



wwPDB EM Validation Summary Report ⓘ

Nov 28, 2024 – 02:23 PM JST

PDB ID : 8K3O
EMDB ID : EMD-36854
Title : Cryo-EM structure of 30S ribosome with cleaved AP-mRNA bound complex I
Authors : Afsar, M.; Shukla, A.; Ramachandran, R.
Deposited on : 2023-07-16
Resolution : 3.88 Å (reported)
Based on initial model : 7NAT

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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

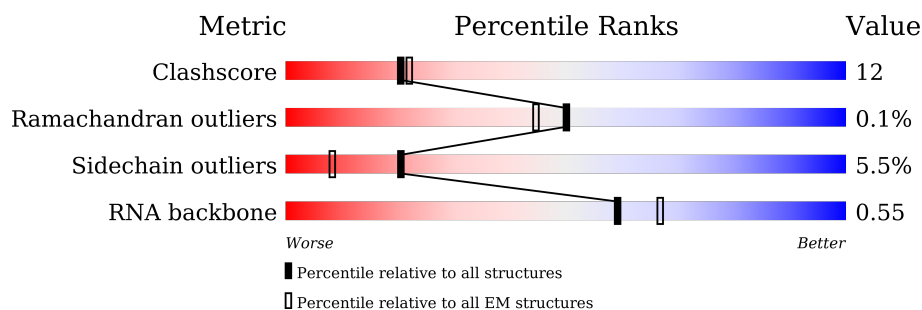
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.88 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	B	241	
2	C	233	
3	D	206	
4	E	167	
5	F	135	
6	G	179	
7	H	130	

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Mol	Chain	Length	Quality of chain
8	I	130	
9	J	103	
10	K	129	
11	L	124	
12	M	118	
13	O	89	
14	P	82	
15	Q	84	
16	R	75	
17	S	92	
18	T	87	
19	V	24	
20	X	71	
21	A	1554	
22	N	101	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 49261 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 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 2 is a protein called 30S ribosomal protein S3.

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

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 5 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	149	Total	C	N	O	S	0	0
			1163	724	222	213	4		

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

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

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	122	Total	C	N	O	S	0	0
			949	587	195	163	4		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	97	Total	C	N	O	S	0	0
			747	466	144	134	3		

- Molecule 13 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	87	Total	C	N	O	S	0	0
			708	436	143	128	1		

- Molecule 14 is a protein called 30S ribosomal protein S16.

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

- Molecule 15 is a protein called 30S ribosomal protein S17.

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

- Molecule 16 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	66	Total	C	N	O	S	0	0
			545	344	102	98	1		

- Molecule 17 is a protein called 30S ribosomal protein S19.

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

- Molecule 18 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	85	Total	C	N	O	S	0	0
			664	411	137	113	3		

- Molecule 19 is a RNA chain called Cleaved AP-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	6	Total	C	N	O	P	0	0
			125	56	19	44	6		

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A	1426	Total 30600	C 13647	N 5618	O 9909	P 1426	0	0

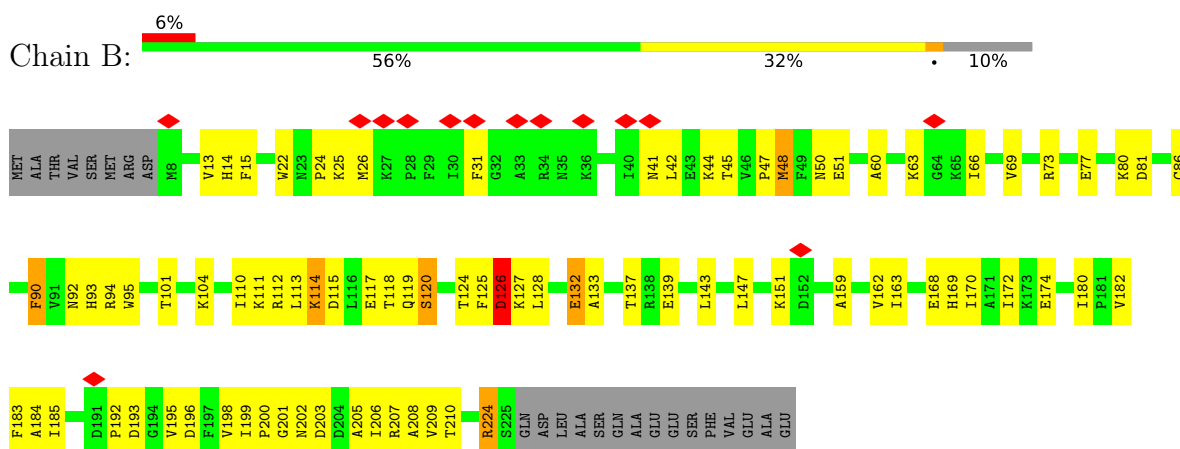
- Molecule 22 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	96	Total 774	C 483	N 160	O 128	S 3	0	0

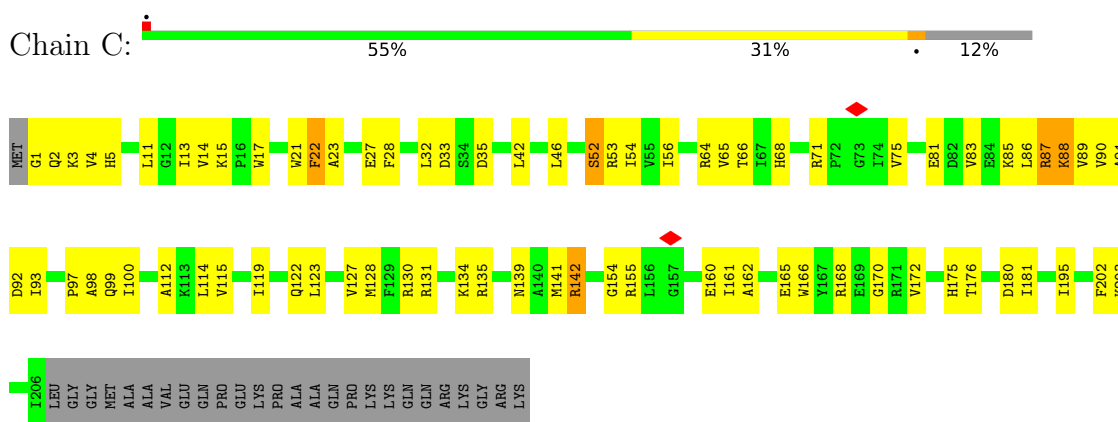
3 Residue-property plots

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.

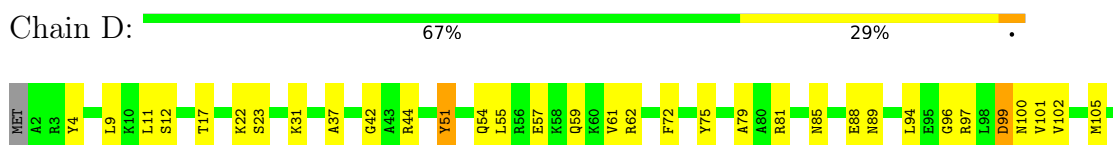
• Molecule 1: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S4

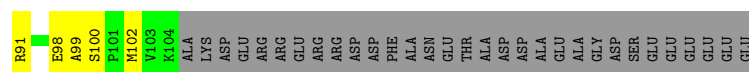
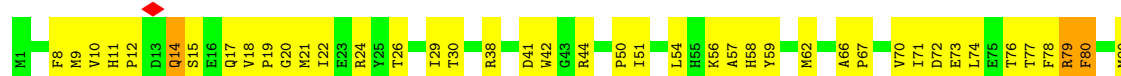




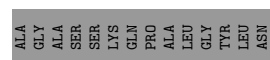
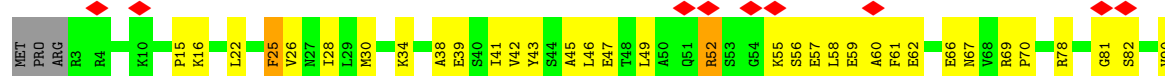
- Molecule 4: 30S ribosomal protein S5



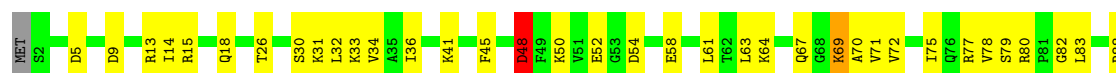
- Molecule 5: 30S ribosomal protein S6, fully modified isoform



- Molecule 6: 30S ribosomal protein S7

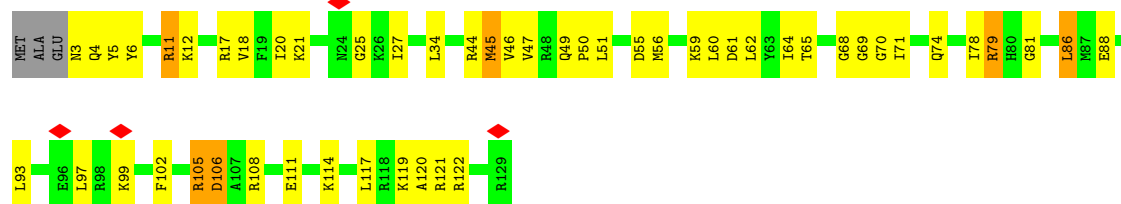


- Molecule 7: 30S ribosomal protein S8



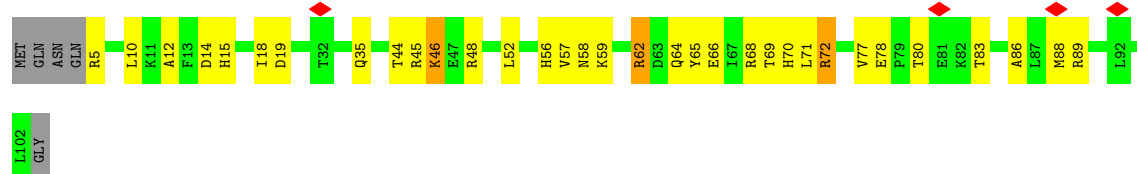
- Molecule 8: 30S ribosomal protein S9

Chain I: 



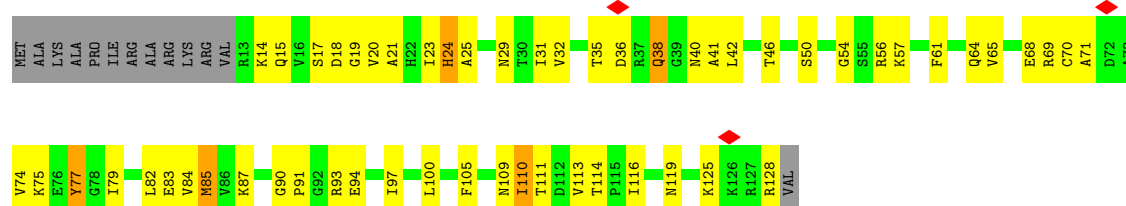
- Molecule 9: 30S ribosomal protein S10

Chain J: 



- Molecule 10: 30S ribosomal protein S11

Chain K: 



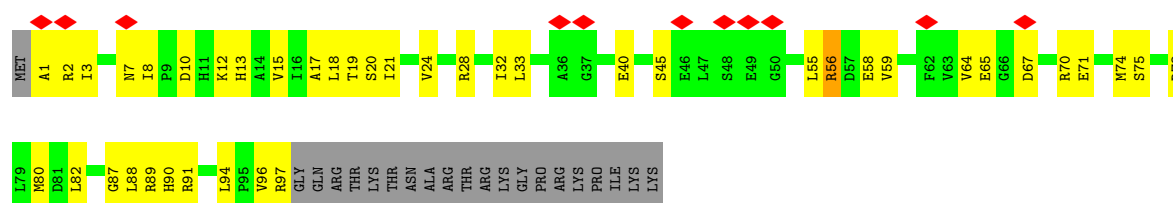
- Molecule 11: 30S ribosomal protein S12

Chain L: 



- Molecule 12: 30S ribosomal protein S13

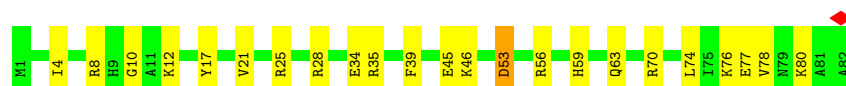
Chain M: 



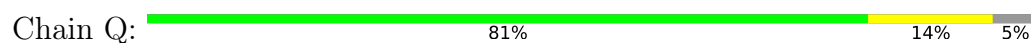
- Molecule 13: 30S ribosomal protein S15



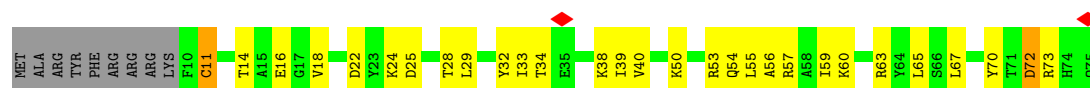
- Molecule 14: 30S ribosomal protein S16



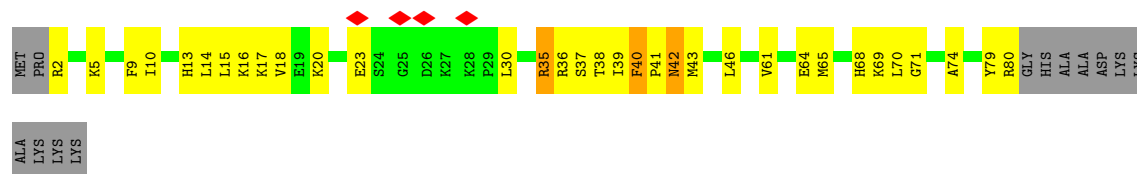
- Molecule 15: 30S ribosomal protein S17



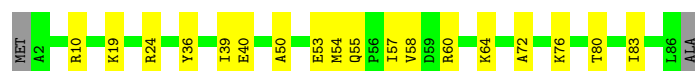
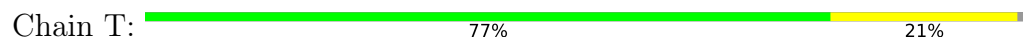
- Molecule 16: 30S ribosomal protein S18



- Molecule 17: 30S ribosomal protein S19

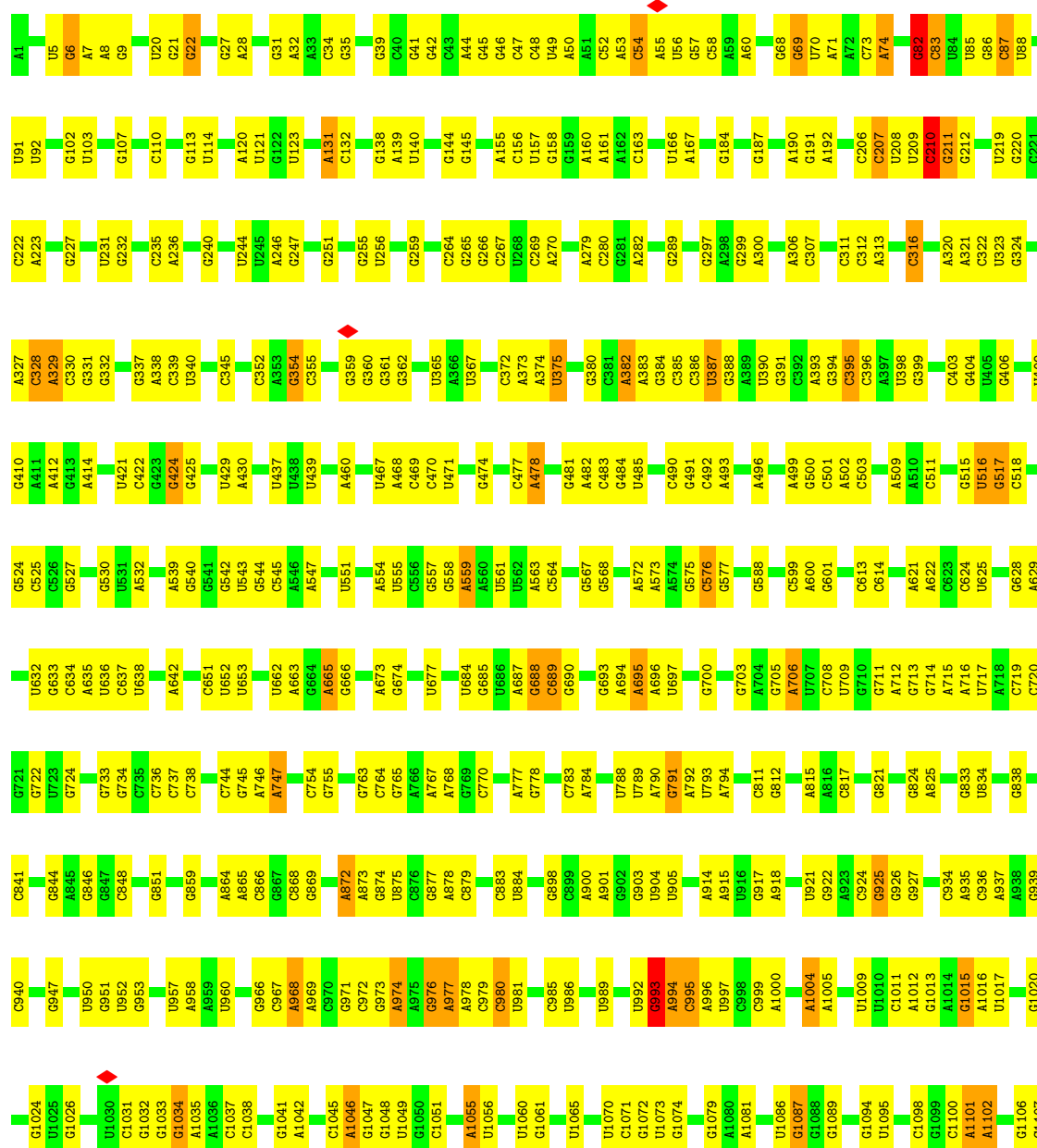


- Molecule 18: 30S ribosomal protein S20



- Molecule 19: Cleaved AP-mRNA







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77582	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.42	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.282	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.38, 1.38, 1.38	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	B	0.34	1/1735 (0.1%)	0.72	5/2338 (0.2%)
2	C	0.27	0/1651	0.64	0/2225
3	D	0.30	0/1665	0.67	1/2227 (0.0%)
4	E	0.29	0/1165	0.65	0/1568
5	F	0.30	0/867	0.66	0/1171
6	G	0.30	0/1176	0.68	0/1577
7	H	0.29	0/989	0.63	2/1326 (0.2%)
8	I	0.30	0/1034	0.73	1/1375 (0.1%)
9	J	0.26	0/796	0.67	0/1077
10	K	0.30	0/885	0.69	1/1195 (0.1%)
11	L	0.29	0/963	0.76	3/1293 (0.2%)
12	M	0.30	0/754	0.73	0/1010
13	O	0.27	0/716	0.69	0/956
14	P	0.25	0/659	0.60	0/884
15	Q	0.25	0/657	0.58	0/881
16	R	0.27	0/554	0.63	0/743
17	S	0.27	0/652	0.67	0/877
18	T	0.28	0/670	0.54	0/888
19	V	0.28	0/138	0.86	0/212
20	X	0.26	0/430	0.69	0/570
21	A	0.21	0/34263	0.82	13/53449 (0.0%)
22	N	0.29	0/785	0.71	0/1043
All	All	0.24	1/53204 (0.0%)	0.77	26/78885 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	I	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	200	PRO	CG-CD	-7.28	1.26	1.50

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	PRO	N-CD-CG	-11.19	86.42	103.20
3	D	174	ASP	CB-CG-OD1	7.74	125.27	118.30
11	L	109	ASP	CB-CG-OD1	6.77	124.40	118.30
1	B	196	ASP	CB-CG-OD1	6.65	124.29	118.30
21	A	754	C	C2-N1-C1'	6.63	126.09	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	I	79	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	B	1704	0	1732	60	0
2	C	1624	0	1699	60	0
3	D	1643	0	1707	48	0
4	E	1152	0	1196	50	0
5	F	848	0	846	40	0
6	G	1163	0	1217	57	0
7	H	979	0	1031	41	0
8	I	1022	0	1070	46	0
9	J	786	0	828	29	0
10	K	869	0	878	48	0
11	L	949	0	1011	25	0
12	M	747	0	793	42	0
13	O	708	0	729	21	0
14	P	649	0	666	19	0
15	Q	648	0	691	5	0
16	R	545	0	560	24	0
17	S	637	0	665	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	T	664	0	714	11	0
19	V	125	0	64	1	0
20	X	425	0	449	6	0
21	A	30600	0	15402	391	0
22	N	774	0	827	42	0
All	All	49261	0	34775	990	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 12.

The worst 5 of 990 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)
4:E:43:ASN:OD1	4:E:44:GLY:N	2.05	0.89
17:S:36:ARG:O	17:S:69:LYS:NZ	2.09	0.86
12:M:70:ARG:HD2	12:M:74:MET:HE2	1.60	0.83
4:E:115:LEU:HD22	4:E:123:VAL:HG11	1.62	0.82
6:G:100:MET:HA	6:G:103:ILE:HD12	1.62	0.81

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	B	216/241 (90%)	189 (88%)	26 (12%)	1 (0%)	25	60
2	C	204/233 (88%)	189 (93%)	15 (7%)	0	100	100
3	D	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
4	E	154/167 (92%)	141 (92%)	13 (8%)	0	100	100
5	F	102/135 (76%)	100 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	147/179 (82%)	144 (98%)	3 (2%)	0	100	100
7	H	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
8	I	125/130 (96%)	114 (91%)	9 (7%)	2 (2%)	8	37
9	J	96/103 (93%)	77 (80%)	19 (20%)	0	100	100
10	K	114/129 (88%)	106 (93%)	8 (7%)	0	100	100
11	L	120/124 (97%)	118 (98%)	2 (2%)	0	100	100
12	M	95/118 (80%)	86 (90%)	9 (10%)	0	100	100
13	O	85/89 (96%)	79 (93%)	6 (7%)	0	100	100
14	P	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
15	Q	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
16	R	64/75 (85%)	64 (100%)	0	0	100	100
17	S	77/92 (84%)	73 (95%)	4 (5%)	0	100	100
18	T	83/87 (95%)	83 (100%)	0	0	100	100
20	X	49/71 (69%)	41 (84%)	8 (16%)	0	100	100
22	N	92/101 (91%)	86 (94%)	6 (6%)	0	100	100
All	All	2311/2576 (90%)	2165 (94%)	143 (6%)	3 (0%)	50	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	I	120	ALA
1	B	124	THR
8	I	55	ASP

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	B	180/199 (90%)	167 (93%)	13 (7%)	12	36
2	C	170/190 (90%)	160 (94%)	10 (6%)	16	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	172/173 (99%)	160 (93%)	12 (7%)	12	36
4	E	119/126 (94%)	115 (97%)	4 (3%)	32	55
5	F	91/116 (78%)	86 (94%)	5 (6%)	18	44
6	G	122/147 (83%)	118 (97%)	4 (3%)	33	56
7	H	104/105 (99%)	100 (96%)	4 (4%)	28	52
8	I	105/107 (98%)	97 (92%)	8 (8%)	11	34
9	J	86/90 (96%)	80 (93%)	6 (7%)	12	36
10	K	89/99 (90%)	83 (93%)	6 (7%)	13	38
11	L	103/104 (99%)	96 (93%)	7 (7%)	13	38
12	M	78/96 (81%)	74 (95%)	4 (5%)	20	45
13	O	75/77 (97%)	74 (99%)	1 (1%)	65	76
14	P	65/65 (100%)	63 (97%)	2 (3%)	35	57
15	Q	74/78 (95%)	68 (92%)	6 (8%)	9	32
16	R	57/65 (88%)	54 (95%)	3 (5%)	19	44
17	S	70/79 (89%)	66 (94%)	4 (6%)	17	43
18	T	65/66 (98%)	64 (98%)	1 (2%)	60	74
20	X	44/61 (72%)	41 (93%)	3 (7%)	13	38
22	N	79/84 (94%)	74 (94%)	5 (6%)	15	40
All	All	1948/2127 (92%)	1840 (94%)	108 (6%)	20	44

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	I	105	ARG
10	K	125	LYS
18	T	54	MET
8	I	122	ARG
9	J	72	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	119	GLN
3	D	152	GLN
5	F	17	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	H	18	GLN
14	P	63	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	V	5/24 (20%)	4 (80%)	2 (40%)
21	A	1424/1554 (91%)	254 (17%)	9 (0%)
All	All	1429/1578 (90%)	258 (18%)	11 (0%)

5 of 258 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	V	67	G
19	V	69	U
19	V	70	C
19	V	71	A
21	A	5	U

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	A	1201	A
21	A	1320	C
21	A	1531	A
21	A	1508	A
21	A	994	A

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 ⓘ

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.

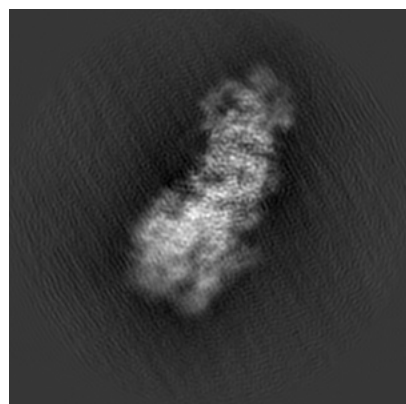
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36854. These allow visual inspection of the internal detail of the map and identification of artifacts.

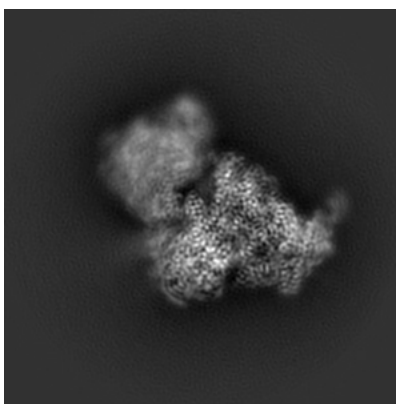
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

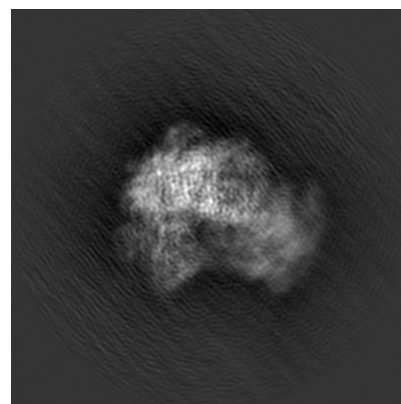
6.1.1 Primary map



X

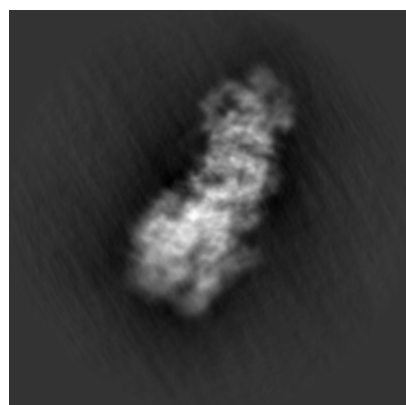


Y

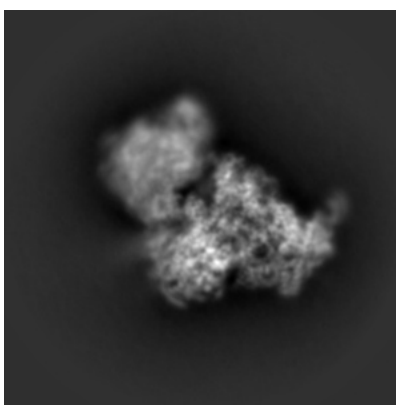


Z

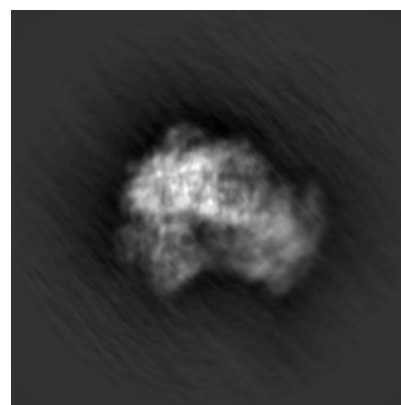
6.1.2 Raw map



X



Y

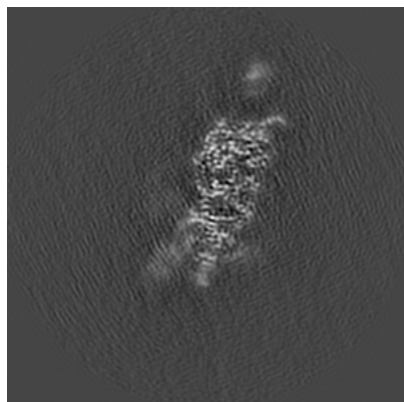


Z

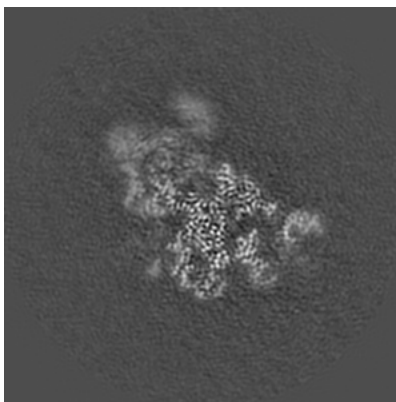
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

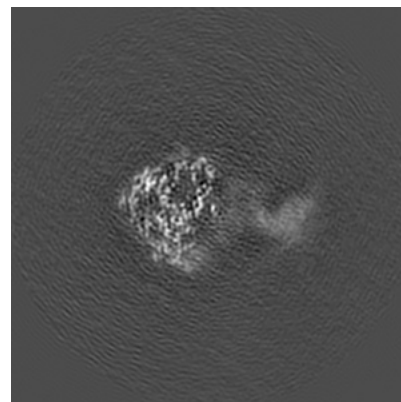
6.2.1 Primary map



X Index: 128

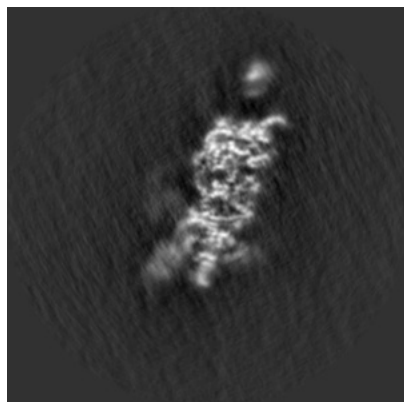


Y Index: 128

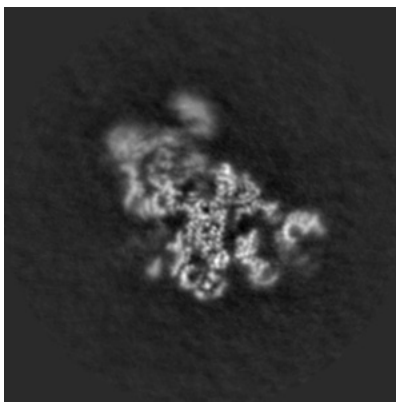


Z Index: 128

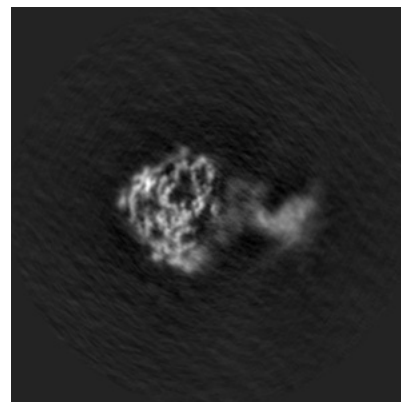
6.2.2 Raw map



X Index: 128



Y Index: 128

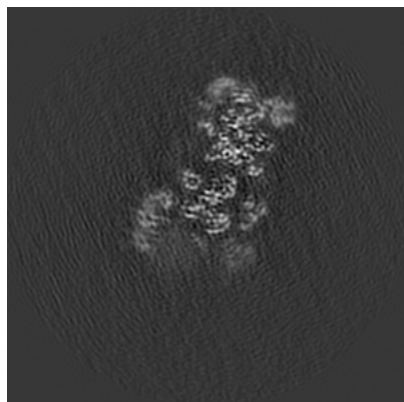


Z Index: 128

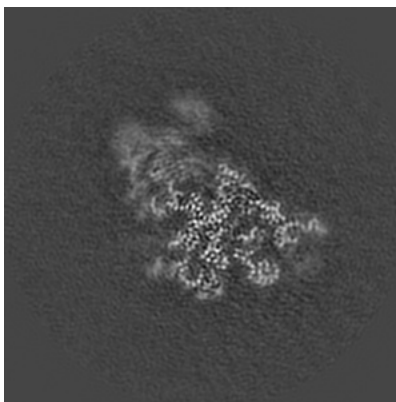
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

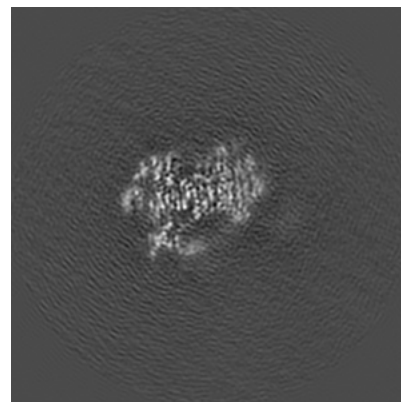
6.3.1 Primary map



X Index: 111

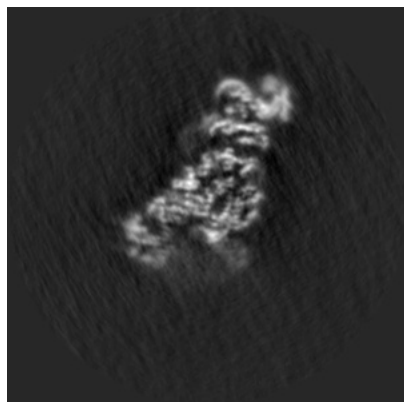


Y Index: 131

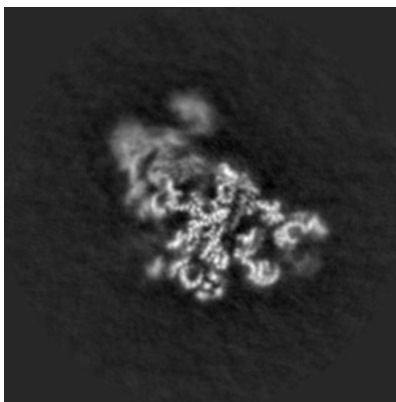


Z Index: 137

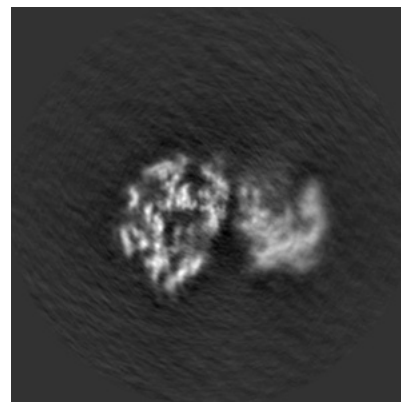
6.3.2 Raw map



X Index: 104



Y Index: 130

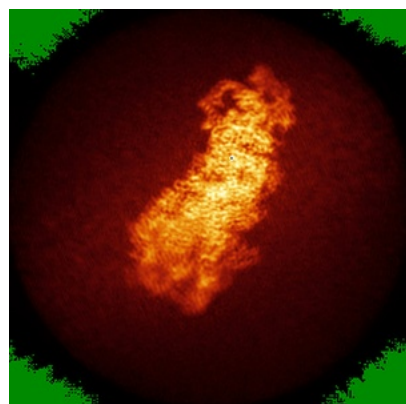


Z Index: 118

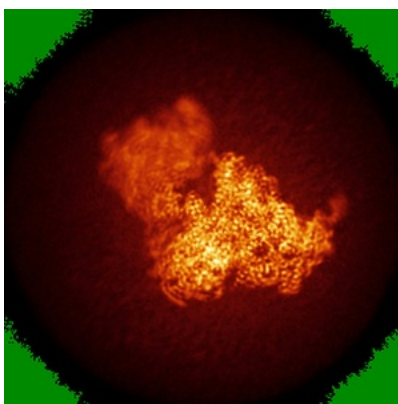
The images above show the largest variance slices of the map in three orthogonal directions.

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

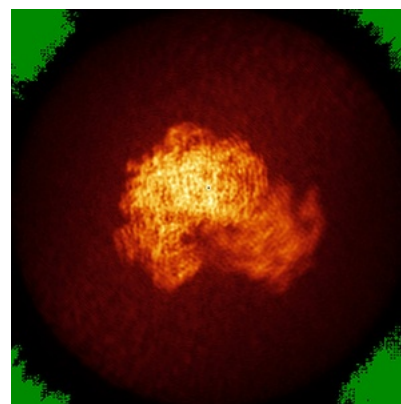
6.4.1 Primary map



X

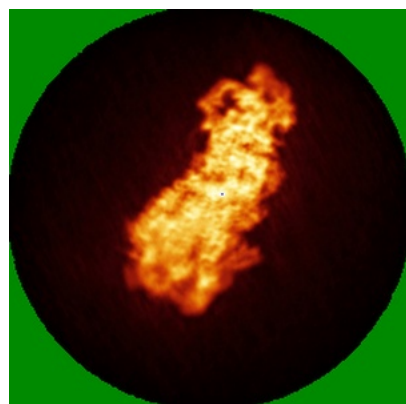


Y



Z

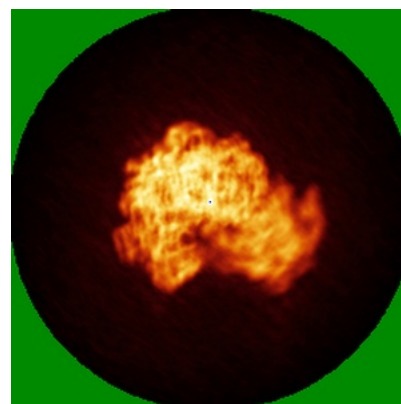
6.4.2 Raw map



X



Y

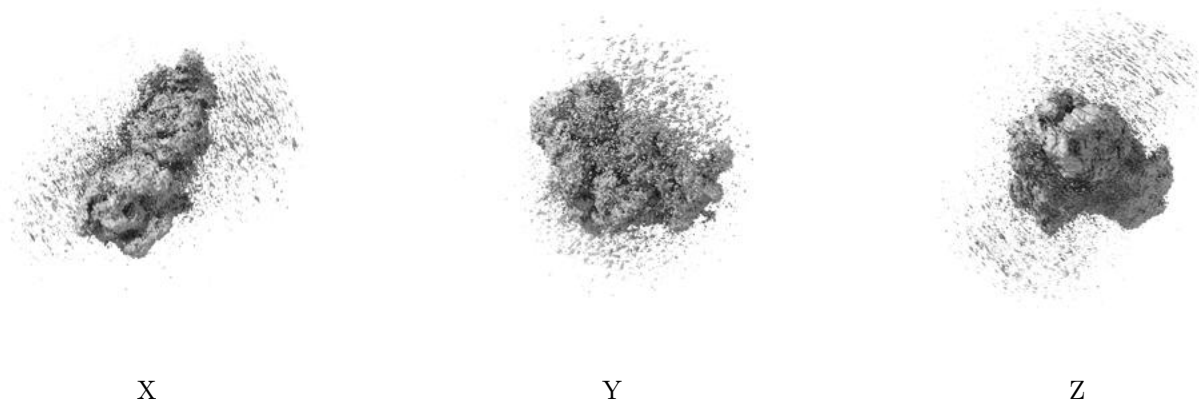


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

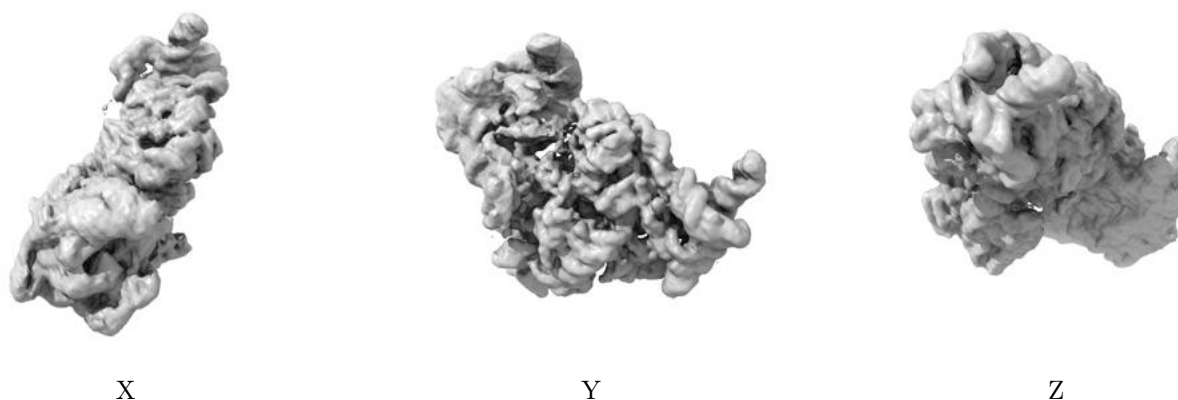
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

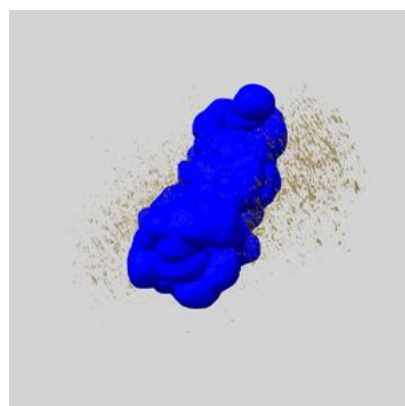
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

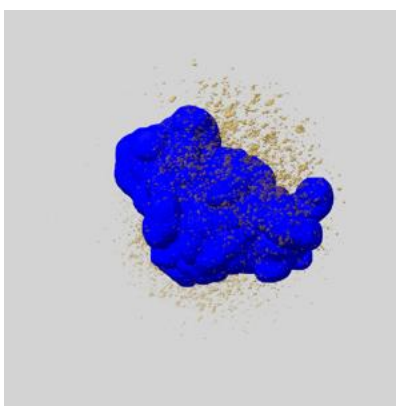
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

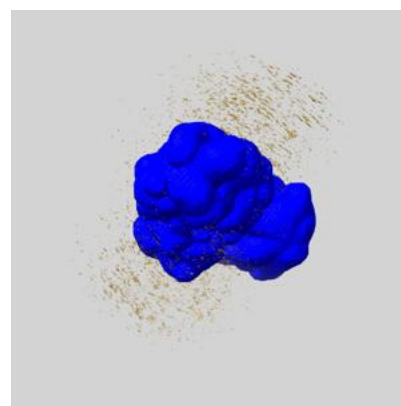
6.6.1 emd_36854_msk_1.map [i](#)



X



Y

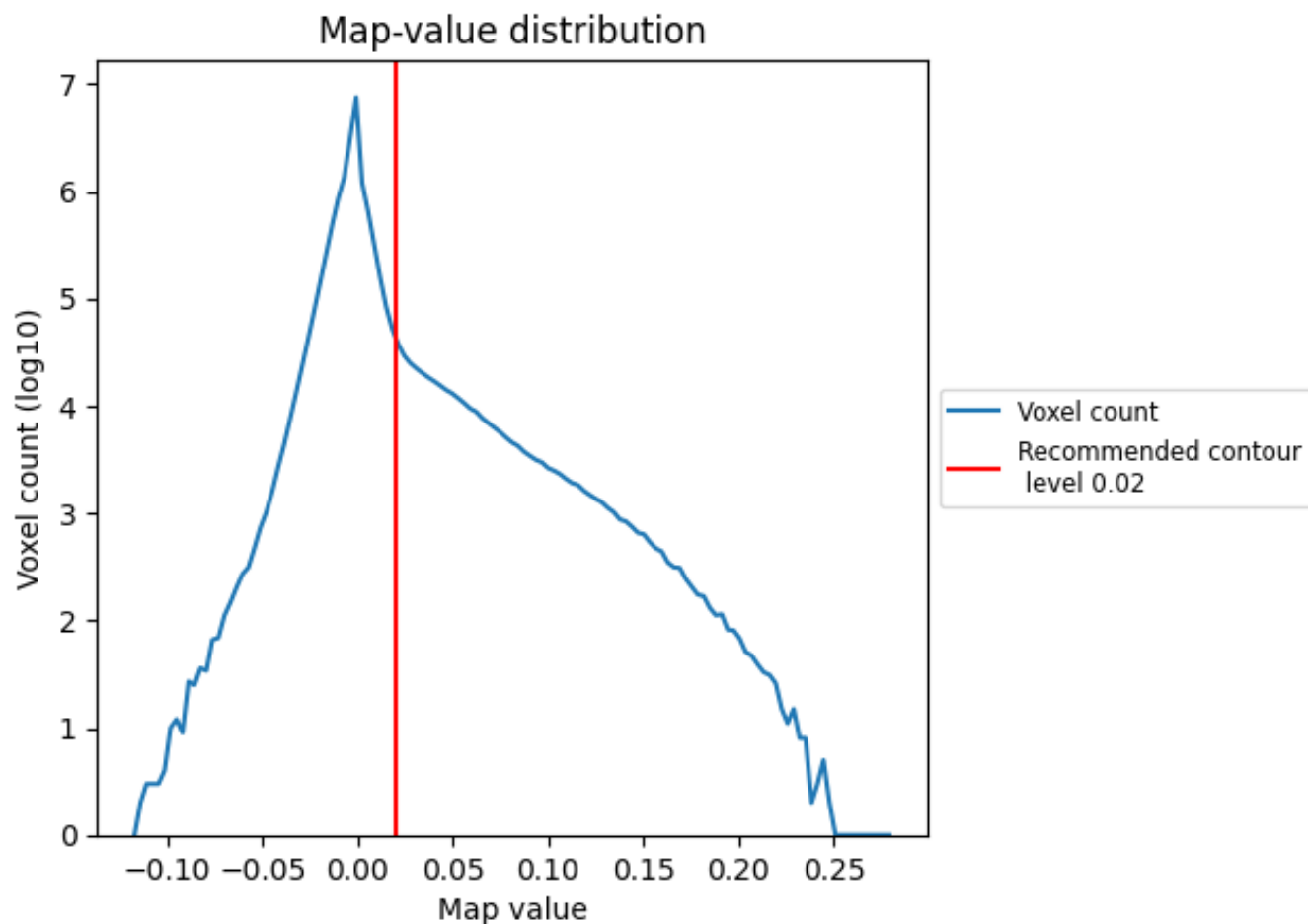


Z

7 Map analysis [i](#)

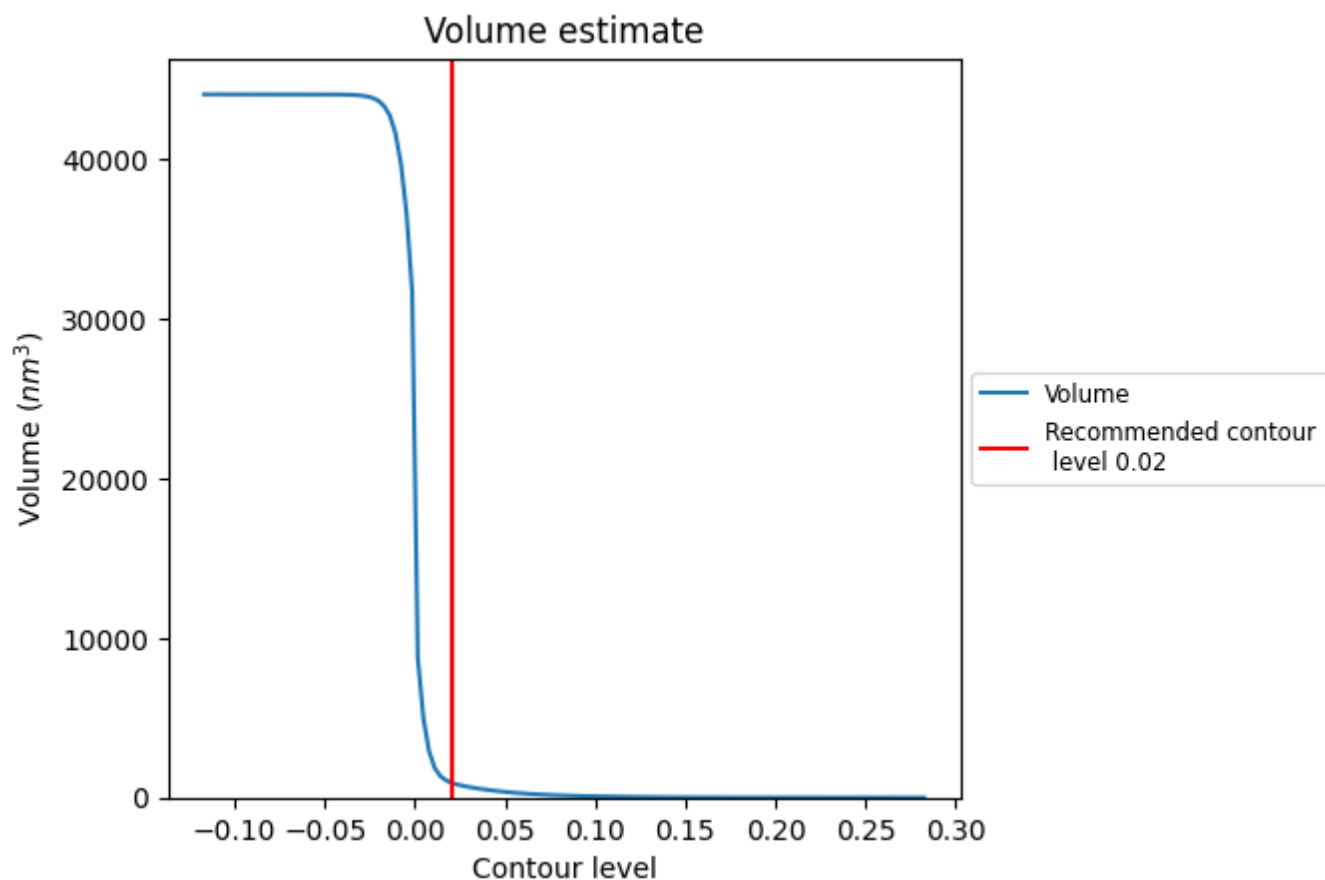
This section contains the results of statistical analysis of the map.

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.

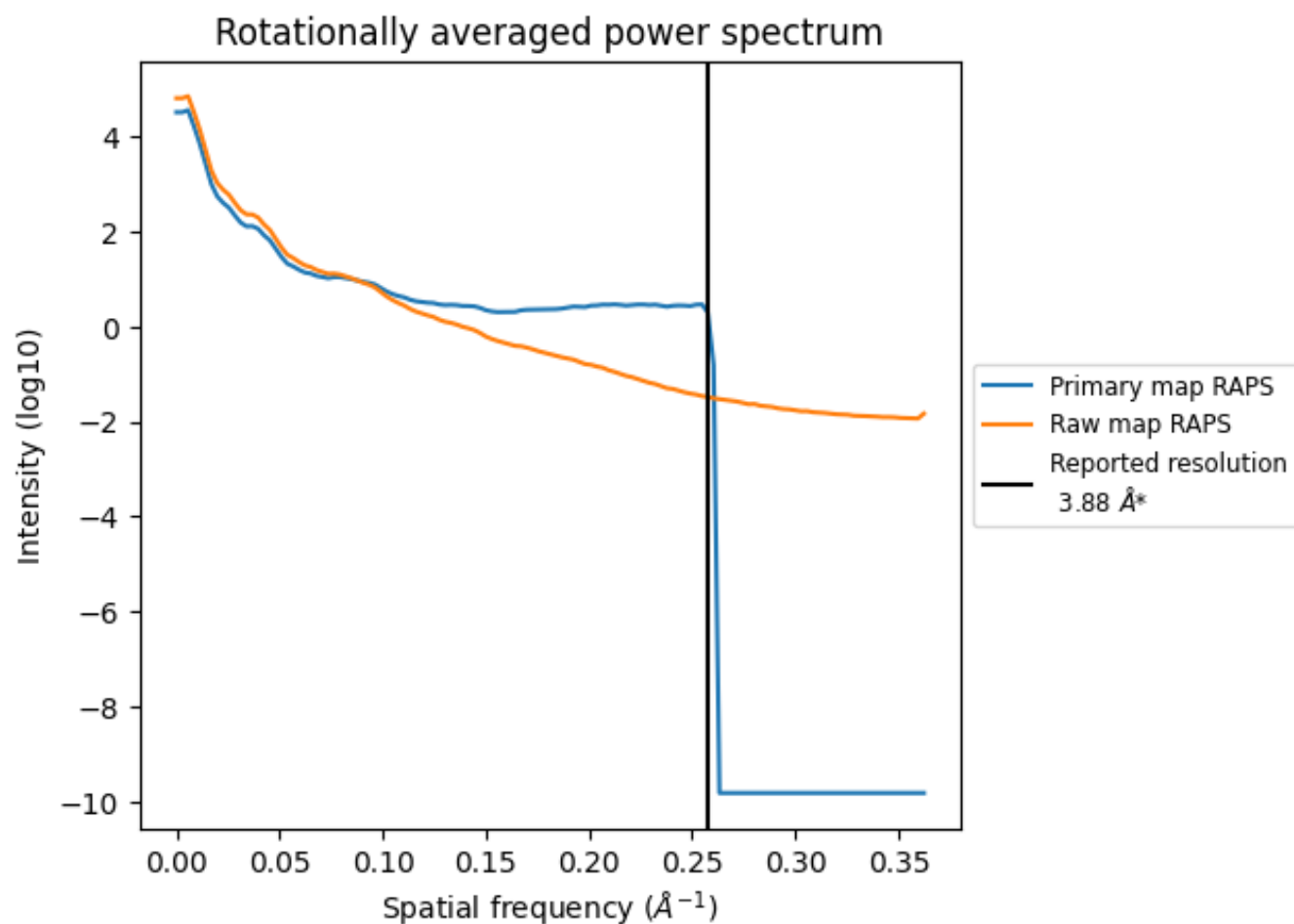
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 942 nm^3 ; this corresponds to an approximate mass of 851 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 ⓘ

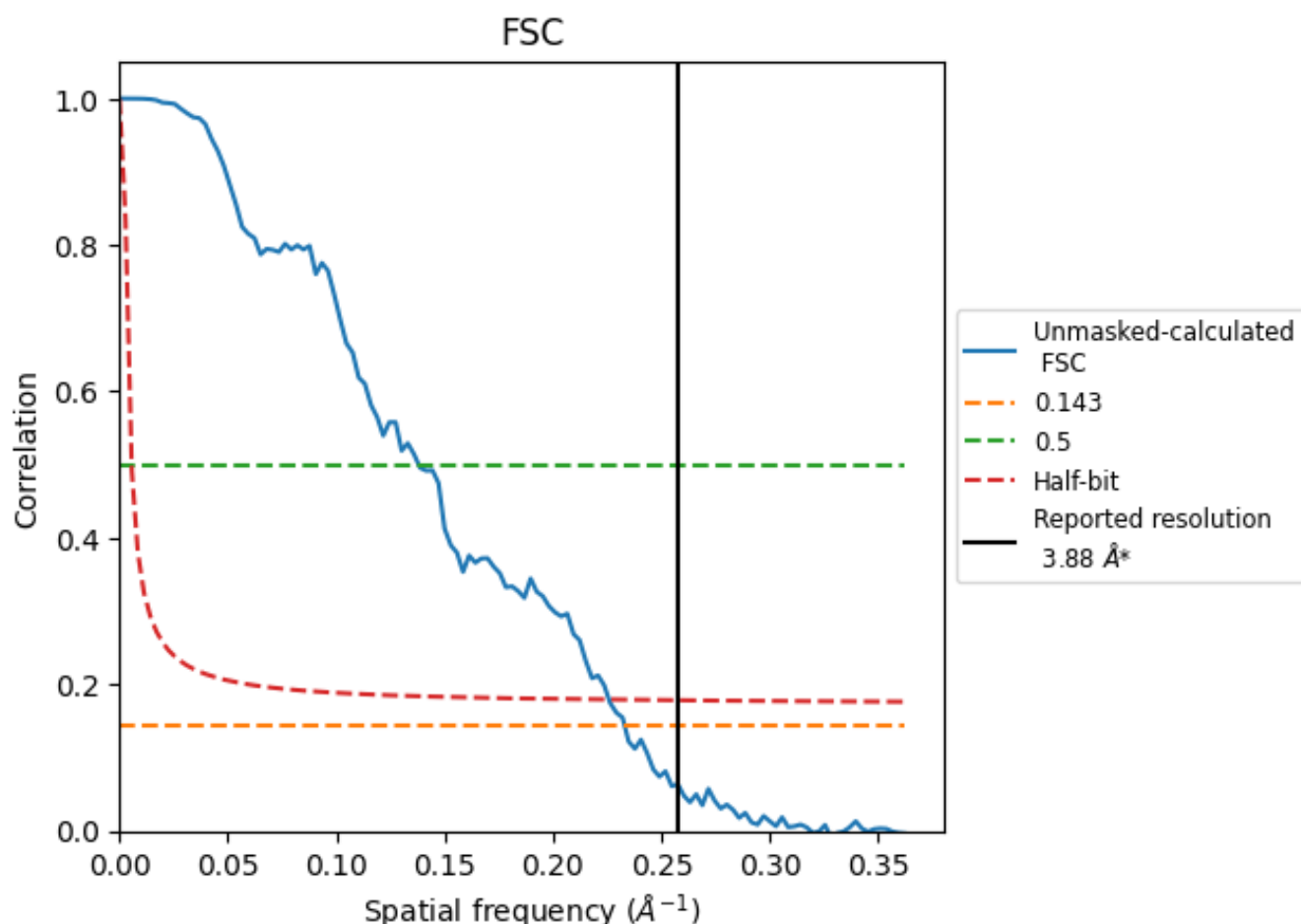


*Reported resolution corresponds to spatial frequency of 0.258 \AA^{-1}

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 0.258 Å⁻¹

8.2 Resolution estimates [i](#)

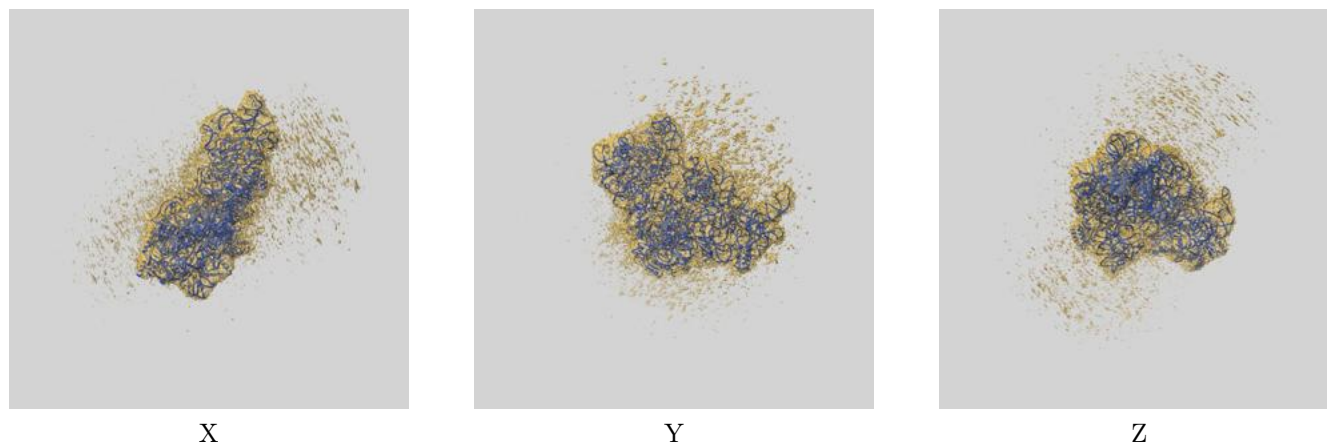
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.88	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.29	7.25	4.43

*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 4.29 differs from the reported value 3.88 by more than 10 %

9 Map-model fit [i](#)

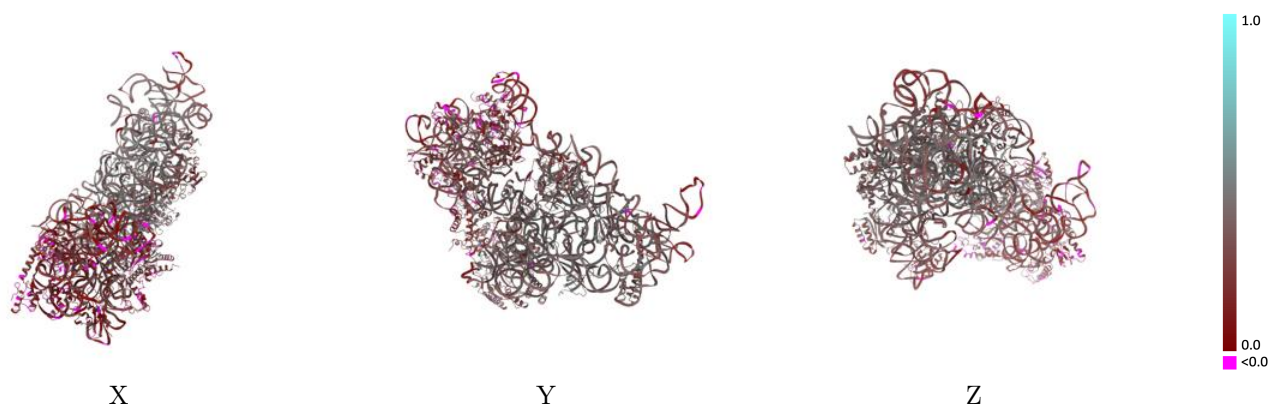
This section contains information regarding the fit between EMDB map EMD-36854 and PDB model 8K3O. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



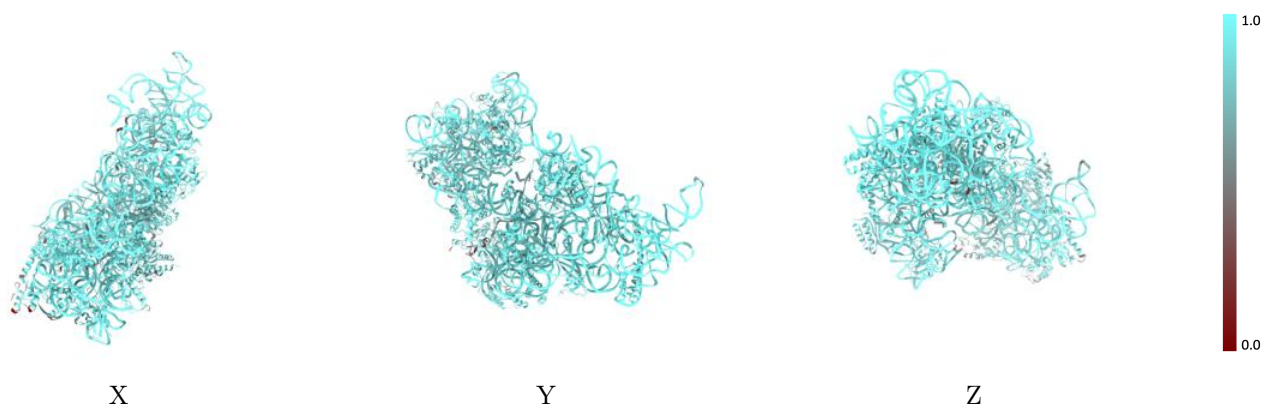
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



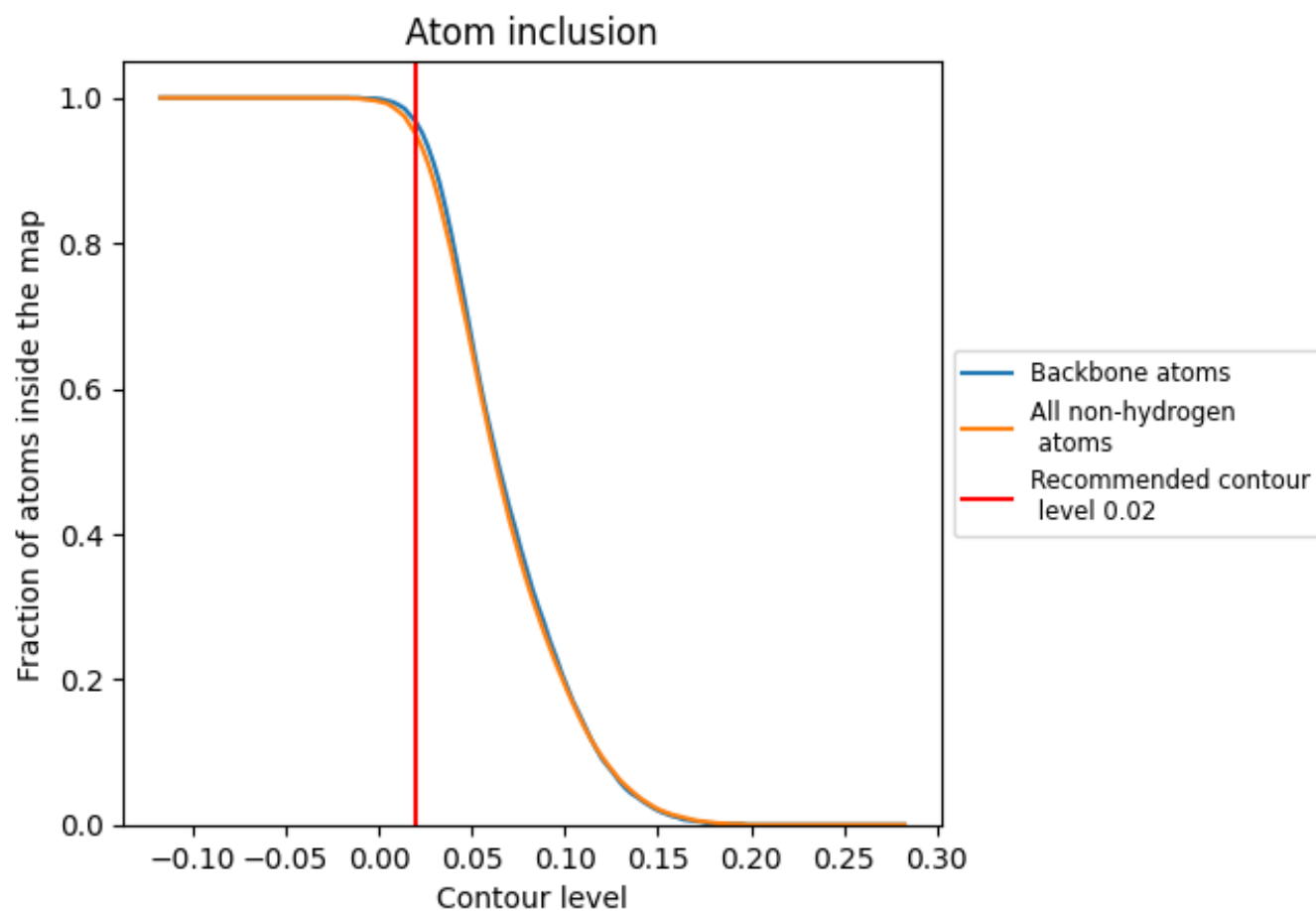
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.3070
A	 0.9780	 0.3160
B	 0.8370	 0.2720
C	 0.9120	 0.2480
D	 0.9530	 0.3690
E	 0.9340	 0.4070
F	 0.9190	 0.3150
G	 0.7770	 0.1260
H	 0.9440	 0.4090
I	 0.8990	 0.1720
J	 0.8950	 0.2100
K	 0.9250	 0.2260
L	 0.9590	 0.4280
M	 0.8120	 0.1490
N	 0.9170	 0.2080
O	 0.9620	 0.3790
P	 0.9490	 0.4150
Q	 0.9600	 0.4360
R	 0.9140	 0.3620
S	 0.8970	 0.1200
T	 0.9780	 0.3940
V	 0.7280	 0.3440
X	 0.7020	 0.2070

