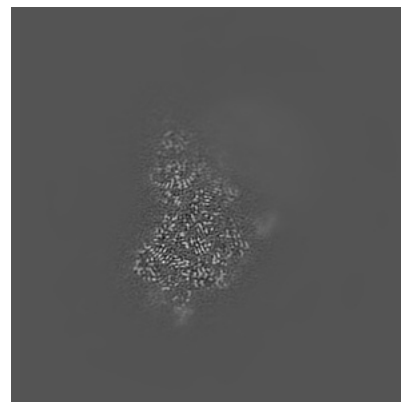
6.2.1 Primary map



X Index: 180

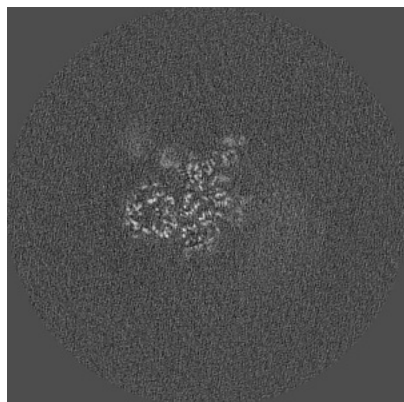


Y Index: 180

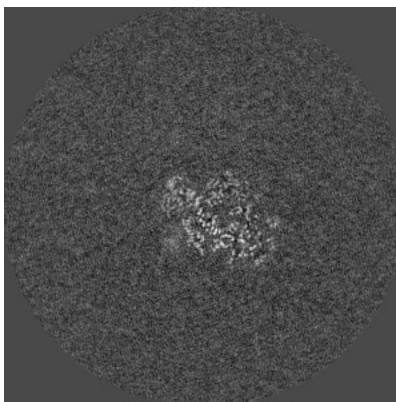


Z Index: 180

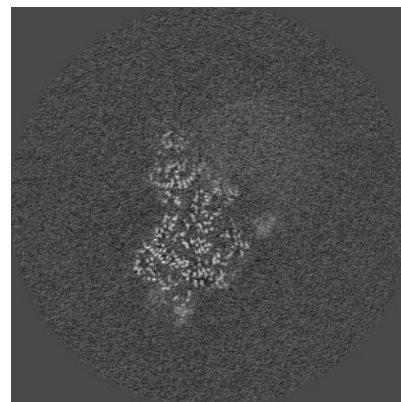
6.2.2 Raw map



X Index: 180



Y Index: 180

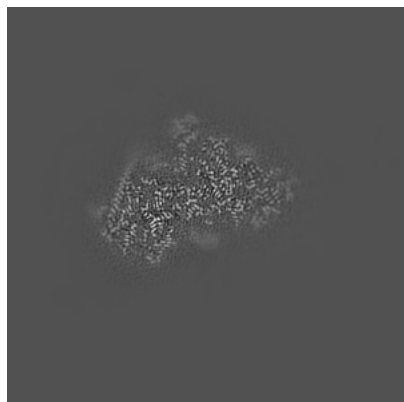


Z Index: 180

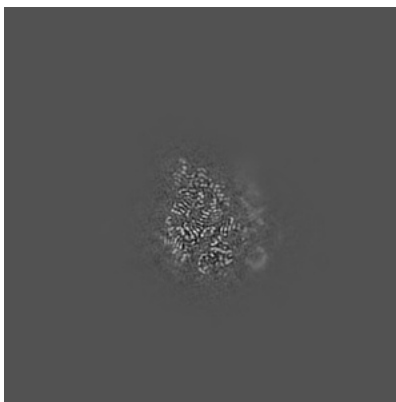
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

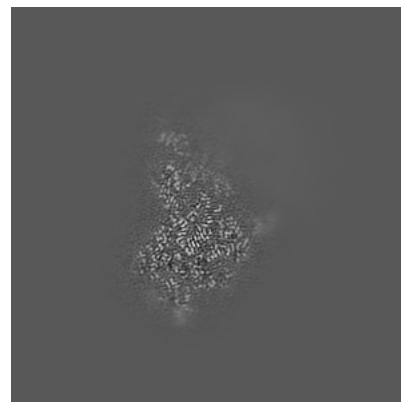
6.3.1 Primary map



X Index: 148

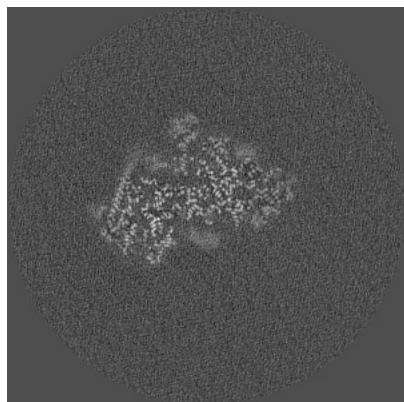


Y Index: 144

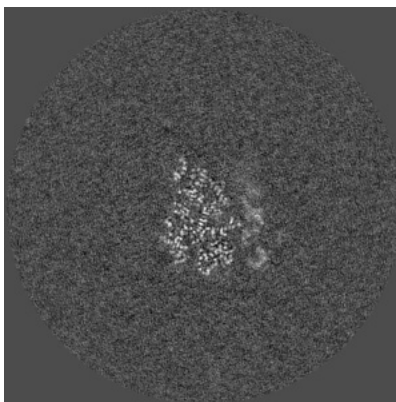


Z Index: 177

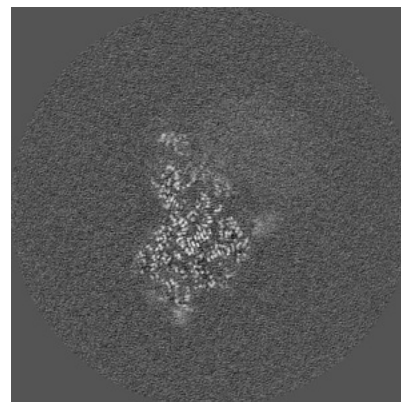
6.3.2 Raw map



X Index: 148



Y Index: 145

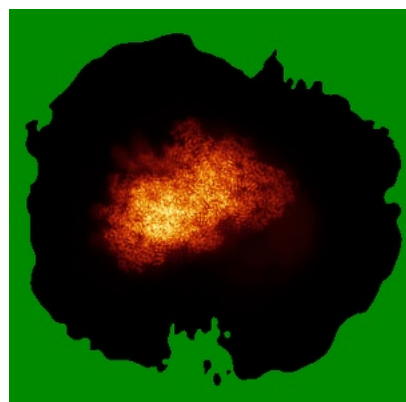


Z Index: 177

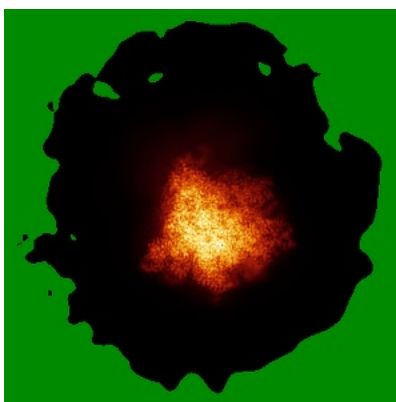
The images above show the largest variance slices of the map in three orthogonal directions.

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

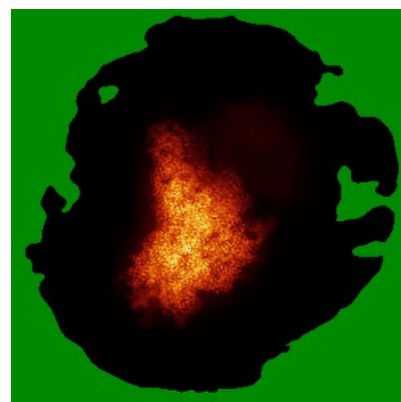
6.4.1 Primary map



X

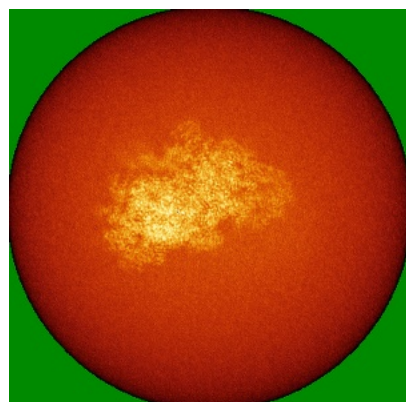


Y

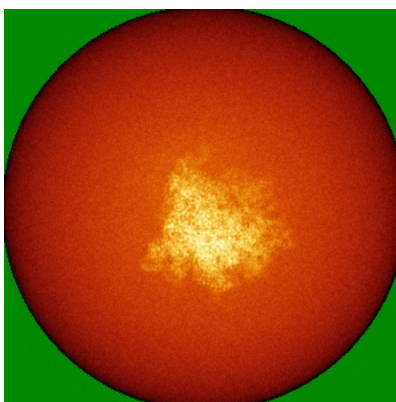


Z

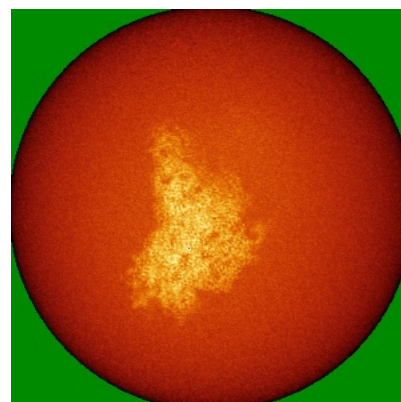
6.4.2 Raw map



X



Y

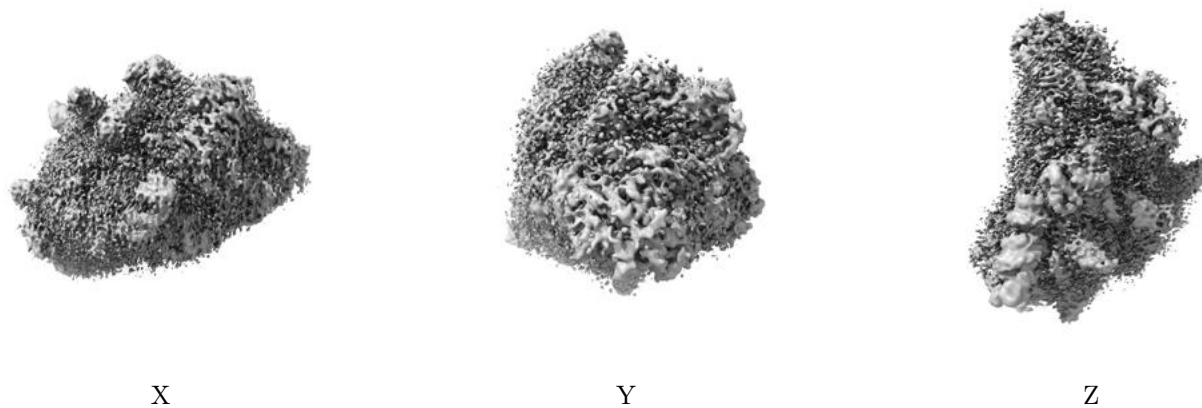


Z

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.

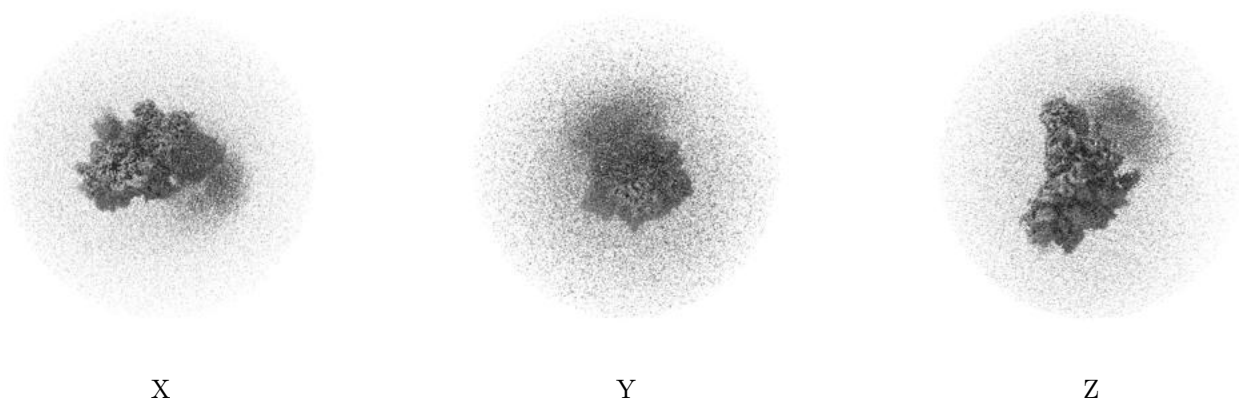
6.5 Orthogonal surface views [i](#)

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.

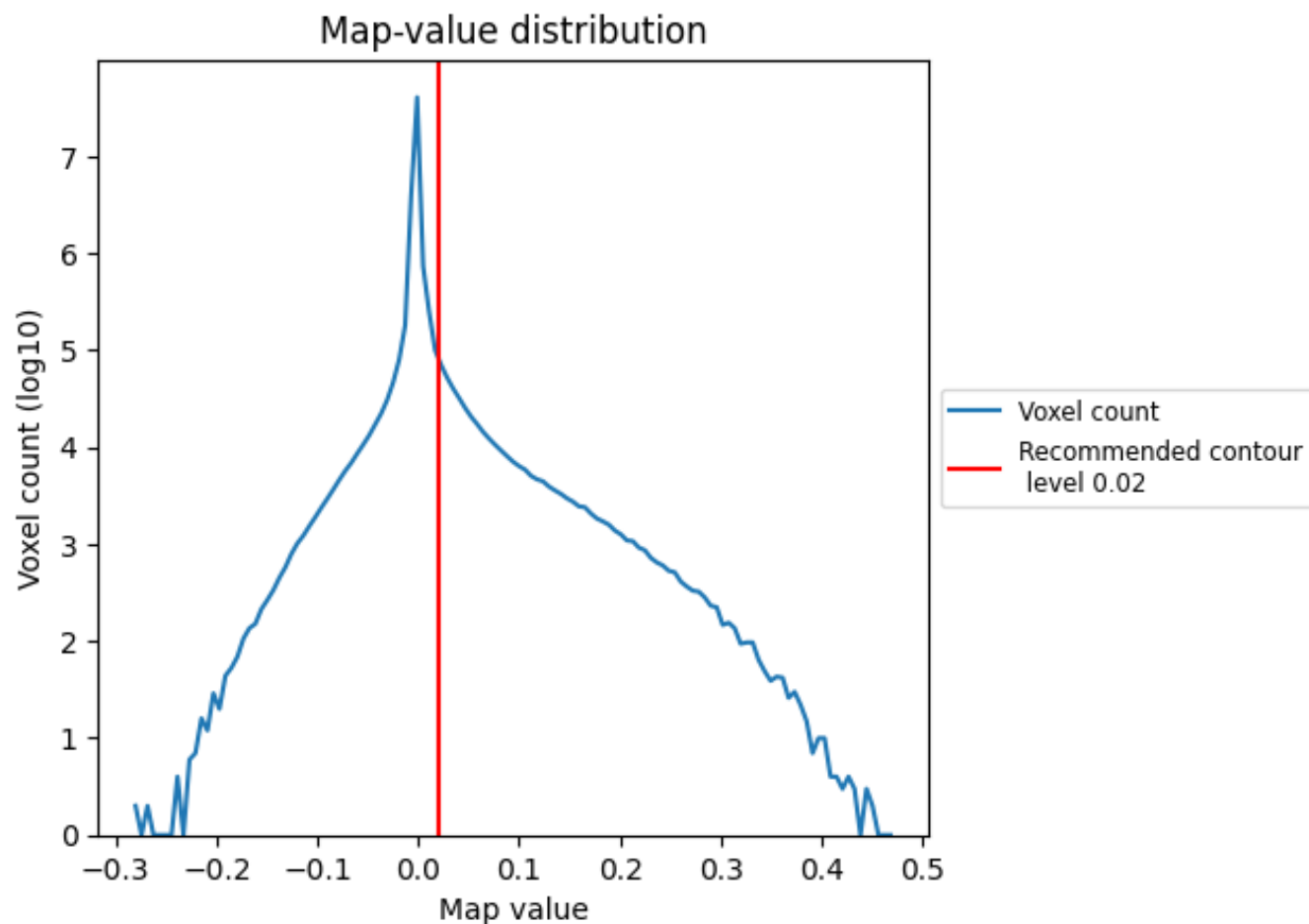
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

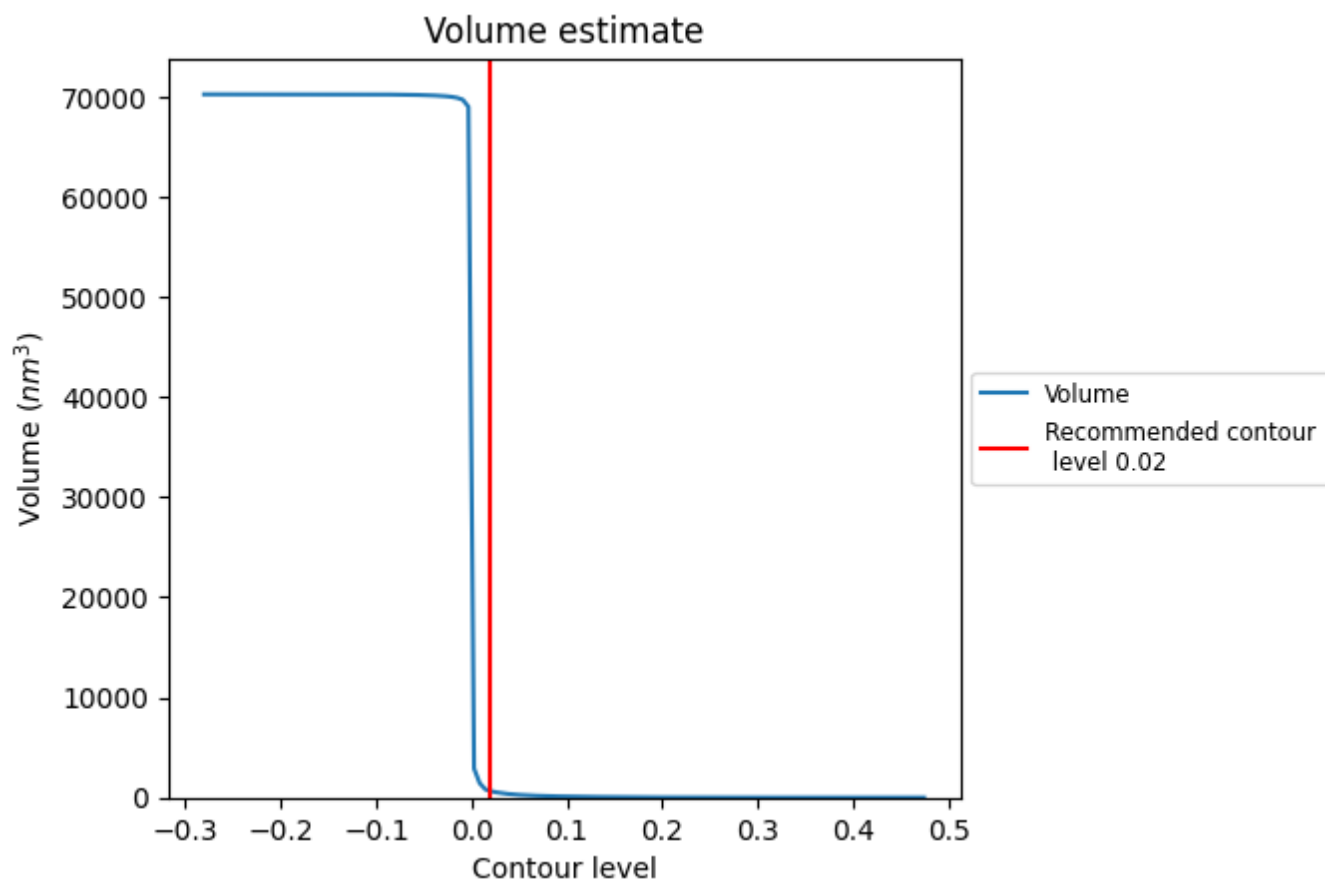
This section contains the results of statistical analysis of the map.

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.

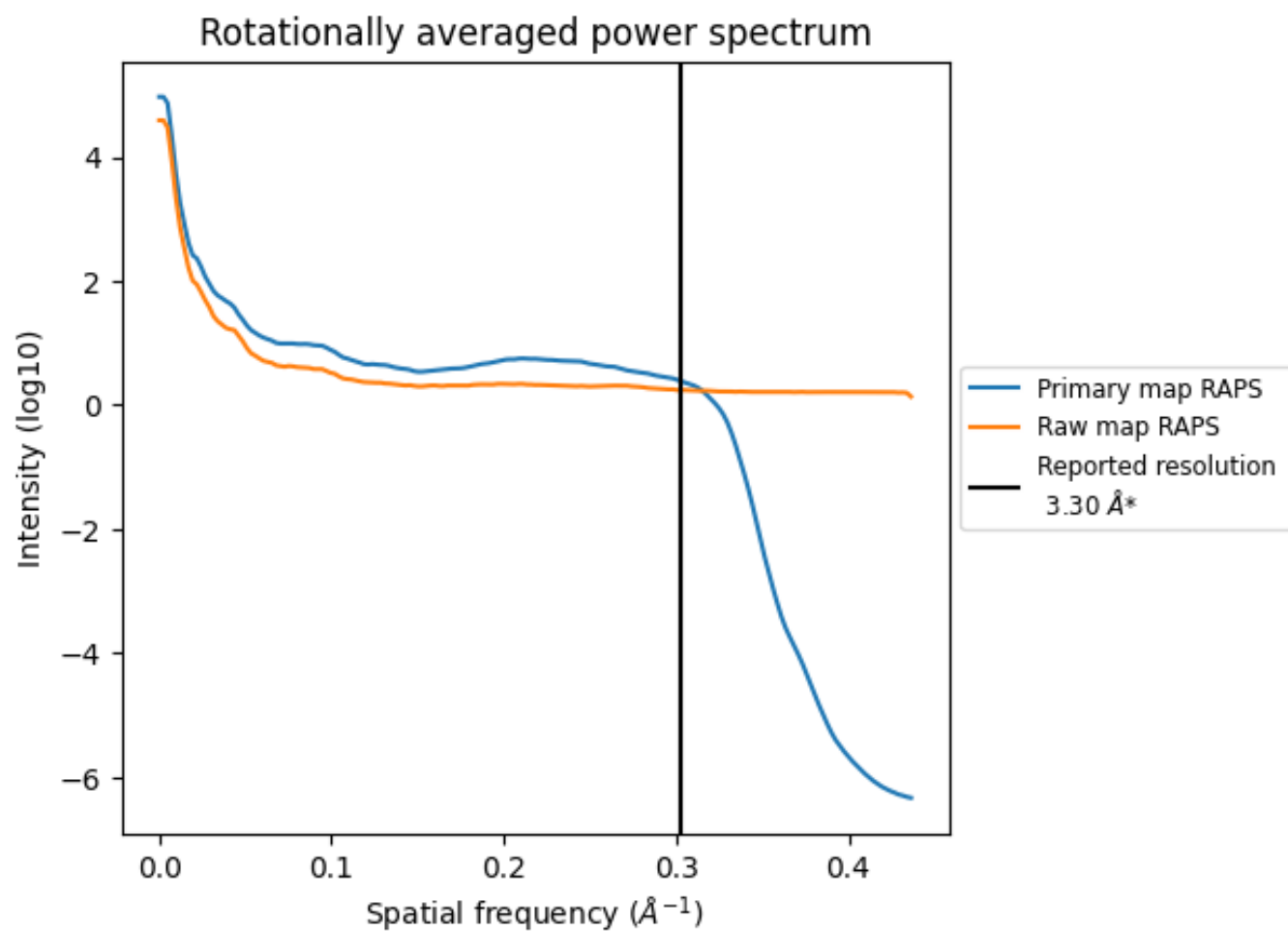
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 652 nm^3 ; this corresponds to an approximate mass of 589 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 ⓘ

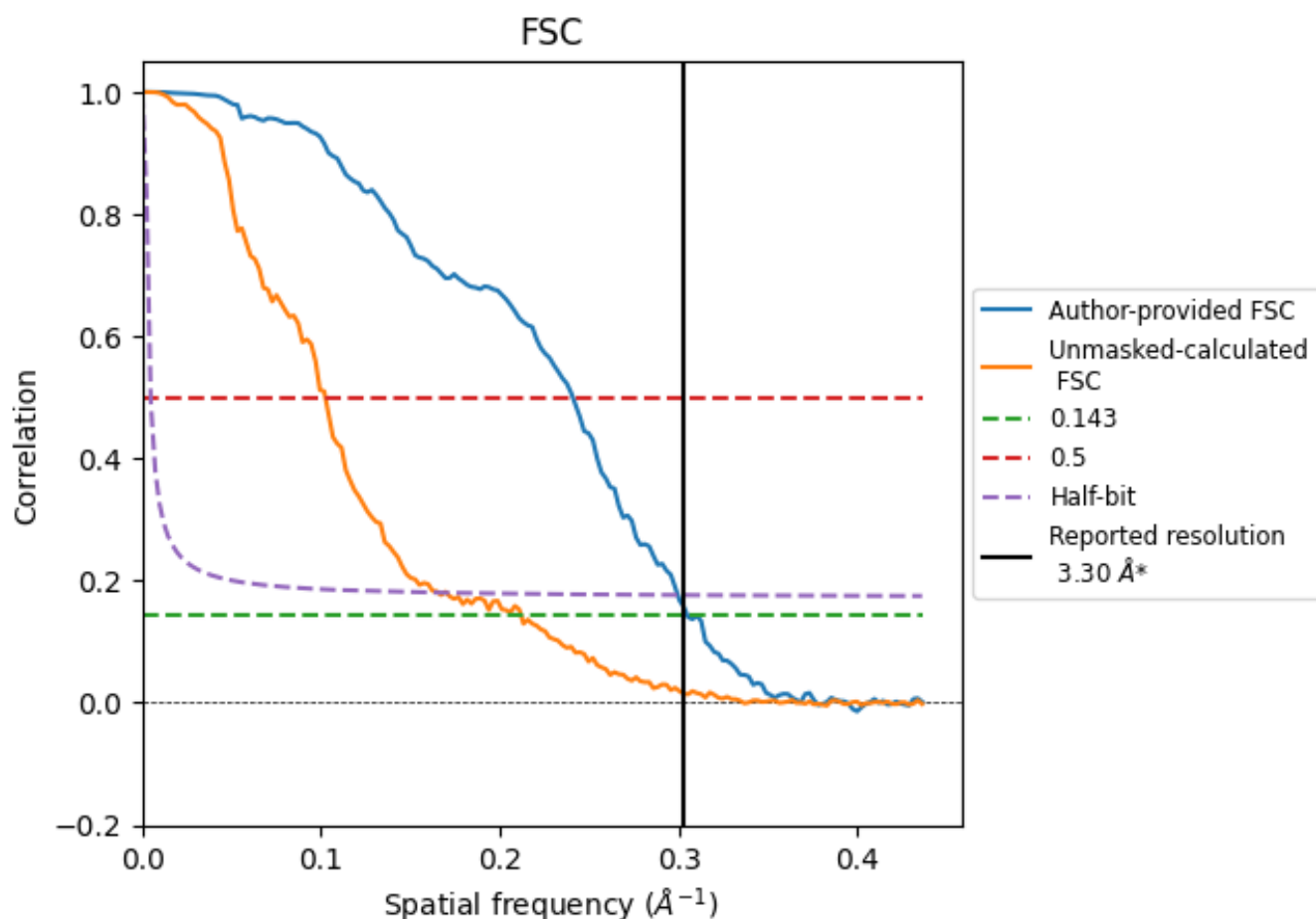


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

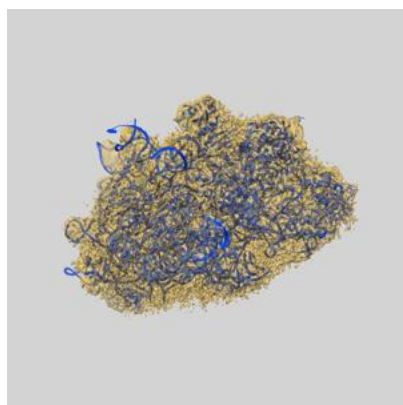
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	4.15	3.34
Unmasked-calculated*	4.72	9.76	6.04

*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 4.72 differs from the reported value 3.3 by more than 10 %

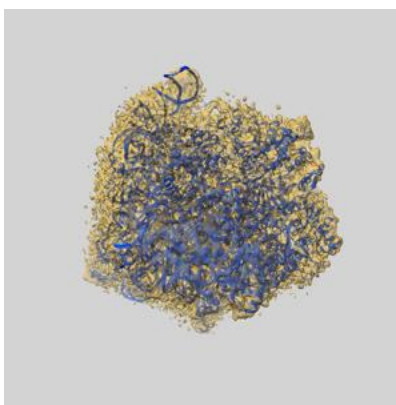
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66679 and PDB model 9XA9. Per-residue inclusion information can be found in section [3](#) on page [8](#).

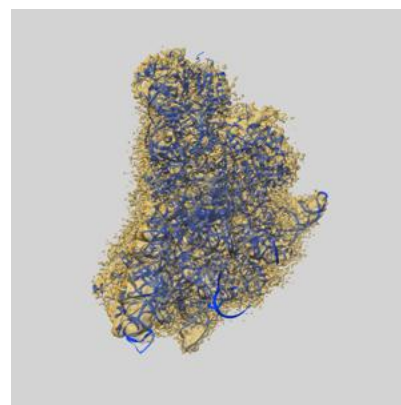
9.1 Map-model overlay [i](#)



X



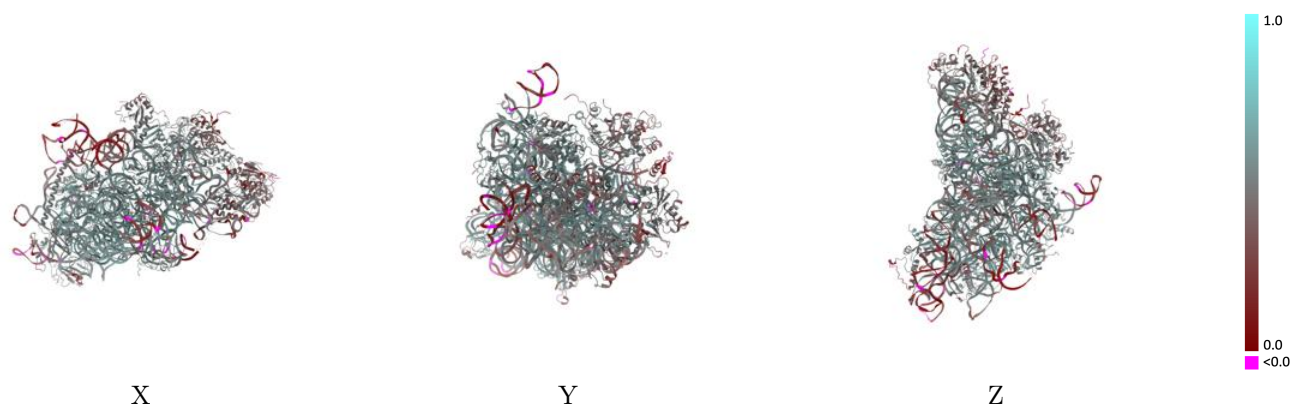
Y



Z

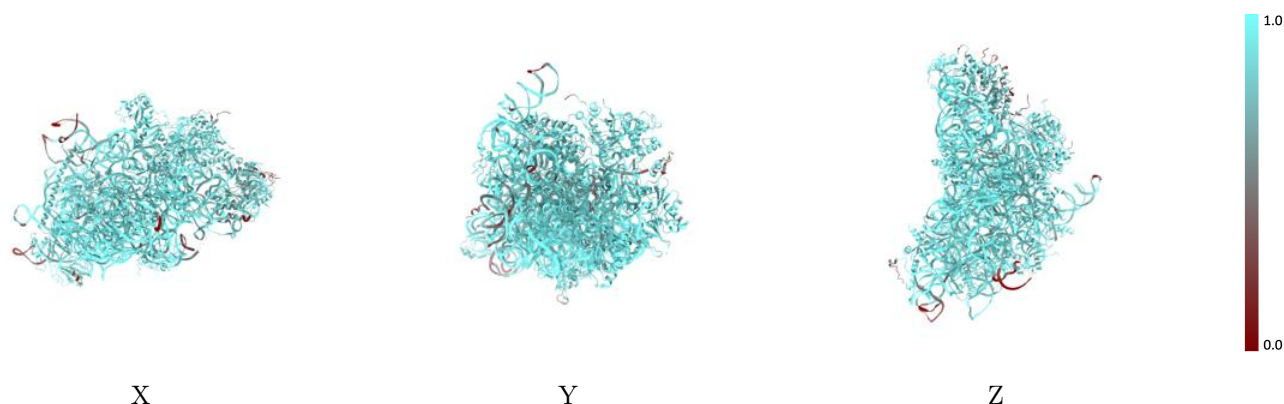
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



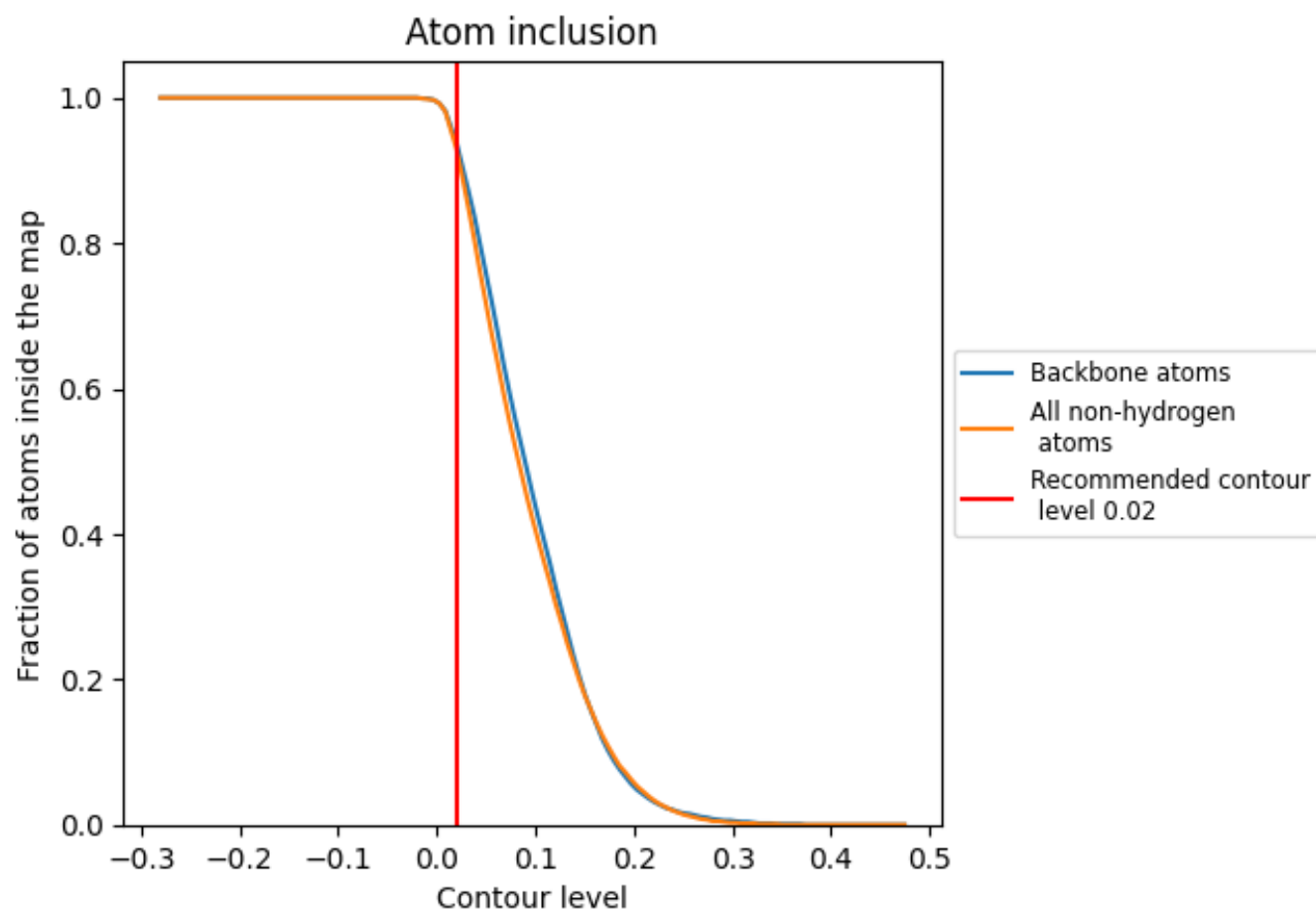
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 94% of all backbone atoms, 93% 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	 0.9290	 0.4920
3	 0.7140	 0.3540
A	 0.9320	 0.4790
D	 0.8790	 0.4500
E	 0.9260	 0.4810
F	 0.9180	 0.5120
H	 0.9800	 0.5770
J	 0.9540	 0.4880
K	 0.9540	 0.4790
L	 0.9380	 0.5290
M	 0.9660	 0.5560
O	 0.9620	 0.5720
Q	 0.9630	 0.5460
R	 0.8720	 0.4430
U	 0.6430	 0.2370
Y	 0.9290	 0.5140
Z	 0.9790	 0.5820
a	 0.9680	 0.5550
b	 0.9290	 0.5090
e	 0.9490	 0.5170
h	 0.9550	 0.5380

