



wwPDB EM Validation Summary Report ⓘ

Sep 24, 2026 – 04:41 pm BST

PDB ID : 9TKN / pdb_00009tkn
EMDB ID : EMD-56034
Title : 30S pre-initiation complex with IF2 and IF1 bound (30S PIC-A)
Authors : Guerra, G.S.; Demo, G.
Deposited on : 2025-12-10
Resolution : 3.10 Å(reported)
Based on initial model : 6WDD

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:

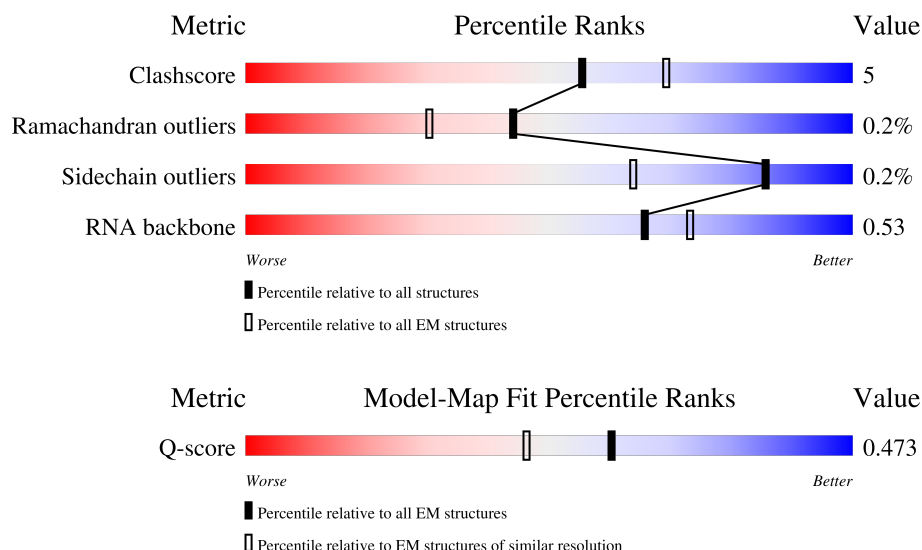
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	241	
2	AB	233	
3	AC	206	

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Mol	Chain	Length	Quality of chain
4	AD	167	
5	AE	135	
6	AF	179	
7	AG	130	
8	AH	130	
9	AI	103	
10	AJ	129	
11	AK	124	
12	AL	118	
13	AM	101	
14	AN	89	
15	AO	82	
16	AP	84	
17	AQ	75	
18	AR	92	
19	AS	87	
20	AT	71	
21	D1	1540	
22	D4	56	
23	D5	77	
24	F1	78	
25	F2	896	

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 58730 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	AA	225	Total	C	N	O	S	0	0
			1756	1111	315	322	8		

- Molecule 2 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 3 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 5 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 7 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 8 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 11 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 12 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 13 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 15 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 17 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 18 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AR	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 19 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 20 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 21 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D1	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D4	5	Total	C	N	O	P	0	0
			109	49	22	33	5		

- Molecule 23 is a RNA chain called tRNA^{fMet}.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D5	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 24 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F1	69	Total	C	N	O	S	0	0
			552	347	98	104	3		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F1	-5	MET	-	initiating methionine	UNP P69222
F1	-4	HIS	-	expression tag	UNP P69222
F1	-3	HIS	-	expression tag	UNP P69222
F1	-2	HIS	-	expression tag	UNP P69222
F1	-1	HIS	-	expression tag	UNP P69222
F1	0	HIS	-	expression tag	UNP P69222
F1	1	HIS	-	expression tag	UNP P69222

- Molecule 25 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F2	597	Total	C	N	O	S	0	0
			4516	2821	795	879	21		

There are 7 discrepancies between the modelled and reference sequences:

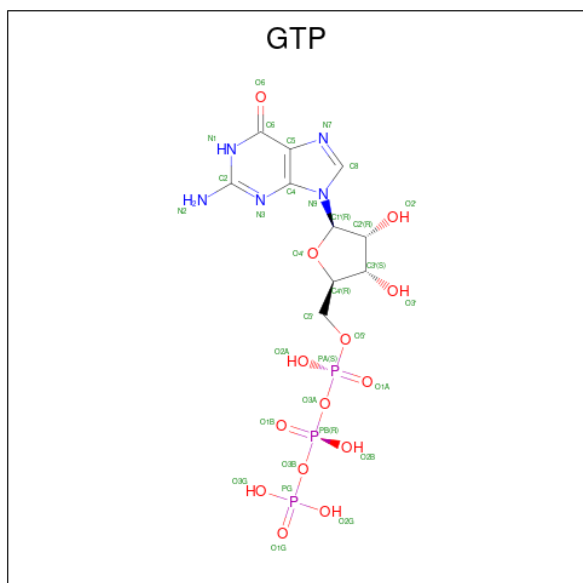
Chain	Residue	Modelled	Actual	Comment	Reference
F2	-5	MET	-	initiating methionine	UNP P0A705

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Chain	Residue	Modelled	Actual	Comment	Reference
F2	-4	HIS	-	expression tag	UNP P0A705
F2	-3	HIS	-	expression tag	UNP P0A705
F2	-2	HIS	-	expression tag	UNP P0A705
F2	-1	HIS	-	expression tag	UNP P0A705
F2	0	HIS	-	expression tag	UNP P0A705
F2	1	HIS	-	expression tag	UNP P0A705

- Molecule 26 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	F2	1	Total	C	N	O	P	0
			32	10	5	14	3	

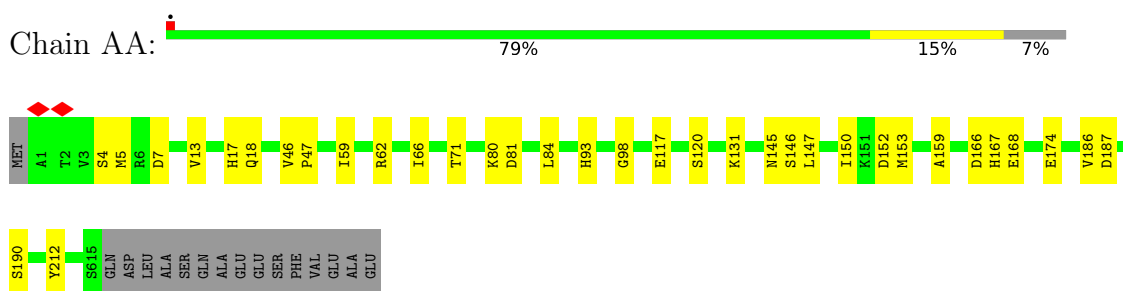
- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	F2	1	Total	Mg	0
			1	1	

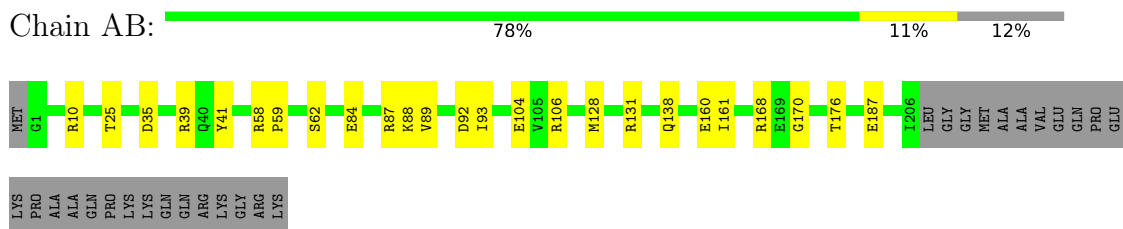
3 Residue-property plots [i](#)

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.

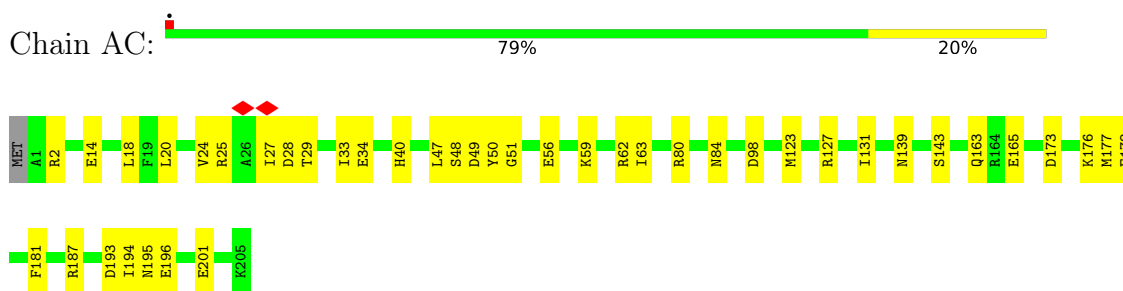
- Molecule 1: Small ribosomal subunit protein uS2



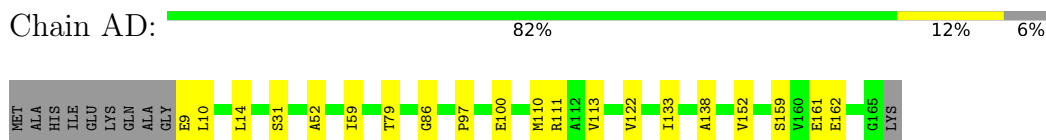
- Molecule 2: Small ribosomal subunit protein uS3



- Molecule 3: Small ribosomal subunit protein uS4

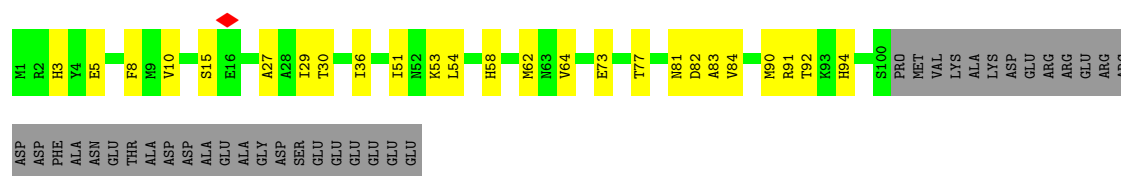


- Molecule 4: Small ribosomal subunit protein uS5



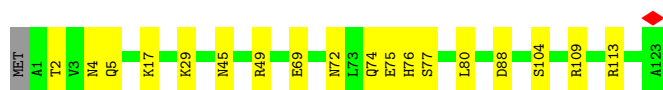
- Molecule 5: Small ribosomal subunit protein bS6, fully modified isoform

Chain AE: 



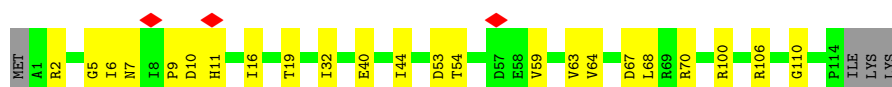
- Molecule 11: Small ribosomal subunit protein uS12

Chain AK: 



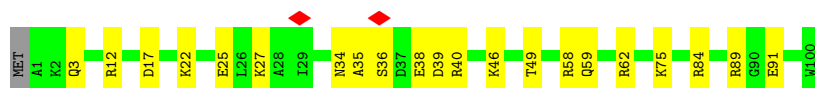
- Molecule 12: Small ribosomal subunit protein uS13

Chain AL: 

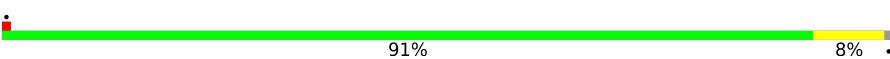


- Molecule 13: Small ribosomal subunit protein uS14

Chain AM: 



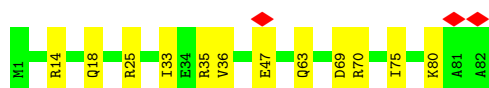
- Molecule 14: Small ribosomal subunit protein uS15

Chain AN: 



- Molecule 15: Small ribosomal subunit protein bS16

Chain AO: 



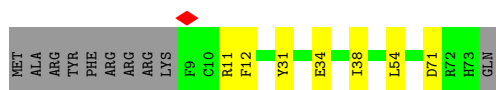
- Molecule 16: Small ribosomal subunit protein uS17

Chain AP: 



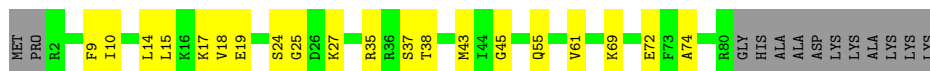
- Molecule 17: Small ribosomal subunit protein bS18

Chain AQ: 



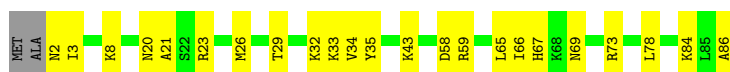
- Molecule 18: Small ribosomal subunit protein uS19

Chain AR: 64% 22% 14%



- Molecule 19: Small ribosomal subunit protein bS20

Chain AS: 71% 26% .



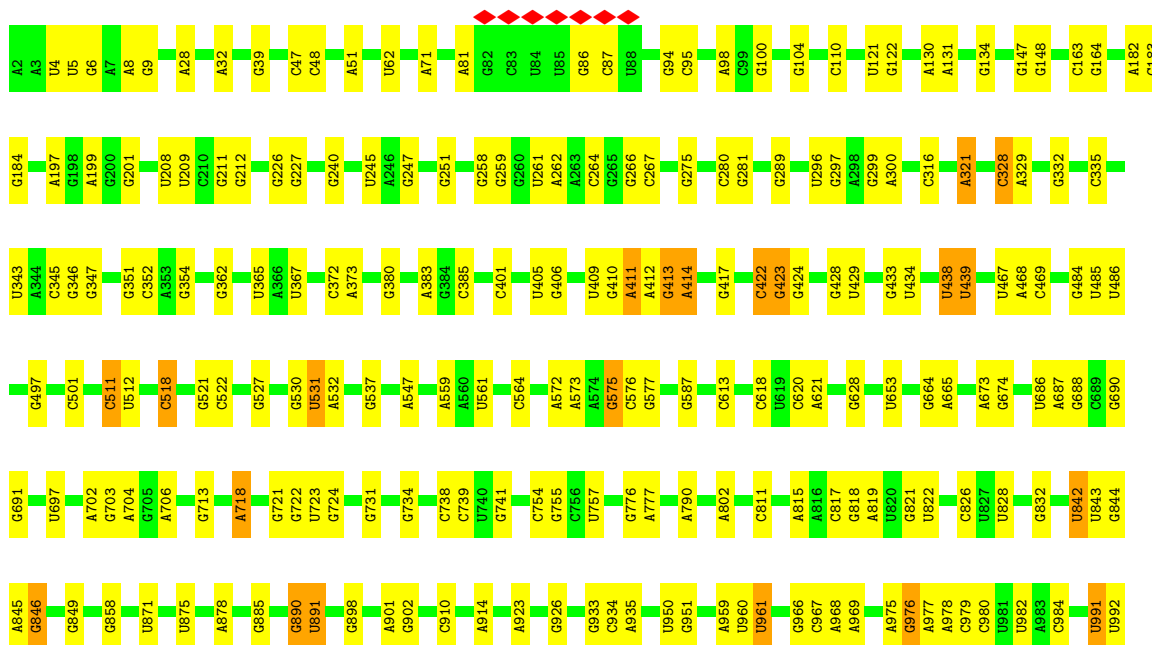
- Molecule 20: Small ribosomal subunit protein bS21

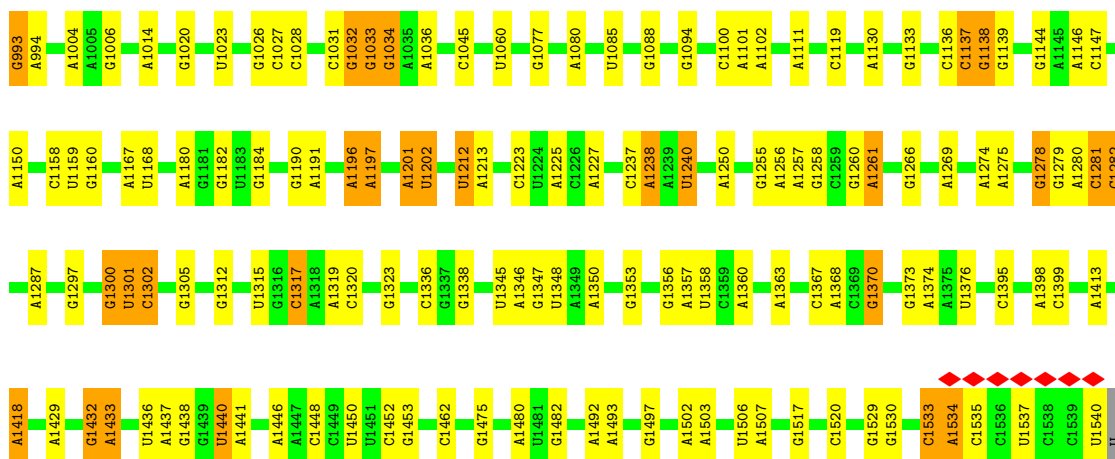
Chain AT: 65% 27% 8%



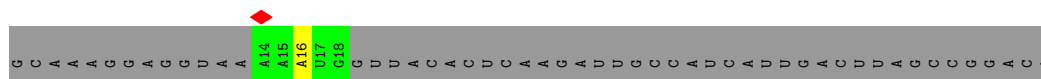
- Molecule 21: 16S Ribosomal RNA

Chain D1: 76% 20% .

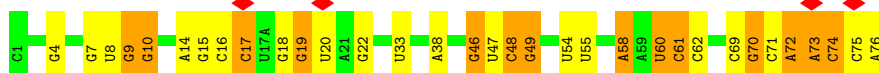




- Molecule 22: mRNA



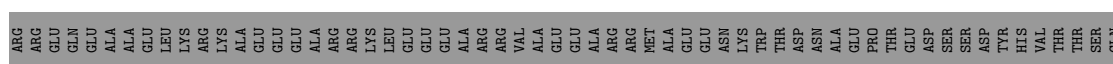
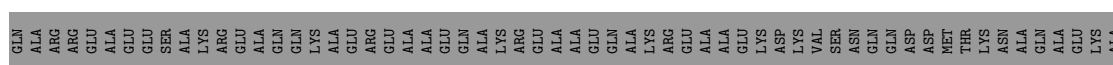
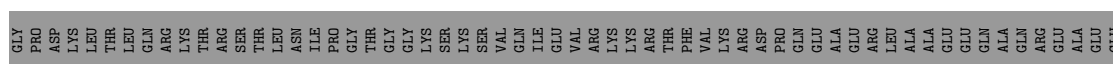
- Molecule 23: tRNA^{fMet}



- Molecule 24: Translation initiation factor IF-1



- Molecule 25: Translation initiation factor IF-2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22197	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	18.570	Depositor
Minimum map value	-4.895	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.787	Depositor
Recommended contour level	3	Depositor
Map size (Å)	400.32, 400.32, 400.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	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, GTP

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	AA	0.20	0/1787	0.37	0/2408
2	AB	0.21	0/1651	0.35	0/2225
3	AC	0.21	0/1665	0.37	0/2227
4	AD	0.23	0/1169	0.42	0/1573
5	AE	0.20	0/835	0.52	0/1128
6	AF	0.19	0/1195	0.37	0/1602
7	AG	0.23	0/989	0.41	0/1326
8	AH	0.21	0/1034	0.41	0/1375
9	AI	0.35	0/796	0.51	0/1077
10	AJ	0.19	0/885	0.45	0/1195
11	AK	0.24	0/969	0.43	0/1300
12	AL	0.20	0/892	0.41	0/1193
13	AM	0.21	0/817	0.42	0/1088
14	AN	0.20	0/722	0.42	0/964
15	AO	0.23	0/659	0.40	0/884
16	AP	0.22	0/657	0.48	0/881
17	AQ	0.21	0/544	0.40	0/731
18	AR	0.18	0/652	0.38	0/877
19	AS	0.21	0/671	0.44	0/888
20	AT	0.23	0/550	0.64	0/728
21	D1	0.23	0/36963	0.29	0/57662
22	D4	0.15	0/122	0.35	0/188
23	D5	0.17	0/1832	0.34	1/2855 (0.0%)
24	F1	0.17	0/559	0.34	0/752
25	F2	0.16	0/4567	0.35	0/6166
All	All	0.22	0/63182	0.33	1/93293 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D5	74	C	P-O3'-C3'	5.25	128.07	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	AA	1756	0	1787	23	0
2	AB	1624	0	1699	15	0
3	AC	1643	0	1710	33	0
4	AD	1156	0	1199	14	0
5	AE	817	0	808	20	0
6	AF	1181	0	1240	25	0
7	AG	979	0	1034	21	0
8	AH	1022	0	1070	14	0
9	AI	786	0	828	11	0
10	AJ	869	0	878	22	0
11	AK	955	0	1019	15	0
12	AL	883	0	944	18	0
13	AM	805	0	847	17	0
14	AN	714	0	737	4	0
15	AO	649	0	666	10	0
16	AP	648	0	691	12	0
17	AQ	535	0	552	6	0
18	AR	637	0	665	13	0
19	AS	665	0	714	20	0
20	AT	544	0	579	14	0
21	D1	33012	0	16618	136	0
22	D4	109	0	55	0	0
23	D5	1640	0	837	26	0
24	F1	552	0	568	9	0
25	F2	4516	0	4604	65	0
26	F2	32	0	12	2	0
27	F2	1	0	0	0	0
All	All	58730	0	42361	487	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.

The worst 5 of 487 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)
23:D5:54:U:C2	23:D5:58:A:N7	2.22	1.06
23:D5:54:U:O2	23:D5:58:A:C5	2.25	0.90
23:D5:54:U:N3	23:D5:58:A:C8	2.41	0.88
23:D5:54:U:C2	23:D5:58:A:C8	2.66	0.84
19:AS:2:ASN:N	21:D1:332:G:OP2	2.13	0.82

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	AA	223/241 (92%)	202 (91%)	21 (9%)	0	100	100
2	AB	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
3	AC	203/206 (98%)	185 (91%)	18 (9%)	0	100	100
4	AD	155/167 (93%)	136 (88%)	18 (12%)	1 (1%)	21	52
5	AE	98/135 (73%)	79 (81%)	19 (19%)	0	100	100
6	AF	149/179 (83%)	140 (94%)	9 (6%)	0	100	100
7	AG	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
8	AH	125/130 (96%)	109 (87%)	16 (13%)	0	100	100
9	AI	96/103 (93%)	81 (84%)	14 (15%)	1 (1%)	12	41
10	AJ	114/129 (88%)	94 (82%)	20 (18%)	0	100	100
11	AK	121/124 (98%)	99 (82%)	22 (18%)	0	100	100
12	AL	112/118 (95%)	98 (88%)	14 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	AM	98/101 (97%)	85 (87%)	13 (13%)	0	100	100
14	AN	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	37
15	AO	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
16	AP	78/84 (93%)	69 (88%)	9 (12%)	0	100	100
17	AQ	63/75 (84%)	58 (92%)	5 (8%)	0	100	100
18	AR	77/92 (84%)	66 (86%)	11 (14%)	0	100	100
19	AS	83/87 (95%)	78 (94%)	5 (6%)	0	100	100
20	AT	63/71 (89%)	42 (67%)	19 (30%)	2 (3%)	3	18
24	F1	67/78 (86%)	64 (96%)	3 (4%)	0	100	100
25	F2	595/896 (66%)	556 (93%)	38 (6%)	1 (0%)	43	73
All	All	3017/3550 (85%)	2701 (90%)	310 (10%)	6 (0%)	44	73

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	AT	8	ASN
4	AD	122	VAL
14	AN	46	LYS
20	AT	36	PHE
25	F2	306	VAL

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	AA	186/199 (94%)	186 (100%)	0	100	100
2	AB	170/190 (90%)	169 (99%)	1 (1%)	78	83
3	AC	172/173 (99%)	172 (100%)	0	100	100
4	AD	119/126 (94%)	119 (100%)	0	100	100
5	AE	87/116 (75%)	87 (100%)	0	100	100
6	AF	124/147 (84%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	104/105 (99%)	104 (100%)	0	100	100
8	AH	105/107 (98%)	105 (100%)	0	100	100
9	AI	86/90 (96%)	83 (96%)	3 (4%)	32	62
10	AJ	89/99 (90%)	89 (100%)	0	100	100
11	AK	103/104 (99%)	103 (100%)	0	100	100
12	AL	92/96 (96%)	92 (100%)	0	100	100
13	AM	83/84 (99%)	83 (100%)	0	100	100
14	AN	76/77 (99%)	75 (99%)	1 (1%)	61	77
15	AO	65/65 (100%)	65 (100%)	0	100	100
16	AP	74/78 (95%)	74 (100%)	0	100	100
17	AQ	56/65 (86%)	56 (100%)	0	100	100
18	AR	70/79 (89%)	70 (100%)	0	100	100
19	AS	65/66 (98%)	65 (100%)	0	100	100
20	AT	55/61 (90%)	55 (100%)	0	100	100
24	F1	63/71 (89%)	63 (100%)	0	100	100
25	F2	481/719 (67%)	481 (100%)	0	100	100
All	All	2525/2917 (87%)	2520 (100%)	5 (0%)	85	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	138	GLN
9	AI	42	LEU
9	AI	44	THR
9	AI	45	ARG
14	AN	34	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
9	AI	20	GLN
25	F2	690	ASN
25	F2	834	ASN
5	AE	94	HIS
5	AE	55	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	D1	1538/1540 (99%)	222 (14%)	13 (0%)
22	D4	4/56 (7%)	1 (25%)	0
23	D5	76/77 (98%)	22 (28%)	1 (1%)
All	All	1618/1673 (96%)	245 (15%)	14 (0%)

5 of 245 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	D1	4	U
21	D1	5	U
21	D1	6	G
21	D1	9	G
21	D1	32	A

5 of 14 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	D1	1201	A
21	D1	1281	C
23	D5	73	A
21	D1	1347	G
21	D1	1432	G

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
26	GTP	F2	901	27	30,34,34	0.84	1 (3%)	46,54,54	1.77	11 (23%)

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
26	GTP	F2	901	27	-	2/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F2	901	GTP	C2-N3	2.21	1.38	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F2	901	GTP	C5-C4-N3	-5.06	120.25	128.46
26	F2	901	GTP	C2-N3-C4	4.48	120.28	112.30
26	F2	901	GTP	PA-O3A-PB	-3.67	120.22	132.83
26	F2	901	GTP	PB-O3B-PG	-3.49	120.84	132.83
26	F2	901	GTP	N9-C4-N3	3.25	132.47	125.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

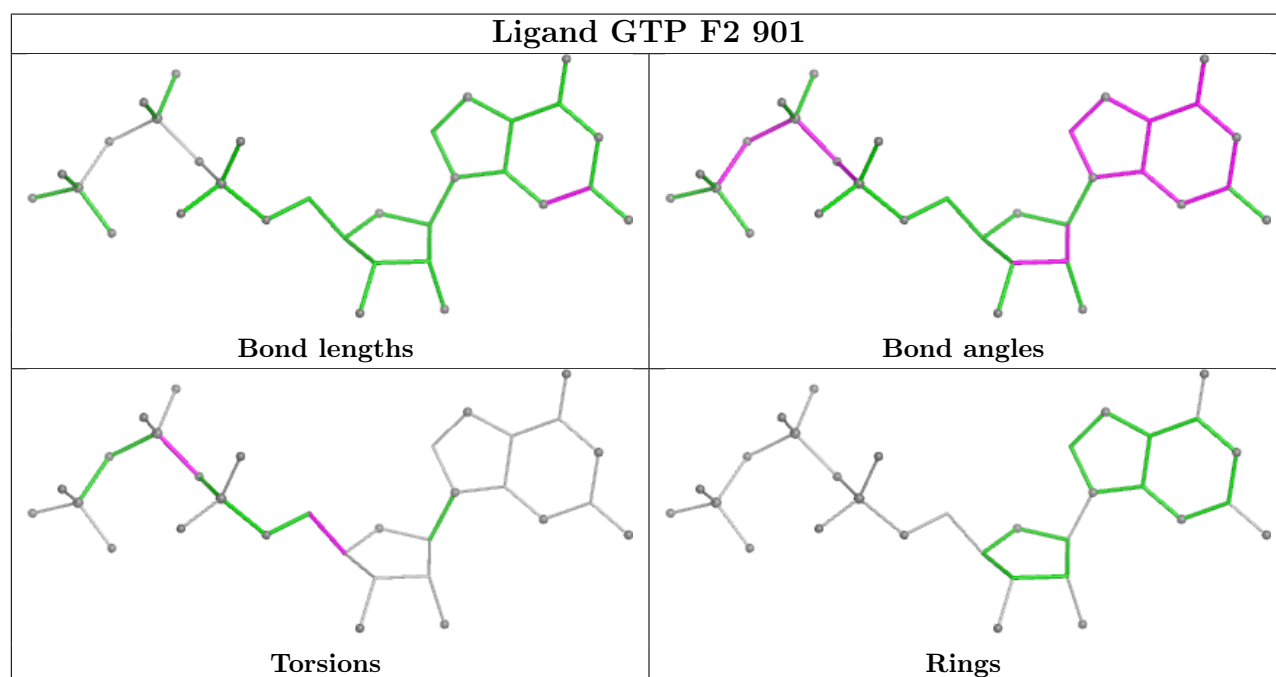
Mol	Chain	Res	Type	Atoms
26	F2	901	GTP	PA-O3A-PB-O2B
26	F2	901	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	F2	901	GTP	2	0

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.

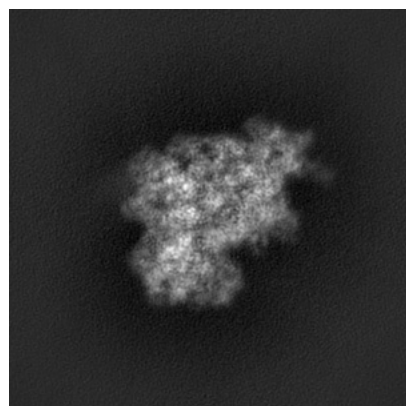
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56034. These allow visual inspection of the internal detail of the map and identification of artifacts.

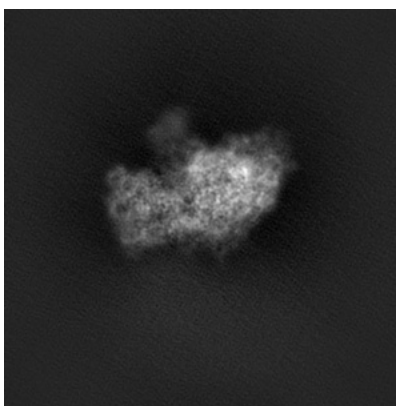
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

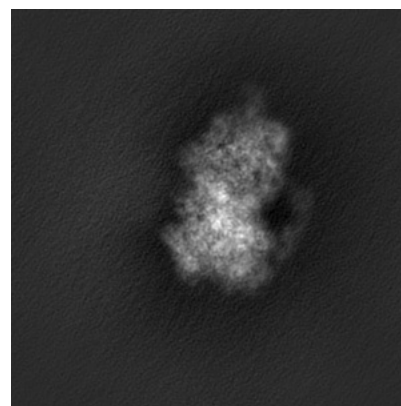
6.1.1 Primary map



X

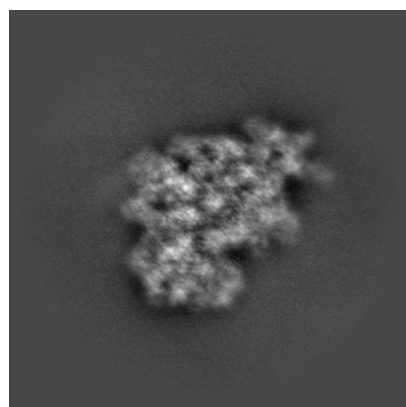


Y

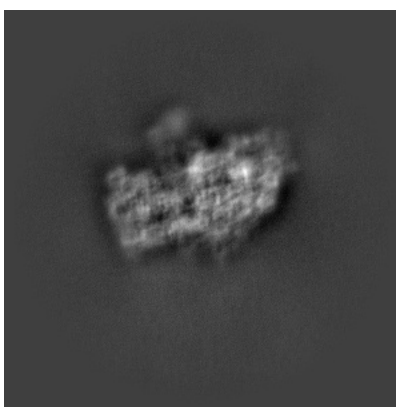


Z

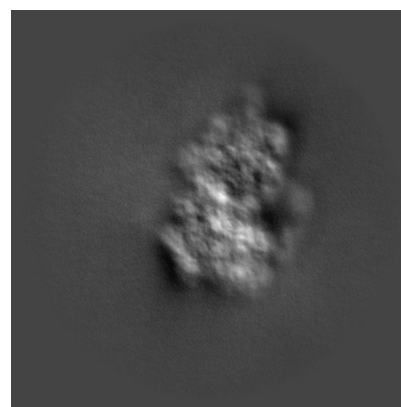
6.1.2 Raw map



X



Y

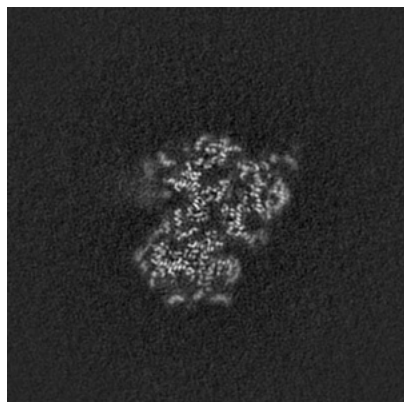


Z

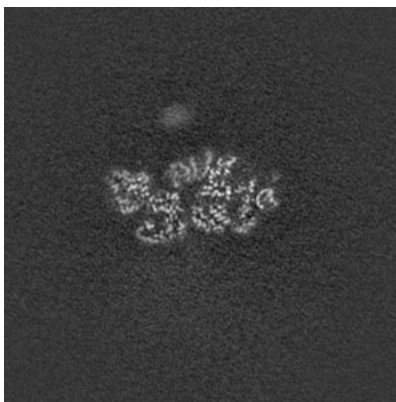
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

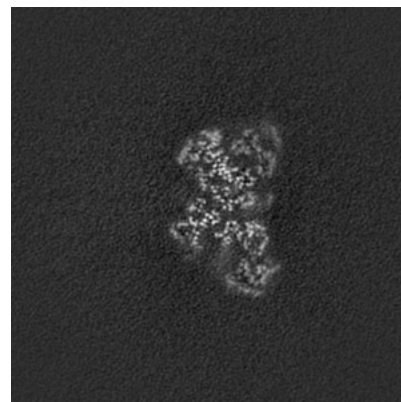
6.2.1 Primary map



X Index: 240

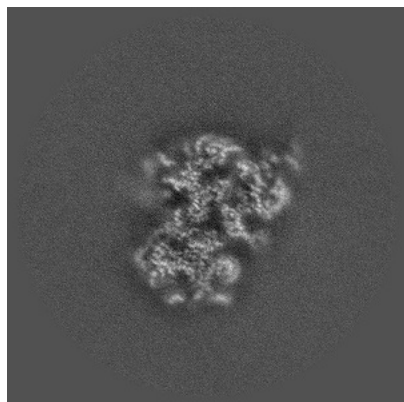


Y Index: 240

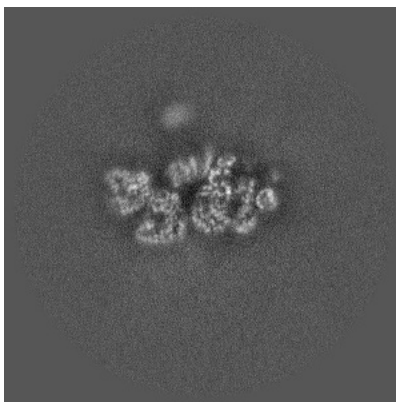


Z Index: 240

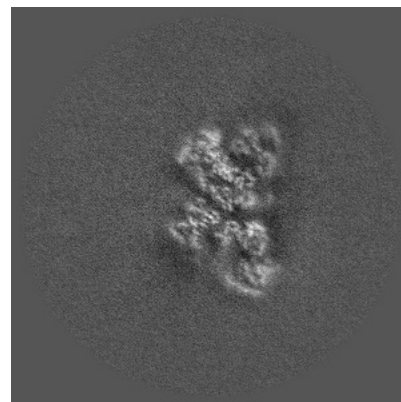
6.2.2 Raw map



X Index: 240



Y Index: 240

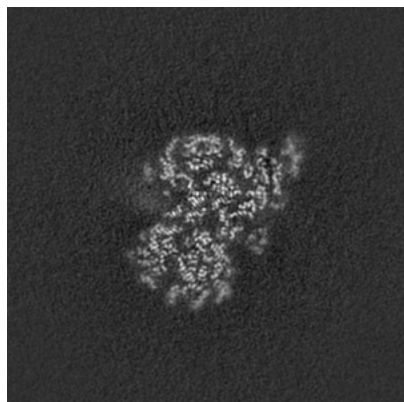


Z Index: 240

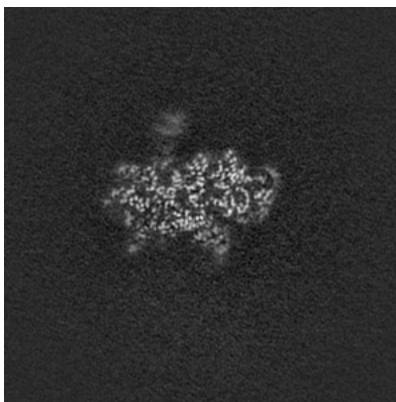
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

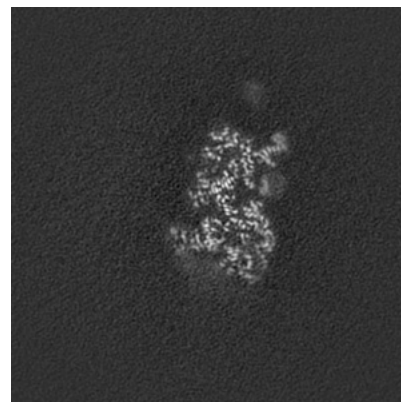
6.3.1 Primary map



X Index: 250

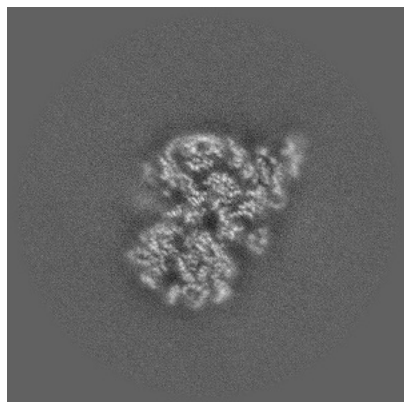


Y Index: 217

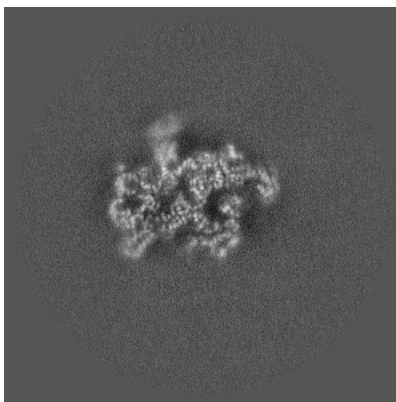


Z Index: 271

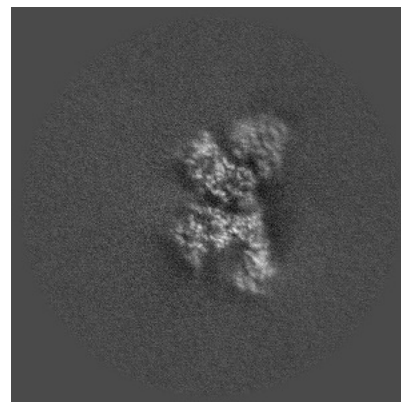
6.3.2 Raw map



X Index: 250



Y Index: 207

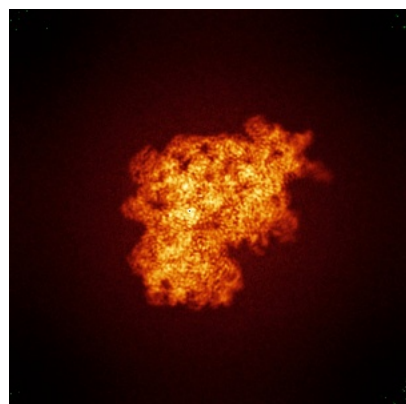


Z Index: 232

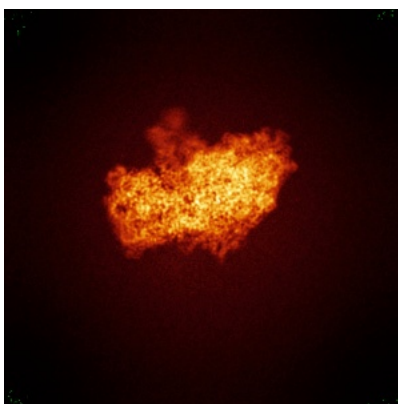
The images above show the largest variance slices of the map in three orthogonal directions.

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

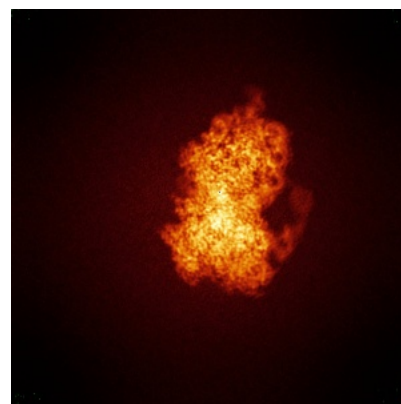
6.4.1 Primary map



X

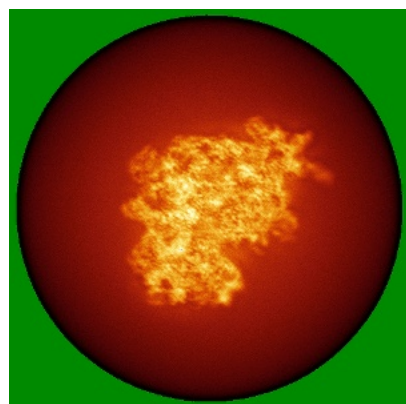


Y

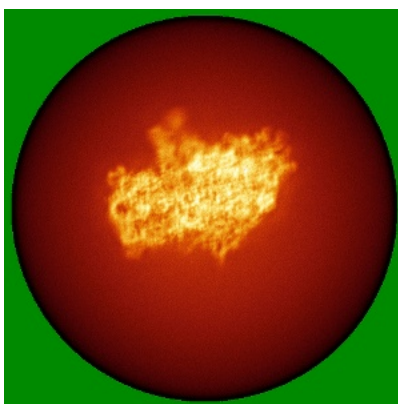


Z

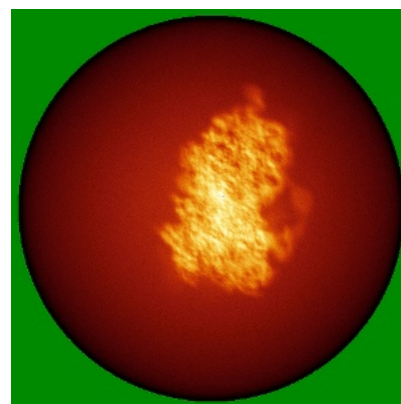
6.4.2 Raw map



X



Y

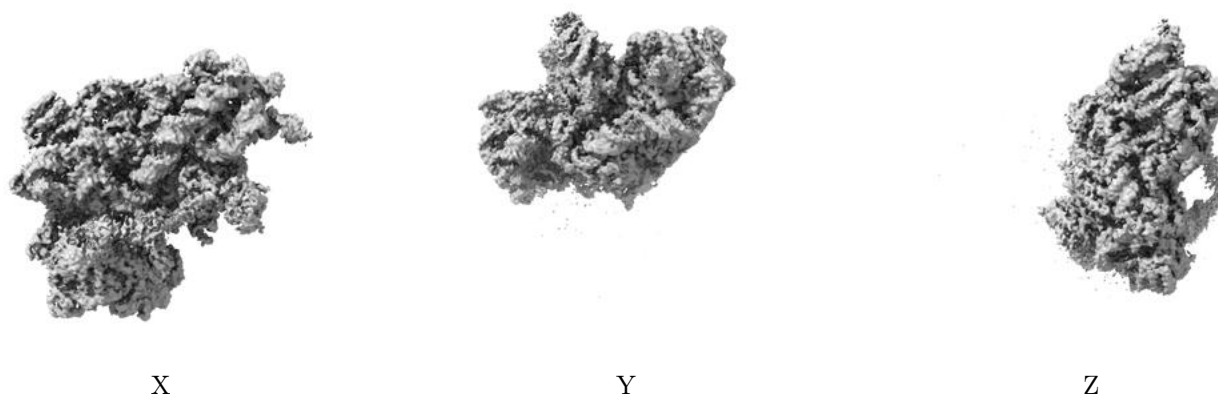


Z

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.

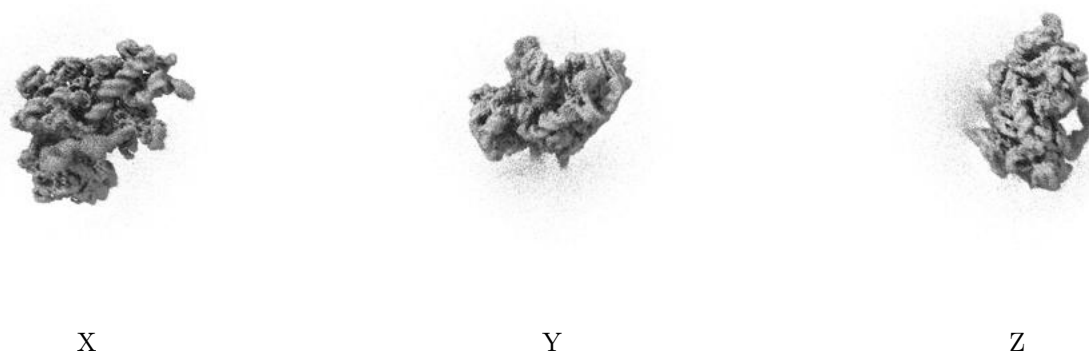
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. 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.

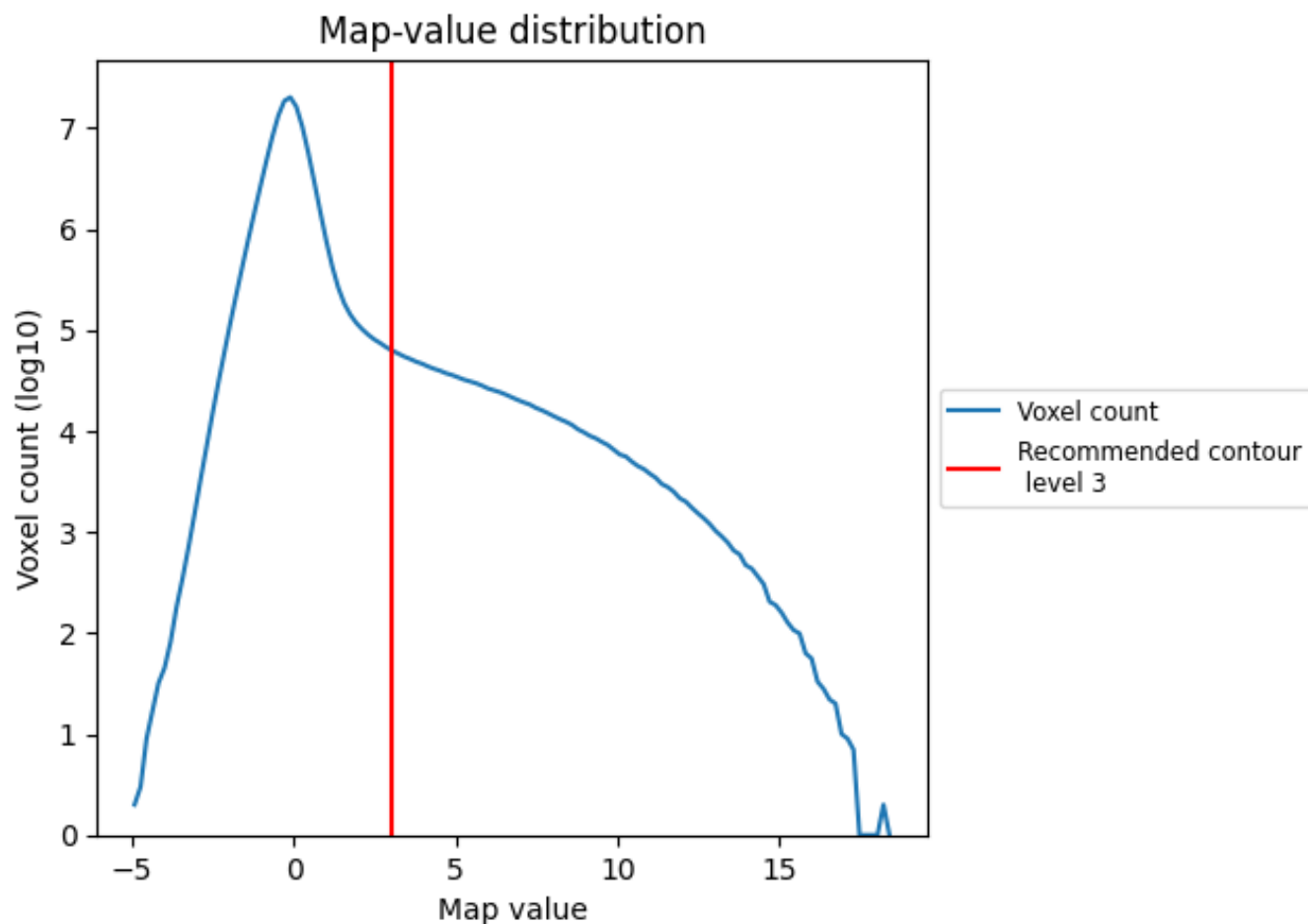
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

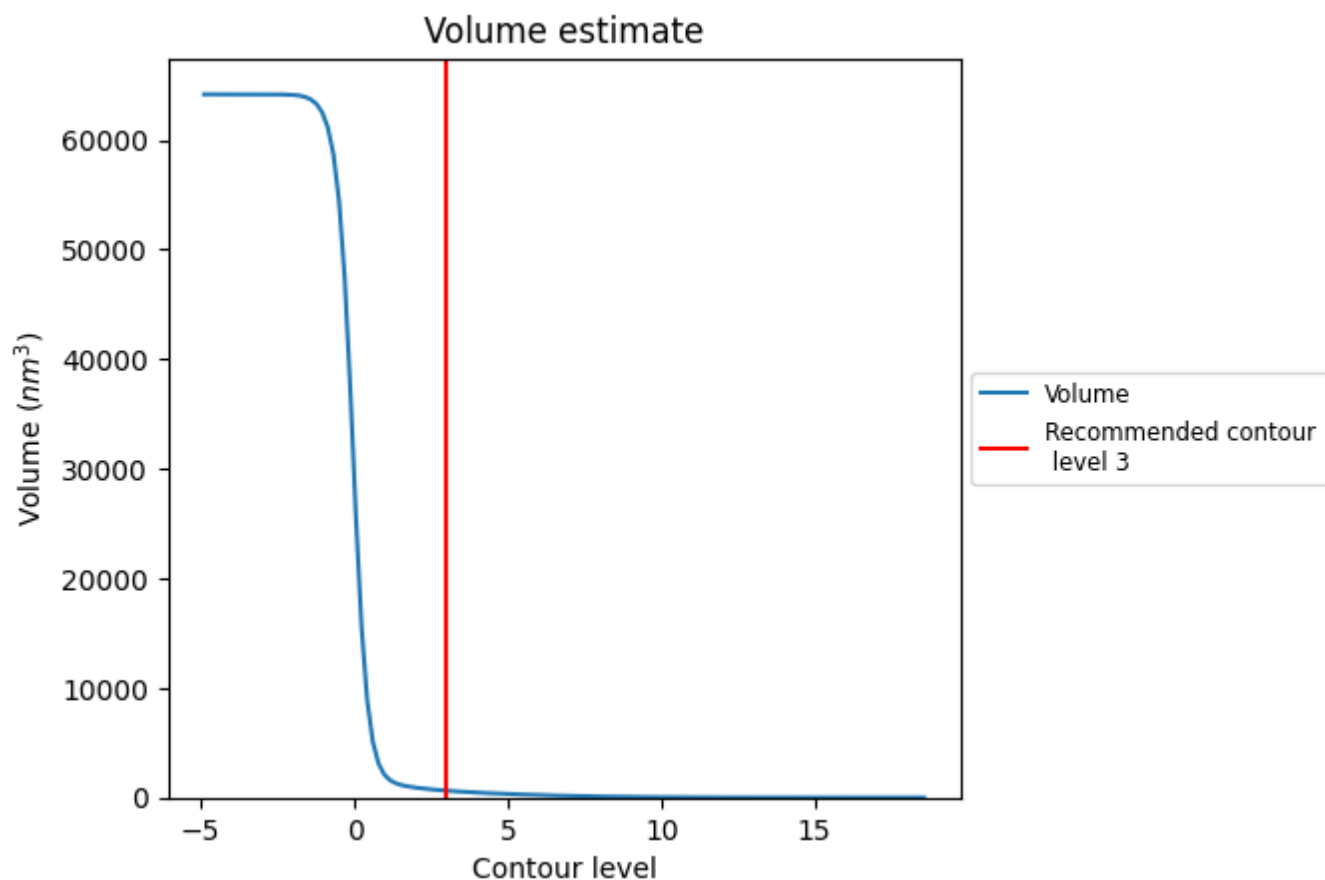
This section contains the results of statistical analysis of the map.

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.

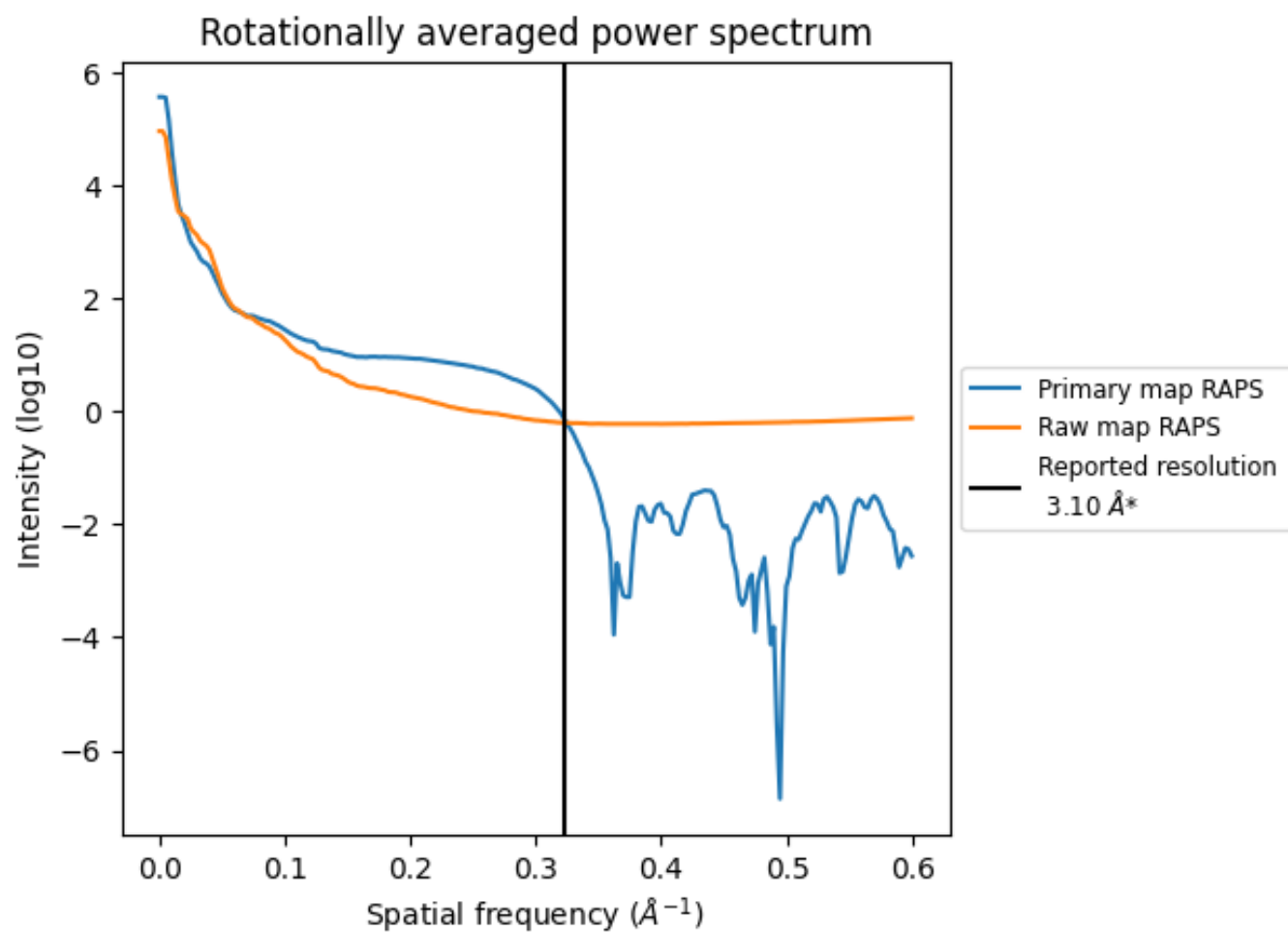
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 630 nm³; this corresponds to an approximate mass of 569 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 ⓘ

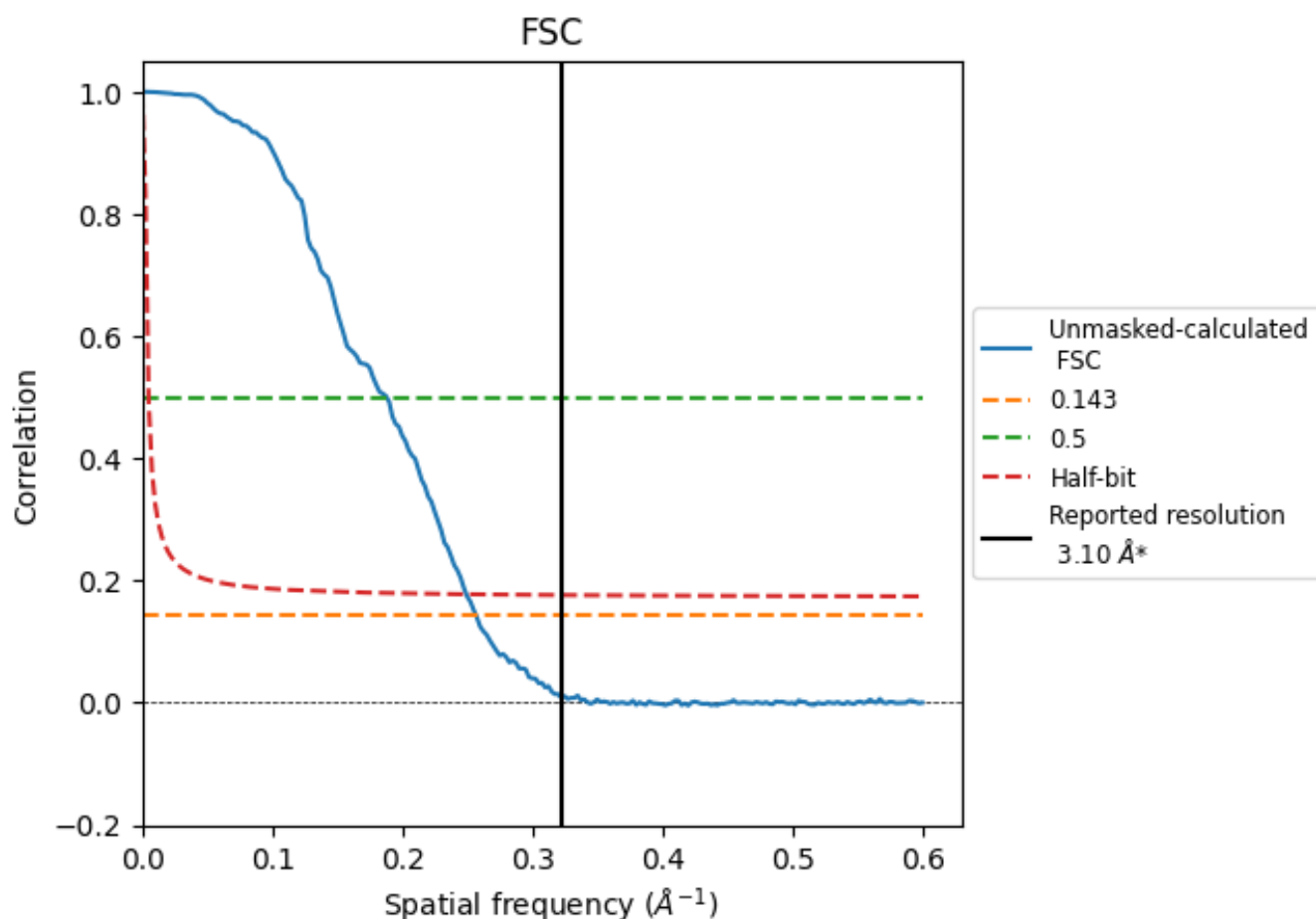


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

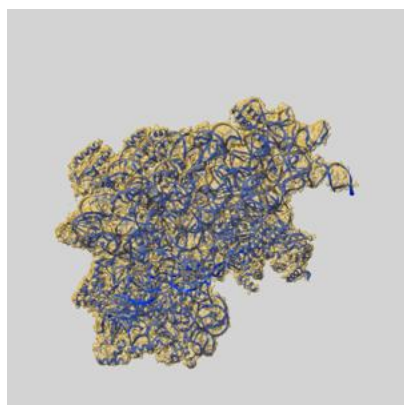
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.90	5.32	4.01

*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 3.90 differs from the reported value 3.1 by more than 10 %

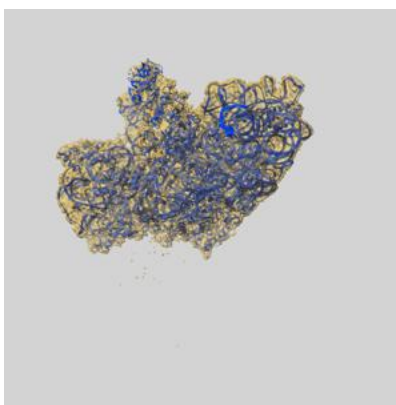
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56034 and PDB model 9TKN. Per-residue inclusion information can be found in section [3](#) on page [9](#).

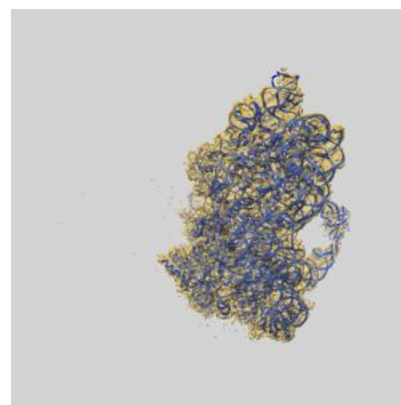
9.1 Map-model overlay [i](#)



X



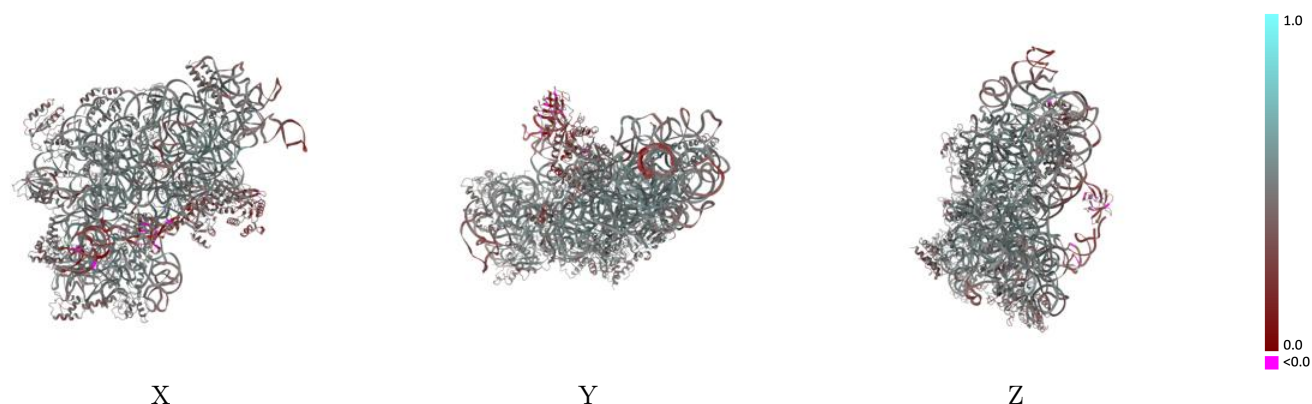
Y



Z

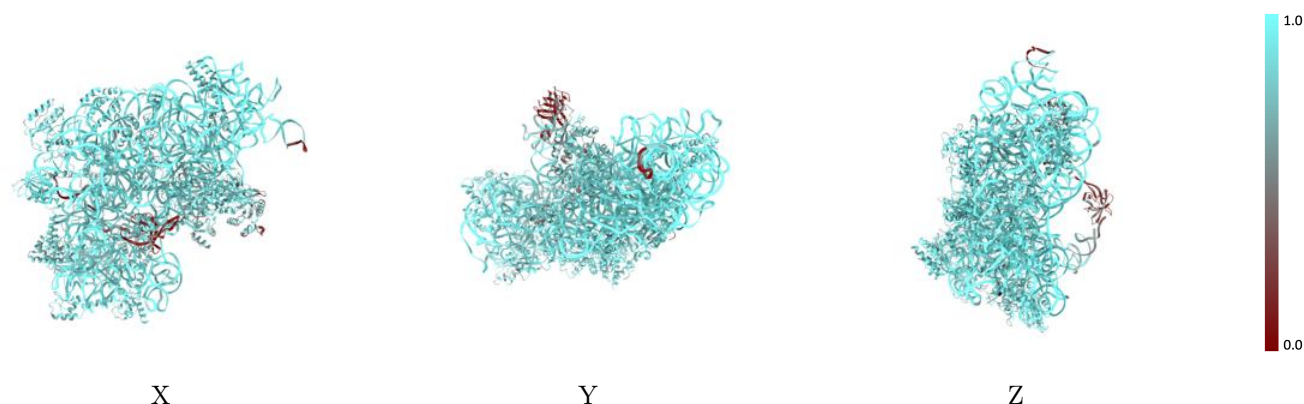
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



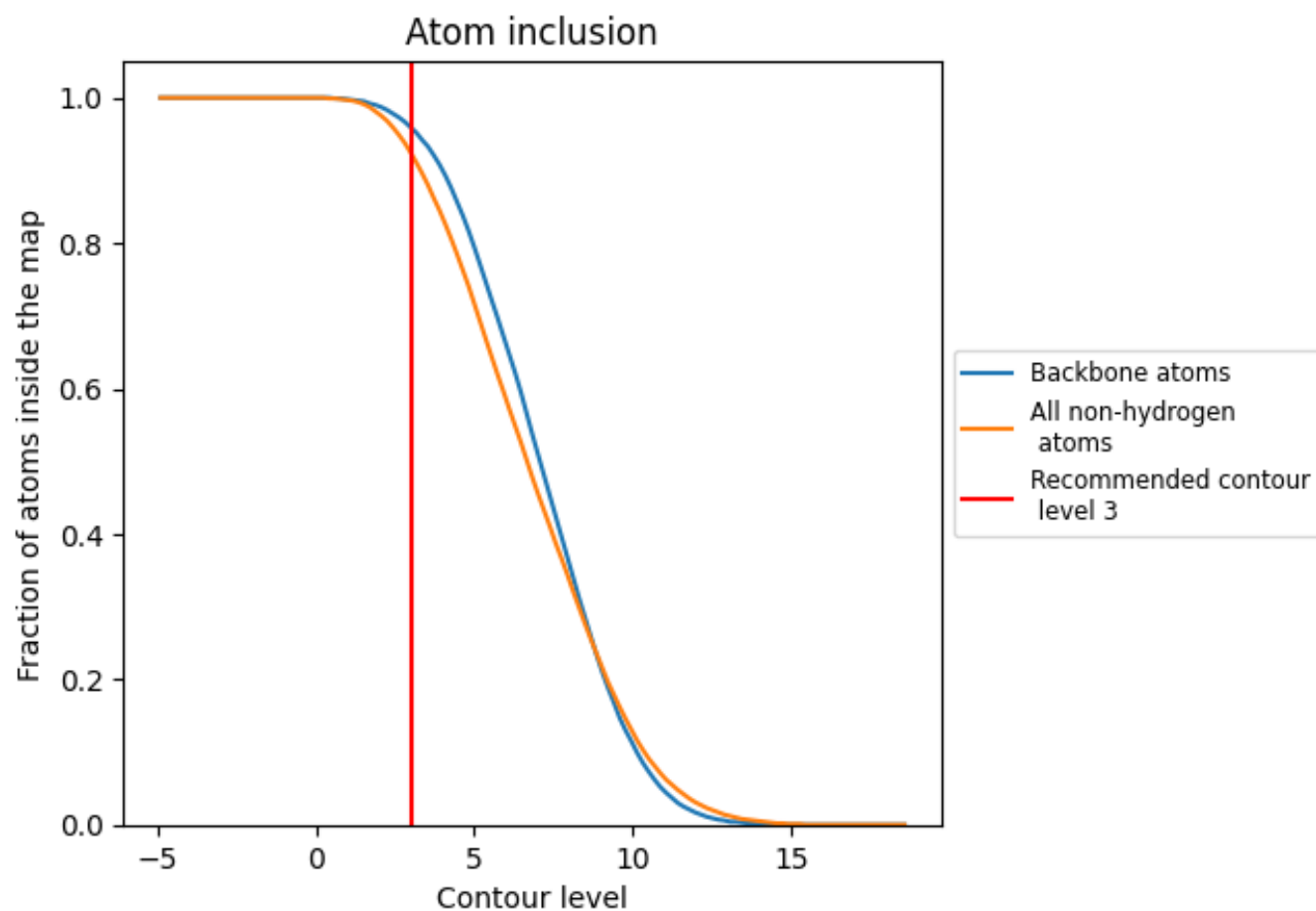
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9240	 0.4730
AA	 0.8840	 0.4640
AB	 0.9070	 0.5010
AC	 0.9040	 0.4800
AD	 0.9380	 0.5090
AE	 0.8540	 0.4250
AF	 0.8420	 0.4480
AG	 0.9420	 0.5100
AH	 0.9160	 0.4840
AI	 0.8540	 0.4600
AJ	 0.9170	 0.4680
AK	 0.9360	 0.5200
AL	 0.8710	 0.4560
AM	 0.9290	 0.4930
AN	 0.9120	 0.4620
AO	 0.9170	 0.5140
AP	 0.9380	 0.5020
AQ	 0.8950	 0.4720
AR	 0.9290	 0.4670
AS	 0.8950	 0.4710
AT	 0.7720	 0.3750
D1	 0.9820	 0.4960
D4	 0.6790	 0.4060
D5	 0.8140	 0.2920
F1	 0.9220	 0.4700
F2	 0.6440	 0.3500

