Full wwPDB EM Validation Report (i)

Jun 20, 2024 – 03:55 AM JST

PDB ID	:	7WTP
EMDB ID	:	EMD-32794
Title	:	Cryo-EM structure of a yeast pre-40S ribosomal subunit - State Tsr1-2 (with Rps2)
Authors	:	Cheng, J.; Lau, B.; Thoms, M.; Ameismeier, M.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on	:	2022-02-05
Resolution	:	3.80 Å(reported)

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 (i) 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 (i)) were used in the production of this report:

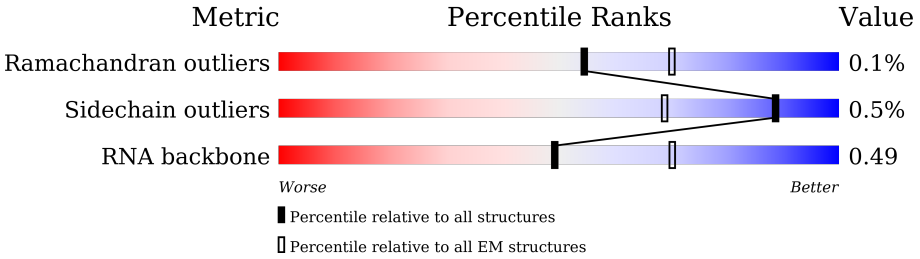
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	C2	1800	49% 19% • 30%
2	SB	255	83% • 15%
3	SC	254	5% 85% • 15%
4	SE	261	98% •
5	SG	236	92% 8%
6	SH	190	94% • • •
7	SI	200	93% • 6%
8	SJ	197	93% • 6%

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Mol	Chain	Length	Quality of chain
9	SL	156	93% 6%
10	SN	151	99%
11	SO	137	93% 7%
12	SW	130	98%
13	SX	145	97%
14	SY	135	95%
15	Sb	82	99%
16	Se	63	11% 60% 40%
17	CA	274	66% 34%
18	CB	275	13% 87%
19	CC	788	11% 84% 16%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 52944 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C2	1255	26763	11971	4765	8772	1255	0	0

- Molecule 2 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SB	216	1722	1091	312	315	4	0	0

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SC	217	1635	1047	289	297	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SE	260	2068	1316	389	360	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SG	218	1755	1102	337	313	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	SH	185	1486	954	266	266	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SI	188	1489	925	298	264	2	0	0

- Molecule 8 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SJ	185	1494	943	289	261	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SL	146	1168	747	221	197	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SN	150	1192	759	224	207	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SO	128	949	582	188	176	3	0	0

- Molecule 12 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SW	129	1021	650	188	180	3	0	0

- Molecule 13 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SX	144	1121	708	220	191	2	0	0

- Molecule 14 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	SY	134	1073	676	208	189	0	0

- Molecule 15 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Sb	81	610	382	110	113	5	0	0

- Molecule 16 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Se	38	313	198	65	49	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	CA	181	1436	917	261	254	4	0	0

- Molecule 18 is a protein called 18S rRNA (guanine(1575)-N(7))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	CB	35	302	189	69	43	1	0	0

- Molecule 19 is a protein called Ribosome biogenesis protein TSR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	CC	661	5346	3413	933	986	14	0	0

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

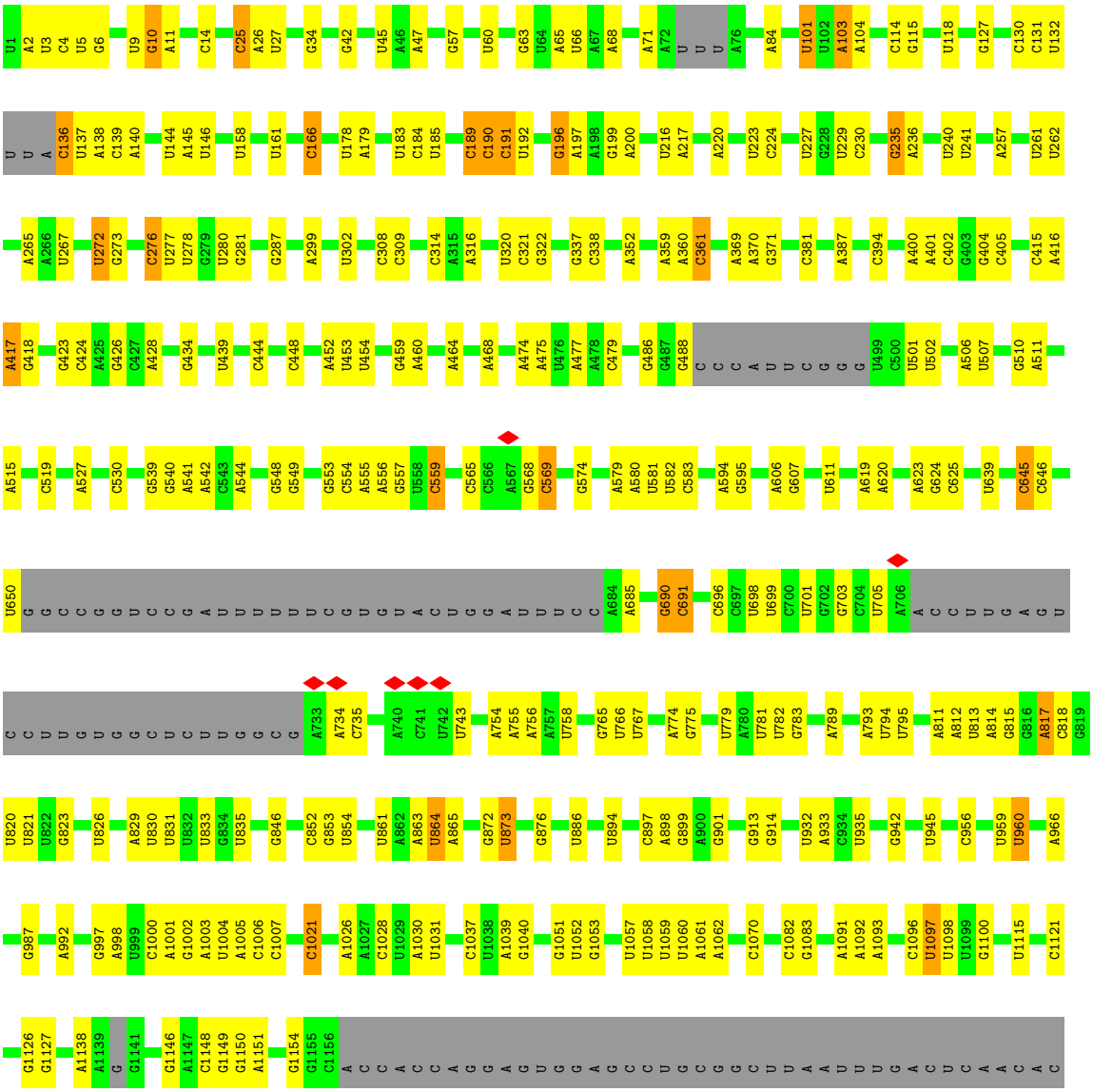
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
20	Sb	1	1	1	0

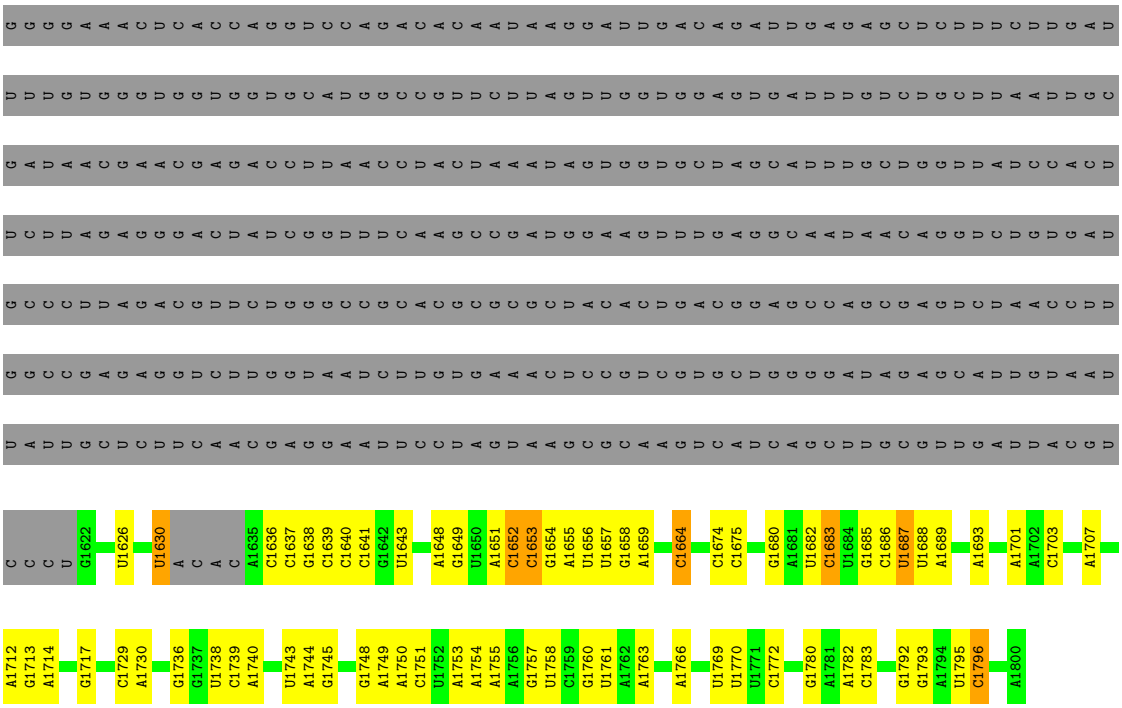
3 Residue-property plots (i)

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: 18S rRNA

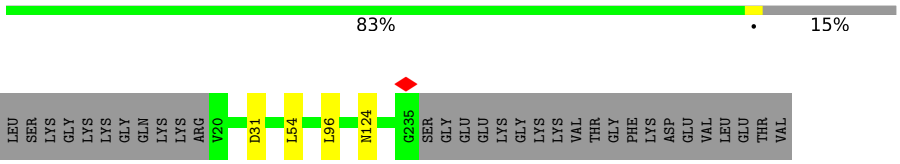
Chain C2: 49% 19% • 30%





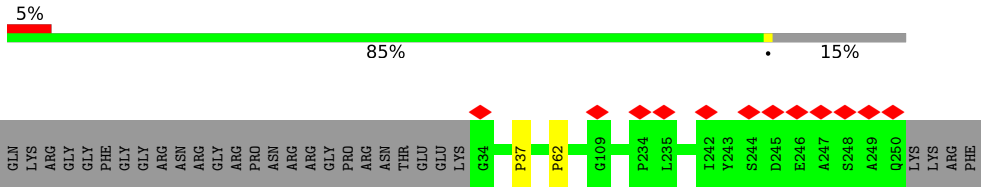
• Molecule 2: 40S ribosomal protein S1-A

Chain SB:



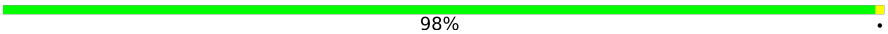
• Molecule 3: 40S ribosomal protein S2

Chain SC:



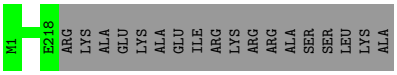
• Molecule 4: 40S ribosomal protein S4-A

Chain SE:



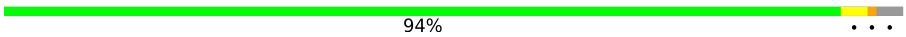
• Molecule 5: 40S ribosomal protein S6-A

Chain SG:



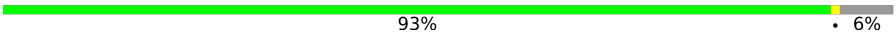
- Molecule 6: 40S ribosomal protein S7-A

Chain SH:



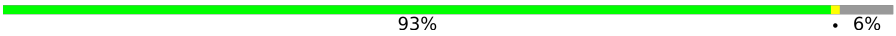
- Molecule 7: 40S ribosomal protein S8-A

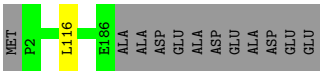
Chain SI:



- Molecule 8: 40S ribosomal protein S9-A

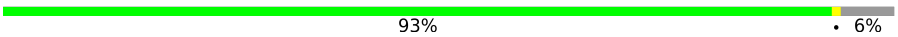
Chain SJ:





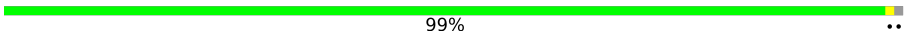
- Molecule 9: 40S ribosomal protein S11-A

Chain SL:



- Molecule 10: 40S ribosomal protein S13

Chain SN:

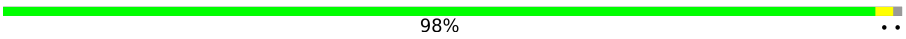


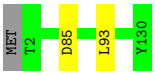
- Molecule 11: 40S ribosomal protein S14-A

Chain SO:

- Molecule 12: 40S ribosomal protein S22-A

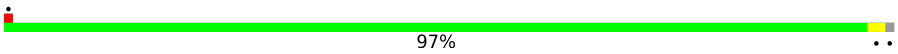
Chain SW:

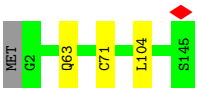




- Molecule 13: 40S ribosomal protein S23-A

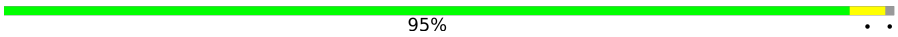
Chain SX:





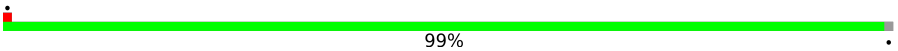
• Molecule 14: 40S ribosomal protein S24-A

Chain SY:



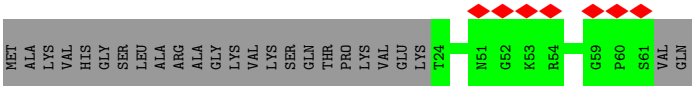
• Molecule 15: 40S ribosomal protein S27-A

Chain Sb:



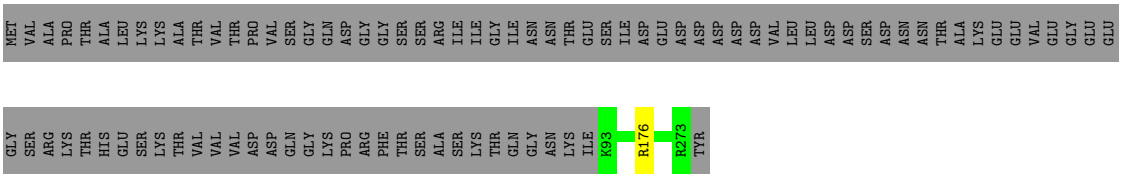
• Molecule 16: 40S ribosomal protein S30-A

Chain Se:



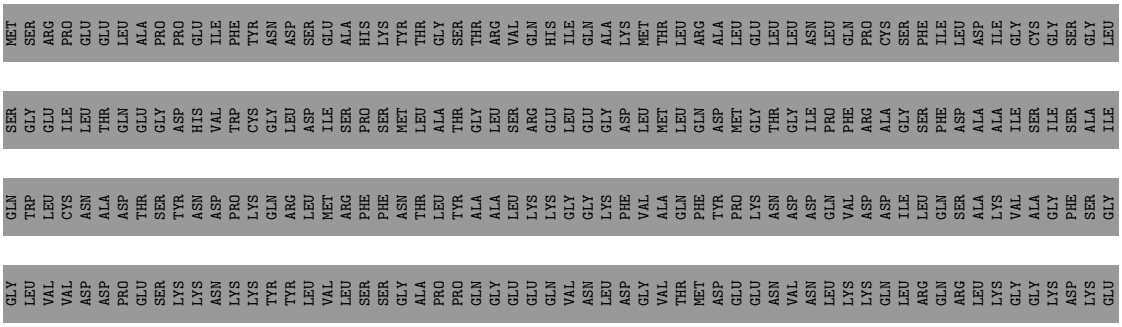
• Molecule 17: Pre-rRNA-processing protein PNO1

Chain CA:



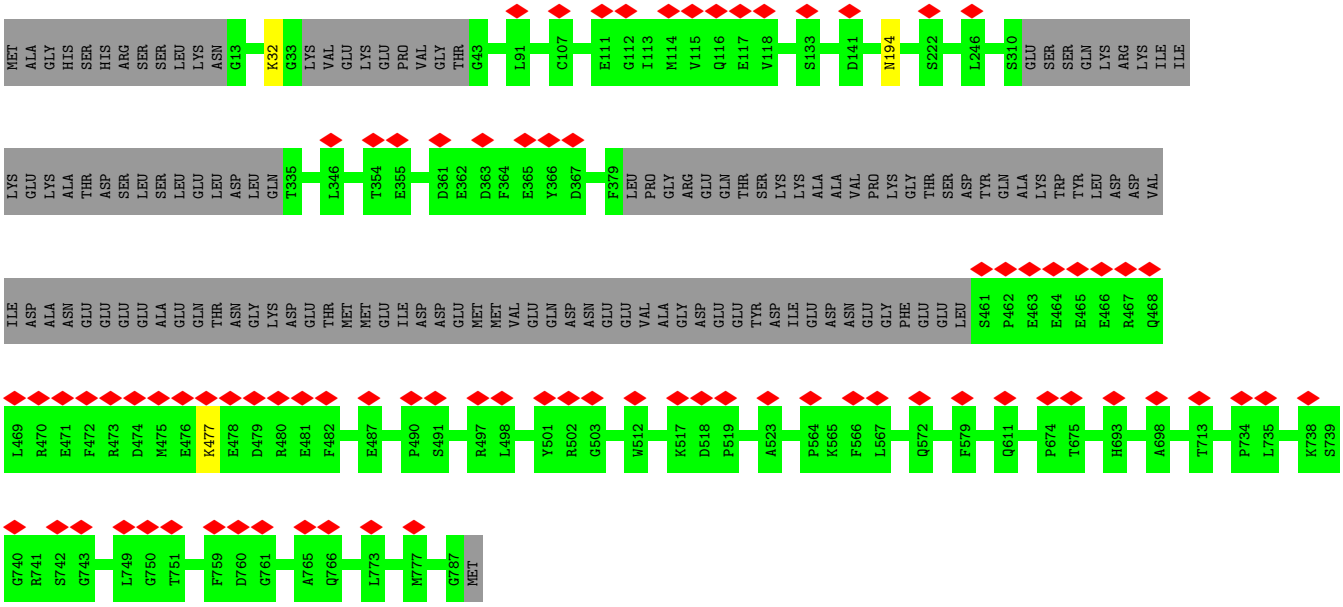
• Molecule 18: 18S rRNA (guanine(1575)-N(7))-methyltransferase

Chain CB:



• Molecule 19: Ribosome biogenesis protein TSR1

Chain CC:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27524	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.252	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	C2	0.80	4/29940 (0.0%)	1.10	123/46636 (0.3%)
2	SB	0.37	0/1748	0.70	3/2352 (0.1%)
3	SC	0.51	3/1665 (0.2%)	0.81	6/2263 (0.3%)
4	SE	0.44	0/2109	0.68	1/2839 (0.0%)
5	SG	0.36	0/1779	0.63	0/2379
6	SH	0.33	0/1511	0.70	1/2036 (0.0%)
7	SI	0.42	0/1514	0.65	0/2021
8	SJ	0.38	0/1519	0.66	1/2035 (0.0%)
9	SL	0.52	0/1194	0.65	0/1610
10	SN	0.45	0/1215	0.70	0/1638
11	SO	0.39	0/960	0.76	1/1290 (0.1%)
12	SW	0.47	0/1038	0.72	2/1395 (0.1%)
13	SX	0.46	0/1139	0.72	2/1518 (0.1%)
14	SY	0.41	0/1087	0.74	1/1449 (0.1%)
15	Sb	0.38	0/620	0.67	0/838
16	Se	0.38	0/319	0.79	0/425
17	CA	0.37	0/1462	0.66	0/1969
18	CB	0.26	0/305	0.65	0/394
19	CC	0.27	0/5469	0.56	0/7383
All	All	0.64	7/56593 (0.0%)	0.94	141/82470 (0.2%)

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
6	SH	0	3
10	SN	0	1
13	SX	0	1
14	SY	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	SC	37	PRO	CG-CD	-11.85	1.11	1.50
3	SC	62	PRO	CG-CD	-9.04	1.20	1.50
1	C2	474	A	N9-C4	-6.09	1.34	1.37
1	C2	118	U	C2-N3	-6.07	1.33	1.37
3	SC	37	PRO	N-CD	5.60	1.55	1.47
1	C2	894	U	C2-N3	-5.11	1.34	1.37
1	C2	1127	G	C2-N3	-5.07	1.28	1.32

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SC	37	PRO	N-CD-CG	-13.41	83.08	103.20
1	C2	190	C	N3-C2-O2	-12.36	113.25	121.90
3	SC	37	PRO	CA-N-CD	-11.69	95.14	111.50
3	SC	62	PRO	N-CD-CG	-11.05	86.63	103.20
1	C2	645	C	N3-C2-O2	-10.80	114.34	121.90
1	C2	956	C	N3-C2-O2	-10.05	114.86	121.90
3	SC	62	PRO	CA-N-CD	-9.86	97.70	111.50
1	C2	118	U	N3-C2-O2	-9.77	115.36	122.20
1	C2	190	C	N1-C2-O2	9.47	124.58	118.90
1	C2	191	C	O4'-C1'-N1	9.44	115.75	108.20
1	C2	191	C	C2-N1-C1'	-8.99	108.92	118.80
1	C2	646	C	C6-N1-C2	-8.68	116.83	120.30
1	C2	956	C	N1-C2-O2	8.44	123.97	118.90
1	C2	646	C	N3-C2-O2	-8.43	116.00	121.90
1	C2	1675	C	N3-C2-O2	-8.29	116.10	121.90
1	C2	894	U	N3-C2-O2	-8.18	116.47	122.20
3	SC	37	PRO	CA-CB-CG	-8.18	88.46	104.00
1	C2	191	C	C6-N1-C1'	7.93	130.32	120.80
1	C2	1121	C	C6-N1-C2	-7.63	117.25	120.30
1	C2	453	U	C2-N1-C1'	7.56	126.77	117.70
1	C2	189	C	N1-C2-O2	7.53	123.42	118.90
2	SB	31	ASP	CB-CG-OD1	7.26	124.83	118.30
1	C2	767	U	N3-C2-O2	-7.22	117.14	122.20
1	C2	479	C	N3-C2-O2	-7.18	116.88	121.90
1	C2	190	C	C6-N1-C2	-7.09	117.47	120.30
1	C2	645	C	N1-C2-O2	7.03	123.12	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C2	1652	C	N1-C2-O2	7.01	123.11	118.90
1	C2	229	U	C2-N1-C1'	6.99	126.09	117.70
1	C2	1657	U	C2-N1-C1'	6.99	126.08	117.70
1	C2	691	C	C2-N1-C1'	6.93	126.42	118.80
1	C2	453	U	N1-C2-O2	6.89	127.62	122.80
8	SJ	116	LEU	CA-CB-CG	6.87	131.10	115.30
1	C2	872	G	N1-C6-O6	-6.85	115.79	119.90
1	C2	184	C	N1-C2-O2	6.80	122.98	118.90
1	C2	872	G	C5-C6-O6	6.80	132.68	128.60
1	C2	101	U	N3-C2-O2	-6.61	117.57	122.20
1	C2	1653	C	N3-C2-O2	-6.57	117.30	121.90
1	C2	453	U	N3-C2-O2	-6.54	117.62	122.20
1	C2	691	C	N1-C2-O2	6.53	122.82	118.90
1	C2	1121	C	N3-C2-O2	-6.52	117.34	121.90
11	SO	66	ASP	CB-CG-OD2	6.52	124.17	118.30
1	C2	1021	C	C2-N1-C1'	6.49	125.94	118.80
1	C2	184	C	N3-C2-O2	-6.46	117.38	121.90
1	C2	1657	U	N3-C2-O2	-6.44	117.69	122.20
1	C2	1657	U	N1-C2-O2	6.40	127.28	122.80
1	C2	236	A	N7-C8-N9	6.40	117.00	113.80
6	SH	9	LEU	CA-CB-CG	6.36	129.92	115.30
1	C2	894	U	N1-C2-O2	6.31	127.22	122.80
1	C2	14	C	N3-C2-O2	-6.31	117.48	121.90
1	C2	479	C	N1-C2-O2	6.30	122.68	118.90
1	C2	530	C	N1-C2-O2	6.29	122.68	118.90
1	C2	272	U	P-O3'-C3'	6.25	127.20	119.70
3	SC	62	PRO	CA-CB-CG	-6.14	92.33	104.00
1	C2	144	U	C2-N1-C1'	6.10	125.02	117.70
1	C2	184	C	C2-N1-C1'	6.08	125.48	118.80
1	C2	530	C	N3-C2-O2	-6.07	117.65	121.90
1	C2	474	A	N3-C4-N9	-5.95	122.64	127.40
1	C2	1683	C	C2-N1-C1'	5.94	125.33	118.80
1	C2	767	U	C2-N1-C1'	5.94	124.82	117.70
1	C2	1686	C	C2-N1-C1'	5.92	125.31	118.80
1	C2	276	C	N3-C2-O2	-5.86	117.80	121.90
1	C2	453	U	C5-C6-N1	5.85	125.63	122.70
2	SB	54	LEU	CA-CB-CG	5.82	128.69	115.30
1	C2	361	C	C5-C6-N1	5.82	123.91	121.00
1	C2	1097	U	OP2-P-O3'	5.82	118.00	105.20
1	C2	1674	C	N1-C2-O2	5.80	122.38	118.90
1	C2	690	G	C5-C6-O6	5.79	132.07	128.60
1	C2	541	A	C2-N3-C4	5.78	113.49	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C2	103	A	P-O3'-C3'	5.78	126.63	119.70
1	C2	474	A	C4-N9-C1'	-5.77	115.92	126.30
1	C2	394	C	C5-C6-N1	5.76	123.88	121.00
12	SW	85	ASP	CB-CG-OD2	5.75	123.48	118.30
1	C2	864	U	C2-N1-C1'	5.69	124.53	117.70
1	C2	1127	G	N3-C2-N2	-5.69	115.92	119.90
1	C2	1097	U	P-O3'-C3'	5.66	126.49	119.70
1	C2	872	G	N9-C4-C5	5.65	107.66	105.40
13	SX	104	LEU	CA-CB-CG	5.65	128.28	115.30
1	C2	645	C	C6-N1-C2	-5.64	118.04	120.30
1	C2	224	C	C6-N1-C2	-5.60	118.06	120.30
1	C2	1674	C	C2-N1-C1'	5.60	124.96	118.80
1	C2	1687	U	N1-C2-O2	5.59	126.72	122.80
1	C2	1683	C	C6-N1-C2	-5.58	118.07	120.30
1	C2	224	C	N3-C2-O2	-5.55	118.01	121.90
1	C2	1664	C	C2-N1-C1'	5.52	124.87	118.80
1	C2	1630	U	O5'-P-OP1	5.50	117.30	110.70
1	C2	625	C	C6-N1-C2	-5.50	118.10	120.30
1	C2	1643	U	C2-N1-C1'	5.50	124.30	117.70
1	C2	474	A	C6-C5-N7	5.48	136.14	132.30
1	C2	236	A	C6-C5-N7	-5.47	128.47	132.30
1	C2	559	C	C2-N1-C1'	5.46	124.81	118.80
1	C2	873	U	N3-C2-O2	-5.45	118.38	122.20
1	C2	901	G	O4'-C1'-N9	5.42	112.54	108.20
1	C2	873	U	N1-C2-O2	5.40	126.58	122.80
1	C2	864	U	N3-C2-O2	-5.39	118.43	122.20
1	C2	1127	G	N9-C4-C5	5.39	107.55	105.40
1	C2	1729	C	N1-C2-O2	5.38	122.13	118.90
1	C2	136	C	P-O3'-C3'	5.36	126.13	119.70
1	C2	1643	U	N1-C2-O2	5.36	126.55	122.80
1	C2	901	G	C4-N9-C1'	5.35	133.46	126.50
1	C2	235	G	N1-C6-O6	-5.35	116.69	119.90
1	C2	690	G	C8-N9-C4	-5.34	104.26	106.40
1	C2	417	A	P-O3'-C3'	5.34	126.10	119.70
1	C2	196	G	N1-C2-N2	-5.33	111.40	116.20
1	C2	474	A	C8-N9-C1'	5.32	137.27	127.70
1	C2	1127	G	C5-C6-O6	5.32	131.79	128.60
1	C2	1652	C	N3-C2-O2	-5.32	118.18	121.90
1	C2	118	U	N1-C2-O2	5.29	126.50	122.80
2	SB	96	LEU	CA-CB-CG	5.29	127.47	115.30
1	C2	1675	C	N1-C2-N3	5.28	122.89	119.20
1	C2	1729	C	N3-C2-O2	-5.26	118.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	SW	93	LEU	CA-CB-CG	5.26	127.39	115.30
1	C2	1664	C	C5-C6-N1	5.24	123.62	121.00
1	C2	1653	C	C6-N1-C2	-5.24	118.20	120.30
1	C2	1675	C	C6-N1-C2	-5.24	118.20	120.30
1	C2	229	U	C5-C6-N1	5.24	125.32	122.70
1	C2	267	U	N3-C2-O2	-5.23	118.54	122.20
1	C2	817	A	P-O3'-C3'	5.23	125.98	119.70
1	C2	1796	C	N1-C2-O2	5.22	122.03	118.90
1	C2	1664	C	N1-C2-O2	5.21	122.02	118.90
1	C2	690	G	N1-C6-O6	-5.20	116.78	119.90
1	C2	1682	U	C2-N1-C1'	5.18	123.91	117.70
1	C2	569	C	N1-C2-O2	5.15	121.99	118.90
1	C2	1037	C	C6-N1-C2	-5.14	118.24	120.30
1	C2	691	C	C5-C6-N1	5.14	123.57	121.00
1	C2	701	U	C2-N1-C1'	5.13	123.86	117.70
1	C2	795	U	C2-N1-C1'	5.13	123.86	117.70
1	C2	474	A	C4-C5-C6	-5.11	114.45	117.00
1	C2	1674	C	N3-C2-O2	-5.10	118.33	121.90
1	C2	758	U	N3-C2-O2	-5.09	118.63	122.20
1	C2	960	U	N3-C2-O2	-5.09	118.64	122.20
14	SY	51	GLU	CA-CB-CG	5.09	124.59	113.40
1	C2	25	C	P-O3'-C3'	5.08	125.79	119.70
1	C2	565	C	N1-C2-O2	5.07	121.94	118.90
1	C2	405	C	C6-N1-C2	-5.06	118.28	120.30
4	SE	261	LEU	CA-CB-CG	5.05	126.92	115.30
1	C2	861	U	C2-N1-C1'	5.04	123.75	117.70
1	C2	10	G	N3-C4-C5	-5.04	126.08	128.60
1	C2	872	G	N1-C2-N3	5.04	126.92	123.90
1	C2	166	C	N1-C2-O2	5.03	121.92	118.90
1	C2	381	C	C6-N1-C2	-5.02	118.29	120.30
13	SX	71	CYS	CA-CB-SG	-5.01	104.97	114.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	SH	31	SER	Peptide
6	SH	64	VAL	Peptide
6	SH	9	LEU	Peptide
10	SN	21	ASN	Peptide
13	SX	63	GLN	Peptide
14	SY	48	TYR	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
2	SB	214/255 (84%)	193 (90%)	21 (10%)	0	100	100
3	SC	215/254 (85%)	194 (90%)	21 (10%)	0	100	100
4	SE	258/261 (99%)	230 (89%)	28 (11%)	0	100	100
5	SG	216/236 (92%)	203 (94%)	13 (6%)	0	100	100
6	SH	183/190 (96%)	164 (90%)	18 (10%)	1 (0%)	29	66
7	SI	184/200 (92%)	173 (94%)	11 (6%)	0	100	100
8	SJ	183/197 (93%)	167 (91%)	16 (9%)	0	100	100
9	SL	144/156 (92%)	126 (88%)	18 (12%)	0	100	100
10	SN	148/151 (98%)	133 (90%)	15 (10%)	0	100	100
11	SO	126/137 (92%)	110 (87%)	16 (13%)	0	100	100
12	SW	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
13	SX	142/145 (98%)	123 (87%)	19 (13%)	0	100	100
14	SY	132/135 (98%)	118 (89%)	11 (8%)	3 (2%)	6	38
15	Sb	79/82 (96%)	67 (85%)	12 (15%)	0	100	100
16	Se	36/63 (57%)	28 (78%)	8 (22%)	0	100	100
17	CA	179/274 (65%)	166 (93%)	13 (7%)	0	100	100
18	CB	33/275 (12%)	28 (85%)	5 (15%)	0	100	100
19	CC	653/788 (83%)	624 (96%)	29 (4%)	0	100	100
All	All	3252/3929 (83%)	2964 (91%)	284 (9%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	SY	32	ARG
14	SY	52	LYS
6	SH	74	GLN
14	SY	79	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
2	SB	192/224 (86%)	191 (100%)	1 (0%)	88	94
3	SC	176/205 (86%)	176 (100%)	0	100	100
4	SE	221/222 (100%)	219 (99%)	2 (1%)	78	88
5	SG	187/201 (93%)	187 (100%)	0	100	100
6	SH	165/170 (97%)	163 (99%)	2 (1%)	71	84
7	SI	150/161 (93%)	148 (99%)	2 (1%)	69	82
8	SJ	158/166 (95%)	158 (100%)	0	100	100
9	SL	129/137 (94%)	128 (99%)	1 (1%)	81	89
10	SN	127/128 (99%)	127 (100%)	0	100	100
11	SO	97/105 (92%)	97 (100%)	0	100	100
12	SW	110/111 (99%)	110 (100%)	0	100	100
13	SX	119/120 (99%)	119 (100%)	0	100	100
14	SY	112/113 (99%)	111 (99%)	1 (1%)	78	88
15	Sb	70/71 (99%)	70 (100%)	0	100	100
16	Se	34/54 (63%)	34 (100%)	0	100	100
17	CA	158/238 (66%)	157 (99%)	1 (1%)	86	92
18	CB	31/233 (13%)	31 (100%)	0	100	100
19	CC	575/703 (82%)	572 (100%)	3 (0%)	88	94
All	All	2811/3362 (84%)	2798 (100%)	13 (0%)	89	94

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	124	ASN
4	SE	108	ARG
4	SE	197	HIS
6	SH	7	LYS
6	SH	83	LYS
7	SI	18	ARG
7	SI	137	LYS
9	SL	67	ARG
14	SY	8	ARG
17	CA	176	ARG
19	CC	32	LYS
19	CC	194	ASN
19	CC	477	LYS

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

Mol	Chain	Res	Type
2	SB	124	ASN
3	SC	94	GLN
6	SH	74	GLN
7	SI	32	GLN
10	SN	101	HIS
13	SX	79	ASN
16	Se	46	ASN
19	CC	194	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C2	1247/1800 (69%)	329 (26%)	13 (1%)

All (329) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C2	2	A
1	C2	3	U
1	C2	4	C
1	C2	5	U
1	C2	6	G
1	C2	9	U
1	C2	10	G

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Mol	Chain	Res	Type
1	C2	11	A
1	C2	25	C
1	C2	26	A
1	C2	27	U
1	C2	34	G
1	C2	42	G
1	C2	45	U
1	C2	47	A
1	C2	57	G
1	C2	60	U
1	C2	63	G
1	C2	65	A
1	C2	66	U
1	C2	68	A
1	C2	71	A
1	C2	84	A
1	C2	101	U
1	C2	104	A
1	C2	114	C
1	C2	115	G
1	C2	127	G
1	C2	130	C
1	C2	131	C
1	C2	132	U
1	C2	137	U
1	C2	138	A
1	C2	140	A
1	C2	145	A
1	C2	146	U
1	C2	158	U
1	C2	161	U
1	C2	166	C
1	C2	178	U
1	C2	179	A
1	C2	183	U
1	C2	185	U
1	C2	189	C
1	C2	190	C
1	C2	191	C
1	C2	192	U
1	C2	196	G
1	C2	197	A

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Mol	Chain	Res	Type
1	C2	199	G
1	C2	200	A
1	C2	216	U
1	C2	217	A
1	C2	220	A
1	C2	223	U
1	C2	227	U
1	C2	230	C
1	C2	235	G
1	C2	240	U
1	C2	241	U
1	C2	257	A
1	C2	261	U
1	C2	262	U
1	C2	265	A
1	C2	272	U
1	C2	273	G
1	C2	276	C
1	C2	277	U
1	C2	278	U
1	C2	280	U
1	C2	281	G
1	C2	287	G
1	C2	299	A
1	C2	302	U
1	C2	308	C
1	C2	309	C
1	C2	314	C
1	C2	316	A
1	C2	320	U
1	C2	321	C
1	C2	322	G
1	C2	337	G
1	C2	338	C
1	C2	352	A
1	C2	359	A
1	C2	360	A
1	C2	361	C
1	C2	369	A
1	C2	370	A
1	C2	371	G
1	C2	387	A

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Mol	Chain	Res	Type
1	C2	400	A
1	C2	401	A
1	C2	402	C
1	C2	404	G
1	C2	415	C
1	C2	416	A
1	C2	418	G
1	C2	423	G
1	C2	424	C
1	C2	426	G
1	C2	428	A
1	C2	434	G
1	C2	439	U
1	C2	444	C
1	C2	448	C
1	C2	452	A
1	C2	454	U
1	C2	459	G
1	C2	460	A
1	C2	464	A
1	C2	468	A
1	C2	475	A
1	C2	477	A
1	C2	486	G
1	C2	488	G
1	C2	501	U
1	C2	502	U
1	C2	506	A
1	C2	507	U
1	C2	510	G
1	C2	511	A
1	C2	515	A
1	C2	519	C
1	C2	527	A
1	C2	539	G
1	C2	540	G
1	C2	542	A
1	C2	544	A
1	C2	548	G
1	C2	549	G
1	C2	553	G
1	C2	554	C

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Mol	Chain	Res	Type
1	C2	555	A
1	C2	556	A
1	C2	557	G
1	C2	559	C
1	C2	568	G
1	C2	569	C
1	C2	574	G
1	C2	579	A
1	C2	580	A
1	C2	581	U
1	C2	582	U
1	C2	583	C
1	C2	594	A
1	C2	595	G
1	C2	606	A
1	C2	607	G
1	C2	611	U
1	C2	619	A
1	C2	620	A
1	C2	623	A
1	C2	624	G
1	C2	639	U
1	C2	645	C
1	C2	650	U
1	C2	685	A
1	C2	690	G
1	C2	691	C
1	C2	696	C
1	C2	698	U
1	C2	699	U
1	C2	703	G
1	C2	705	U
1	C2	734	A
1	C2	735	C
1	C2	743	U
1	C2	754	A
1	C2	755	A
1	C2	756	A
1	C2	765	G
1	C2	766	U
1	C2	774	A
1	C2	775	G

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Mol	Chain	Res	Type
1	C2	779	U
1	C2	781	U
1	C2	782	U
1	C2	783	G
1	C2	789	A
1	C2	793	A
1	C2	794	U
1	C2	811	A
1	C2	812	A
1	C2	813	U
1	C2	814	A
1	C2	815	G
1	C2	818	C
1	C2	820	U
1	C2	821	U
1	C2	823	G
1	C2	826	U
1	C2	829	A
1	C2	830	U
1	C2	831	U
1	C2	833	U
1	C2	835	U
1	C2	846	G
1	C2	852	C
1	C2	853	G
1	C2	854	U
1	C2	863	A
1	C2	864	U
1	C2	865	A
1	C2	873	U
1	C2	876	G
1	C2	886	U
1	C2	897	C
1	C2	898	A
1	C2	899	G
1	C2	913	G
1	C2	914	G
1	C2	932	U
1	C2	933	A
1	C2	935	U
1	C2	942	G
1	C2	945	U

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Mol	Chain	Res	Type
1	C2	959	U
1	C2	960	U
1	C2	966	A
1	C2	987	G
1	C2	992	A
1	C2	998	A
1	C2	1000	C
1	C2	1001	A
1	C2	1002	G
1	C2	1003	A
1	C2	1004	U
1	C2	1005	A
1	C2	1006	C
1	C2	1007	C
1	C2	1021	C
1	C2	1026	A
1	C2	1028	C
1	C2	1030	A
1	C2	1031	U
1	C2	1039	A
1	C2	1040	G
1	C2	1052	U
1	C2	1053	G
1	C2	1057	U
1	C2	1058	U
1	C2	1059	U
1	C2	1060	U
1	C2	1061	A
1	C2	1062	A
1	C2	1070	C
1	C2	1082	C
1	C2	1083	G
1	C2	1091	A
1	C2	1092	A
1	C2	1093	A
1	C2	1096	C
1	C2	1097	U
1	C2	1098	U
1	C2	1100	G
1	C2	1115	U
1	C2	1126	G
1	C2	1138	A

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Mol	Chain	Res	Type
1	C2	1146	G
1	C2	1148	C
1	C2	1149	G
1	C2	1150	G
1	C2	1151	A
1	C2	1154	G
1	C2	1626	U
1	C2	1630	U
1	C2	1636	C
1	C2	1637	C
1	C2	1638	G
1	C2	1639	C
1	C2	1640	C
1	C2	1641	C
1	C2	1648	A
1	C2	1649	G
1	C2	1651	A
1	C2	1652	C
1	C2	1653	C
1	C2	1654	G
1	C2	1655	A
1	C2	1656	U
1	C2	1658	G
1	C2	1659	A
1	C2	1664	C
1	C2	1680	G
1	C2	1683	C
1	C2	1685	G
1	C2	1687	U
1	C2	1688	U
1	C2	1689	A
1	C2	1693	A
1	C2	1701	A
1	C2	1703	C
1	C2	1707	A
1	C2	1712	A
1	C2	1713	G
1	C2	1714	A
1	C2	1717	G
1	C2	1730	A
1	C2	1736	G
1	C2	1738	U

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Mol	Chain	Res	Type
1	C2	1739	C
1	C2	1740	A
1	C2	1743	U
1	C2	1744	A
1	C2	1745	G
1	C2	1748	G
1	C2	1749	A
1	C2	1750	A
1	C2	1751	C
1	C2	1753	A
1	C2	1754	A
1	C2	1755	A
1	C2	1757	G
1	C2	1758	U
1	C2	1760	G
1	C2	1761	U
1	C2	1763	A
1	C2	1766	A
1	C2	1769	U
1	C2	1770	U
1	C2	1772	C
1	C2	1780	G
1	C2	1782	A
1	C2	1783	C
1	C2	1792	G
1	C2	1793	G
1	C2	1795	U
1	C2	1796	C

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C2	25	C
1	C2	103	A
1	C2	136	C
1	C2	139	C
1	C2	272	U
1	C2	417	A
1	C2	555	A
1	C2	755	A
1	C2	817	A
1	C2	997	G

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Mol	Chain	Res	Type
1	C2	1051	G
1	C2	1097	U
1	C2	1652	C

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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.

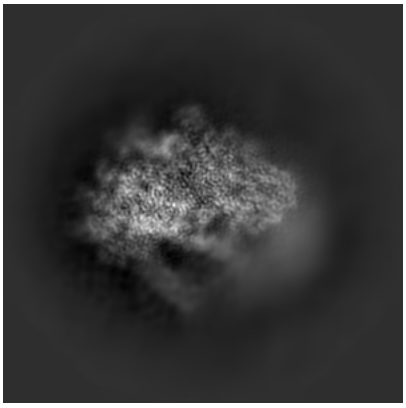
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32794. These allow visual inspection of the internal detail of the map and identification of artifacts.

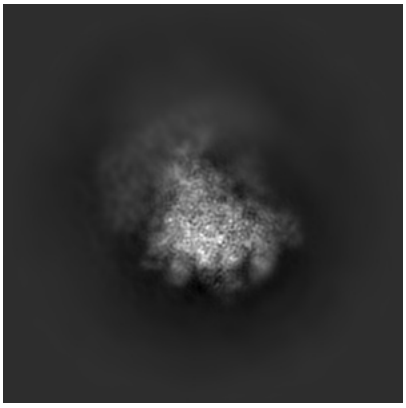
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

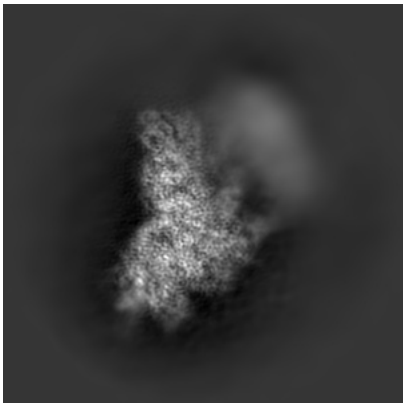
6.1.1 Primary map



X



Y

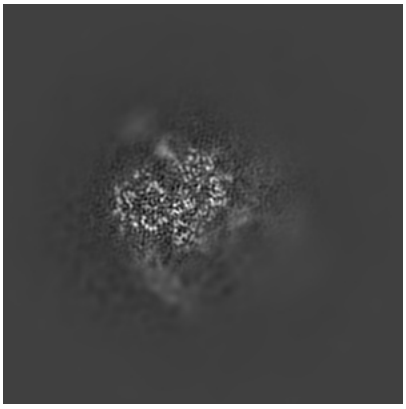


Z

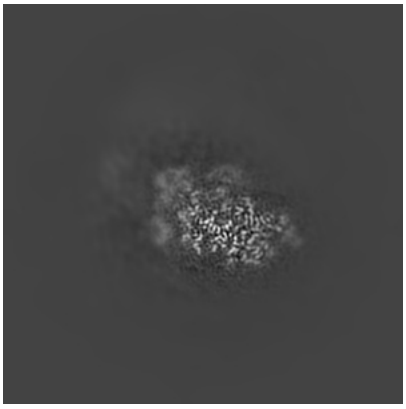
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

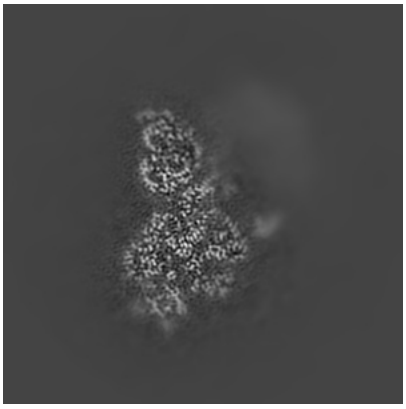
6.2.1 Primary map



X Index: 180



Y Index: 180

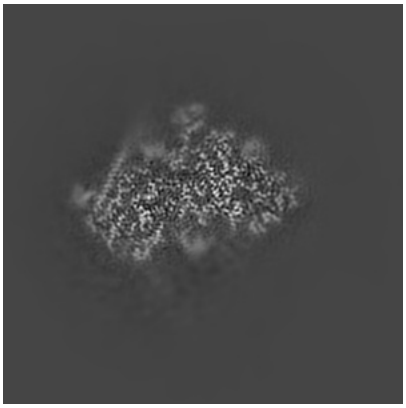


Z Index: 180

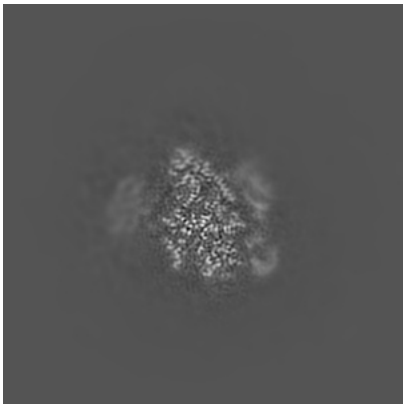
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

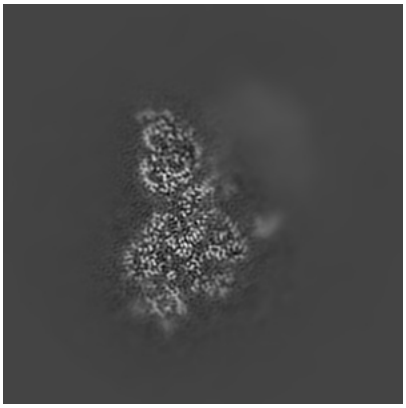
6.3.1 Primary map



X Index: 147



Y Index: 143

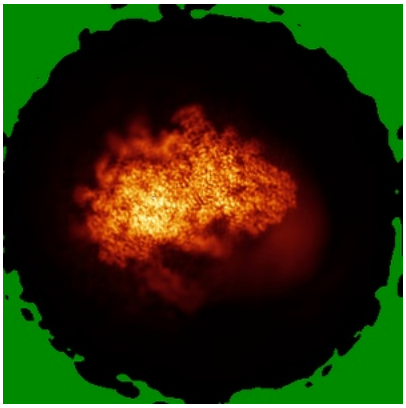


Z Index: 180

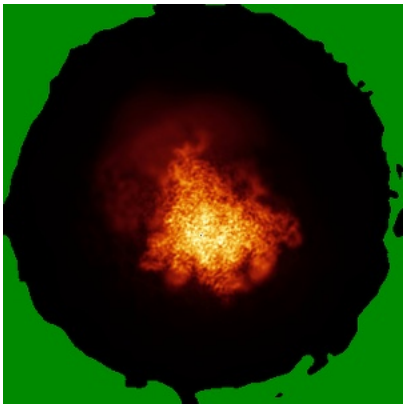
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

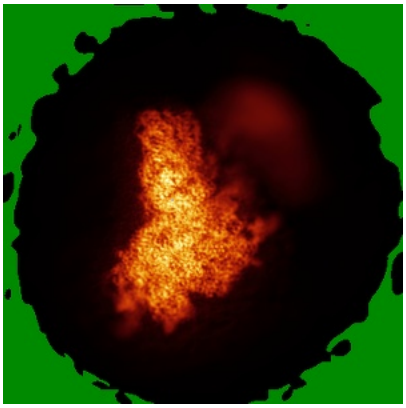
6.4.1 Primary map



X



Y



Z

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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

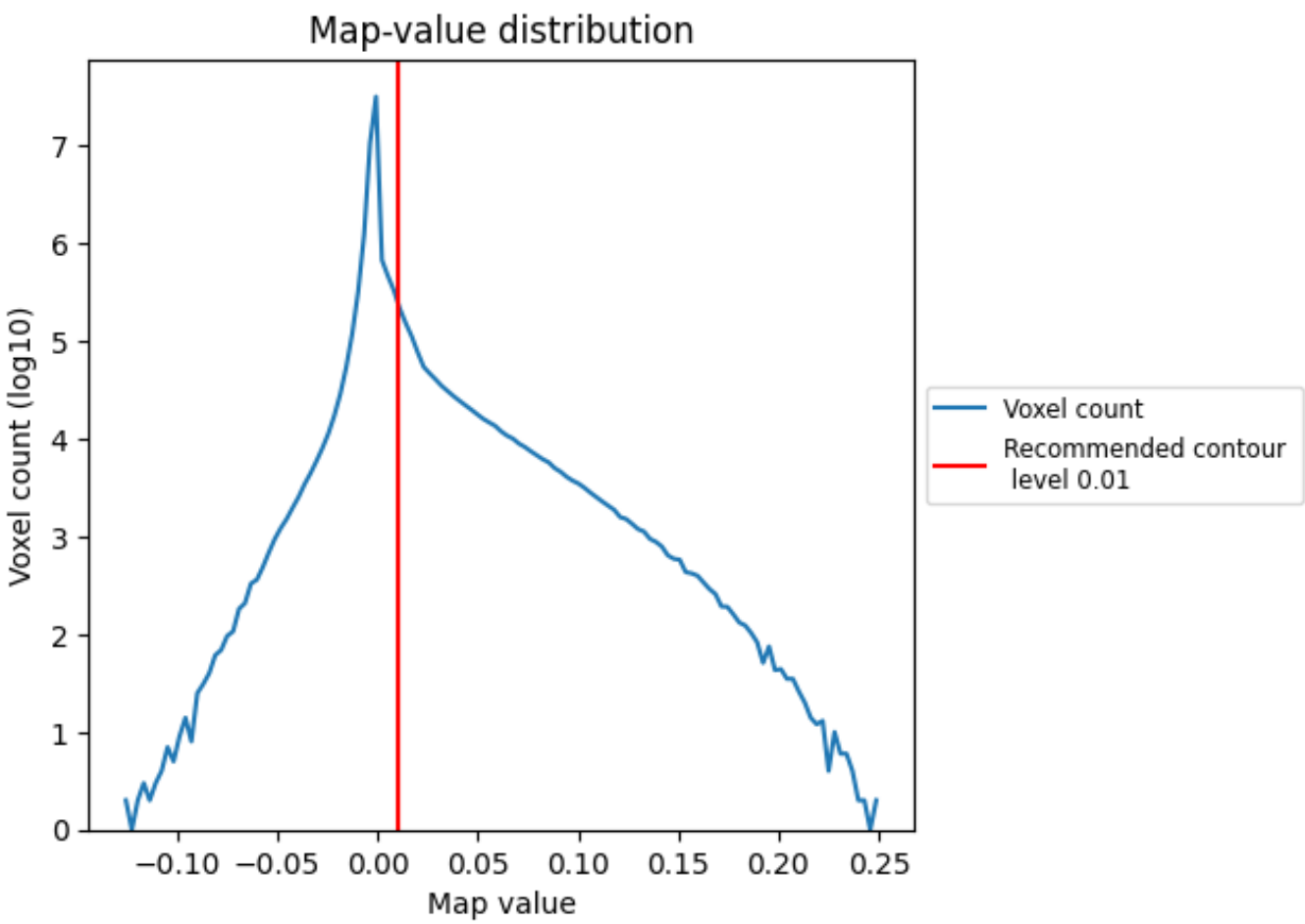
6.6 Mask visualisation (i)

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

7 Map analysis (i)

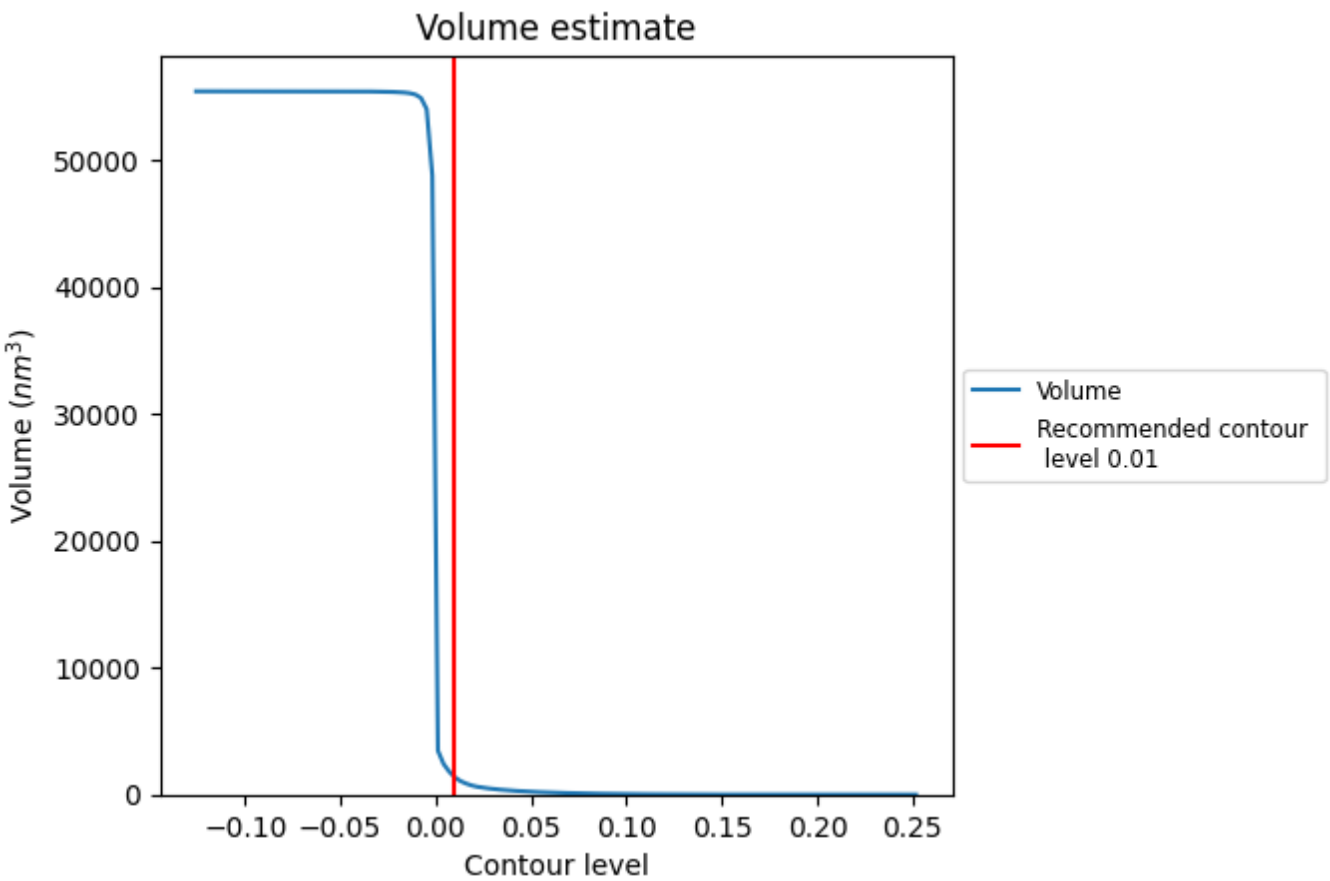
This section contains the results of statistical analysis of the map.

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.

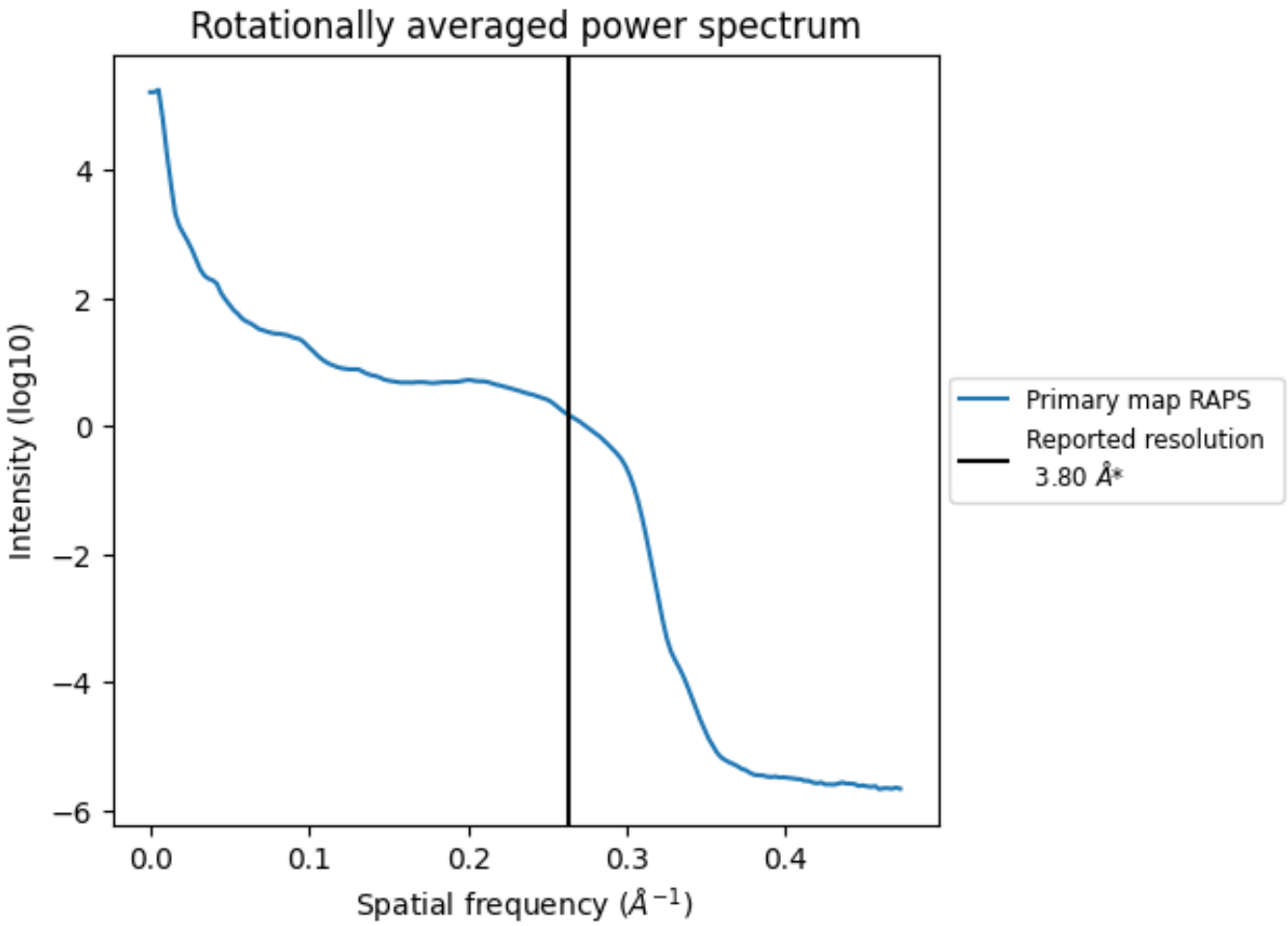
7.2 Volume estimate (i)



The volume at the recommended contour level is 1359 nm^3; this corresponds to an approximate mass of 1228 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 (i)

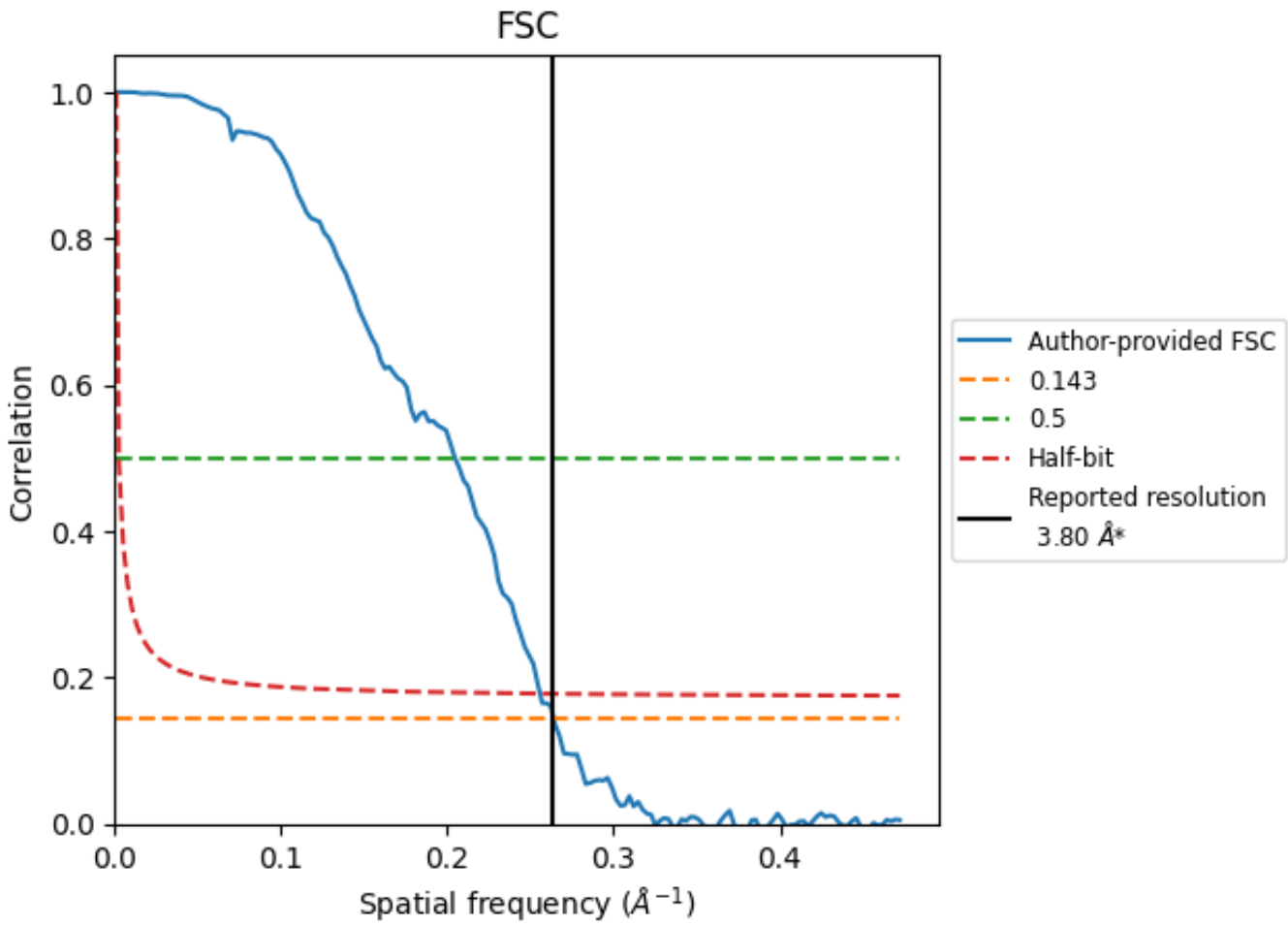


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



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

8.2 Resolution estimates (i)

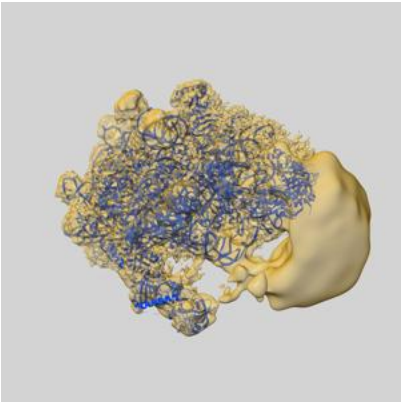
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.79	4.89	3.91
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

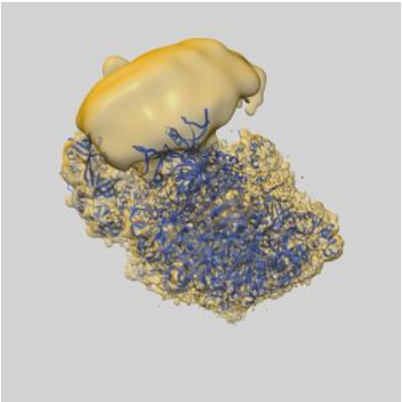
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32794 and PDB model 7WTP. Per-residue inclusion information can be found in section 3 on page 7.

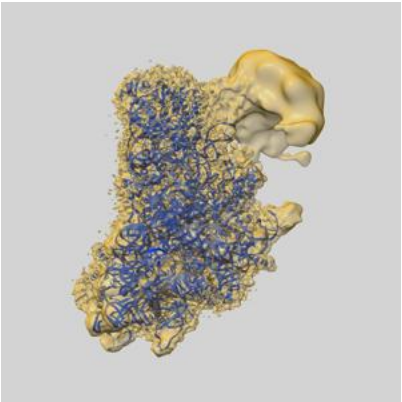
9.1 Map-model overlay (i)



X



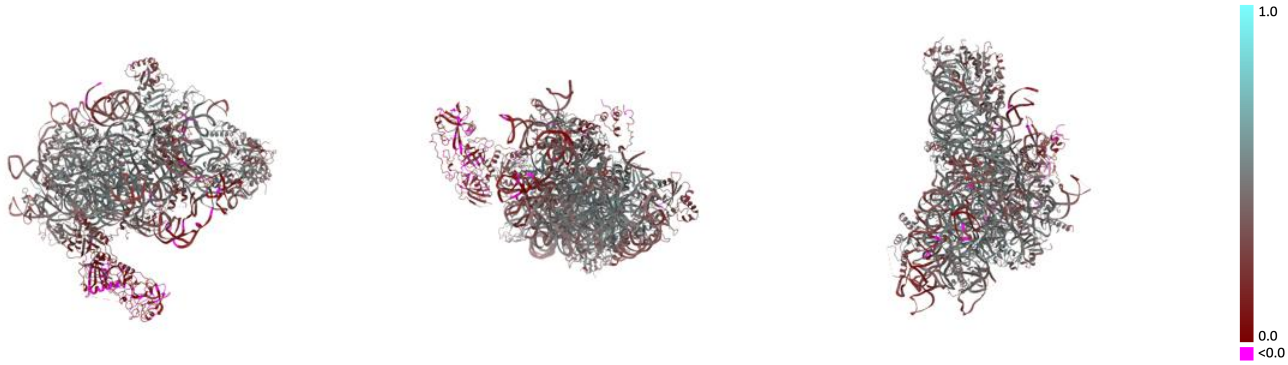
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

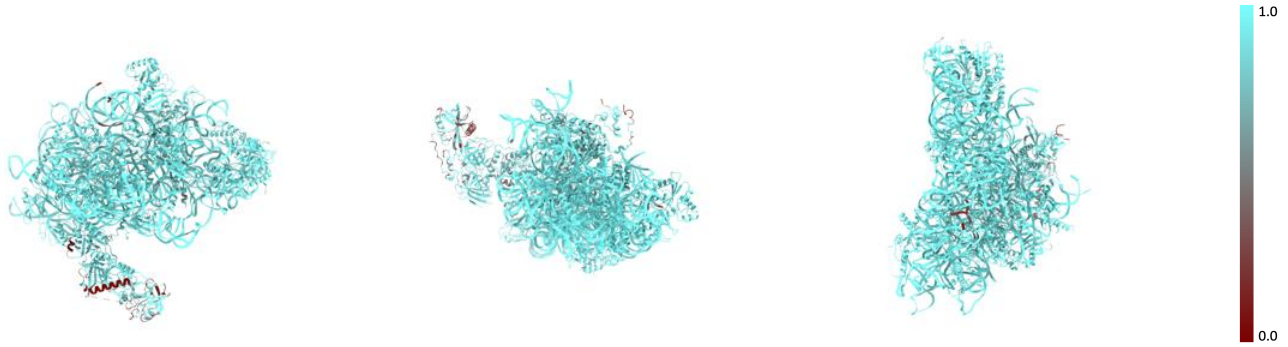
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

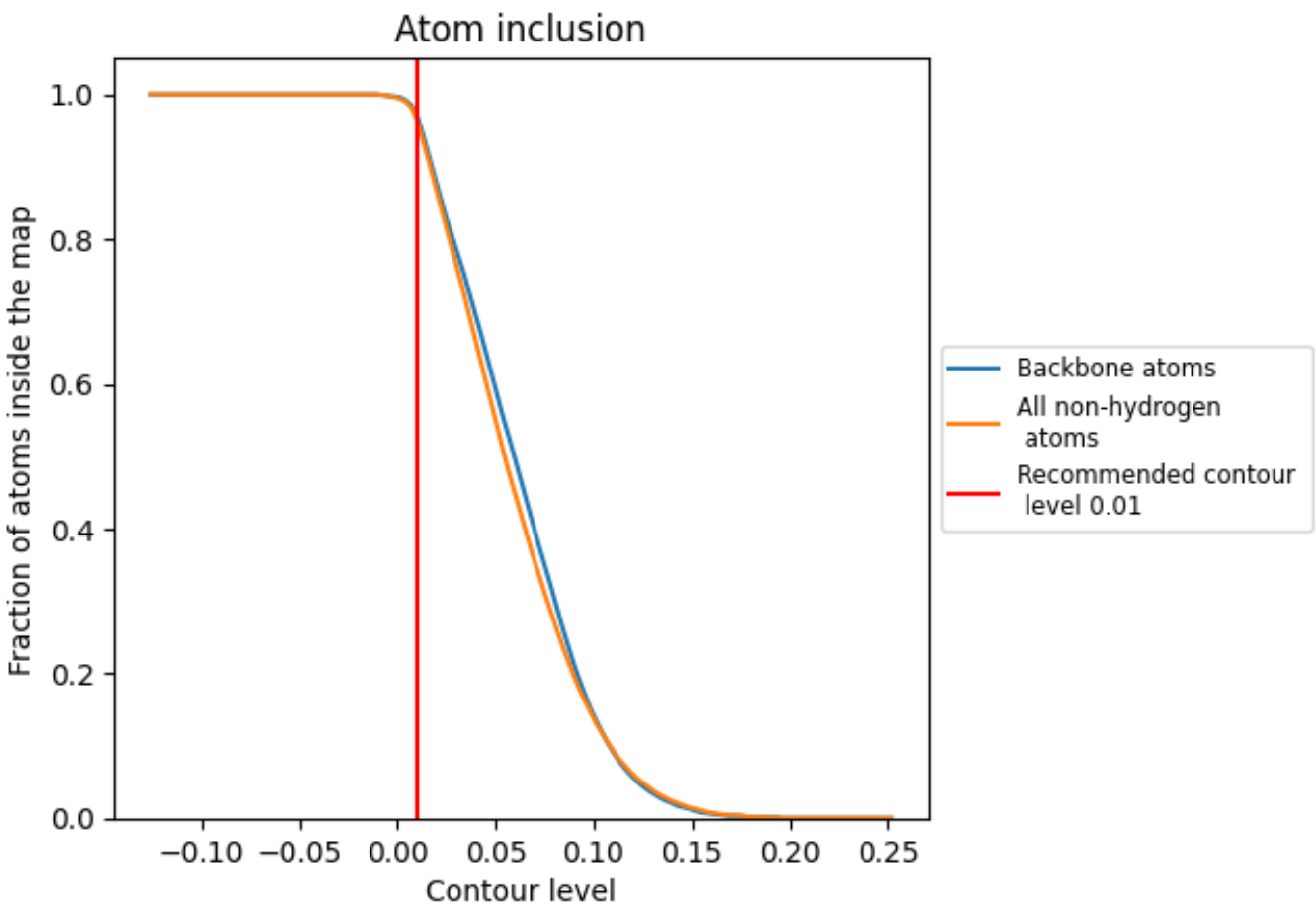
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9650	0.3990
C2	0.9900	0.4150
CA	0.9870	0.4050
CB	0.9060	0.3240
CC	0.7980	0.1620
SB	0.9810	0.4510
SC	0.8720	0.3060
SE	0.9910	0.4990
SG	0.9930	0.4150
SH	0.9830	0.3670
SI	0.9940	0.4770
SJ	0.9890	0.4600
SL	0.9880	0.5150
SN	0.9950	0.4820
SO	0.9790	0.4430
SW	0.9970	0.5100
SX	0.9740	0.4480
SY	0.9910	0.4530
Sb	0.9900	0.4600
Se	0.8360	0.3640