wwPDB EM Validation Summary Report

May 25, 2024 – 08:41 AM EDT

PDB ID	:	7NAF
EMDB ID	:	EMD-24271
Title	:	State E2 nucleolar 60S ribosomal biogenesis intermediate - Spb1-MTD local model
Authors	:	Cruz, V.E.; Sekulski, K.; Peddada, N.; Erzberger, J.P.
Deposited on	:	2021-06-21
Resolution	:	3.13 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:

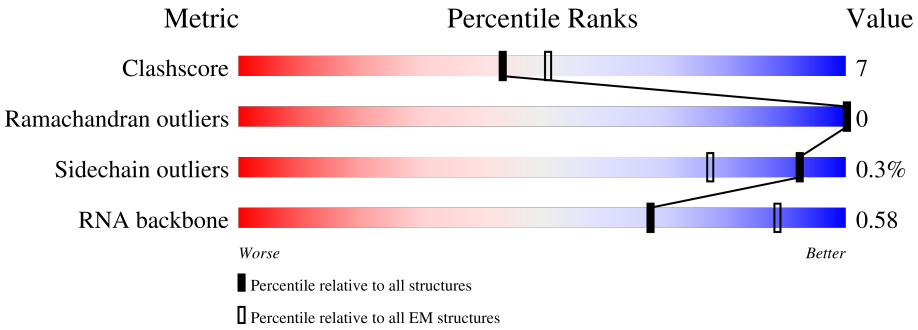
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.13 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)
Clashscore	158937	4297
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	1	378	10% 59% 35% 6%
2	5	105	44% 91% 9%
3	8	39	18% 90% 10%
4	V	134	89% 11%
5	u	65	100%
6	w	389	15% 93% 7%
7	b	74	16% 100%

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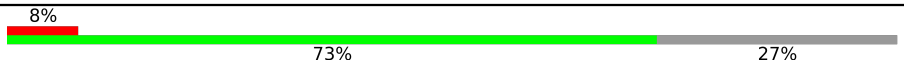
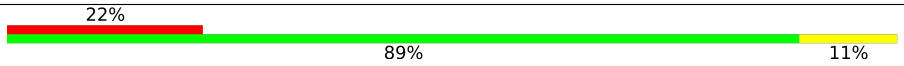
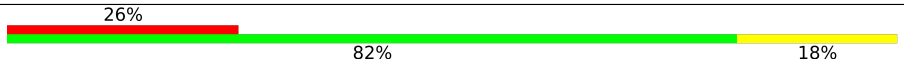
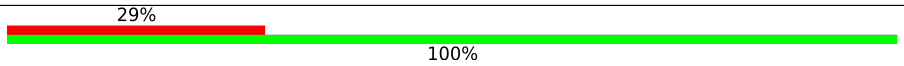
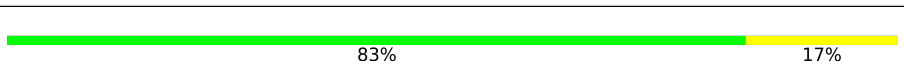
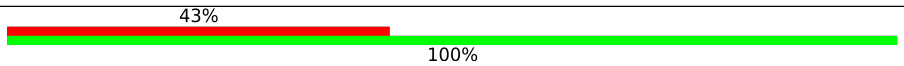
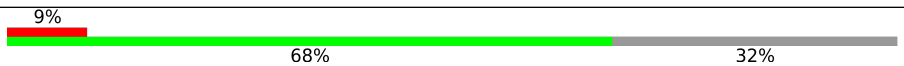
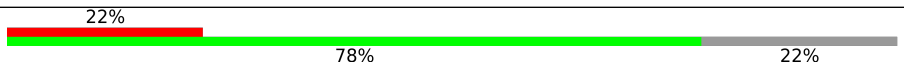
Mol	Chain	Length	Quality of chain
8	d	60	
9	U	18	
10	R	62	
11	c	41	
12	B	376	
13	z	6	
14	s	7	
15	y	245	
16	q	36	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 18868 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 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	378	8046	3597	1413	2658	378	0	0

- Molecule 2 is a protein called Ribosomal RNA-processing protein 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	5	105	918	568	183	166	1	0	0

- Molecule 3 is a protein called Nucleolar complex protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	8	39	332	204	74	54	0	0

- Molecule 4 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	V	134	993	623	187	176	7	0	0

- Molecule 5 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	u	65	543	346	109	81	7	0	0

- Molecule 6 is a protein called 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	w	361	2959	1883	524	534	18	0	0

- Molecule 7 is a protein called 60S ribosome biogenesis factor Nog1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	74	Total	C	N	O	S	0	0
			613	387	123	99	4		

- Molecule 8 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	d	44	Total	C	N	O	0	0
			369	236	77	56		

- Molecule 9 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	18	Total	C	N	O	0	0
			165	110	29	26		

- Molecule 10 is a protein called 60S ribosome ribosomal protein L19A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	R	62	Total	C	N	O	0	0
			529	343	108	78		

- Molecule 11 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	c	41	Total	C	N	O	0	0
			310	203	53	54		

- Molecule 12 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	190	Total	C	N	O	S	0	0
			1493	942	284	261	6		

- Molecule 13 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	z	6	Total	C	N	O	0	0
			44	27	10	7		

- Molecule 14 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	s	7	Total	C	N	O	S	0	0
			66	39	18	8	1		

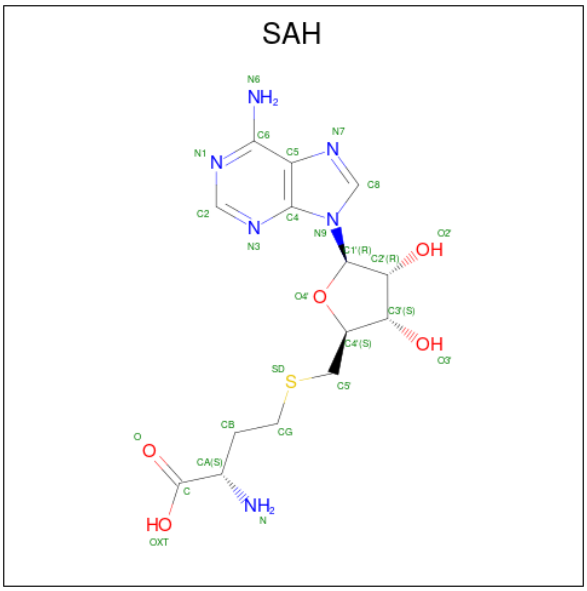
- Molecule 15 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	y	167	Total	C	N	O	S	0	0
			1250	777	217	249	7		

- Molecule 16 is a protein called 25S rRNA (cytosine(2870)-C(5))-methyltransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	q	28	Total	C	N	O	0	0
			210	134	37	39		

- Molecule 17 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	w	1	Total	C	N	O	S	0
			26	14	6	5	1	

- Molecule 18 is water.

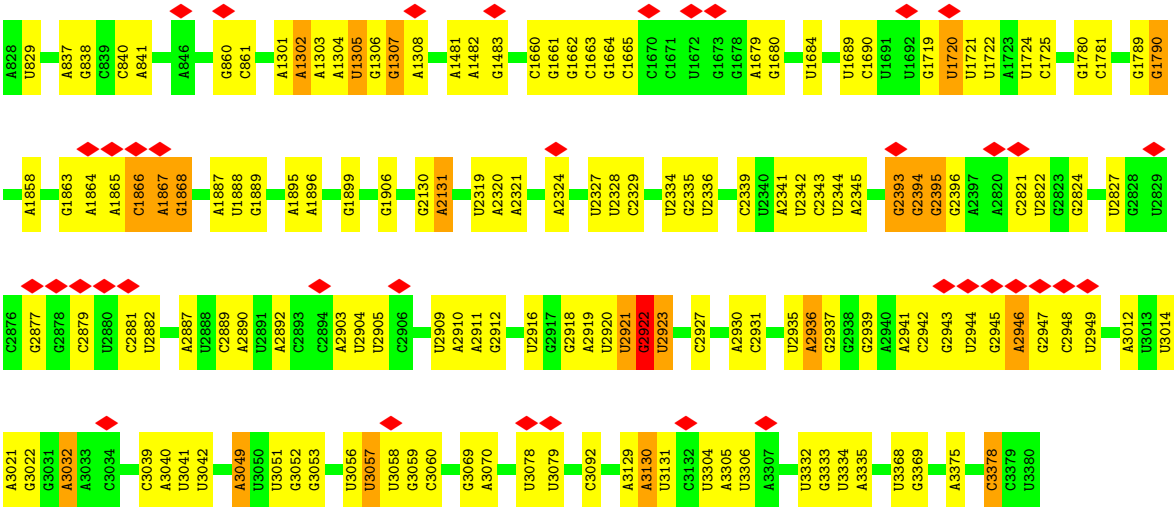
Mol	Chain	Residues	Atoms		AltConf
18	w	2	Total	O	0
			2	2	

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.

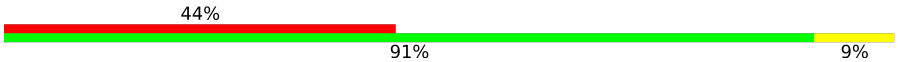
• Molecule 1: 25S rRNA

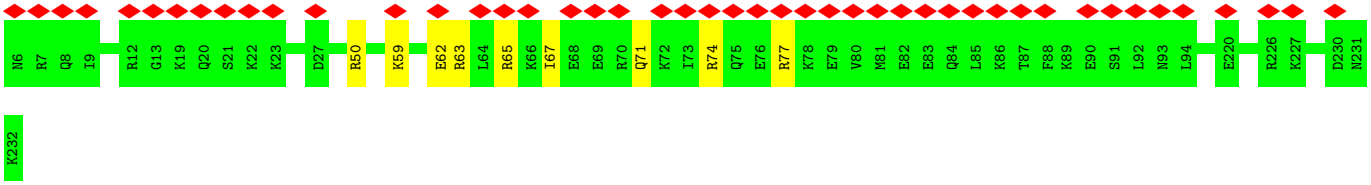
Chain 1:



• Molecule 2: Ribosomal RNA-processing protein 17

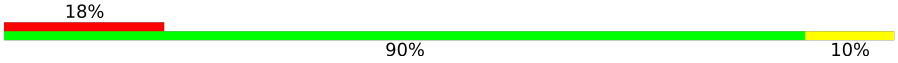
Chain 5:

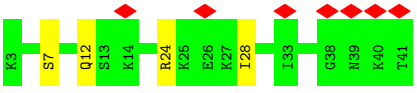




• Molecule 3: Nucleolar complex protein 2

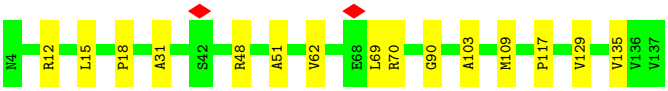
Chain 8:





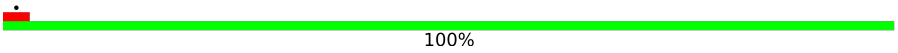
• Molecule 4: 60S ribosomal protein L23-A

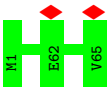
Chain V:



• Molecule 5: Ribosome biogenesis protein RLP24

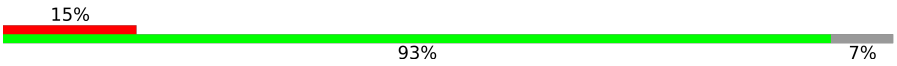
Chain u:

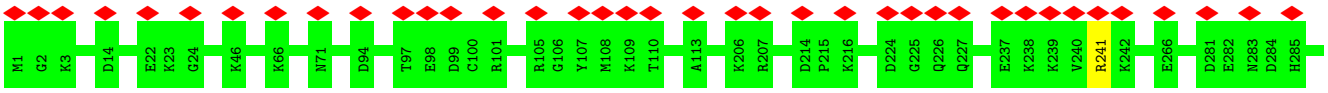


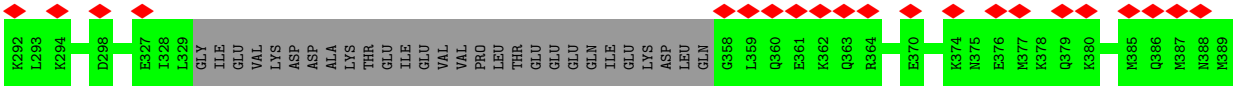


• Molecule 6: 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase

Chain w:

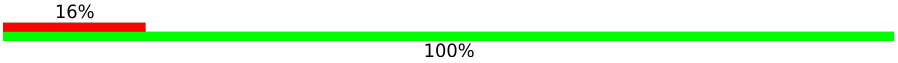


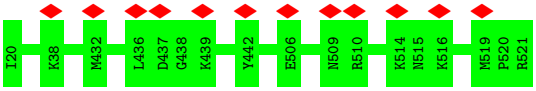




• Molecule 7: 60S ribosome biogenesis factor Nog1

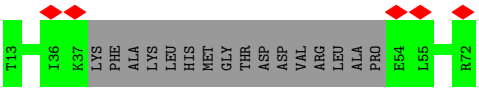
Chain b:





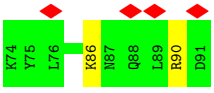
• Molecule 8: 60S ribosomal protein L31-A

Chain d:



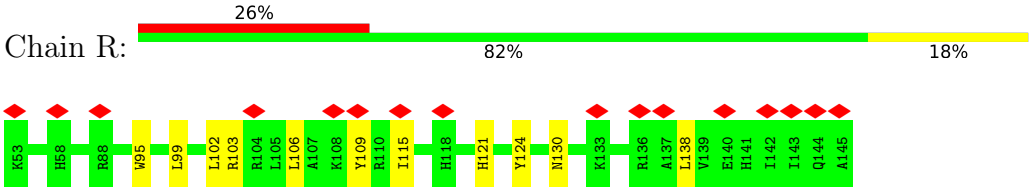
• Molecule 9: 60S ribosomal protein L22-A

Chain U:



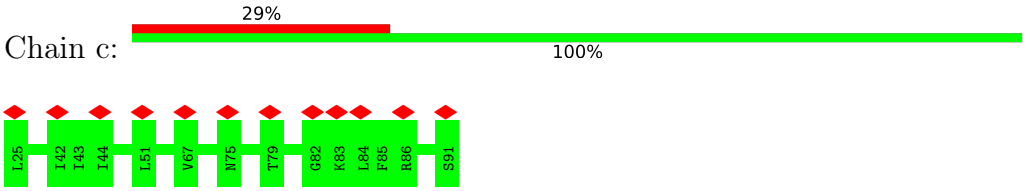
• Molecule 10: 60S ribosome ribosomal protein L19A

Chain R:



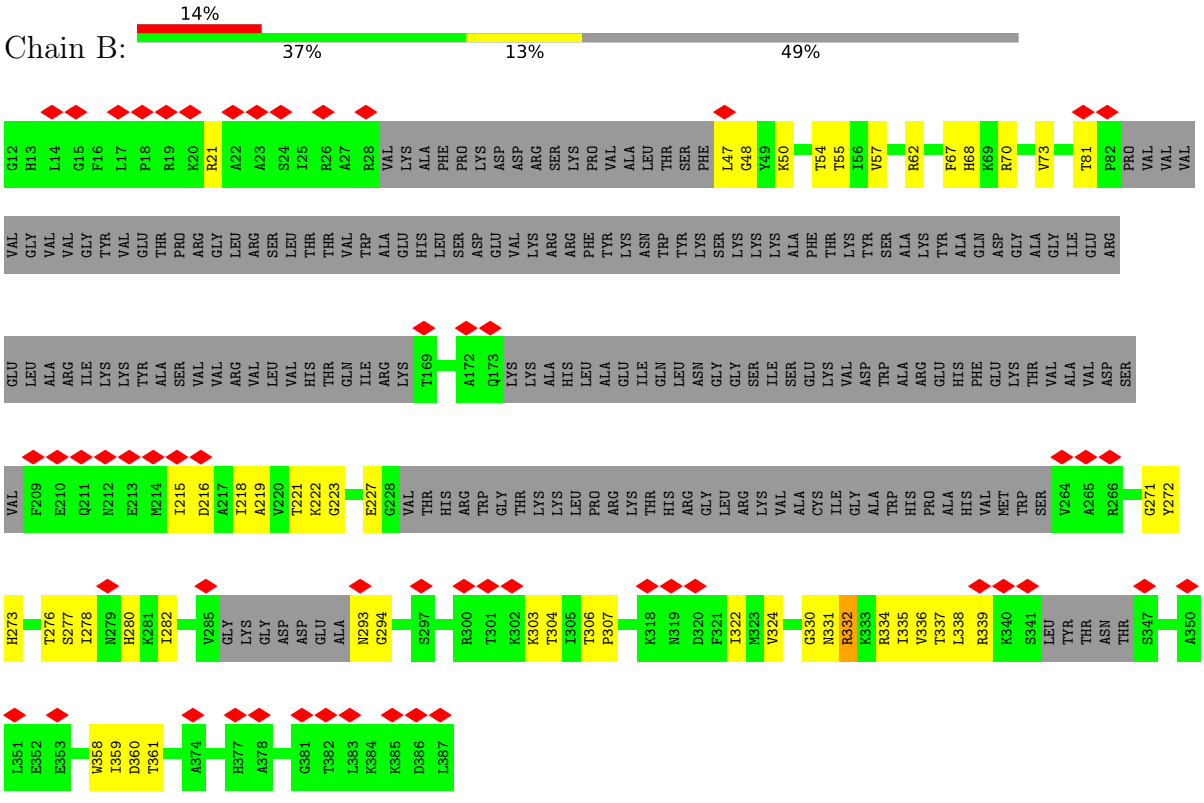
• Molecule 11: 60S ribosomal protein L30

Chain c:



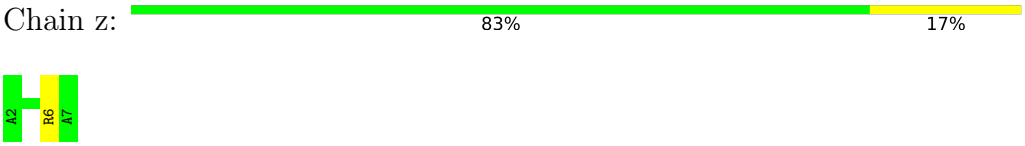
• Molecule 12: 60S ribosomal protein L3

Chain B:



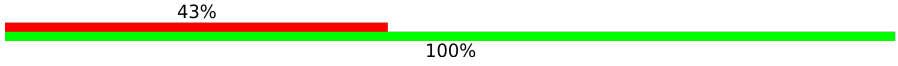
• Molecule 13: UPF0642 protein YBL028C

Chain z:



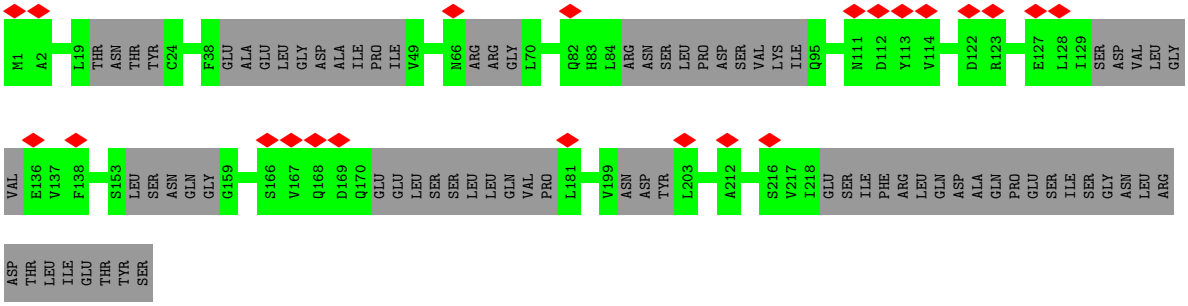
• Molecule 14: Nuclear GTP-binding protein NUG1

Chain s:



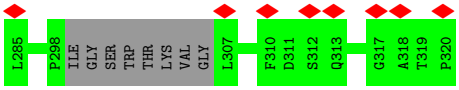
• Molecule 15: Eukaryotic translation initiation factor 6

Chain y:



• Molecule 16: 25S rRNA (cytosine(2870)-C(5))-methyltransferase

Chain q:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	198000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.2	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.102	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	453.6, 453.6, 453.6	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, OMU, OMG, SAH, A2M

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	1	0.23	0/8872	0.75	3/13766 (0.0%)
2	5	0.25	0/924	0.53	0/1214
3	8	0.23	0/334	0.51	0/434
4	V	0.27	0/1008	0.54	0/1356
5	u	0.26	0/558	0.51	0/740
6	w	0.25	0/3012	0.47	0/4038
7	b	0.24	0/619	0.54	0/821
8	d	0.25	0/374	0.52	0/495
9	U	0.24	0/167	0.38	0/219
10	R	0.24	0/538	0.49	0/717
11	c	0.25	0/313	0.46	0/420
12	B	0.26	0/1516	0.53	0/2021
13	z	0.21	0/43	0.54	0/55
14	s	0.25	0/65	0.73	0/82
15	y	0.25	0/1257	0.52	0/1698
16	q	0.24	0/212	0.45	0/289
All	All	0.24	0/19812	0.64	3/28365 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	3306	U	C2-N1-C1'	6.10	125.02	117.70
1	1	3306	U	N1-C2-O2	5.30	126.51	122.80
1	1	3306	U	N3-C2-O2	-5.11	118.62	122.20

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	1	8046	0	4083	81	0
2	5	918	0	957	7	0
3	8	332	0	373	3	0
4	V	993	0	1040	10	0
5	u	543	0	557	0	0
6	w	2959	0	3053	0	0
7	b	613	0	670	0	0
8	d	369	0	403	0	0
9	U	165	0	186	2	0
10	R	529	0	576	11	0
11	c	310	0	321	0	0
12	B	1493	0	1534	32	0
13	z	44	0	51	0	0
14	s	66	0	80	0	0
15	y	1250	0	1243	0	0
16	q	210	0	217	0	0
17	w	26	0	19	0	0
18	w	2	0	0	0	0
All	All	18868	0	15363	126	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 7.

The worst 5 of 126 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)
1:1:1720:U:H2'	10:R:103:ARG:HD3	1.71	0.71
1:1:1680:G:OP2	9:U:90:ARG:NH2	2.24	0.69
1:1:3021:A:H61	1:1:3032:A:H3'	1.59	0.67
12:B:47:LEU:HD12	12:B:335:ILE:HD11	1.76	0.67
4:V:109:MET:HE3	4:V:129:VAL:HA	1.79	0.64

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	
2	5	99/105 (94%)	92 (93%)	7 (7%)	0	100	100
3	8	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
4	V	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
5	u	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
6	w	357/389 (92%)	329 (92%)	28 (8%)	0	100	100
7	b	68/74 (92%)	66 (97%)	2 (3%)	0	100	100
8	d	40/60 (67%)	40 (100%)	0	0	100	100
9	U	16/18 (89%)	16 (100%)	0	0	100	100
10	R	56/62 (90%)	54 (96%)	2 (4%)	0	100	100
11	c	35/41 (85%)	35 (100%)	0	0	100	100
12	B	176/376 (47%)	173 (98%)	3 (2%)	0	100	100
13	z	4/6 (67%)	4 (100%)	0	0	100	100
14	s	5/7 (71%)	5 (100%)	0	0	100	100
15	y	149/245 (61%)	145 (97%)	4 (3%)	0	100	100
16	q	24/36 (67%)	23 (96%)	1 (4%)	0	100	100
All	All	1261/1657 (76%)	1208 (96%)	53 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	5	100/100 (100%)	100 (100%)	0	100 100
3	8	37/37 (100%)	37 (100%)	0	100 100
4	V	103/103 (100%)	103 (100%)	0	100 100
5	u	56/56 (100%)	56 (100%)	0	100 100
6	w	328/354 (93%)	327 (100%)	1 (0%)	92 97
7	b	66/66 (100%)	66 (100%)	0	100 100
8	d	38/51 (74%)	38 (100%)	0	100 100
9	U	18/18 (100%)	18 (100%)	0	100 100
10	R	56/56 (100%)	56 (100%)	0	100 100
11	c	32/32 (100%)	32 (100%)	0	100 100
12	B	156/313 (50%)	155 (99%)	1 (1%)	86 94
13	z	4/4 (100%)	3 (75%)	1 (25%)	0 2
14	s	7/7 (100%)	7 (100%)	0	100 100
15	y	141/211 (67%)	141 (100%)	0	100 100
16	q	24/30 (80%)	24 (100%)	0	100 100
All	All	1166/1438 (81%)	1163 (100%)	3 (0%)	92 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	w	241	ARG
12	B	332	ARG
13	z	6	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
6	w	235	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	354/378 (93%)	70 (19%)	2 (0%)

5 of 70 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	860	G
1	1	861	C
1	1	1302	A
1	1	1303	A
1	1	1304	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1302	A
1	1	1307	G

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	OMG	1	2922	1	18,26,27	1.33	2 (11%)	19,38,41	1.49	2 (10%)
1	PSU	1	2923	1	18,21,22	1.21	3 (16%)	22,30,33	1.60	2 (9%)
1	OMU	1	2921	1	19,22,23	0.76	0	26,31,34	0.92	2 (7%)
1	A2M	1	2946	1	18,25,26	1.47	2 (11%)	18,36,39	1.07	1 (5%)

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
1	OMG	1	2922	1	-	3/5/27/28	0/3/3/3
1	PSU	1	2923	1	-	4/7/25/26	0/2/2/2
1	OMU	1	2921	1	-	2/9/27/28	0/2/2/2
1	A2M	1	2946	1	-	1/5/27/28	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2946	A2M	O5'-C5'	-4.45	1.33	1.44
1	1	2922	OMG	C6-N1	4.05	1.43	1.37
1	1	2923	PSU	C2-N1	3.12	1.41	1.36
1	1	2922	OMG	C2-N2	2.53	1.40	1.34
1	1	2923	PSU	C4-N3	2.46	1.43	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2923	PSU	C6-C5-C4	4.89	121.62	118.20
1	1	2922	OMG	O6-C6-N1	-4.08	115.83	120.65
1	1	2922	OMG	O6-C6-C5	3.34	130.90	124.37
1	1	2923	PSU	O2-C2-N1	-2.65	119.87	122.79
1	1	2921	OMU	CM2-O2'-C2'	-2.37	108.30	114.52

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	2922	OMG	O4'-C4'-C5'-O5'
1	1	2922	OMG	C3'-C4'-C5'-O5'
1	1	2922	OMG	C1'-C2'-O2'-CM2
1	1	2923	PSU	C3'-C4'-C5'-O5'
1	1	2923	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2922	OMG	1	0
1	1	2921	OMU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
17	SAH	w	801	-	24,28,28	1.21	3 (12%)	25,40,40	1.71	5 (20%)

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
17	SAH	w	801	-	-	3/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	w	801	SAH	C2-N3	3.97	1.38	1.32
17	w	801	SAH	C2-N1	2.47	1.38	1.33
17	w	801	SAH	OXT-C	-2.17	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	w	801	SAH	N3-C2-N1	-5.39	120.25	128.68
17	w	801	SAH	C5'-SD-CG	-3.89	90.60	102.27
17	w	801	SAH	C3'-C2'-C1'	2.77	105.15	100.98
17	w	801	SAH	OXT-C-O	-2.69	117.99	124.09
17	w	801	SAH	OXT-C-CA	2.28	121.17	113.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

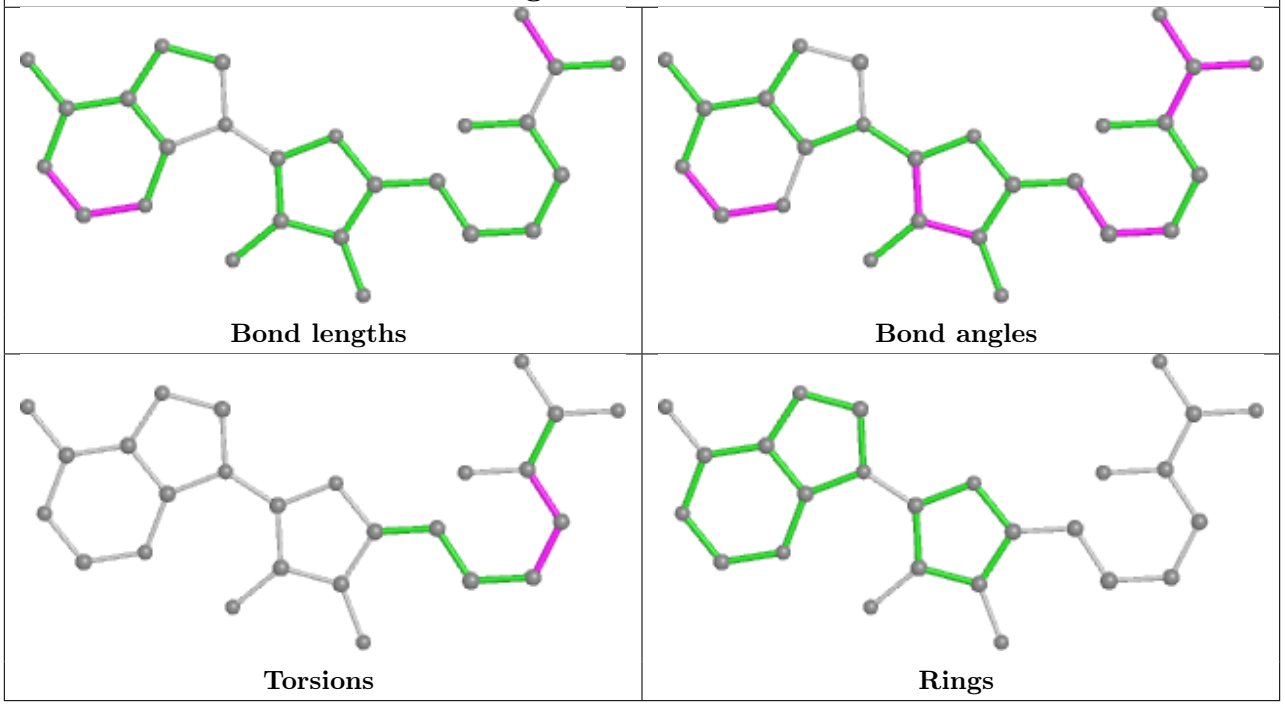
Mol	Chain	Res	Type	Atoms
17	w	801	SAH	N-CA-CB-CG
17	w	801	SAH	C-CA-CB-CG
17	w	801	SAH	CA-CB-CG-SD

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 then 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.

Ligand SAH w 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	23
7	b	2
2	5	2
10	R	2
11	c	2

The worst 5 of 31 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	864:G	O3'	1301:A	P	85.70
1	1	1308:A	O3'	1456:A	P	72.27
1	b	56:GLY	C	432:MET	N	72.22
1	5	94:LEU	C	212:LYS	N	66.39
1	b	442:TYR	C	496:ILE	N	56.37

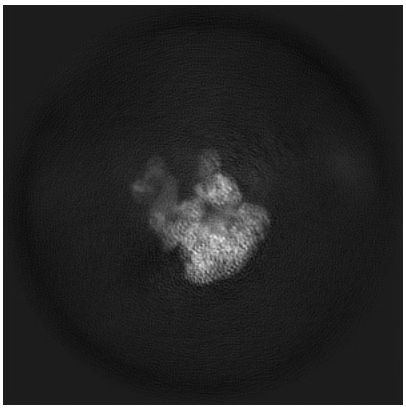
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24271. These allow visual inspection of the internal detail of the map and identification of artifacts.

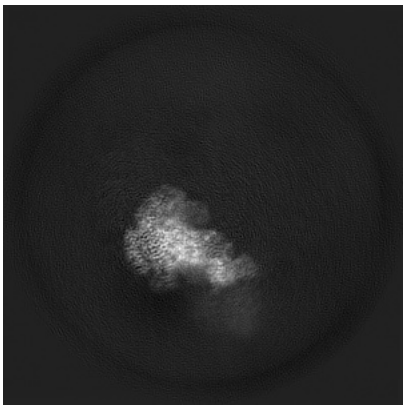
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

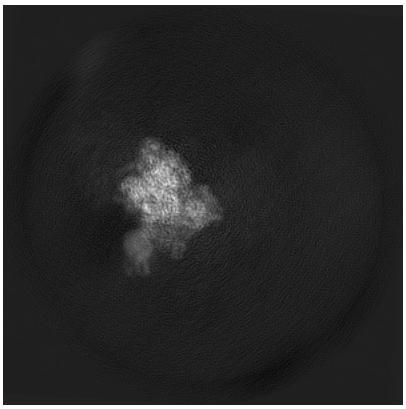
6.1.1 Primary map



X

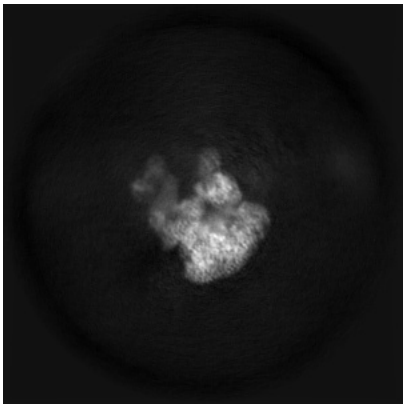


Y

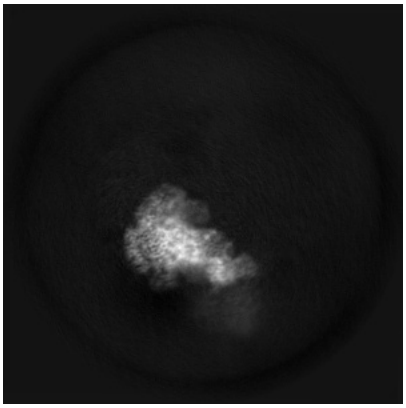


Z

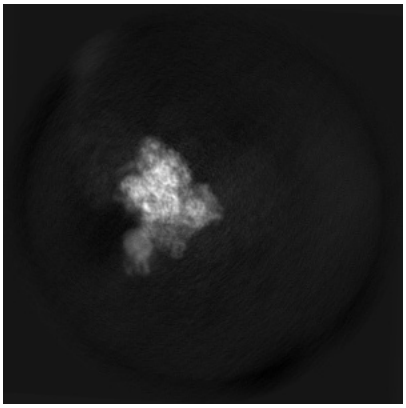
6.1.2 Raw map



X



Y

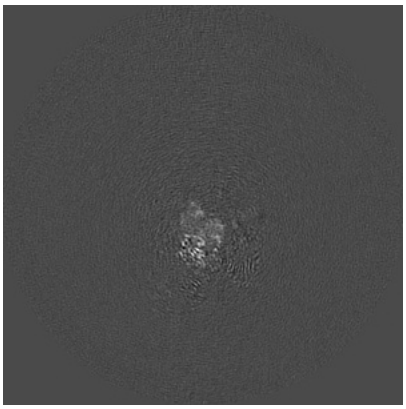


Z

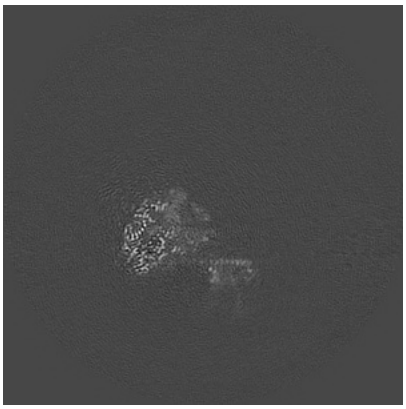
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

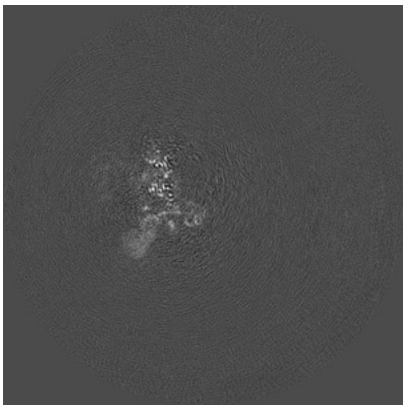
6.2.1 Primary map



X Index: 210

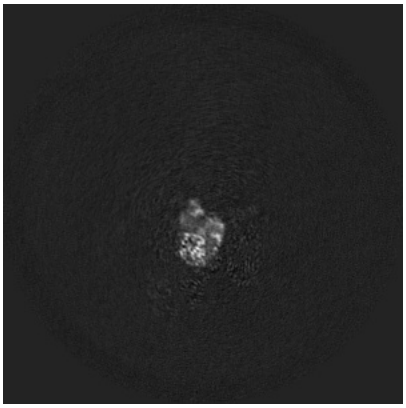


Y Index: 210

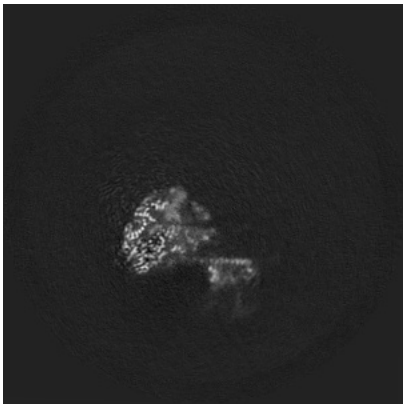


Z Index: 210

6.2.2 Raw map



X Index: 210



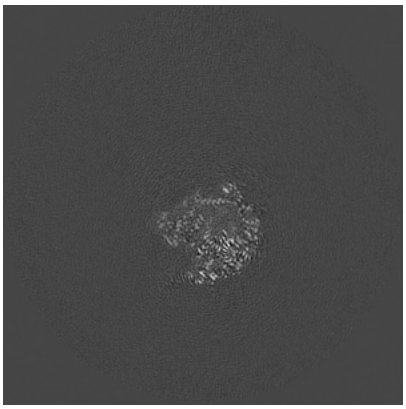
Y Index: 210

Z Index: 210

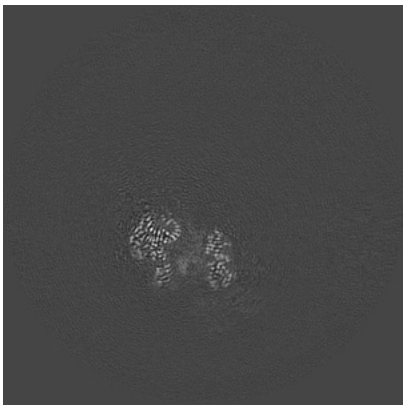
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

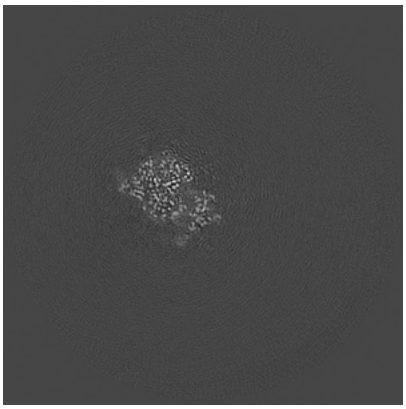
6.3.1 Primary map



X Index: 174

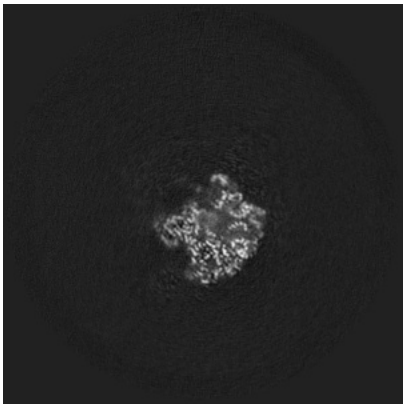


Y Index: 233

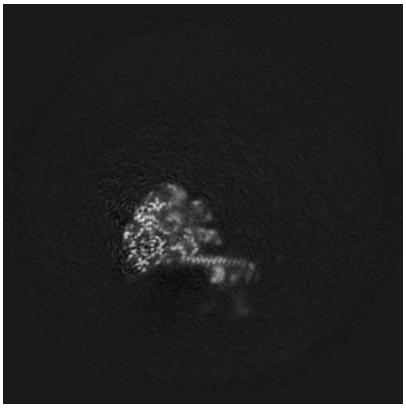


Z Index: 162

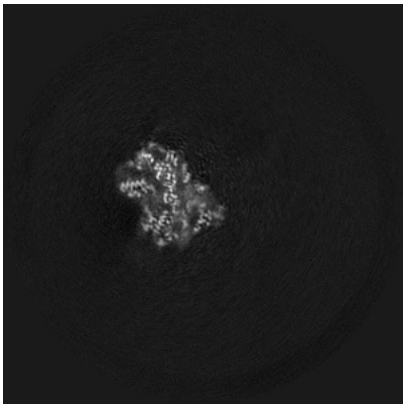
6.3.2 Raw map



X Index: 168



Y Index: 206

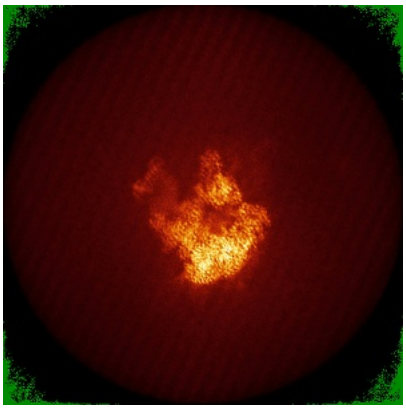


Z Index: 173

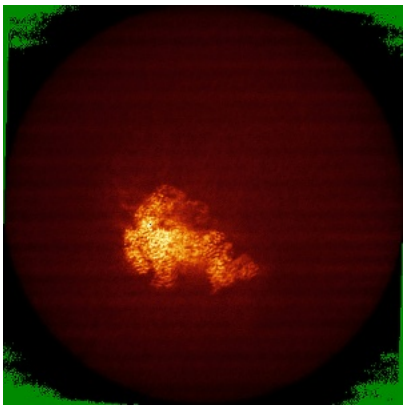
The images above show the largest variance slices of the map in three orthogonal directions.

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

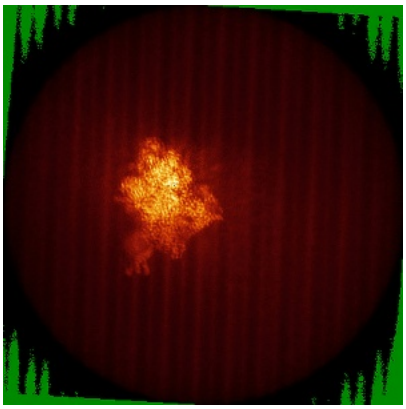
6.4.1 Primary map



X

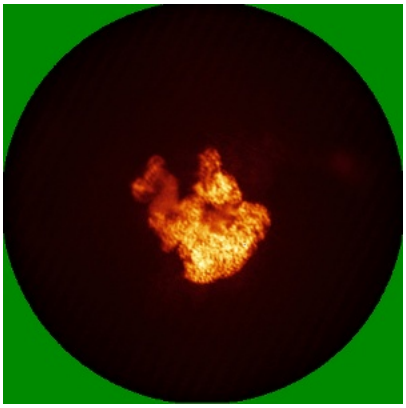


Y



Z

6.4.2 Raw map



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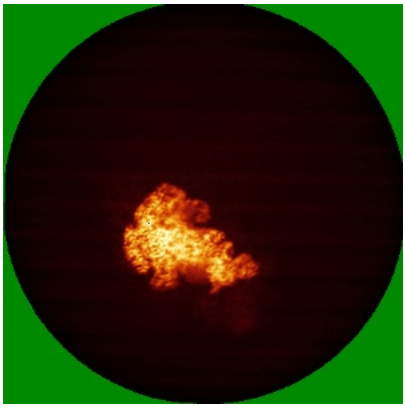

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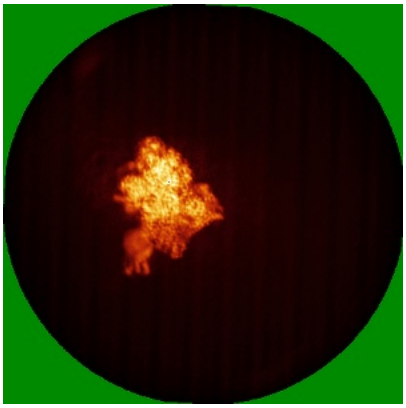


Z

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 0.018. 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

X Y Z

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.

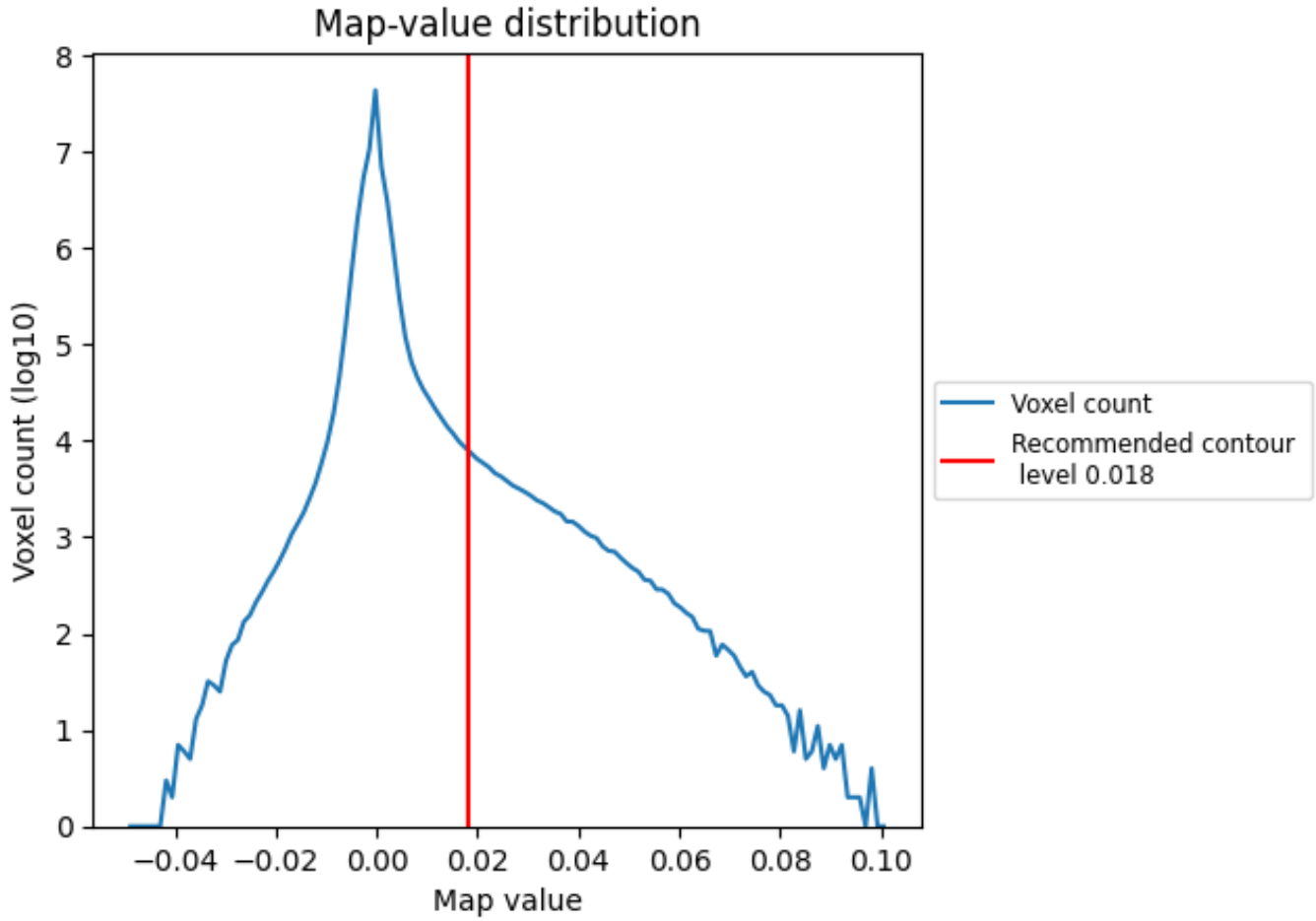
6.6 Mask visualisation (i)

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

7 Map analysis

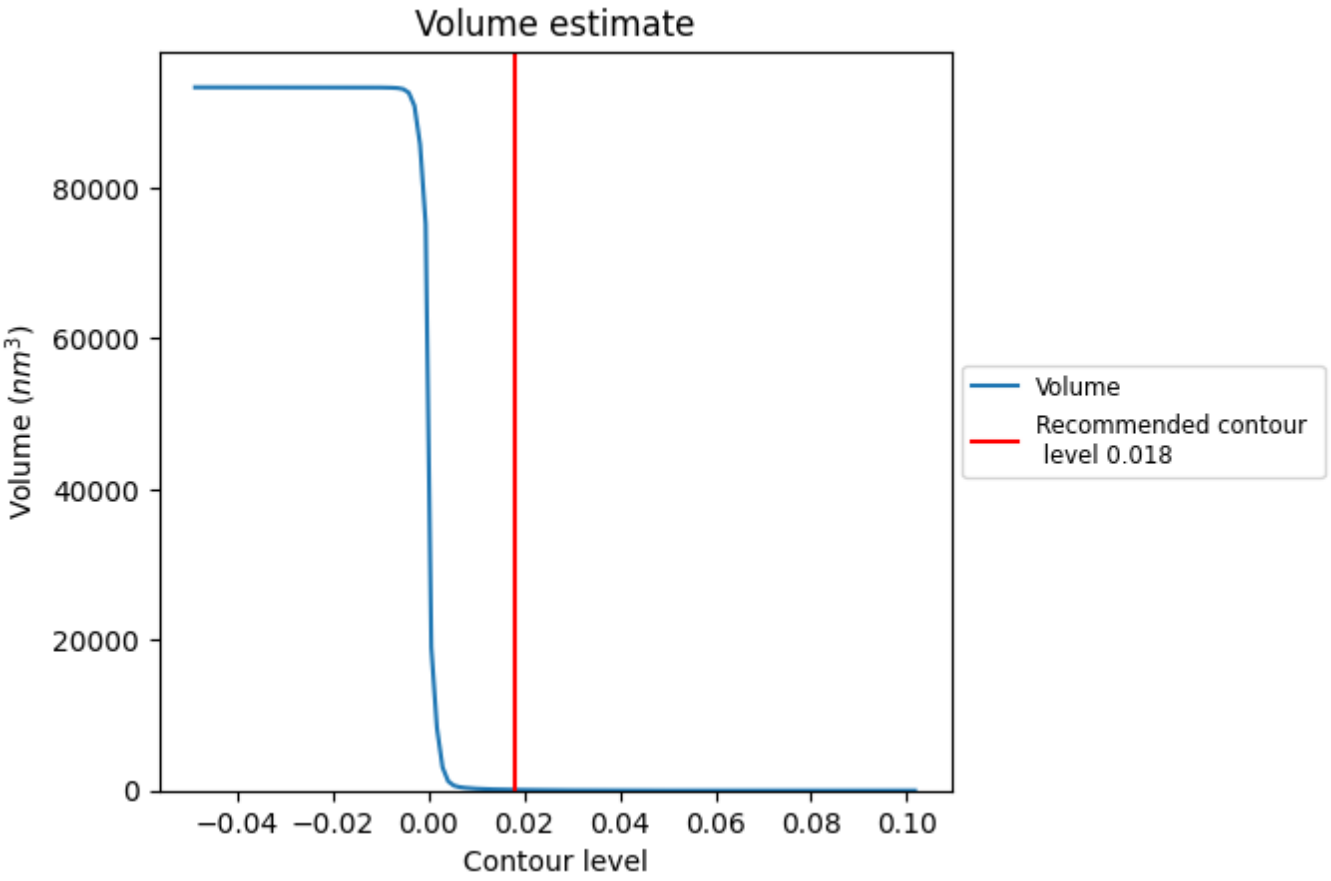
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

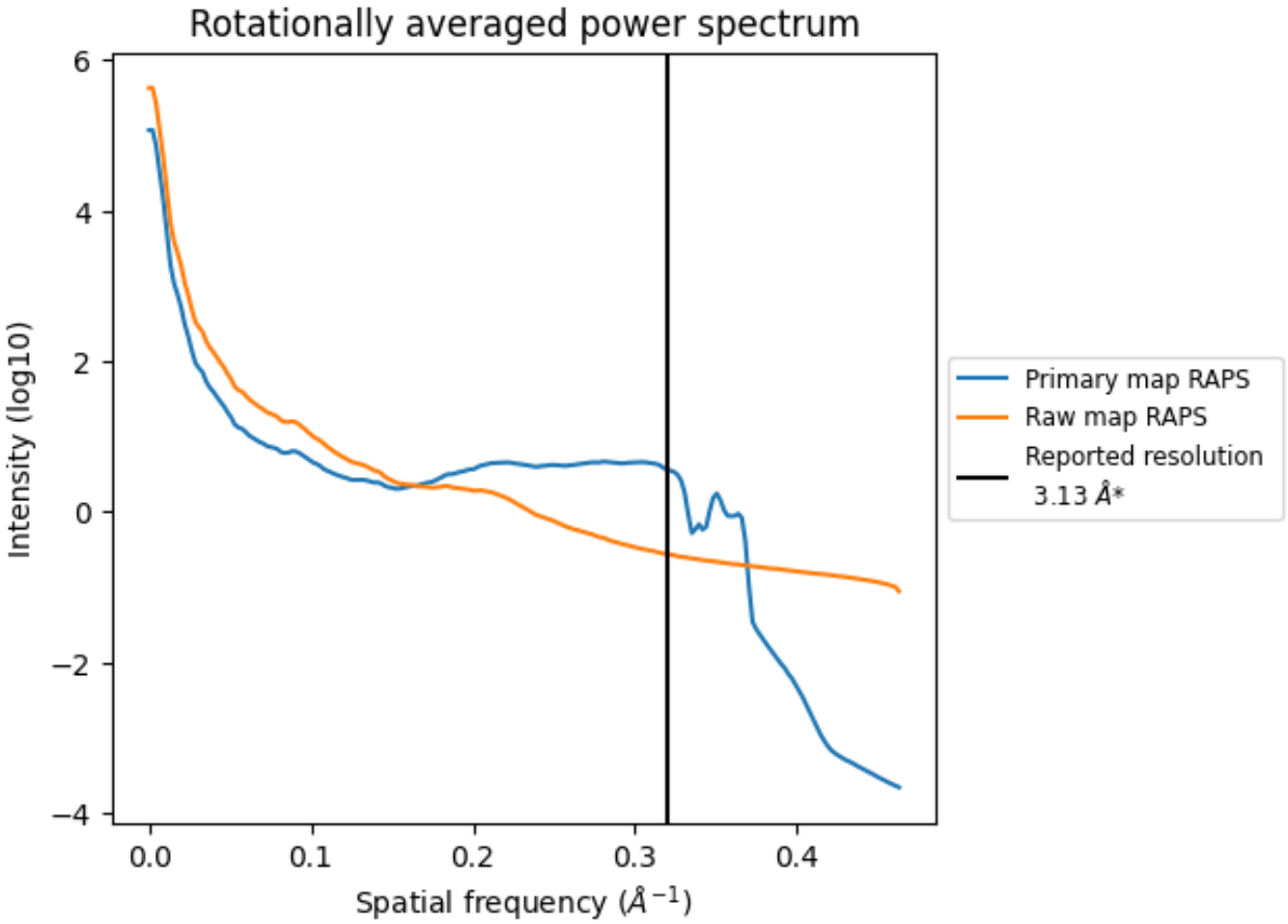
7.2 Volume estimate (i)



The volume at the recommended contour level is 101 nm^3; this corresponds to an approximate mass of 92 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)

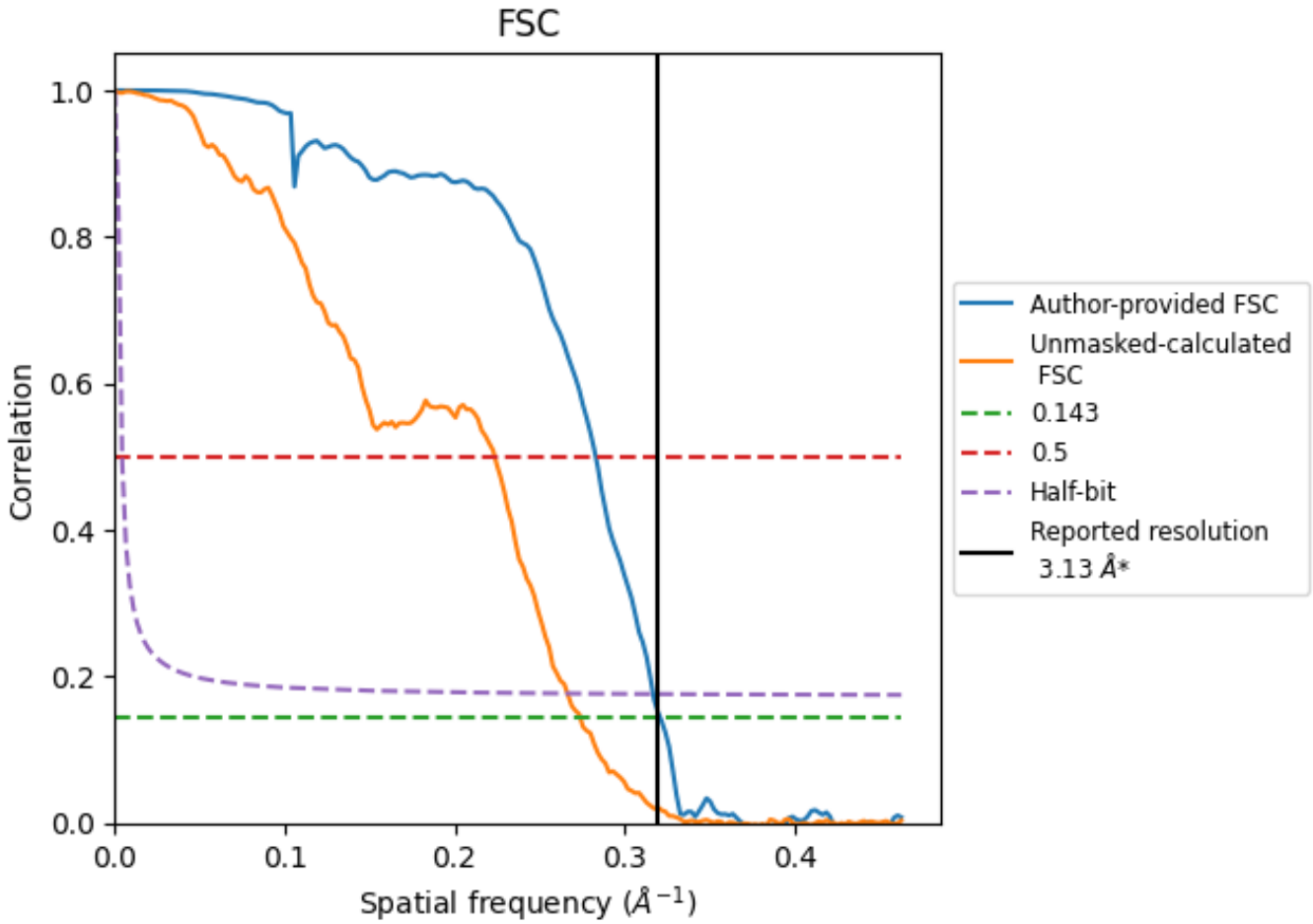


*Reported resolution corresponds to spatial frequency of 0.319 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.319 Å^{-1}

8.2 Resolution estimates (i)

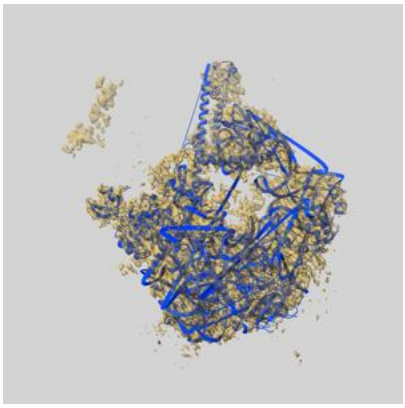
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.11	3.53	3.16
Unmasked-calculated*	3.65	4.47	3.75

*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 3.65 differs from the reported value 3.13 by more than 10 %

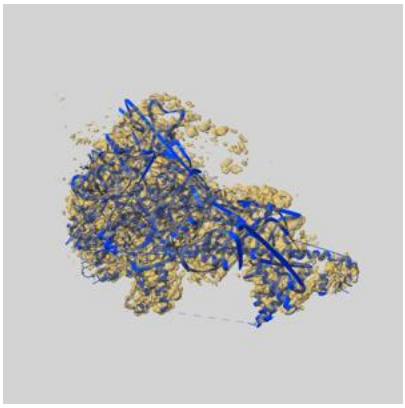
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24271 and PDB model 7NAF. Per-residue inclusion information can be found in section 3 on page 7.

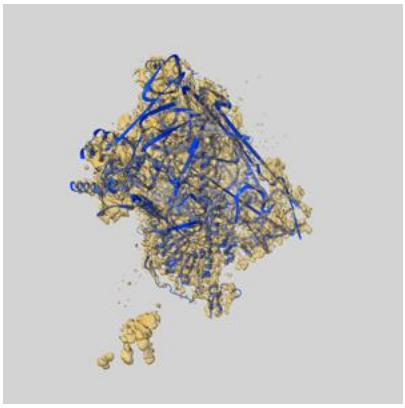
9.1 Map-model overlay



X



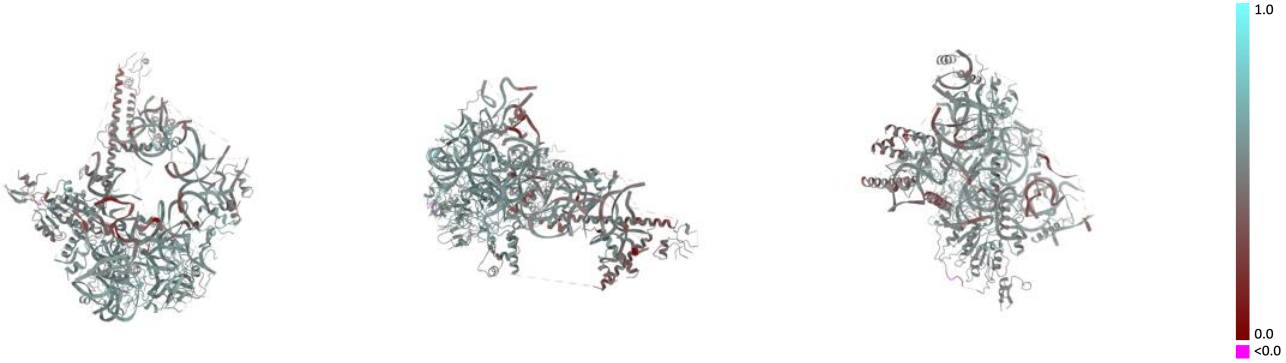
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

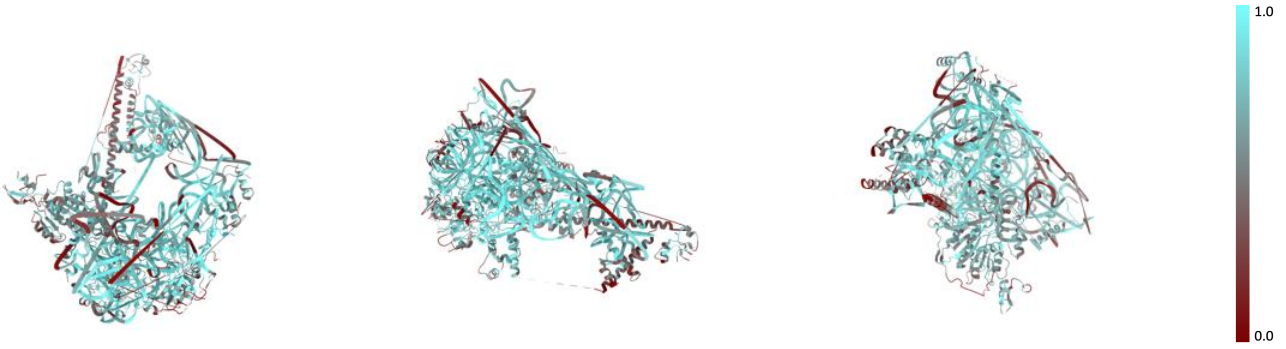
9.2 Q-score mapped to coordinate model (i)



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.

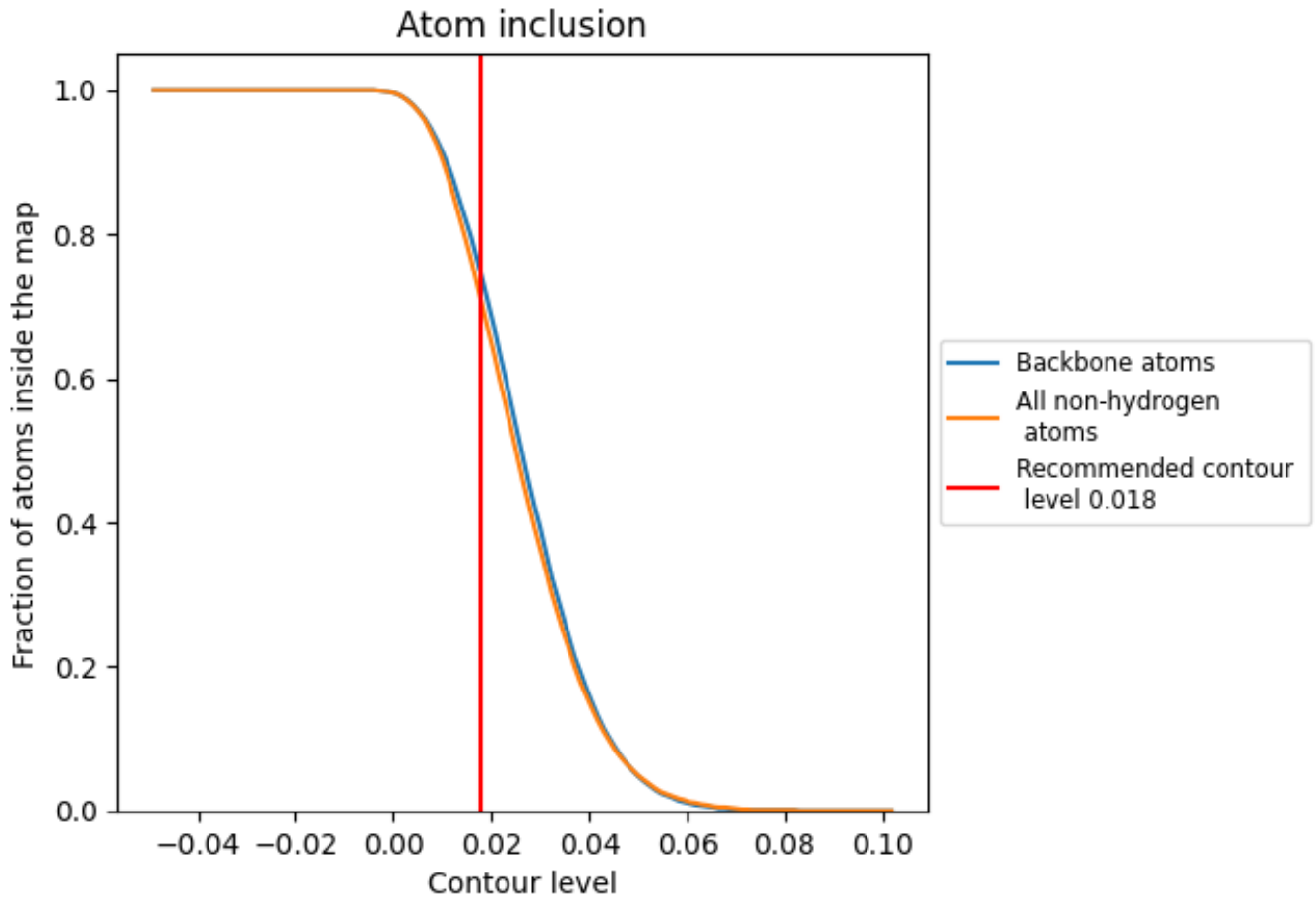
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 70% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7050	0.5130
1	0.7850	0.5100
5	0.4480	0.4370
8	0.6460	0.5140
B	0.6330	0.5420
R	0.5660	0.4690
U	0.5690	0.4830
V	0.8300	0.5720
b	0.6550	0.5120
c	0.5350	0.4550
d	0.7100	0.5460
q	0.5190	0.4710
s	0.5000	0.4840
u	0.8850	0.5760
w	0.6280	0.5030
y	0.7120	0.5330
z	0.6910	0.5720