



Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 09:08 PM EDT

PDB ID : 5U4J
EMDB ID : EMD-8506
Title : Structural Basis of Co-translational Quality Control by ArfA and RF2 Bound to Ribosome
Authors : Zeng, F.; Chen, Y.; Remis, J.; Shekhar, M.; Phillips, J.C.; Tajkhorshid, E.; Jin, H.
Deposited on : 2016-12-04
Resolution : 3.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

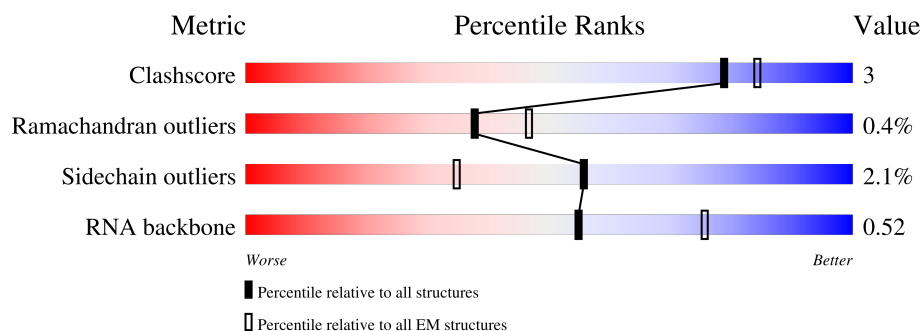
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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 $\leq 5\%$. 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	a	1533	 15% 5% 80%
2	A	2904	 100%
3	c	233	 9% 91%
4	d	206	 15% 32% 68%
5	e	167	 13% 80% 19%
6	z	18	 17% 28% 6% 67%
7	x	77	 19% 81%

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Mol	Chain	Length	Quality of chain
8	l	124	<div><div></div><div>18%</div><div>98%</div><div></div></div>
9	v	383	<div><div></div><div>21%</div><div>34%</div><div></div><div>66%</div></div>
10	w	57	<div><div></div><div>25%</div><div>72%</div><div>11%</div><div>18%</div></div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 11360 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	307	Total	C	N	O	P	0	0
			6591	2944	1198	2142	307		

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	11	Total	C	N	O	P	0	0
			233	105	42	75	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	887	A	U	conflict	GB 42756

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	c	21	Total	C	N	O	0	0
			169	105	32	32		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	65	Total	C	N	O	S	0	0
			523	327	106	89	1		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	136	Total	C	N	O	S	0	0
			1001	625	190	182	4		

- Molecule 6 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	z	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 7 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	x	15	Total	C	N	O	P	0	0
			315	141	54	105	15		

- Molecule 8 is a protein called 30S ribosomal protein S12.

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

- Molecule 9 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	v	132	Total	C	N	O	S	0	0
			1054	659	182	208	5		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-17	HIS	-	expression tag	UNP P07012
v	-16	HIS	-	expression tag	UNP P07012
v	-15	HIS	-	expression tag	UNP P07012
v	-14	HIS	-	expression tag	UNP P07012
v	-13	HIS	-	expression tag	UNP P07012
v	-12	HIS	-	expression tag	UNP P07012
v	-11	SER	-	expression tag	UNP P07012
v	-10	ALA	-	expression tag	UNP P07012
v	-9	ALA	-	expression tag	UNP P07012
v	-8	LEU	-	expression tag	UNP P07012
v	-7	GLU	-	expression tag	UNP P07012
v	-6	VAL	-	expression tag	UNP P07012
v	-5	LEU	-	expression tag	UNP P07012
v	-4	PHE	-	expression tag	UNP P07012
v	-3	GLN	-	expression tag	UNP P07012
v	-2	GLY	-	expression tag	UNP P07012
v	-1	PRO	-	expression tag	UNP P07012
v	0	GLY	-	expression tag	UNP P07012

- Molecule 10 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	w	47	Total	C	N	O	S	0	0
			388	239	82	66	1		

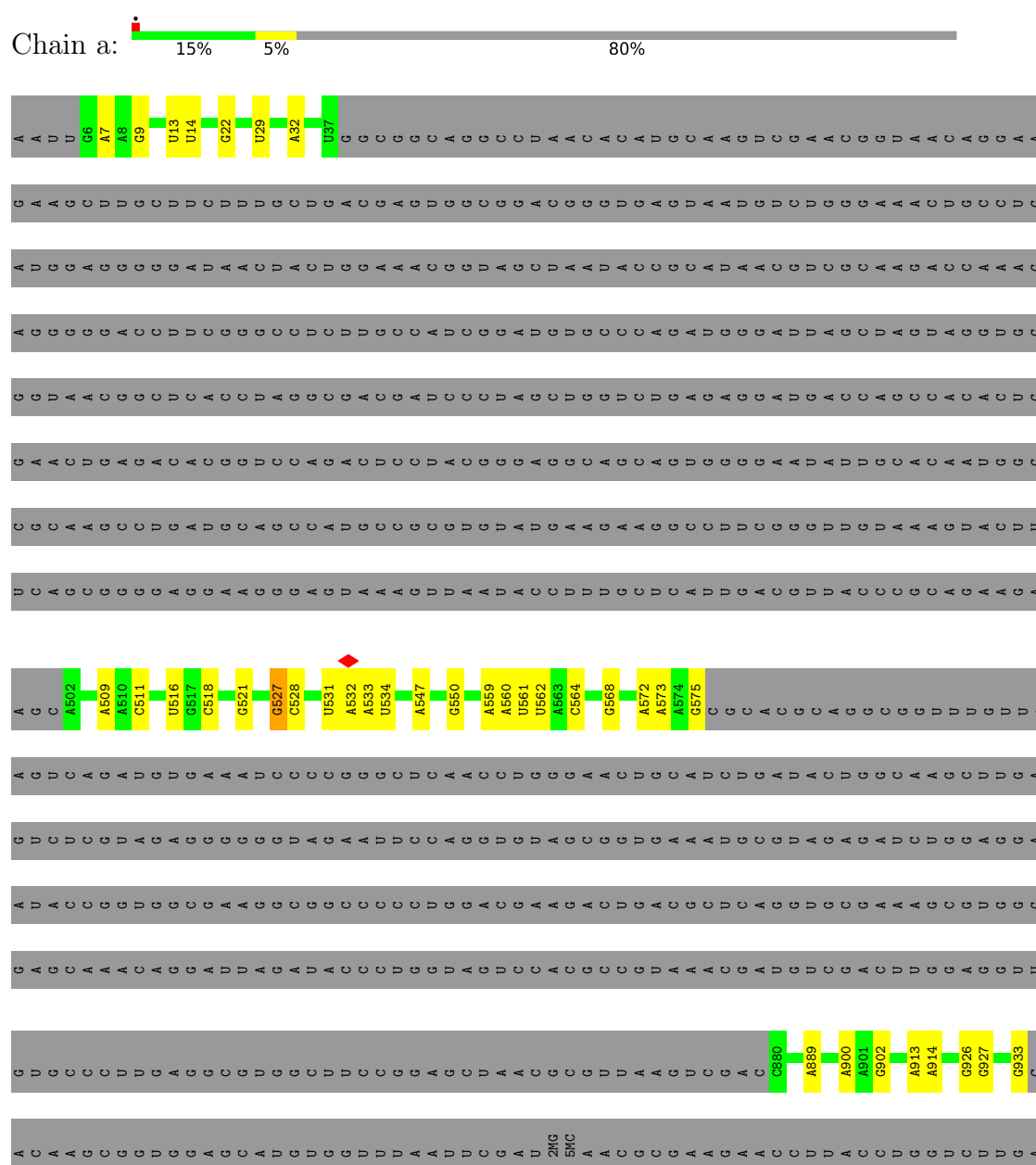
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	-1	GLY	-	expression tag	UNP P36675
w	0	SER	-	expression tag	UNP P36675

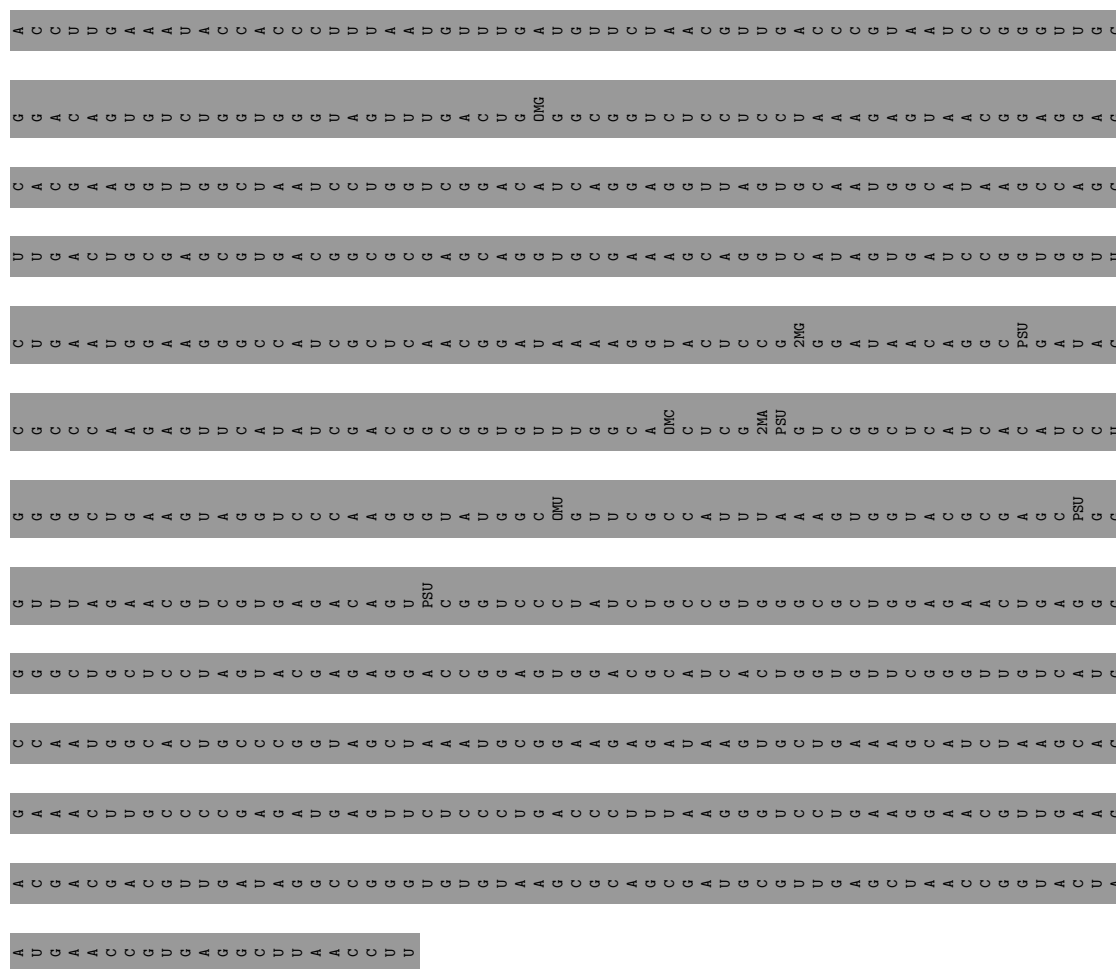
3 Residue-property plots [i](#)

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.

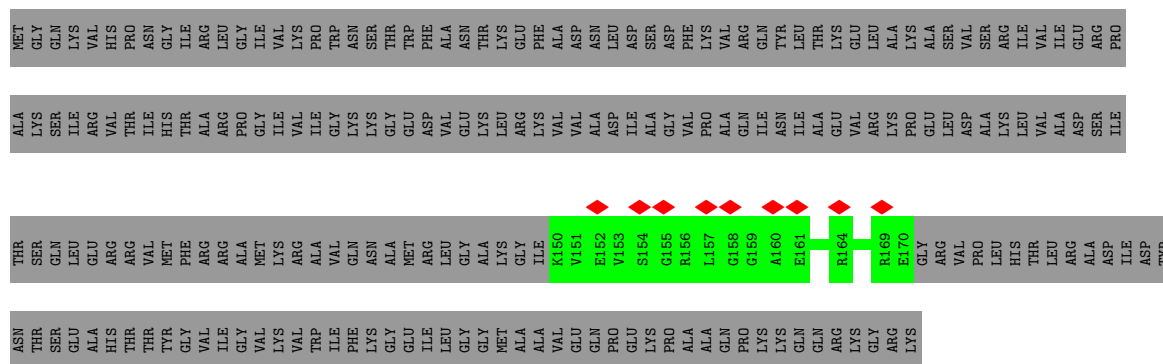
• Molecule 1: 16S rRNA



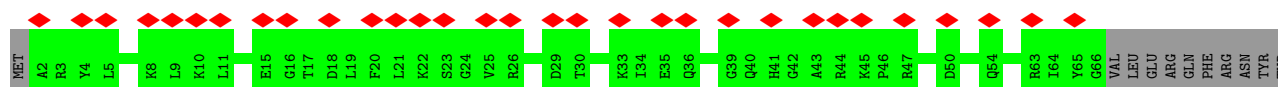
WORLDWIDE
PDB
PROTEIN DATA BANK



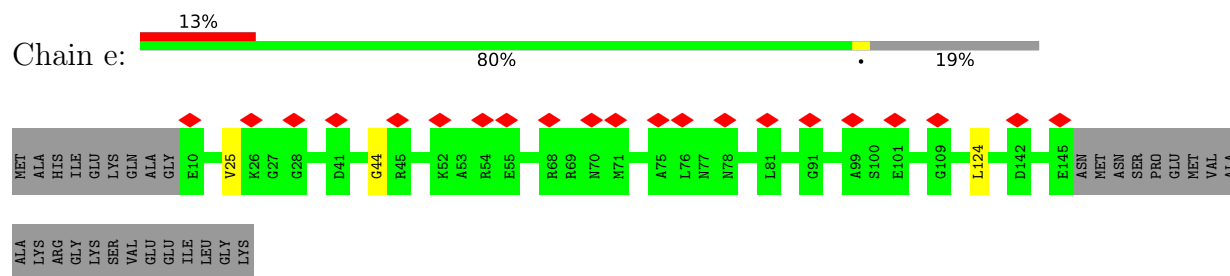
- Molecule 3: 30S ribosomal protein S3



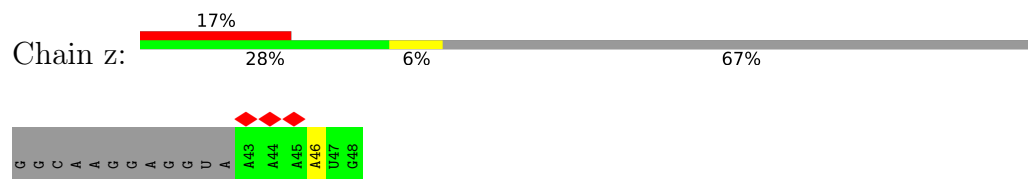
- Molecule 4: 30S ribosomal protein S4



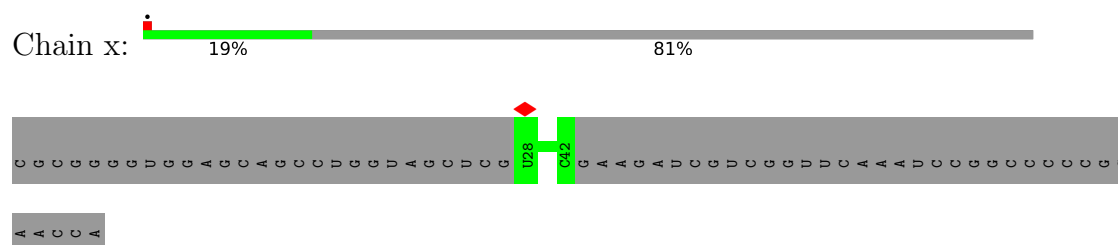
- Molecule 5: 30S ribosomal protein S5



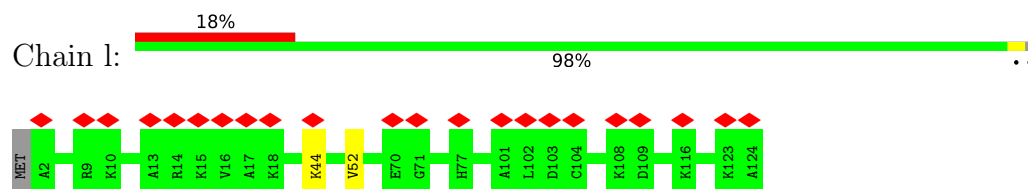
- Molecule 6: mRNA



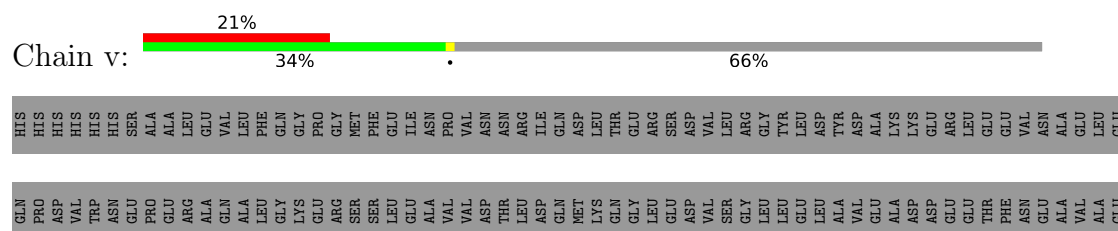
- Molecule 7: P-site tRNA fMet

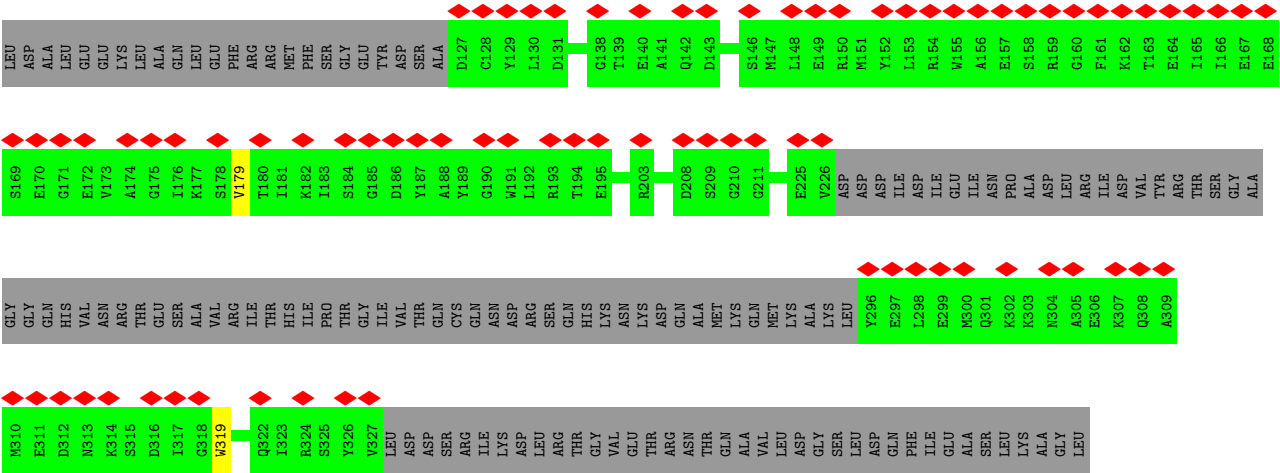


- Molecule 8: 30S ribosomal protein S12

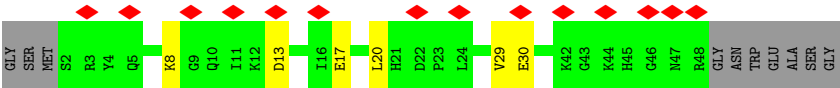


- Molecule 9: Peptide chain release factor 2





● Molecule 10: Alternative ribosome-rescue factor A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	155440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	83822	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.236	Depositor
Minimum map value	-0.193	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	458.112, 458.112, 458.112	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.193, 1.193, 1.193	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: 2MG, MA6, 5MC, 4OC, UR3, PSU, G7M

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	a	0.23	0/7167	0.64	3/11159 (0.0%)
2	A	0.18	0/216	0.63	0/334
3	c	0.37	0/171	0.51	0/228
4	d	0.37	0/530	0.55	0/704
5	e	0.36	0/1013	0.56	0/1365
6	z	0.19	0/147	0.59	0/227
7	x	0.20	0/350	0.63	0/542
8	l	0.35	0/969	0.59	0/1300
9	v	0.39	0/1075	0.52	0/1443
10	w	0.34	0/394	0.69	2/519 (0.4%)
All	All	0.28	0/12032	0.62	5/17821 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	527	G7M	O3'-P-O5'	9.93	122.87	104.00
10	w	8	LYS	CB-CA-C	5.74	121.87	110.40
1	a	528	C	OP1-P-OP2	-5.62	111.17	119.60
10	w	20	LEU	CA-CB-CG	5.23	127.33	115.30
1	a	1070	U	C2'-C3'-O3'	5.02	121.73	113.70

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	a	6591	0	3340	0	0
2	A	233	0	119	0	0
3	c	169	0	165	0	0
4	d	523	0	558	0	0
5	e	1001	0	1039	0	0
6	z	131	0	66	0	0
7	x	315	0	163	0	0
8	l	955	0	1016	0	0
9	v	1054	0	1004	0	0
10	w	388	0	400	0	0
All	All	11360	0	7870	0	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 3.

There are no clashes within the asymmetric unit.

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	
3	c	19/233 (8%)	18 (95%)	1 (5%)	0	100	100
4	d	63/206 (31%)	62 (98%)	1 (2%)	0	100	100
5	e	134/167 (80%)	123 (92%)	10 (8%)	1 (1%)	22	59
8	l	121/124 (98%)	114 (94%)	6 (5%)	1 (1%)	19	56
9	v	128/383 (33%)	121 (94%)	7 (6%)	0	100	100
10	w	45/57 (79%)	41 (91%)	4 (9%)	0	100	100
All	All	510/1170 (44%)	479 (94%)	29 (6%)	2 (0%)	38	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	l	44	LYS
5	e	44	GLY

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	
3	c	16/190 (8%)	16 (100%)	0	100	100
4	d	54/173 (31%)	54 (100%)	0	100	100
5	e	102/126 (81%)	100 (98%)	2 (2%)	55	74
8	l	103/104 (99%)	102 (99%)	1 (1%)	76	86
9	v	110/325 (34%)	108 (98%)	2 (2%)	59	77
10	w	40/46 (87%)	36 (90%)	4 (10%)	7	32
All	All	425/964 (44%)	416 (98%)	9 (2%)	56	74

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	25	VAL
5	e	124	LEU
8	l	52	VAL
9	v	179	VAL
9	v	319	TRP
10	w	13	ASP
10	w	17	GLU
10	w	29	VAL
10	w	30	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
5	e	132	ASN

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Mol	Chain	Res	Type
9	v	214	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	297/1533 (19%)	68 (22%)	0
2	A	10/2904 (0%)	2 (20%)	1 (10%)
6	z	5/18 (27%)	1 (20%)	0
7	x	14/77 (18%)	0	0
All	All	326/4532 (7%)	71 (21%)	1 (0%)

All (71) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	7	A
1	a	9	G
1	a	13	U
1	a	14	U
1	a	22	G
1	a	29	U
1	a	32	A
1	a	509	A
1	a	511	C
1	a	518	C
1	a	521	G
1	a	527	G7M
1	a	531	U
1	a	532	A
1	a	533	A
1	a	534	U
1	a	547	A
1	a	550	G
1	a	559	A
1	a	560	A
1	a	561	U
1	a	562	U
1	a	564	C
1	a	568	G
1	a	572	A
1	a	573	A
1	a	575	G

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Mol	Chain	Res	Type
1	a	889	A
1	a	900	A
1	a	902	G
1	a	913	A
1	a	914	A
1	a	926	G
1	a	927	G
1	a	933	G
1	a	1054	C
1	a	1056	U
1	a	1064	G
1	a	1065	U
1	a	1066	C
1	a	1071	C
1	a	1074	G
1	a	1081	A
1	a	1085	U
1	a	1193	G
1	a	1196	A
1	a	1197	A
1	a	1395	C
1	a	1397	C
1	a	1404	C
1	a	1419	G
1	a	1422	G
1	a	1491	G
1	a	1492	A
1	a	1493	A
1	a	1494	G
1	a	1499	A
1	a	1502	A
1	a	1503	A
1	a	1504	G
1	a	1505	G
1	a	1506	U
1	a	1515	G
1	a	1516	2MG
1	a	1517	G
1	a	1528	U
1	a	1529	G
1	a	1530	G
2	A	1913	A

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Mol	Chain	Res	Type
2	A	1914	C
6	z	46	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	1913	A

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

10 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	4OC	a	1402	1	20,23,24	0.87	2 (10%)	26,32,35	1.29	6 (23%)
1	G7M	a	527	1	20,26,27	1.14	2 (10%)	17,39,42	1.00	0
2	PSU	A	1911	2	18,21,22	1.39	3 (16%)	22,30,33	1.91	5 (22%)
2	PSU	A	1917	2	18,21,22	1.40	3 (16%)	22,30,33	1.95	5 (22%)
1	MA6	a	1519	1	19,26,27	1.22	3 (15%)	18,38,41	2.04	6 (33%)
1	5MC	a	1407	1	18,22,23	1.01	1 (5%)	26,32,35	1.26	5 (19%)
1	MA6	a	1518	1	19,26,27	1.25	2 (10%)	18,38,41	2.23	5 (27%)
1	PSU	a	516	1	18,21,22	1.40	3 (16%)	22,30,33	2.03	5 (22%)
1	2MG	a	1516	1	18,26,27	1.00	1 (5%)	16,38,41	1.23	3 (18%)
1	UR3	a	1498	1	19,22,23	1.23	2 (10%)	26,32,35	1.67	2 (7%)

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	4OC	a	1402	1	-	2/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	a	527	1	-	0/3/25/26	0/3/3/3
2	PSU	A	1911	2	-	0/7/25/26	0/2/2/2
2	PSU	A	1917	2	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	5/7/29/30	0/3/3/3
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	4/7/29/30	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	2/5/27/28	0/3/3/3
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1911	PSU	C6-C5	4.29	1.40	1.35
1	a	516	PSU	C6-C5	4.24	1.40	1.35
2	A	1917	PSU	C6-C5	4.23	1.40	1.35
1	a	1407	5MC	C6-C5	3.09	1.39	1.34
1	a	1498	UR3	C2-N1	3.01	1.42	1.38
1	a	527	G7M	C5-C4	2.81	1.44	1.39
1	a	1519	MA6	C5-C4	2.74	1.48	1.40
1	a	1518	MA6	C5-C4	2.69	1.48	1.40
1	a	1518	MA6	C6-N1	2.56	1.36	1.33
1	a	1519	MA6	C6-N1	2.37	1.36	1.33
1	a	527	G7M	C6-N1	-2.30	1.34	1.37
1	a	516	PSU	C4-N3	-2.23	1.34	1.38
2	A	1917	PSU	C4-N3	-2.22	1.34	1.38
2	A	1911	PSU	C4-N3	-2.17	1.34	1.38
2	A	1917	PSU	C4-C5	2.13	1.50	1.44
1	a	1516	2MG	O4'-C1'	2.12	1.44	1.41
1	a	516	PSU	C4-C5	2.10	1.50	1.44
1	a	1498	UR3	C6-C5	2.07	1.39	1.35
1	a	1402	4OC	C4-N3	2.07	1.36	1.32
1	a	1519	MA6	O4'-C1'	2.06	1.44	1.41
1	a	1402	4OC	C6-C5	2.05	1.39	1.35
2	A	1911	PSU	C4-C5	2.01	1.49	1.44

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1518	MA6	N1-C6-N6	7.07	124.49	117.06
1	a	1498	UR3	C4-N3-C2	-6.12	118.80	124.56

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	516	PSU	N1-C2-N3	5.91	121.82	115.13
2	A	1917	PSU	N1-C2-N3	5.74	121.63	115.13
2	A	1911	PSU	N1-C2-N3	5.70	121.59	115.13
1	a	1519	MA6	N1-C6-N6	4.91	122.23	117.06
1	a	516	PSU	C4-N3-C2	-3.79	120.88	126.34
2	A	1917	PSU	C4-N3-C2	-3.72	120.97	126.34
2	A	1911	PSU	C4-N3-C2	-3.71	120.99	126.34
1	a	516	PSU	O2-C2-N1	-3.51	118.93	122.79
1	a	1519	MA6	N3-C2-N1	-3.42	123.34	128.68
1	a	516	PSU	C3'-C2'-C1'	3.31	105.49	101.64
2	A	1911	PSU	O2-C2-N1	-3.28	119.18	122.79
2	A	1917	PSU	O2-C2-N1	-3.27	119.19	122.79
1	a	1518	MA6	N3-C2-N1	-3.25	123.59	128.68
1	a	1519	MA6	C9-N6-C6	-3.10	110.13	119.51
2	A	1917	PSU	C3'-C2'-C1'	3.08	105.22	101.64
1	a	1519	MA6	C4-C5-N7	-2.91	106.37	109.40
1	a	1407	5MC	O2-C2-N3	-2.77	117.83	122.33
1	a	1407	5MC	C5-C4-N3	-2.76	118.70	121.67
1	a	1402	4OC	O2-C2-N3	-2.63	118.05	122.33
1	a	1518	MA6	C3'-C2'-C1'	2.62	104.92	100.98
1	a	1518	MA6	C9-N6-C6	-2.60	111.64	119.51
1	a	1519	MA6	C10-N6-C9	-2.52	108.02	116.12
1	a	1516	2MG	C5-C6-N1	2.44	118.26	113.95
1	a	1516	2MG	C3'-C2'-C1'	2.41	104.61	100.98
1	a	1518	MA6	C4-C5-N7	-2.41	106.89	109.40
2	A	1911	PSU	C3'-C2'-C1'	2.35	104.37	101.64
2	A	1917	PSU	C6-C5-C4	-2.32	116.58	118.20
1	a	1407	5MC	C5-C6-N1	-2.30	120.97	123.34
1	a	1402	4OC	C6-C5-C4	2.29	119.77	116.96
1	a	1519	MA6	C10-N6-C6	-2.22	112.78	119.51
1	a	1407	5MC	O4'-C1'-N1	2.22	113.44	108.36
1	a	1516	2MG	C8-N7-C5	2.20	107.18	102.99
1	a	1407	5MC	CM5-C5-C6	-2.20	119.91	122.85
1	a	1402	4OC	C5-C4-N4	-2.16	118.21	122.61
1	a	1402	4OC	O4'-C1'-N1	2.15	113.29	108.36
2	A	1911	PSU	C6-C5-C4	-2.15	116.70	118.20
1	a	1498	UR3	O4'-C1'-N1	2.05	113.04	108.36
1	a	516	PSU	C6-C5-C4	-2.04	116.77	118.20
1	a	1402	4OC	C5-C4-N3	-2.04	119.32	122.59
1	a	1402	4OC	C2'-C1'-N1	-2.01	110.32	114.22

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1402	4OC	O4'-C4'-C5'-O5'
1	a	1402	4OC	C3'-C4'-C5'-O5'
1	a	1518	MA6	C5-C6-N6-C9
1	a	1518	MA6	C5-C6-N6-C10
1	a	1519	MA6	O4'-C4'-C5'-O5'
1	a	1519	MA6	C3'-C4'-C5'-O5'
1	a	1519	MA6	C5-C6-N6-C9
1	a	1518	MA6	N1-C6-N6-C9
1	a	1519	MA6	N1-C6-N6-C9
1	a	1518	MA6	N1-C6-N6-C10
1	a	1519	MA6	C4'-C5'-O5'-P
1	a	1516	2MG	C4'-C5'-O5'-P
1	a	1516	2MG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

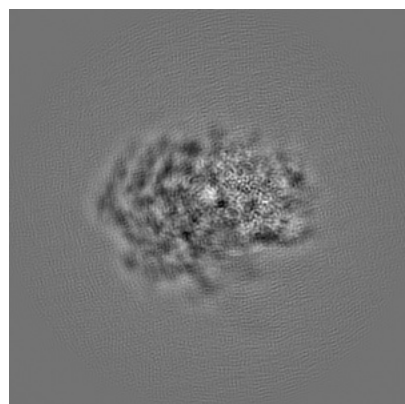
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8506. These allow visual inspection of the internal detail of the map and identification of artifacts.

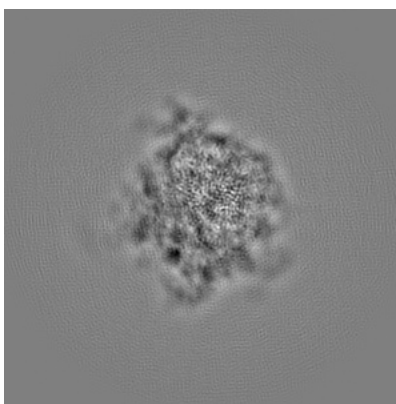
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

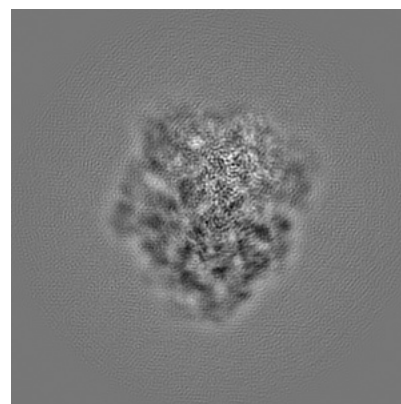
6.1.1 Primary map



X

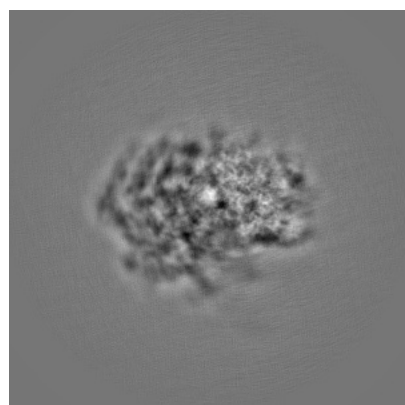


Y

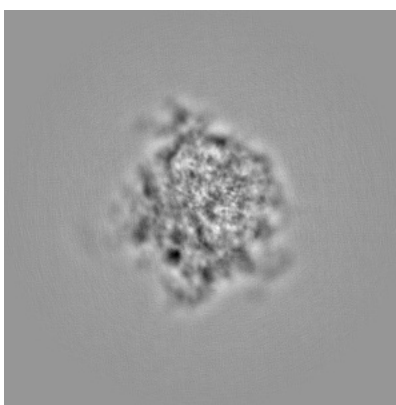


Z

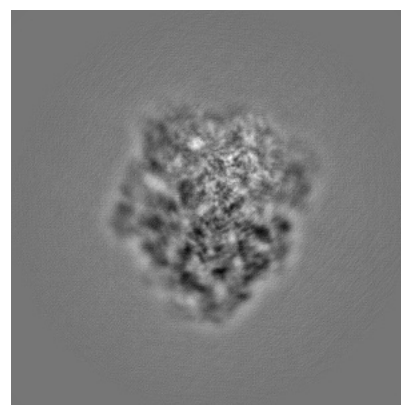
6.1.2 Raw map



X



Y

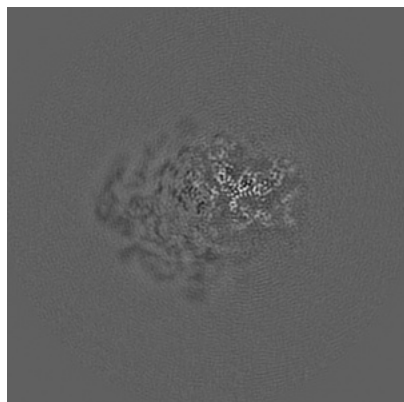


Z

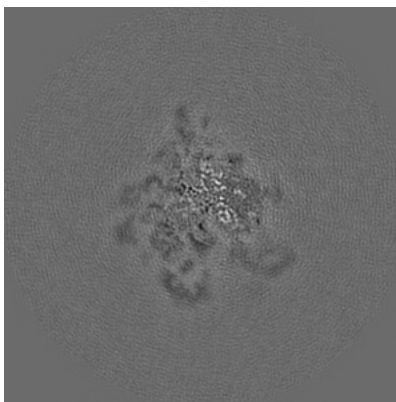
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

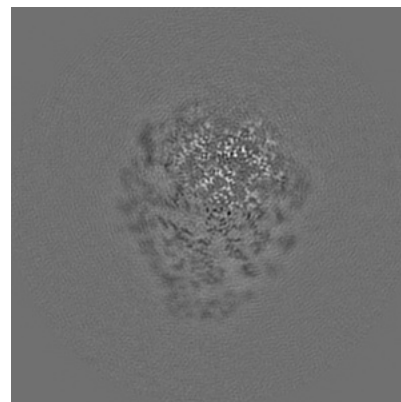
6.2.1 Primary map



X Index: 192

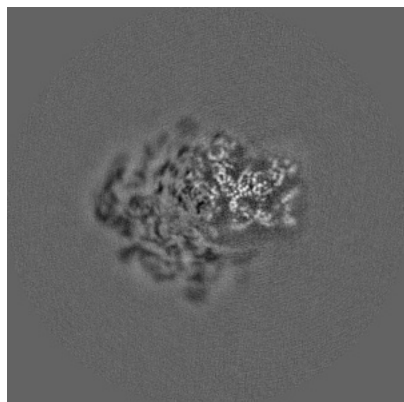


Y Index: 192

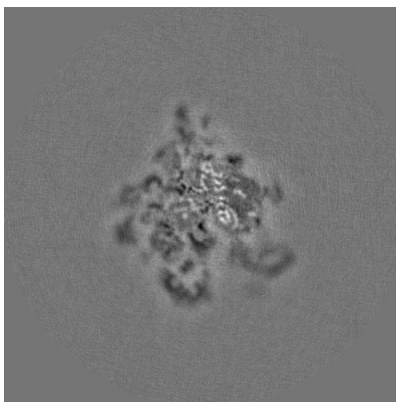


Z Index: 192

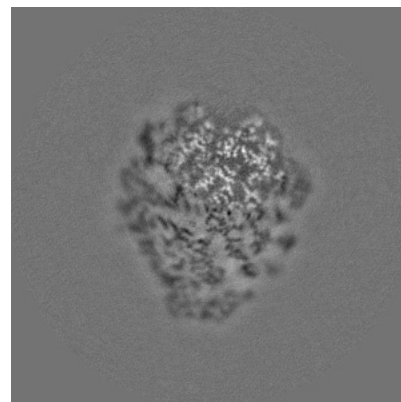
6.2.2 Raw map



X Index: 192



Y Index: 192

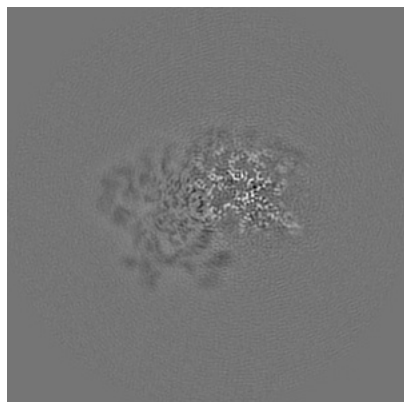


Z Index: 192

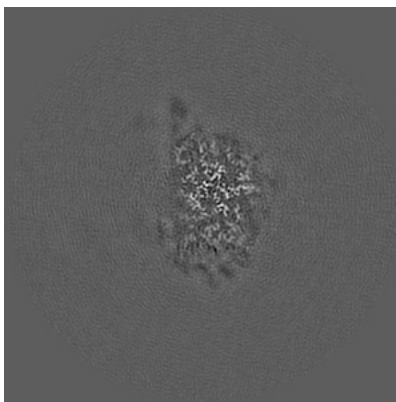
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

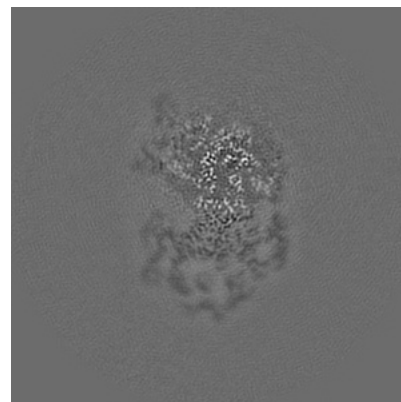
6.3.1 Primary map



X Index: 208

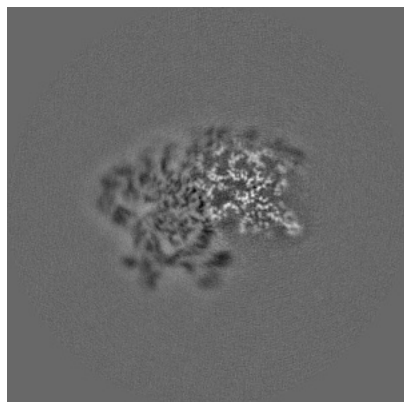


Y Index: 241

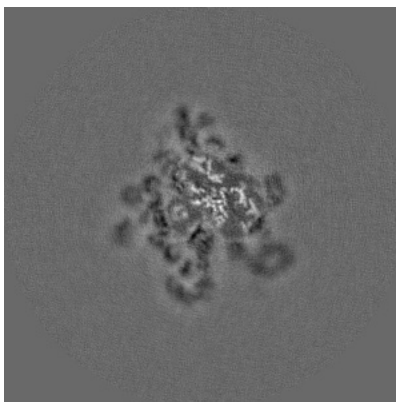


Z Index: 208

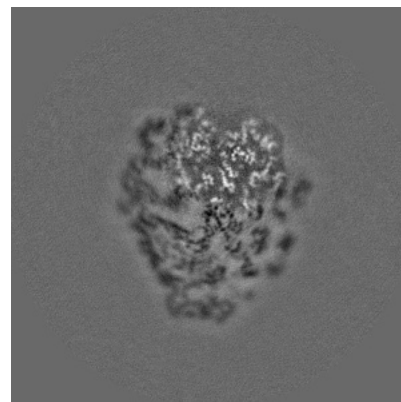
6.3.2 Raw map



X Index: 208



Y Index: 197

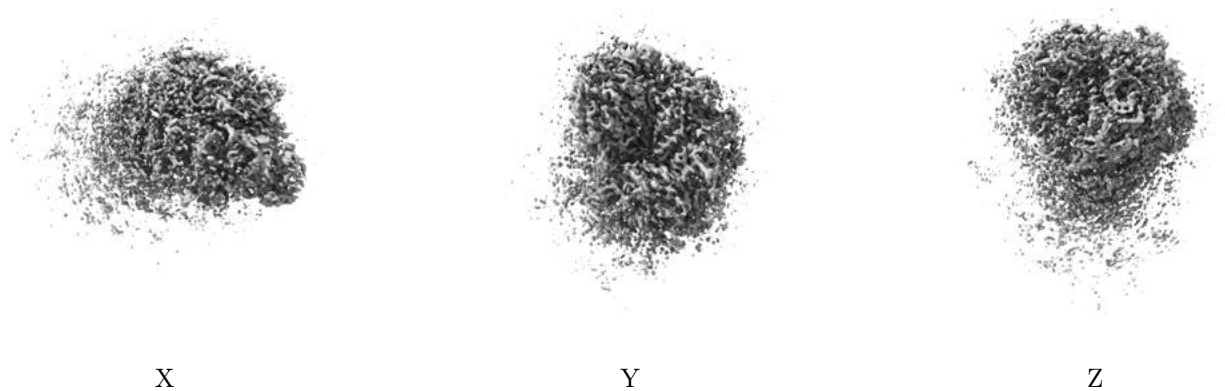


Z Index: 195

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

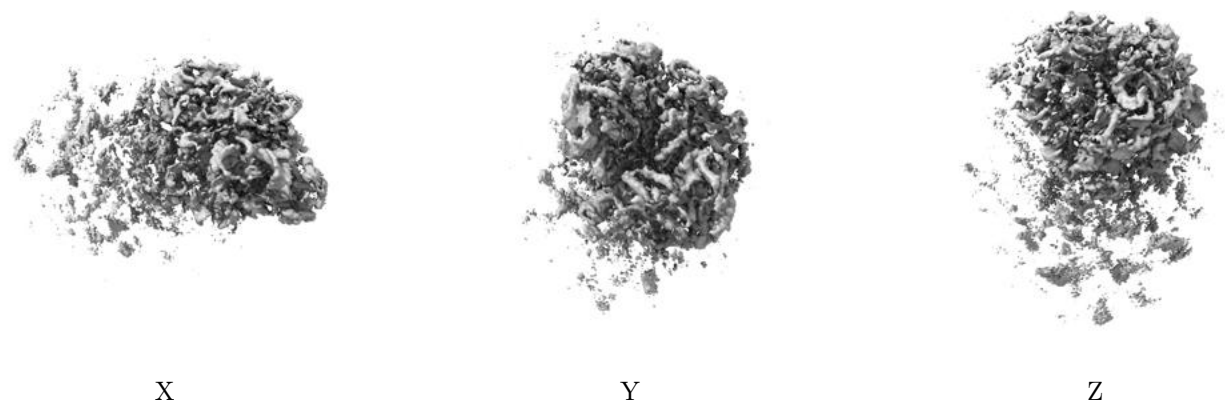
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

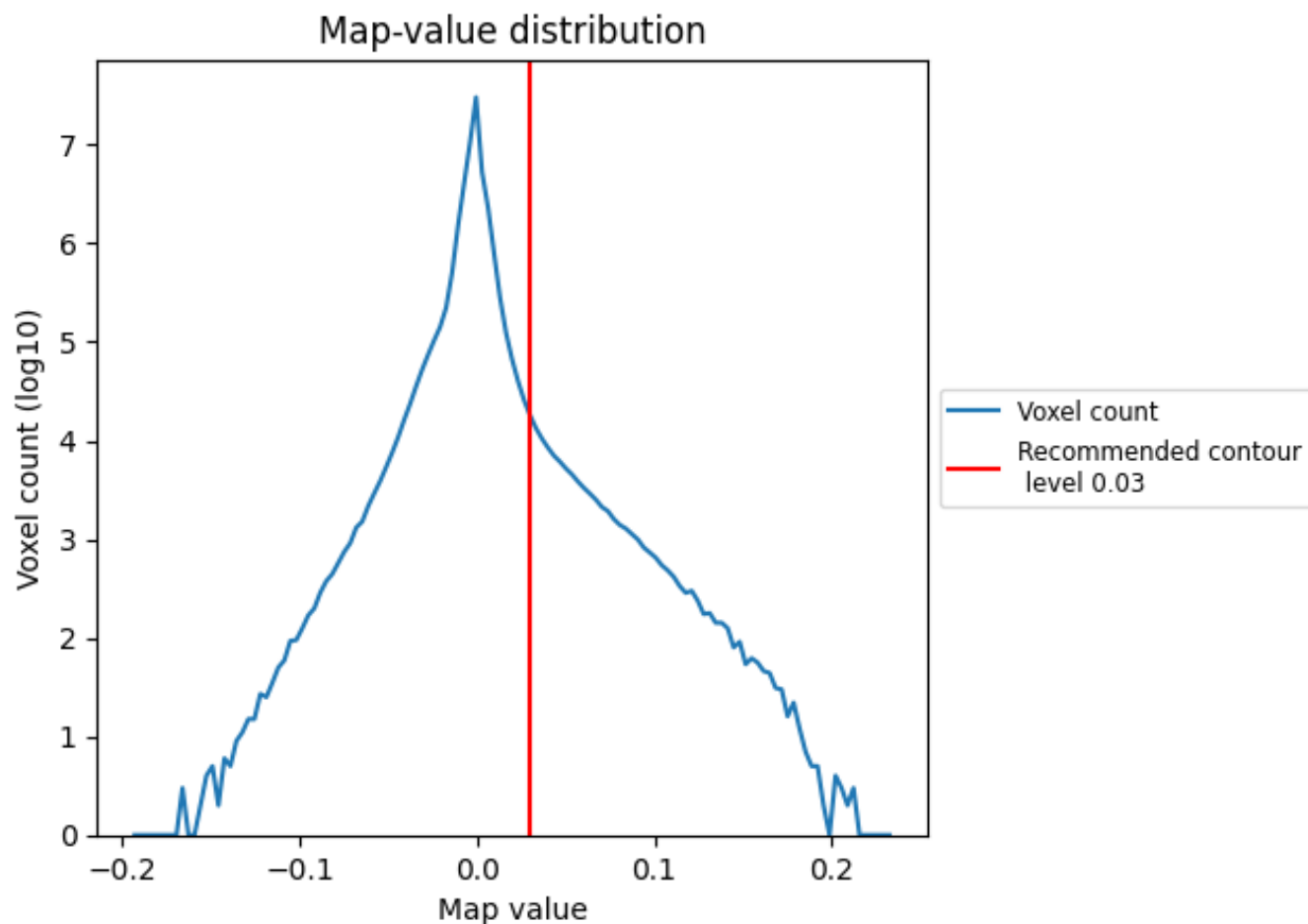
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

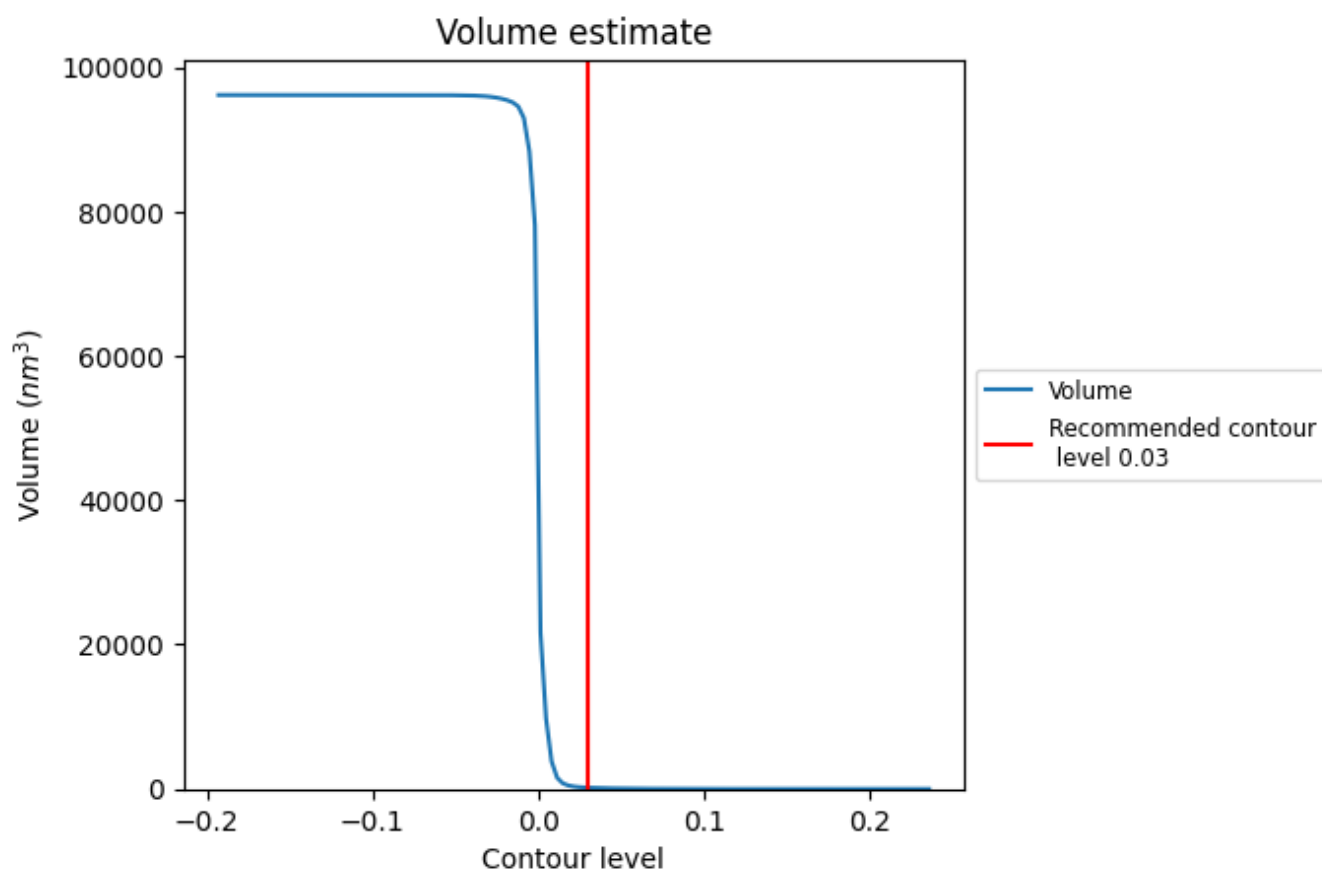
This section contains the results of statistical analysis of the map.

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.

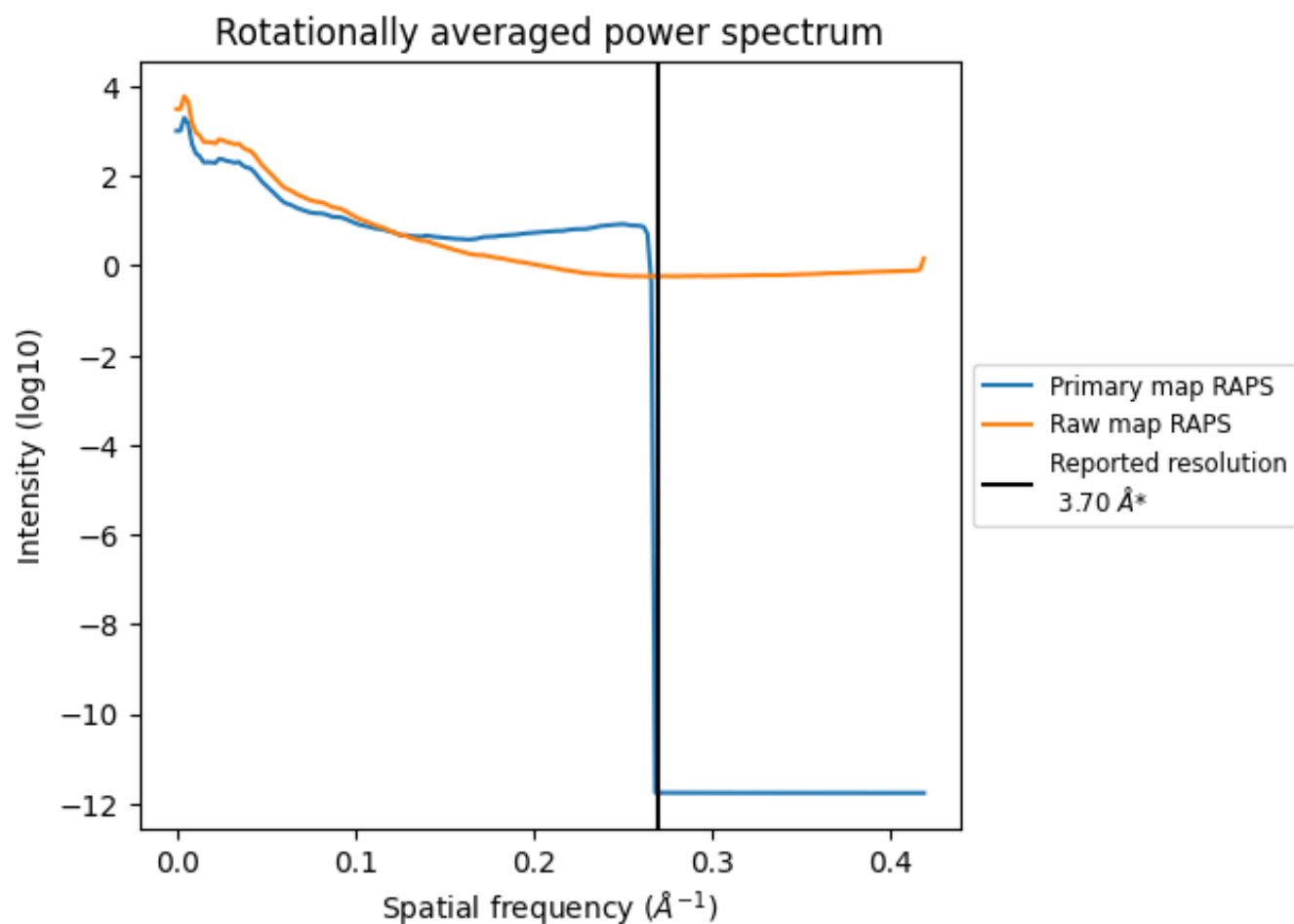
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 175 nm³; this corresponds to an approximate mass of 158 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 ⓘ

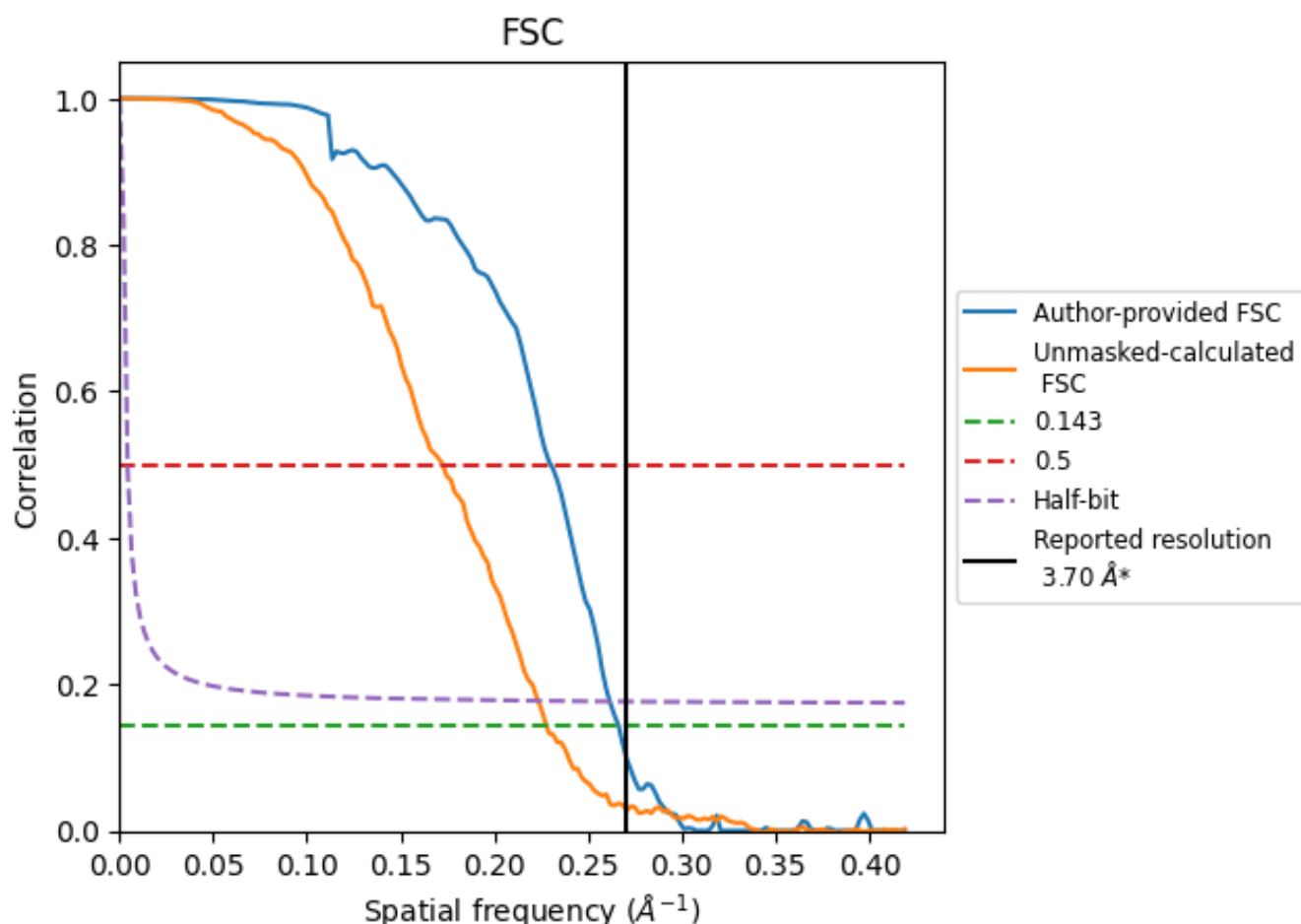


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

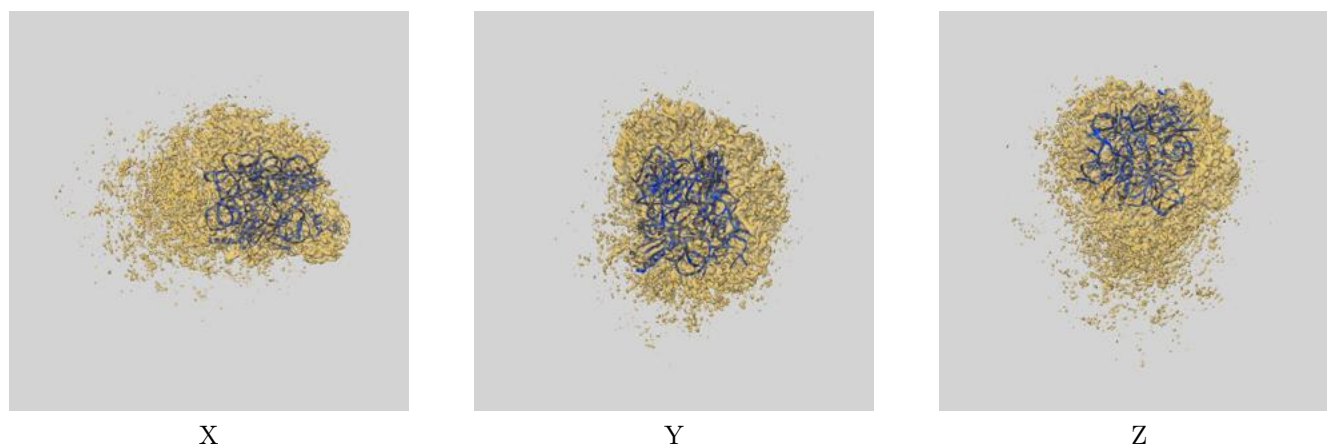
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.75	4.35	3.82
Unmasked-calculated*	4.39	5.80	4.48

*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 4.39 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

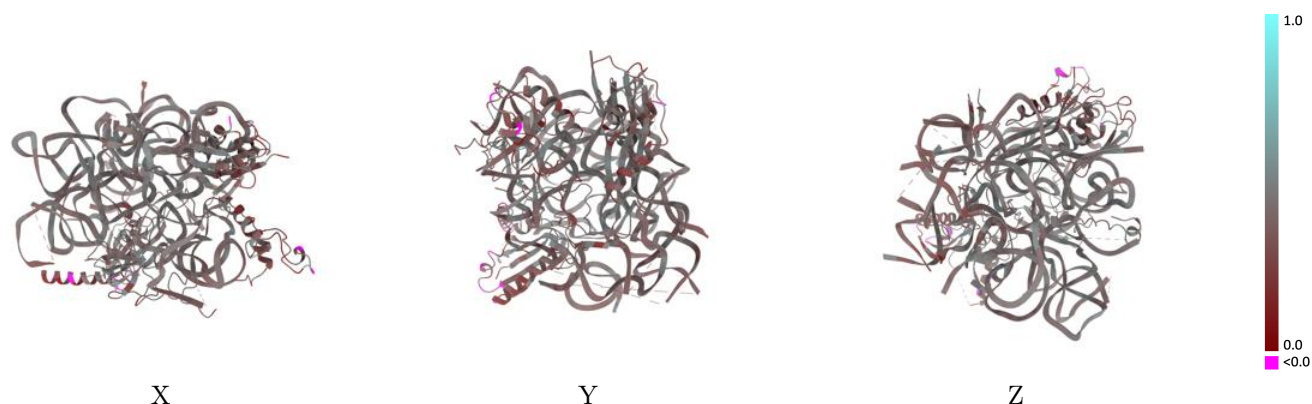
This section contains information regarding the fit between EMDB map EMD-8506 and PDB model 5U4J. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



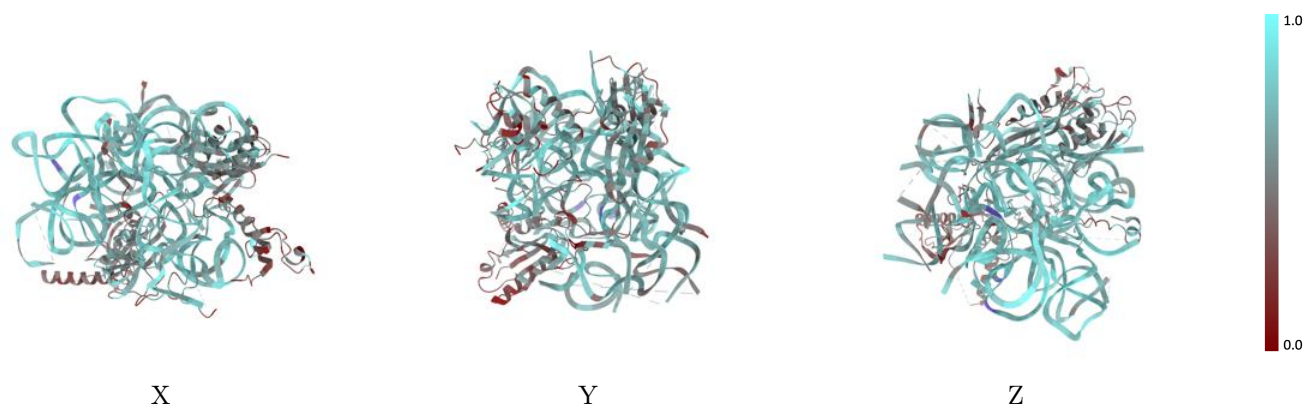
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



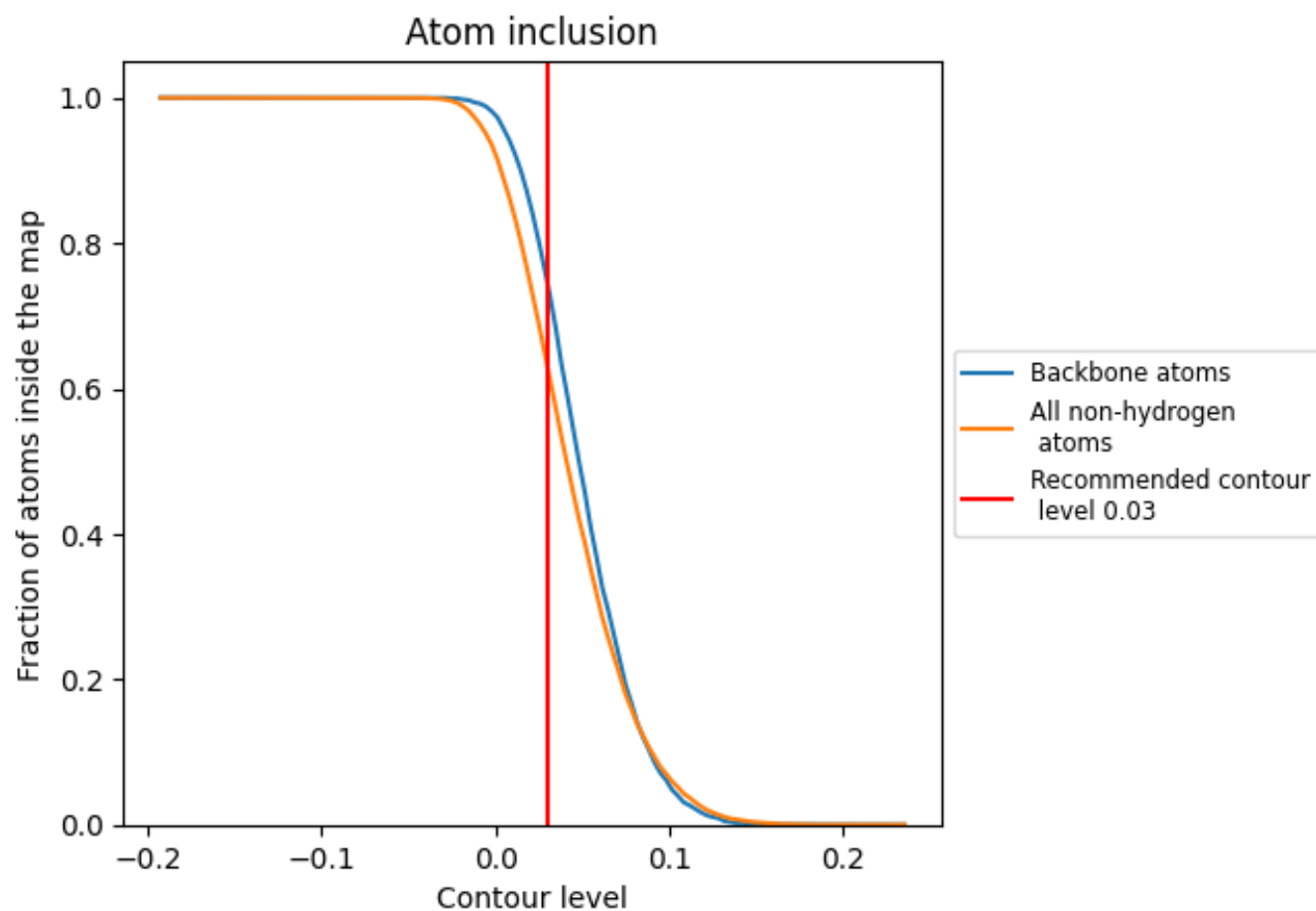
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 63% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6317	<div></div> 0.4020
A	<div></div> 0.7167	<div></div> 0.4250
a	<div></div> 0.7302	<div></div> 0.4250
c	<div></div> 0.4596	<div></div> 0.4170
d	<div></div> 0.3924	<div></div> 0.3230
e	<div></div> 0.5352	<div></div> 0.3870
l	<div></div> 0.5744	<div></div> 0.4250
v	<div></div> 0.3463	<div></div> 0.3040
w	<div></div> 0.4973	<div></div> 0.3770
x	<div></div> 0.6254	<div></div> 0.3840
z	<div></div> 0.4122	<div></div> 0.3480

1.0

0.0

<0.0