



wwPDB EM Validation Summary Report ⓘ

Apr 6, 2024 – 03:06 PM EDT

PDB ID : 8FVY
EMDB ID : EMD-29495
Title : 40S subunit of the Giardia lamblia 80S ribosome
Authors : Eiler, D.R.; Wimberly, B.T.; Bilodeau, D.Y.; Rissland, O.S.; Kieft, J.S.
Deposited on : 2023-01-20
Resolution : 2.94 Å(reported)

This is a wwPDB EM Validation Summary 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:

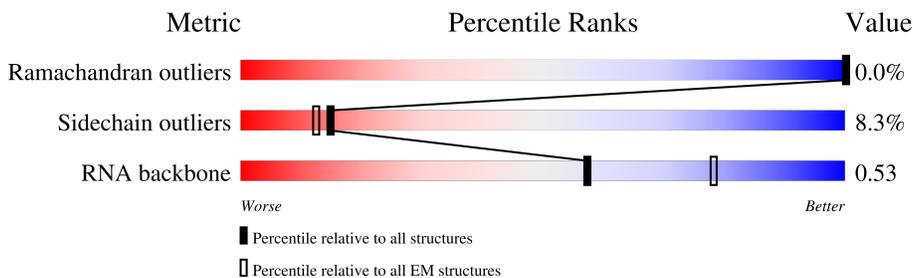
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.94 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 $\leq 5\%$. 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	2	1451	
2	A	245	
3	B	248	
4	C	242	
5	D	217	
6	E	268	
7	F	190	
8	G	248	

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Mol	Chain	Length	Quality of chain
9	H	201	75% 7% 18%
10	I	174	89% 7%
11	J	189	80% 6% 13%
12	K	134	72% 6% 22%
13	L	199	80% 6% 15%
14	N	154	94% 6%
15	O	145	88% 8%
16	P	145	69% 6% 26%
17	Q	158	92% 8%
18	R	137	55% 41%
19	S	154	86% 6% 7%
20	T	158	78% 9% 13%
21	U	126	75% 6% 18%
22	V	89	82% 9% 9%
23	W	130	94% 5%
24	X	143	93% 7%
25	Y	132	89% 8%
26	Z	88	69% 14% 17%
27	a	109	83% 5% 12%
28	b	124	51% 6% 44%
29	c	64	81% 12% 6%
30	d	137	61% 38%
31	f	137	22% 74%
32	g	74	76% 24%
33	M	125	12% 74% 8% 18%

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Mol	Chain	Length	Quality of chain
34	e	69	 <p>70% 6% 25%</p>

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 119930 atoms, of which 52077 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	H	N	O			P
1	2	1441	46630	13746	15711	5742	9991	1440	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	932	C	U	conflict	GB 2333213660

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	A	199	3230	1030	1632	279	281	8	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	B	224	3657	1144	1847	335	318	13	0	0

- Molecule 4 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	C	209	3267	1028	1651	292	292	4	0	0

- Molecule 5 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	D	209	3354	1044	1698	305	291	16	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	E	258	4212	1323	2144	378	354	13	0	0

- Molecule 7 is a protein called SSU ribosomal protein S7P (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	F	190	2958	914	1487	279	268	10	0	0

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	G	216	3532	1081	1814	328	298	11	0	0

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	H	165	2689	848	1367	227	241	6	0	0

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	I	167	2659	820	1349	251	236	3	0	0

- Molecule 11 is a protein called Ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	J	164	2733	834	1400	260	233	6	0	0

- Molecule 12 is a protein called Ribosomal protein S10B.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	K	105	1700	556	841	144	156	3	0	0

- Molecule 13 is a protein called SSU ribosomal protein S17P.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	L	170	2826	885	1427	275	232	7	0	0

- Molecule 14 is a protein called Ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	N	153	2532	780	1304	237	206	5	0	0

- Molecule 15 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	O	139	2113	645	1058	210	196	4	0	0

- Molecule 16 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	P	108	1825	564	942	172	139	8	0	0

- Molecule 17 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	Q	158	2537	768	1302	244	219	4	0	0

- Molecule 18 is a protein called Ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	R	81	1350	405	699	130	114	2	0	0

- Molecule 19 is a protein called Ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	S	143	2294	701	1156	228	202	7	0	0

- Molecule 20 is a protein called SSU ribosomal protein S19E (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	T	137	2163	683	1089	203	185	3	0	0

- Molecule 21 is a protein called Ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	U	103	1668	522	849	148	144	5	0	0

- Molecule 22 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	V	81	1214	377	607	112	112	6	0	0

- Molecule 23 is a protein called SSU ribosomal protein S8P (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	W	129	2104	659	1074	192	176	3	0	0

- Molecule 24 is a protein called SSU ribosomal protein S12P.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	X	143	2310	703	1195	223	185	4	0	0

- Molecule 25 is a protein called Ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	Y	122	1988	613	1019	181	168	7	0	0

- Molecule 26 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	Z	73	1183	366	605	104	102	6	0	0

- Molecule 27 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	a	96	Total	C	H	N	O	S	0	0
			1575	480	795	161	132	7		

- Molecule 28 is a protein called Ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace	
28	b	70	Total	C	H	N	O	S	0	0
			1078	349	532	92	101	4		

- Molecule 29 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace	
29	c	60	Total	C	H	N	O	S	0	0
			957	293	483	91	88	2		

- Molecule 30 is a protein called Ribosomal protein S29A.

Mol	Chain	Residues	Atoms					AltConf	Trace	
30	d	85	Total	C	H	N	O	S	0	0
			1336	425	654	129	121	7		

- Molecule 31 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
31	f	35	Total	C	H	N	O	S	0	0
			535	165	265	53	48	4		

- Molecule 32 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
32	g	74	Total	C	H	N	O	P	0	0
			2314	701	745	274	521	73		

- Molecule 33 is a protein called Ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace	
33	M	103	Total	C	H	N	O	S	0	0
			1679	532	843	148	148	8		

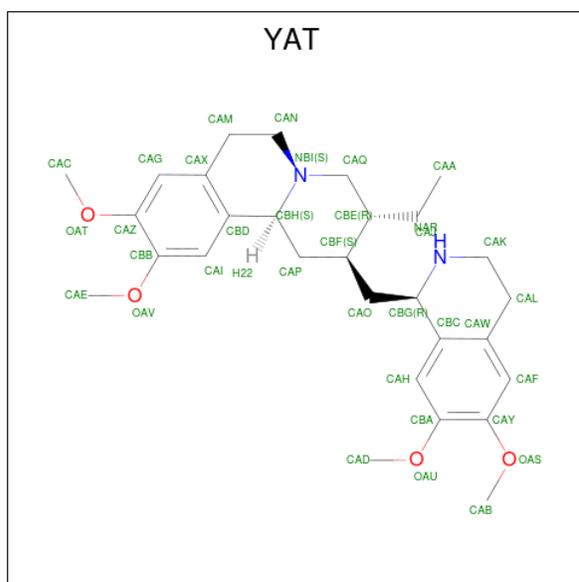
- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
34	e	52	886	269	453	93	71	0	0

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
35	2	23	23	23	0

- Molecule 36 is emetine (three-letter code: YAT) (formula: C₂₉H₄₀N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
36	2	1	75	29	40	2	4	0

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
37	a	1	1	1	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
38	2	591	591	591	0

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Mol	Chain	Residues	Atoms		AltConf
38	B	1	Total 1	O 1	0
38	C	6	Total 6	O 6	0
38	D	6	Total 6	O 6	0
38	E	10	Total 10	O 10	0
38	F	12	Total 12	O 12	0
38	G	2	Total 2	O 2	0
38	H	1	Total 1	O 1	0
38	I	10	Total 10	O 10	0
38	K	7	Total 7	O 7	0
38	L	4	Total 4	O 4	0
38	N	9	Total 9	O 9	0
38	O	3	Total 3	O 3	0
38	P	2	Total 2	O 2	0
38	Q	12	Total 12	O 12	0
38	R	2	Total 2	O 2	0
38	S	10	Total 10	O 10	0
38	T	10	Total 10	O 10	0
38	U	6	Total 6	O 6	0
38	W	4	Total 4	O 4	0
38	X	5	Total 5	O 5	0
38	Z	6	Total 6	O 6	0

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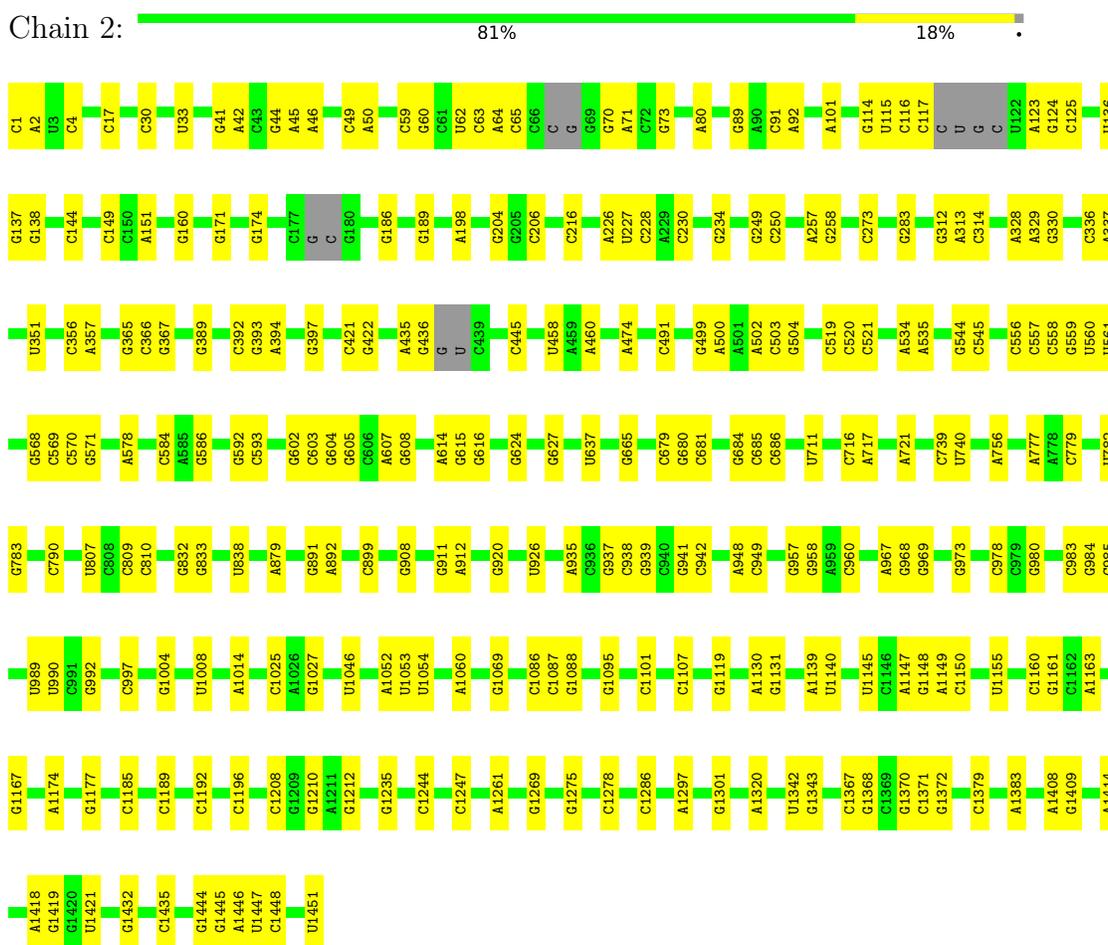
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Mol	Chain	Residues	Atoms		AltConf
38	a	6	Total 6	O 6	0
38	b	1	Total 1	O 1	0
38	d	6	Total 6	O 6	0
38	f	1	Total 1	O 1	0
38	g	2	Total 2	O 2	0
38	M	7	Total 7	O 7	0
38	e	1	Total 1	O 1	0

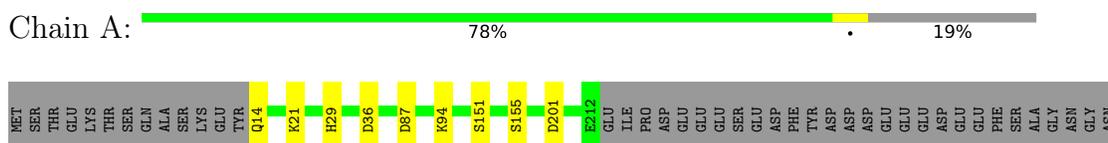
3 Residue-property plots [i](#)

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

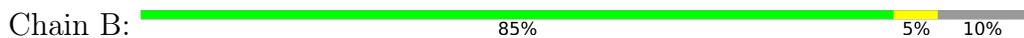


- Molecule 2: 40S ribosomal protein SA



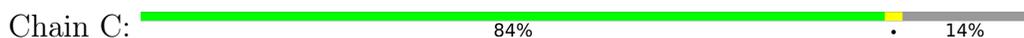
LEU
PHE
ASP
GLU
TYR

• Molecule 3: 40S ribosomal protein S3a



MET ALA ILE GLY SER ASN LYS THR PRO GLY LYS LYS LYS LYS ILE T14 E26 Y85 D93 M103 M125 E175 K178 K196 E199 Q202 K219 W223 T224 V237 ARG ASN LEU ALA GLY GLN SER ILE GLN

• Molecule 4: Ribosomal protein S2



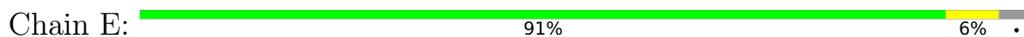
MET GLN ALA GLU SER ALA PRO ARG PRO ARG ARG ARG ARG ARG ARG ARG E25 K67 E73 V115 A116 M117 K124 D144 Q235 ASP ILE THR MET SER LEU ALA ASP

• Molecule 5: Ribosomal protein S3



MET PRO ARG I4 V5 R6 D20 E62 R71 R82 D95 R100 R130 E141 R152 K157 E176 K191 D206 A212 PHE SER ARG GLN LYS

• Molecule 6: 40S ribosomal protein S4



M1 R11 R39 T98 R108 L123 V126 L139 R148 D170 E171 S204 T220 C223 D231 K249 T258 ALA LYS ARG GLY GLY ALA TYR GLU

• Molecule 7: SSU ribosomal protein S7P (Fragment)



M1 S2 L3 K17 L23 R41 D126 K146 K172 S181 S188 R189 R190

• Molecule 8: 40S ribosomal protein S6

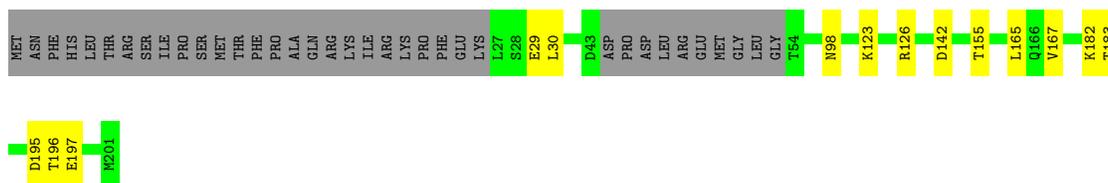


MET PRO LYS G4 K8 S12 V15 L22 W23 F27 E49 Y70 Q71 S76 Q77 L81 C89 R93 S102 V118 L119 V120 G123 LEU THR ASP VAL V134 R138 F151 GLY LEU PRO THR T156 E168 L169 I170 LYS GLU LEU GLY HIS

GLU VAL THR LEU LYS ASN GLY K184 K187 Y188 M214 L218 Q219 R230 K233 Y240 LYS PRO ALA LYS ARG THR VAL GLU

• Molecule 9: 40S ribosomal protein S7

Chain H:  75% 7% 18%



- Molecule 10: 40S ribosomal protein S8

Chain I:  89% 7%



- Molecule 11: Ribosomal protein S9

Chain J:  80% 6% 13%



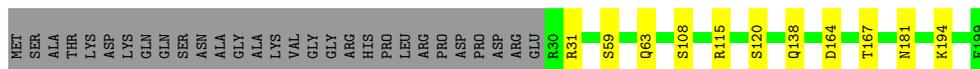
- Molecule 12: Ribosomal protein S10B

Chain K:  72% 6% 22%



- Molecule 13: SSU ribosomal protein S17P

Chain L:  80% 6% 15%



- Molecule 14: Ribosomal protein S13

Chain N:  94% 6%



- Molecule 15: Ribosomal protein S14

Chain O:  88% 8%





- Molecule 23: SSU ribosomal protein S8P (Fragment)

Chain W: 94% 5%



- Molecule 24: SSU ribosomal protein S12P

Chain X: 93% 7%



- Molecule 25: Ribosomal protein S24

Chain Y: 89% 8%



- Molecule 26: 40S ribosomal protein S25

Chain Z: 69% 14% 17%



- Molecule 27: 40S ribosomal protein S26

Chain a: 83% 5% 12%

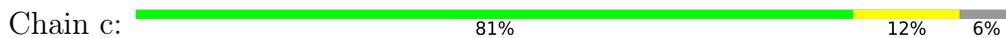


- Molecule 28: Ribosomal protein S27

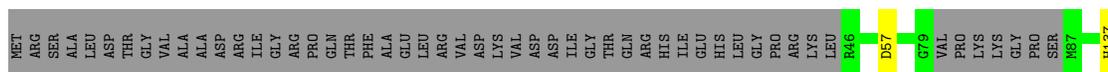
Chain b: 51% 6% 44%



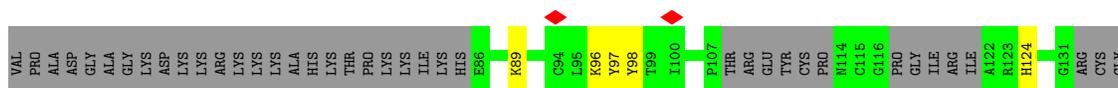
- Molecule 29: Ribosomal protein S28



• Molecule 30: Ribosomal protein S29A



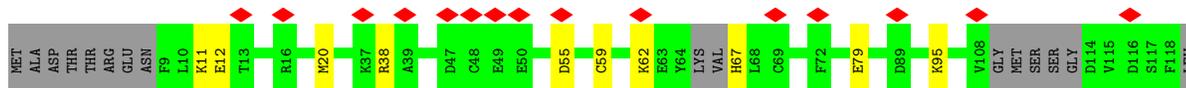
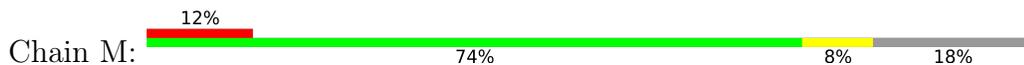
• Molecule 31: Ribosomal protein S27a



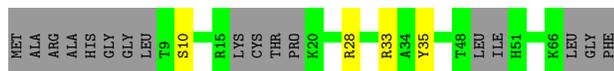
• Molecule 32: tRNA



• Molecule 33: Ribosomal protein S12



• Molecule 34: 40S ribosomal protein S30



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	289618	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	72.26	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.990	Depositor
Minimum map value	-1.460	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.152	Depositor
Recommended contour level	0.0895	Depositor
Map size (Å)	369.495, 369.495, 369.495	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8211, 0.8211, 0.8211	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: MG, YAT, 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	2	0.58	2/34573 (0.0%)	0.85	12/53952 (0.0%)
2	A	0.32	0/1633	0.52	0/2219
3	B	0.34	0/1845	0.57	0/2488
4	C	0.35	0/1649	0.52	0/2225
5	D	0.63	0/1682	0.63	0/2259
6	E	0.32	0/2114	0.56	0/2852
7	F	0.70	0/1494	0.61	0/2010
8	G	0.30	0/1739	0.58	0/2317
9	H	0.33	0/1345	0.53	0/1815
10	I	0.34	0/1330	0.58	0/1784
11	J	0.30	0/1351	0.57	0/1807
12	K	0.76	0/884	0.61	0/1204
13	L	0.39	0/1429	0.59	0/1912
14	N	0.36	0/1252	0.56	0/1681
15	O	0.35	0/1070	0.62	0/1436
16	P	0.61	0/898	0.64	0/1198
17	Q	0.67	0/1247	0.67	0/1666
18	R	0.54	0/657	0.65	0/877
19	S	0.61	0/1154	0.63	0/1549
20	T	0.75	0/1098	0.63	0/1476
21	U	0.65	0/835	0.62	0/1128
22	V	0.33	0/615	0.54	0/825
23	W	0.35	0/1047	0.56	0/1412
24	X	0.33	0/1130	0.61	0/1512
25	Y	0.30	0/983	0.53	0/1314
26	Z	0.68	0/584	0.69	0/779
27	a	0.39	0/792	0.58	0/1065
28	b	0.35	0/558	0.47	0/757
29	c	0.61	0/477	0.68	0/638
30	d	0.55	0/696	0.64	0/932
31	f	0.36	0/273	0.62	0/362
32	g	0.27	0/1751	0.76	0/2727

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	M	0.45	0/848	0.63	0/1132
34	e	0.30	0/438	0.61	0/578
All	All	0.52	2/71471 (0.0%)	0.74	12/103888 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
17	Q	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	189	G	N3-C4	5.77	1.39	1.35
1	2	189	G	C5-C4	5.55	1.42	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	189	G	C6-N1-C2	18.29	136.07	125.10
1	2	189	G	N1-C2-N3	-12.29	116.53	123.90
1	2	189	G	C5-C6-N1	-11.83	105.58	111.50
1	2	30	C	O5'-P-OP1	-9.75	96.93	105.70
1	2	189	G	C2-N3-C4	7.65	115.72	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	Q	57	VAL	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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	197/245 (80%)	192 (98%)	5 (2%)	0	100	100
3	B	222/248 (90%)	216 (97%)	6 (3%)	0	100	100
4	C	207/242 (86%)	202 (98%)	5 (2%)	0	100	100
5	D	207/217 (95%)	190 (92%)	17 (8%)	0	100	100
6	E	256/268 (96%)	246 (96%)	10 (4%)	0	100	100
7	F	188/190 (99%)	173 (92%)	15 (8%)	0	100	100
8	G	208/248 (84%)	198 (95%)	10 (5%)	0	100	100
9	H	161/201 (80%)	155 (96%)	6 (4%)	0	100	100
10	I	163/174 (94%)	159 (98%)	4 (2%)	0	100	100
11	J	162/189 (86%)	158 (98%)	4 (2%)	0	100	100
12	K	103/134 (77%)	93 (90%)	9 (9%)	1 (1%)	15	43
13	L	168/199 (84%)	163 (97%)	5 (3%)	0	100	100
14	N	151/154 (98%)	149 (99%)	2 (1%)	0	100	100
15	O	137/145 (94%)	134 (98%)	3 (2%)	0	100	100
16	P	104/145 (72%)	99 (95%)	5 (5%)	0	100	100
17	Q	156/158 (99%)	142 (91%)	14 (9%)	0	100	100
18	R	79/137 (58%)	78 (99%)	1 (1%)	0	100	100
19	S	141/154 (92%)	122 (86%)	19 (14%)	0	100	100
20	T	135/158 (85%)	127 (94%)	8 (6%)	0	100	100
21	U	101/126 (80%)	94 (93%)	7 (7%)	0	100	100
22	V	79/89 (89%)	78 (99%)	1 (1%)	0	100	100
23	W	127/130 (98%)	115 (91%)	12 (9%)	0	100	100
24	X	141/143 (99%)	133 (94%)	8 (6%)	0	100	100
25	Y	118/132 (89%)	110 (93%)	8 (7%)	0	100	100
26	Z	71/88 (81%)	63 (89%)	8 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	a	94/109 (86%)	93 (99%)	1 (1%)	0	100	100
28	b	66/124 (53%)	63 (96%)	3 (4%)	0	100	100
29	c	58/64 (91%)	53 (91%)	5 (9%)	0	100	100
30	d	81/137 (59%)	66 (82%)	15 (18%)	0	100	100
31	f	29/137 (21%)	21 (72%)	7 (24%)	1 (3%)	3	13
33	M	97/125 (78%)	81 (84%)	16 (16%)	0	100	100
34	e	46/69 (67%)	45 (98%)	1 (2%)	0	100	100
All	All	4253/5079 (84%)	4011 (94%)	240 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	K	71	ALA
31	f	124	HIS

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	A	175/217 (81%)	166 (95%)	9 (5%)	24	53
3	B	202/220 (92%)	189 (94%)	13 (6%)	17	43
4	C	173/201 (86%)	167 (96%)	6 (4%)	36	67
5	D	174/182 (96%)	160 (92%)	14 (8%)	12	32
6	E	227/232 (98%)	212 (93%)	15 (7%)	16	42
7	F	156/157 (99%)	146 (94%)	10 (6%)	17	43
8	G	185/213 (87%)	158 (85%)	27 (15%)	3	9
9	H	148/181 (82%)	134 (90%)	14 (10%)	8	24
10	I	141/148 (95%)	129 (92%)	12 (8%)	10	29
11	J	146/164 (89%)	134 (92%)	12 (8%)	11	31
12	K	94/119 (79%)	87 (93%)	7 (7%)	13	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	L	146/171 (85%)	135 (92%)	11 (8%)	13	35
14	N	129/130 (99%)	120 (93%)	9 (7%)	15	39
15	O	107/113 (95%)	96 (90%)	11 (10%)	7	21
16	P	97/128 (76%)	89 (92%)	8 (8%)	11	31
17	Q	130/130 (100%)	118 (91%)	12 (9%)	9	26
18	R	72/123 (58%)	67 (93%)	5 (7%)	15	40
19	S	122/131 (93%)	112 (92%)	10 (8%)	11	31
20	T	113/133 (85%)	99 (88%)	14 (12%)	4	13
21	U	92/110 (84%)	84 (91%)	8 (9%)	10	29
22	V	64/72 (89%)	56 (88%)	8 (12%)	4	13
23	W	114/115 (99%)	107 (94%)	7 (6%)	18	45
24	X	114/114 (100%)	104 (91%)	10 (9%)	10	28
25	Y	106/113 (94%)	101 (95%)	5 (5%)	26	57
26	Z	65/79 (82%)	53 (82%)	12 (18%)	1	4
27	a	90/103 (87%)	85 (94%)	5 (6%)	21	50
28	b	64/112 (57%)	57 (89%)	7 (11%)	6	18
29	c	53/57 (93%)	45 (85%)	8 (15%)	3	8
30	d	73/116 (63%)	71 (97%)	2 (3%)	44	74
31	f	28/112 (25%)	24 (86%)	4 (14%)	3	9
33	M	93/112 (83%)	83 (89%)	10 (11%)	6	19
34	e	46/58 (79%)	42 (91%)	4 (9%)	10	29
All	All	3739/4366 (86%)	3430 (92%)	309 (8%)	15	30

5 of 309 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	V	69	ARG
29	c	30	MET
23	W	57	ARG
26	Z	29	GLU
33	M	59	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
33	M	105	HIS
33	M	67	HIS
19	S	128	HIS
14	N	62	GLN
24	X	97	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1437/1451 (99%)	249 (17%)	12 (0%)
32	g	73/74 (98%)	18 (24%)	0
All	All	1510/1525 (99%)	267 (17%)	12 (0%)

5 of 267 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	33	U
1	2	41	G

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	558	C
1	2	604	G
1	2	989	U
1	2	679	C
1	2	312	G

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

Of 25 ligands modelled in this entry, 24 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	YAT	2	1524	-	39,39,39	3.07	18 (46%)	51,56,56	2.52	17 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	YAT	2	1524	-	-	8/14/49/49	0/5/5/5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	2	1524	YAT	CAN-CAM	-10.32	1.31	1.51
36	2	1524	YAT	CAN-NBI	9.72	1.66	1.47
36	2	1524	YAT	CAQ-NBI	4.17	1.54	1.47
36	2	1524	YAT	OAT-CAZ	4.02	1.43	1.37
36	2	1524	YAT	CBC-CBG	3.88	1.55	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	2	1524	YAT	CAN-NBI-CAQ	11.96	132.61	110.29
36	2	1524	YAT	CAQ-CBE-CBF	4.54	117.15	108.17
36	2	1524	YAT	CAP-CBH-CBD	-4.35	106.88	113.07
36	2	1524	YAT	CBE-CAQ-NBI	3.83	117.25	112.23
36	2	1524	YAT	CAL-CAK-NAR	3.38	113.73	109.04

There are no chirality outliers.

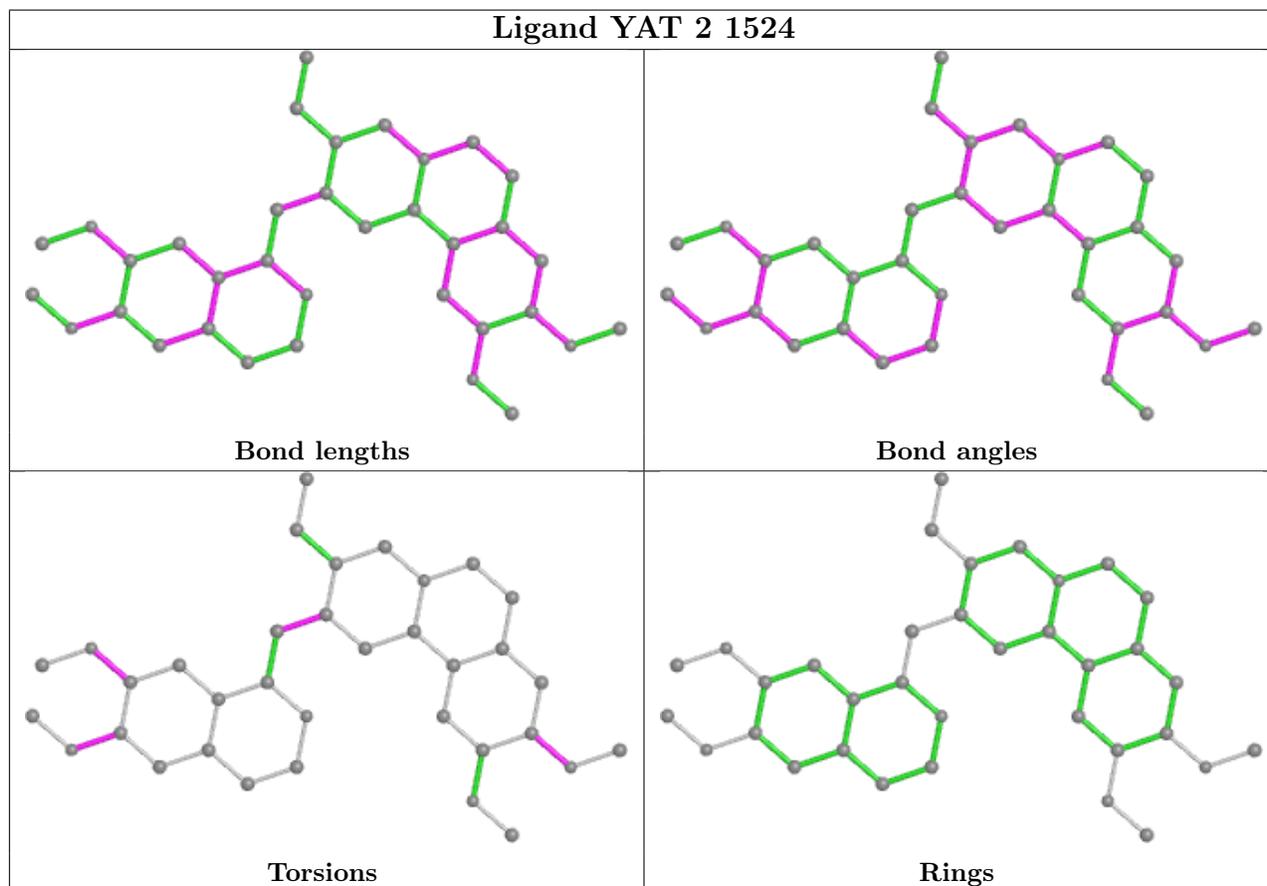
5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	2	1524	YAT	CAY-CBA-OAU-CAD
36	2	1524	YAT	CAG-CAZ-OAT-CAC
36	2	1524	YAT	CAF-CAY-OAS-CAB
36	2	1524	YAT	CAH-CBA-OAU-CAD
36	2	1524	YAT	CBB-CAZ-OAT-CAC

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

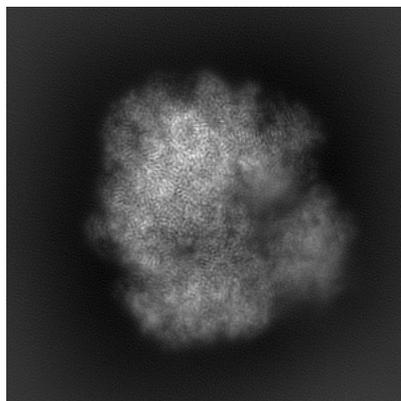
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29495. These allow visual inspection of the internal detail of the map and identification of artifacts.

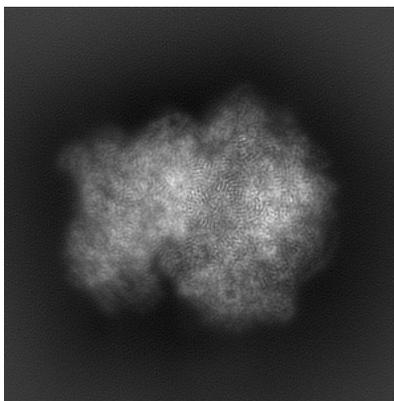
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

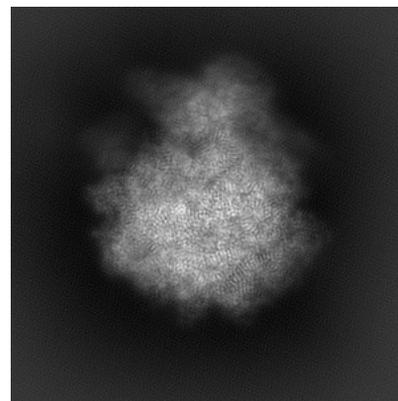
6.1.1 Primary map



X

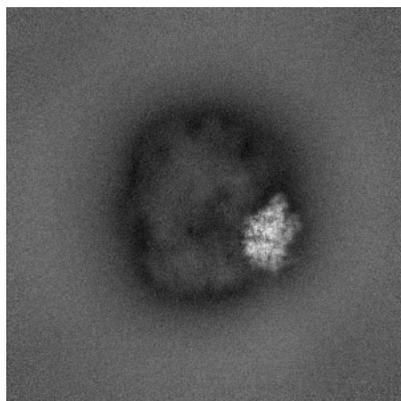


Y

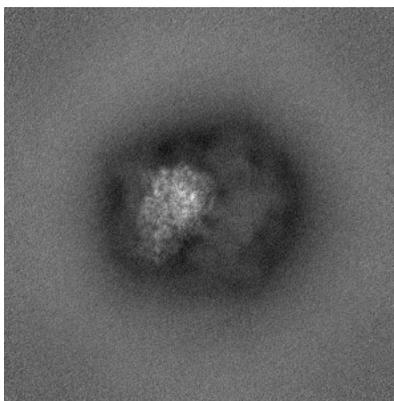


Z

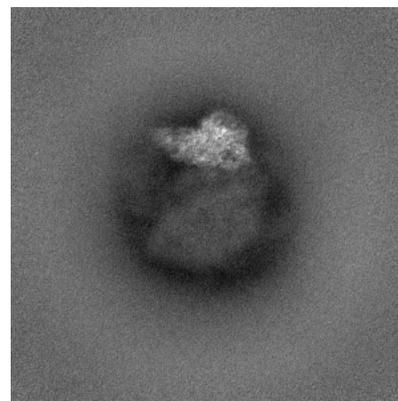
6.1.2 Raw map



X



Y

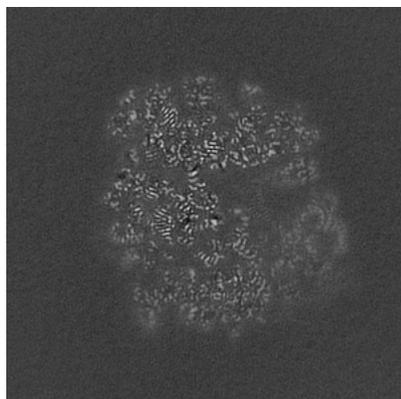


Z

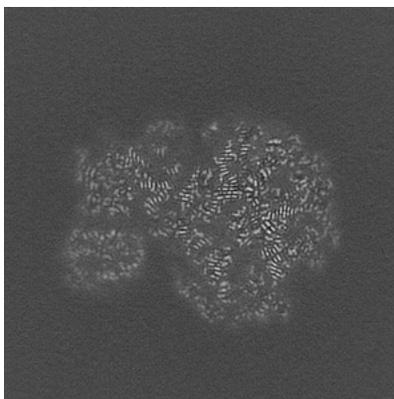
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

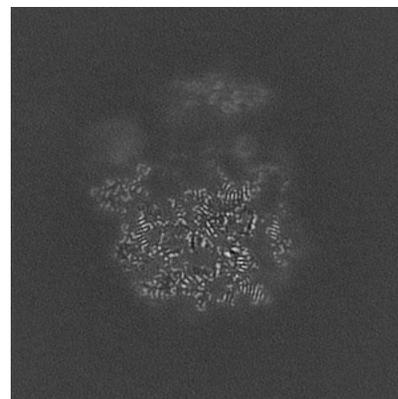
6.2.1 Primary map



X Index: 225

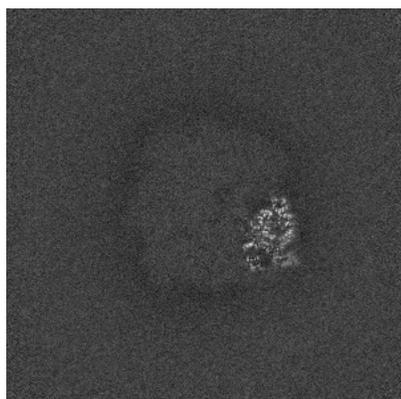


Y Index: 225

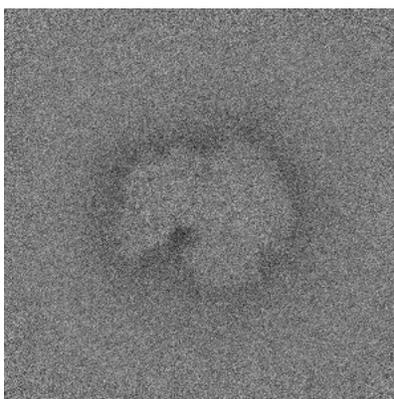


Z Index: 225

6.2.2 Raw map



X Index: 351



Y Index: 351

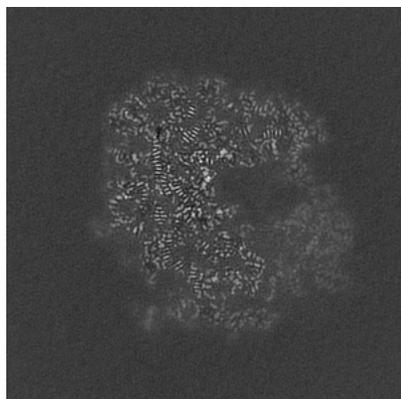


Z Index: 351

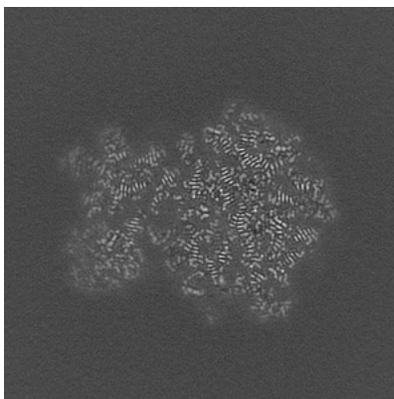
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

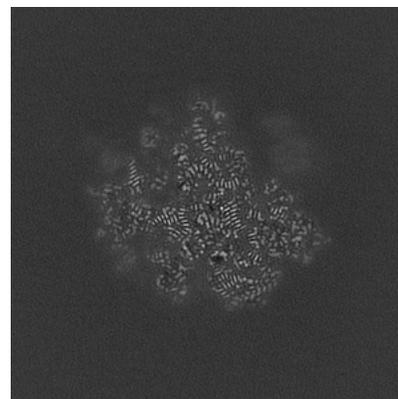
6.3.1 Primary map



X Index: 239

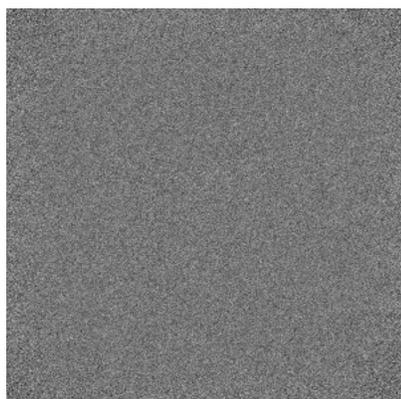


Y Index: 217

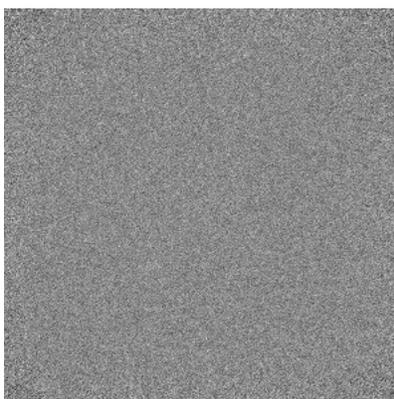


Z Index: 280

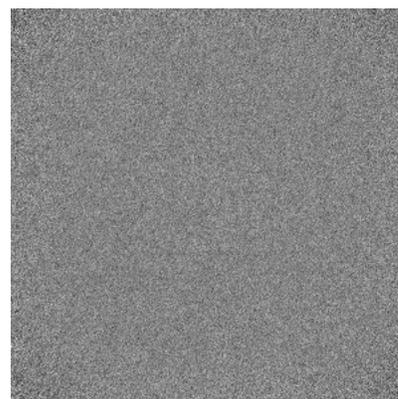
6.3.2 Raw map



X Index: 0



Y Index: 0

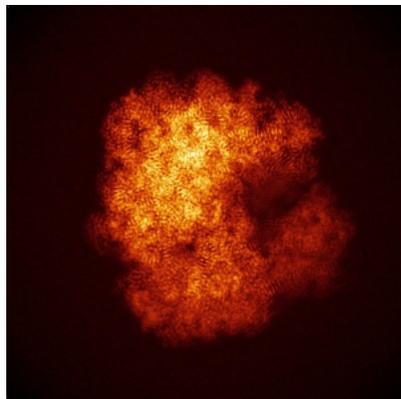


Z Index: 0

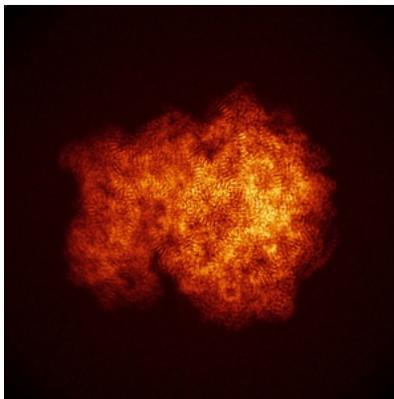
The images above show the largest variance slices of the map in three orthogonal directions.

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

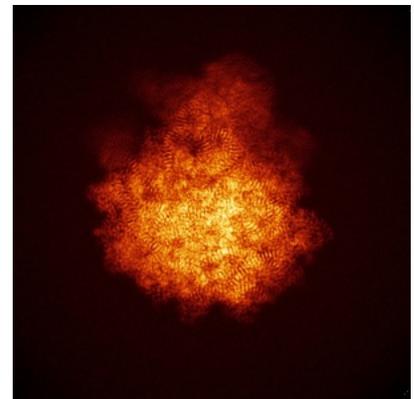
6.4.1 Primary map



X

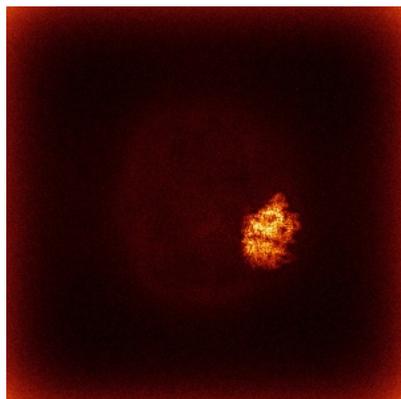


Y

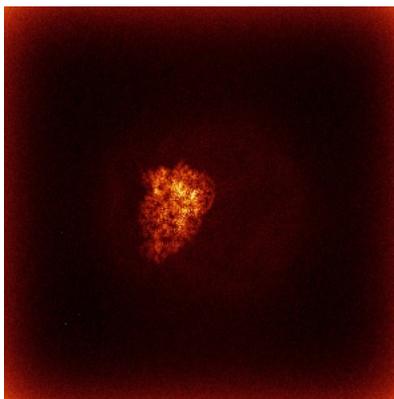


Z

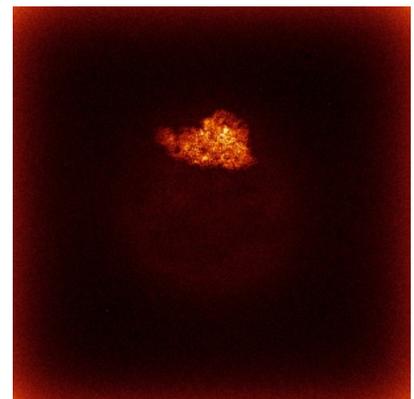
6.4.2 Raw map



X



Y

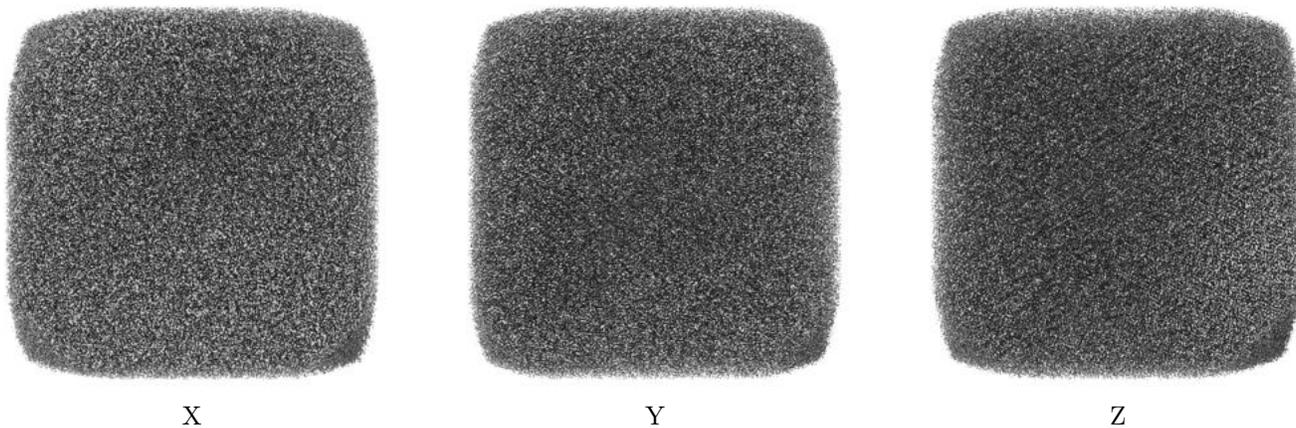


Z

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.

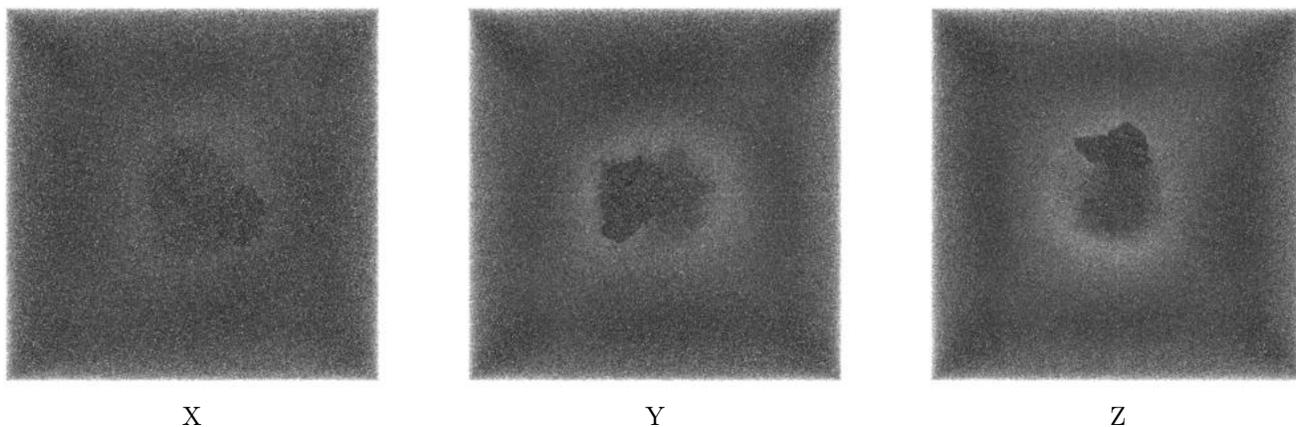
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0895. 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.

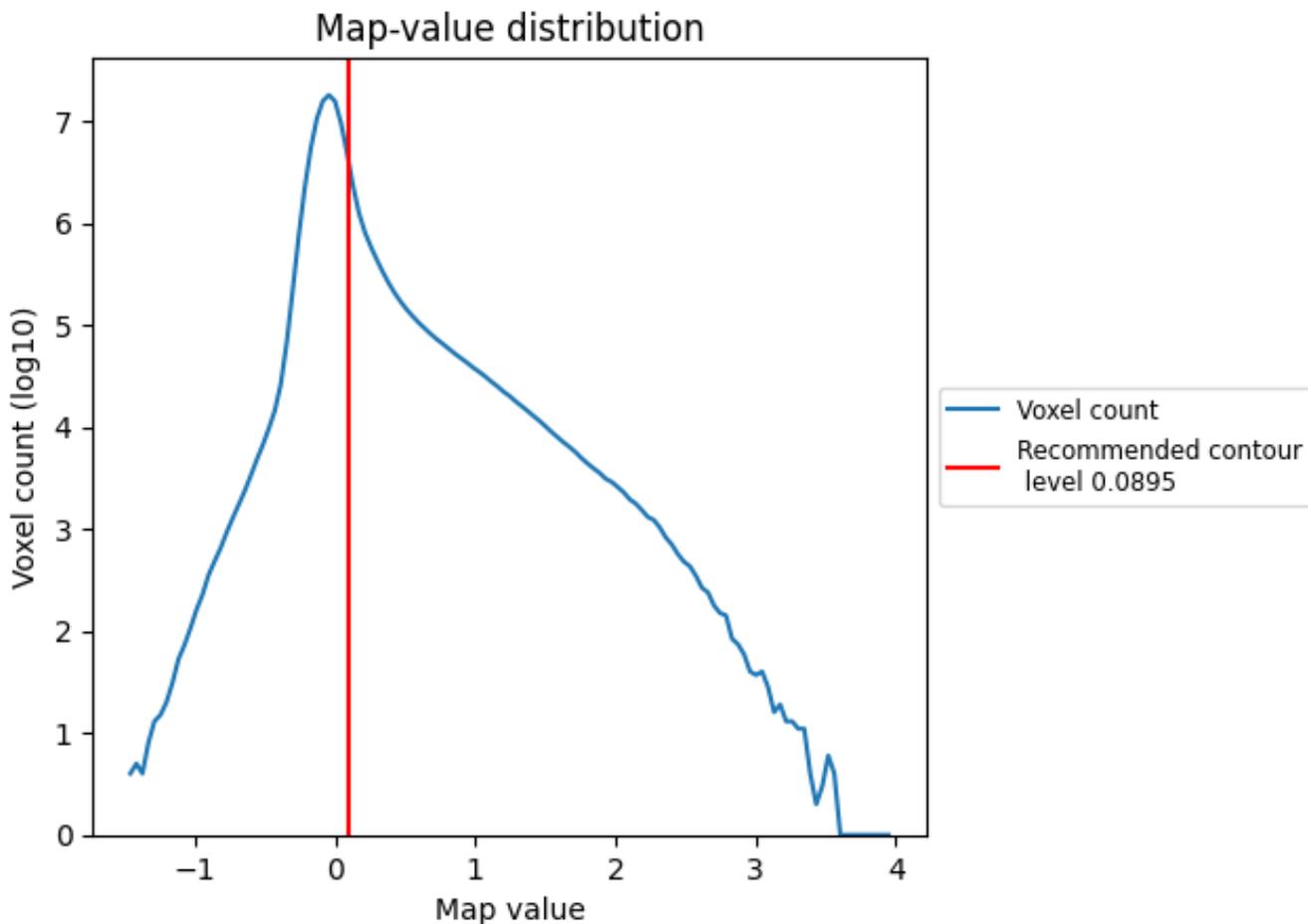
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

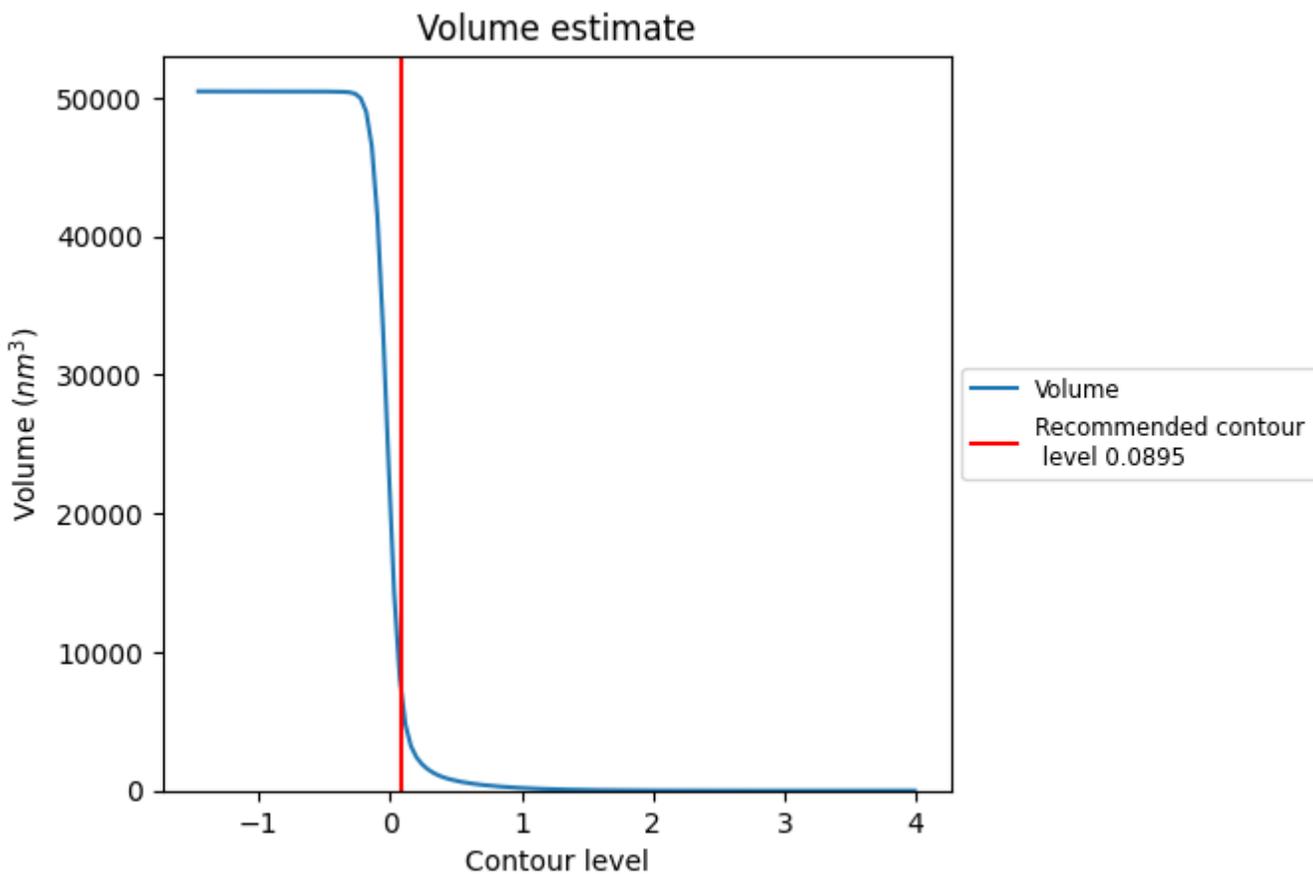
This section contains the results of statistical analysis of the map.

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.

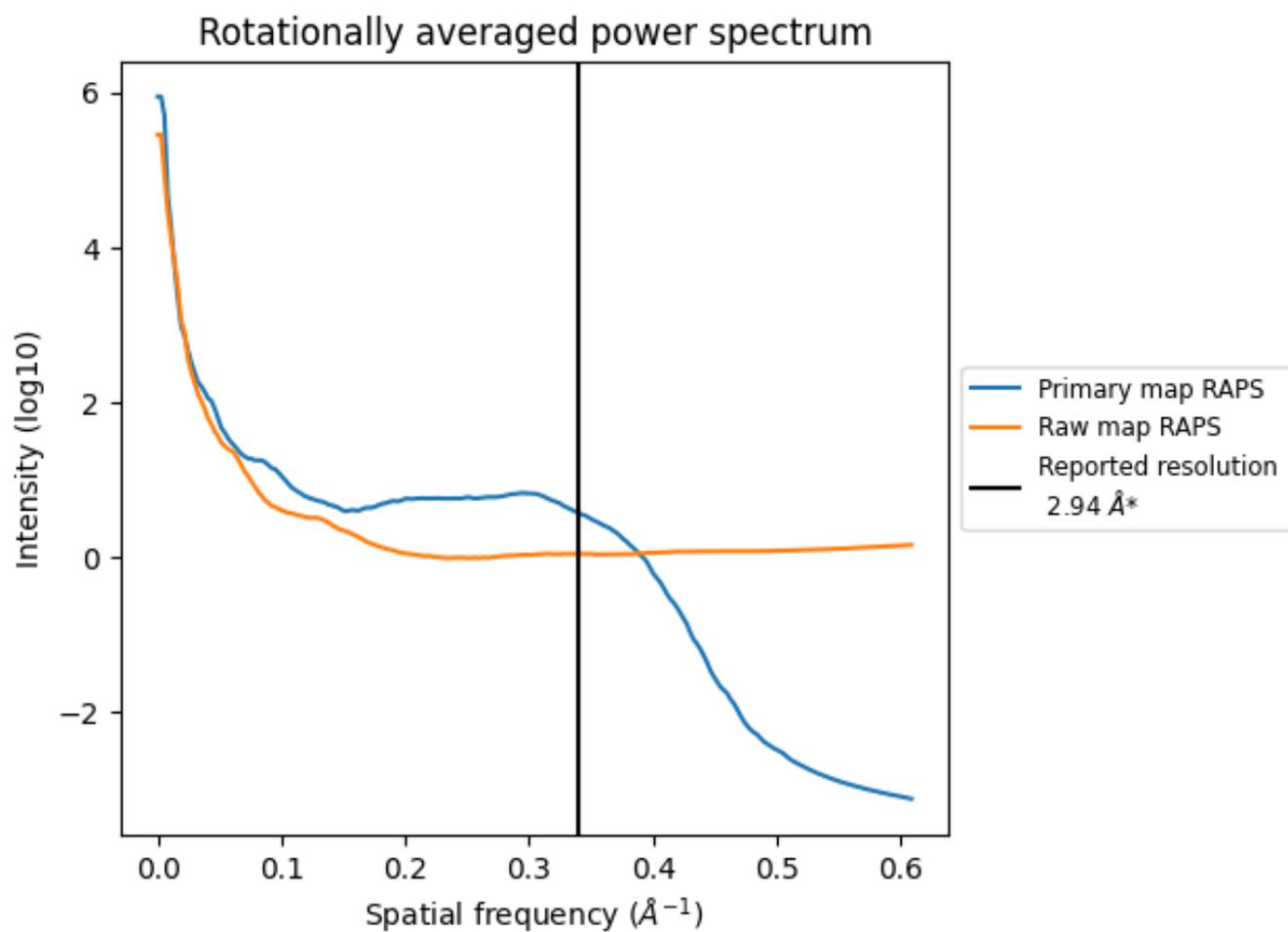
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 6823 nm³; this corresponds to an approximate mass of 6164 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](#)

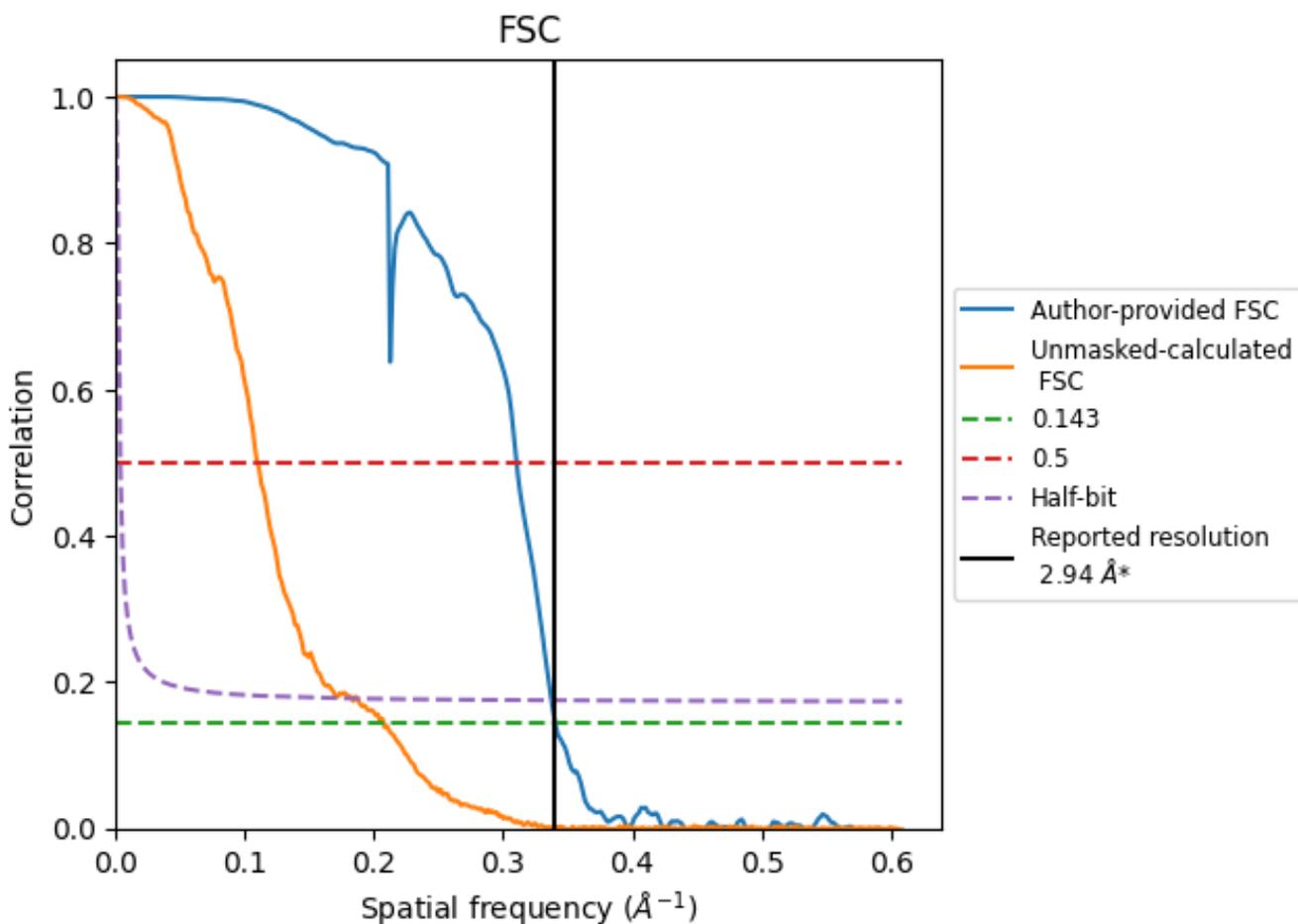


*Reported resolution corresponds to spatial frequency of 0.340 Å⁻¹

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 0.340 Å⁻¹

8.2 Resolution estimates [i](#)

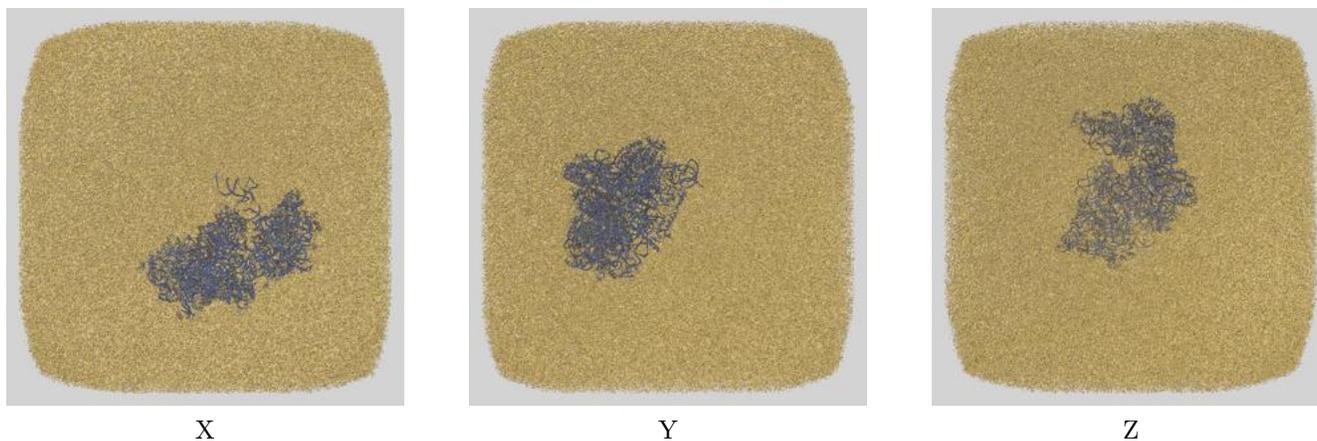
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.94	3.22	2.96
Unmasked-calculated*	4.82	9.13	5.47

*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 4.82 differs from the reported value 2.94 by more than 10 %

9 Map-model fit [i](#)

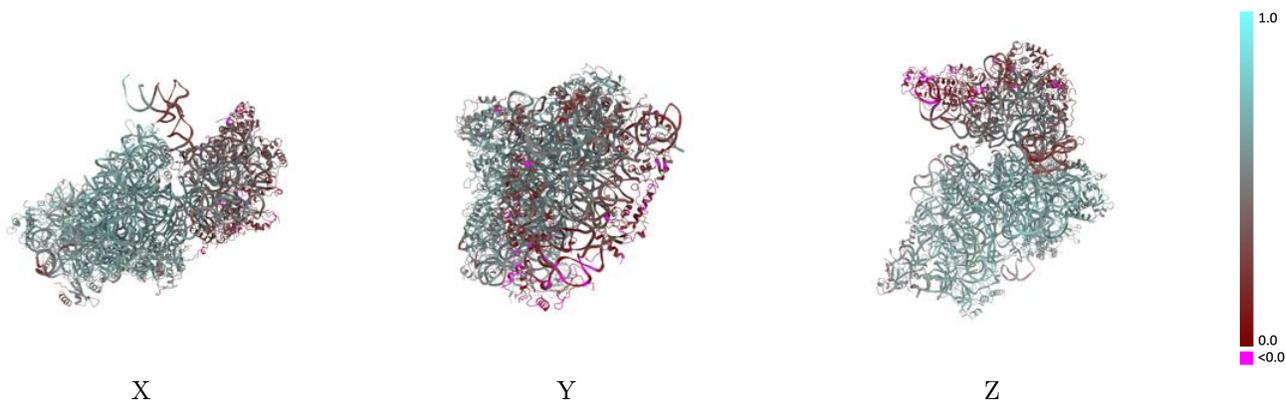
This section contains information regarding the fit between EMDB map EMD-29495 and PDB model 8FVY. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



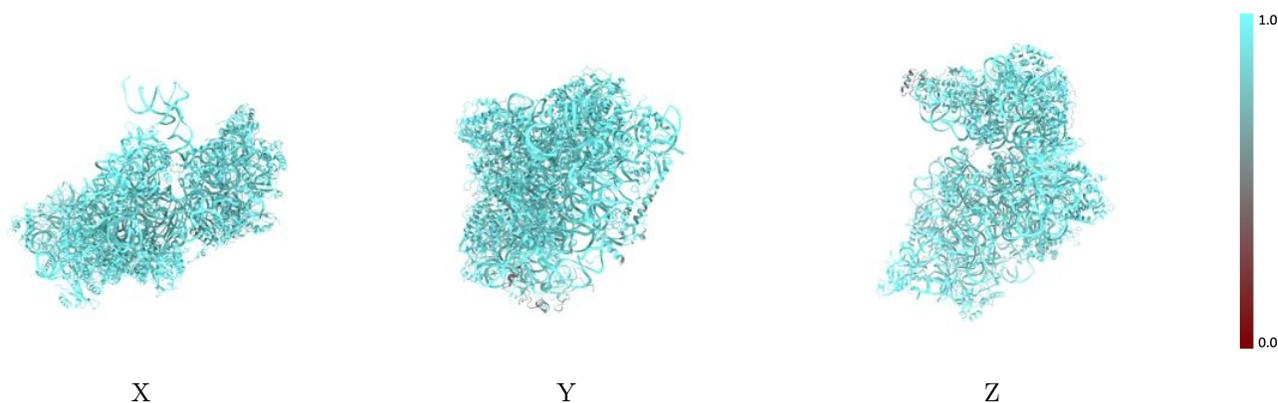
The images above show the 3D surface view of the map at the recommended contour level 0.0895 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



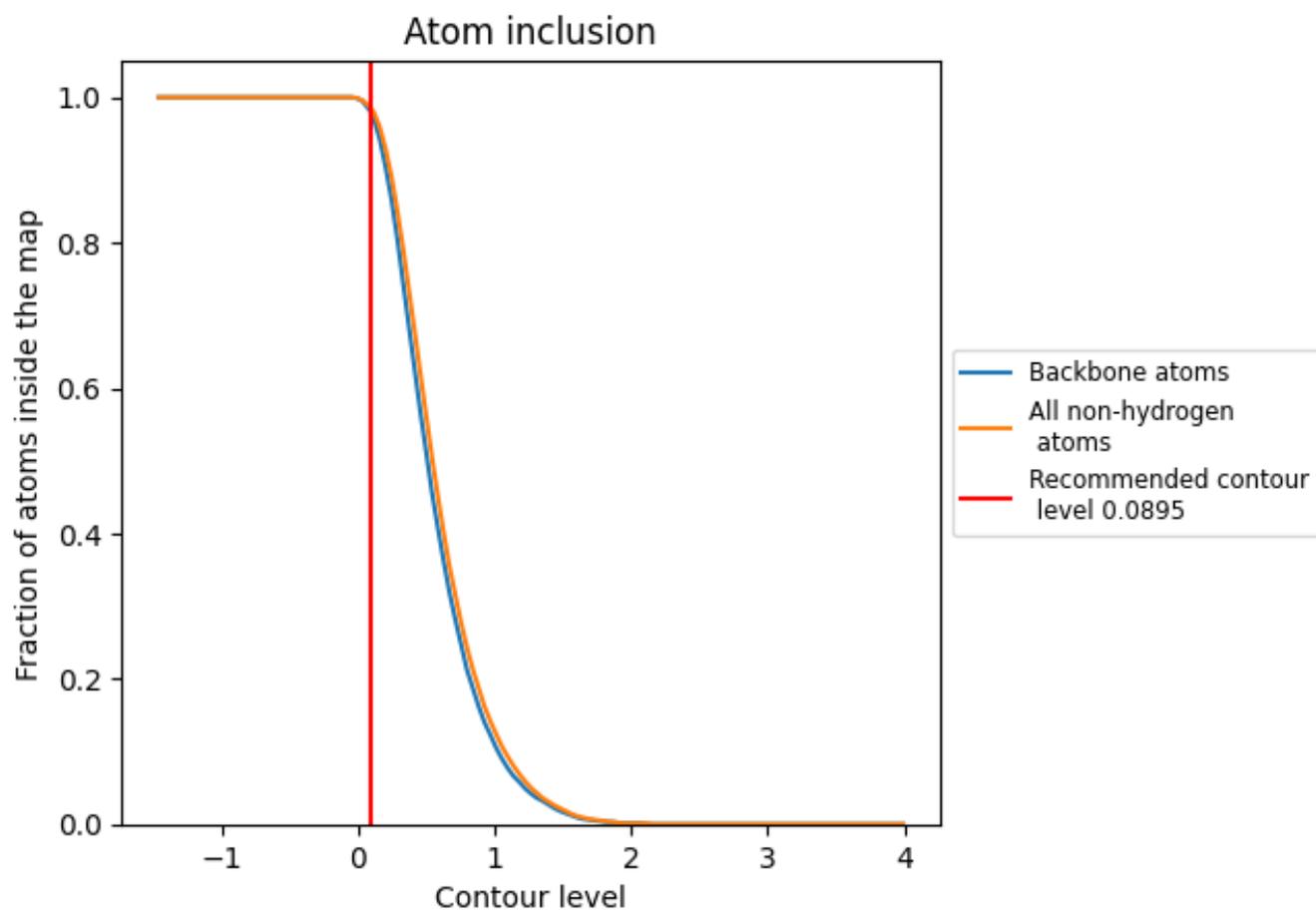
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0895).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 99% 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 (0.0895) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9860	 0.5100
2	 0.9980	 0.5630
A	 0.9970	 0.5450
B	 0.9960	 0.5910
C	 0.9980	 0.5950
D	 0.9580	 0.3470
E	 1.0000	 0.5950
F	 0.9860	 0.4100
G	 0.9900	 0.5010
H	 0.9950	 0.5190
I	 0.9960	 0.6120
J	 0.9980	 0.5700
K	 0.9250	 0.2060
L	 0.9960	 0.6260
M	 0.6630	 0.0740
N	 0.9990	 0.5970
O	 0.9980	 0.6060
P	 0.9350	 0.2040
Q	 0.9850	 0.3720
R	 0.9750	 0.3270
S	 0.9370	 0.1920
T	 0.9910	 0.3780
U	 0.9540	 0.3480
V	 0.9920	 0.5600
W	 0.9980	 0.6180
X	 0.9920	 0.5800
Y	 0.9940	 0.5060
Z	 0.9580	 0.2960
a	 1.0000	 0.6300
b	 0.9940	 0.5620
c	 0.9760	 0.4110
d	 0.9560	 0.2930
e	 0.9300	 0.3190
f	 0.6720	 0.0420
g	 0.9640	 0.3130

