



wwPDB EM Validation Summary Report ⓘ

Jun 9, 2026 – 04:44 pm BST

PDB ID : 9SS1 / pdb_00009ss1
EMDB ID : EMD-55173
Title : 30S ribosomal subunit RimM-KO with IF1 and IF3 (State II)
Authors : Hassan, A.H.; Demo, G.
Deposited on : 2025-09-25
Resolution : 2.90 Å(reported)
Based on initial model : 6WDE

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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

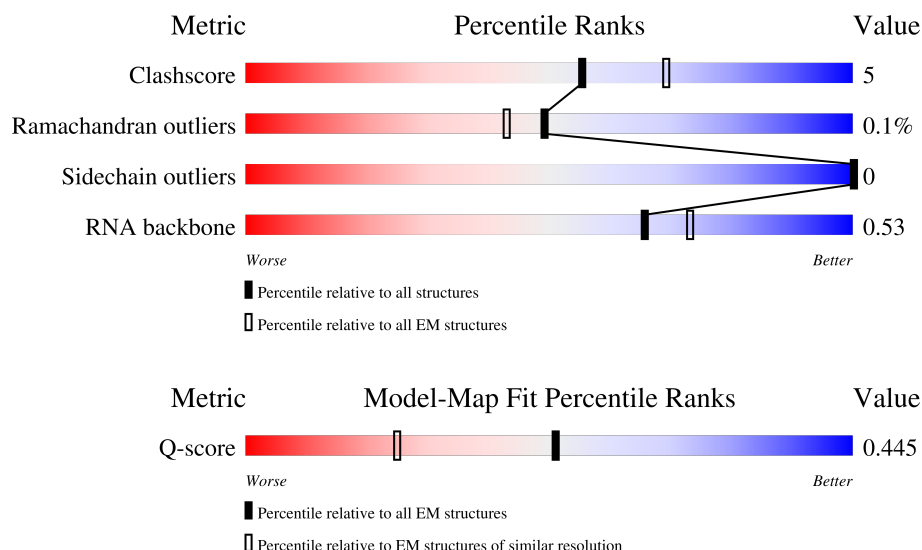
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	AA	241	<div> <div>43%</div> <div> <div>81%</div> <div>12%</div> <div>7%</div> </div> </div>
2	AC	206	<div> <div>80%</div> <div>19%</div> </div>
3	AD	167	<div> <div>75%</div> <div>19%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
4	AE	135	
5	AF	179	
6	AG	130	
7	AH	130	
8	AJ	129	
9	AK	124	
10	AL	118	
11	AN	89	
12	AO	82	
13	AP	84	
14	AQ	75	
15	AR	92	
16	AS	87	
17	AT	71	
18	D1	1540	
19	F1	72	
20	F3	180	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49967 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	225	Total	C	N	O	S	0	0
			1756	1111	315	322	8		

- Molecule 2 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 3 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 4 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 6 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AH	111	Total	C	N	O	S	0	0
			882	548	171	160	3		

- Molecule 8 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AL	92	Total	C	N	O	S	0	0
			724	447	151	123	3		

- Molecule 11 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 12 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 14 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 17 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 18 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D1	1525	Total	C	N	O	P	0	0
			32716	14592	5999	10601	1524		

- Molecule 19 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F1	70	Total	C	N	O	S	0	0
			557	350	99	105	3		

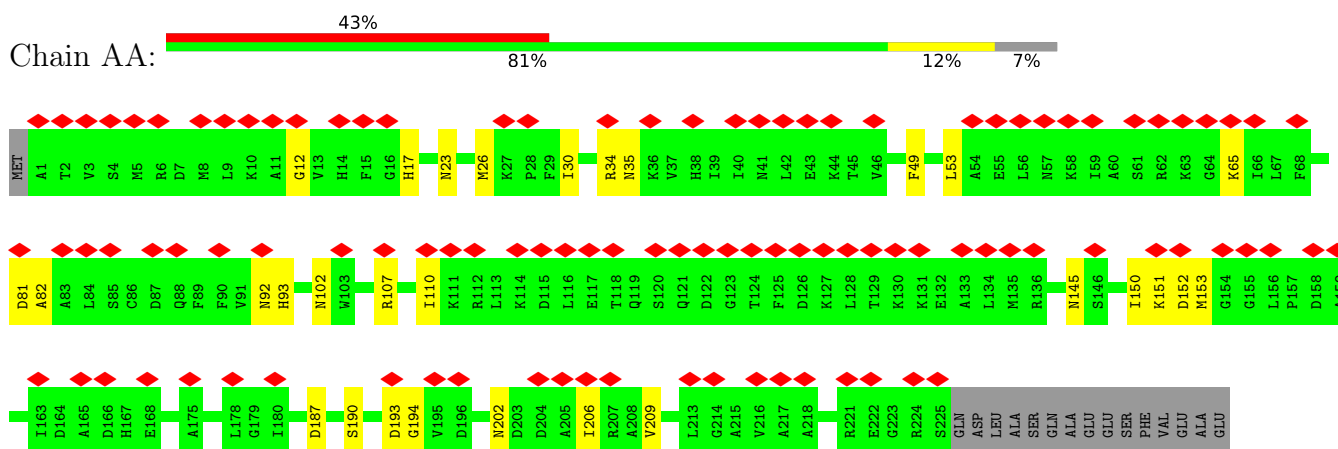
- Molecule 20 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F3	167	Total	C	N	O	S	0	0
			1340	842	241	251	6		

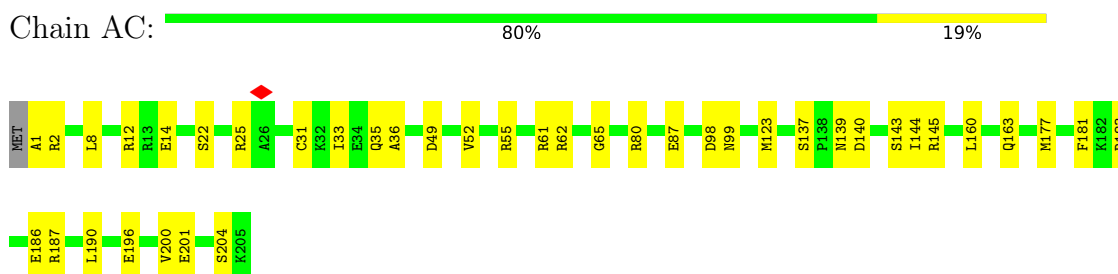
3 Residue-property plots

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.

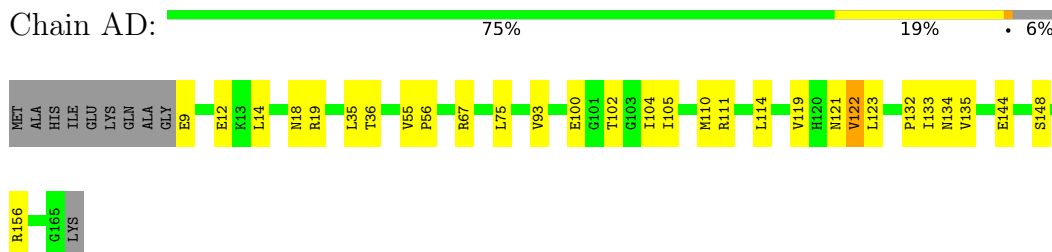
- Molecule 1: Small ribosomal subunit protein uS2



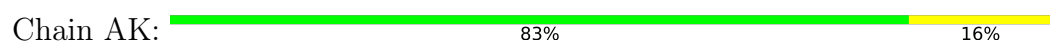
- Molecule 2: Small ribosomal subunit protein uS4



- Molecule 3: Small ribosomal subunit protein uS5

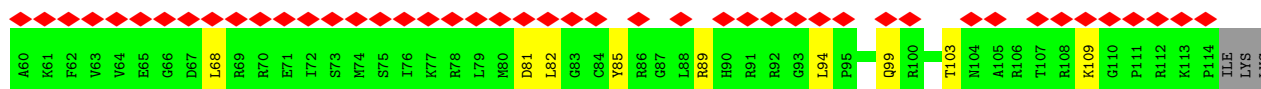
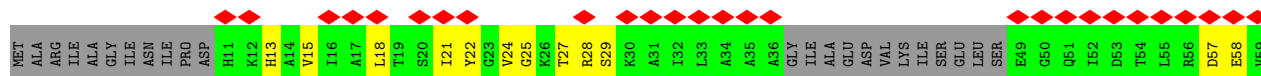


- Molecule 4: Small ribosomal subunit protein bS6, fully modified isoform

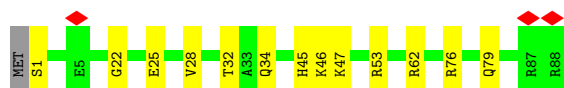
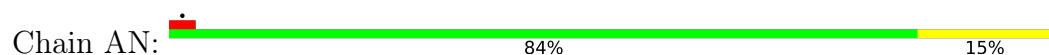




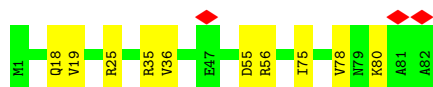
- Molecule 10: Small ribosomal subunit protein uS13



- Molecule 11: Small ribosomal subunit protein uS15



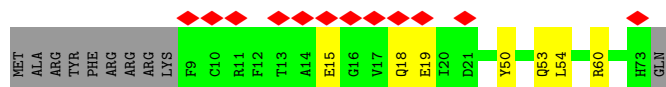
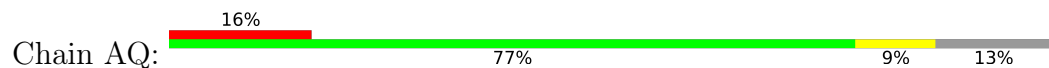
- Molecule 12: Small ribosomal subunit protein bS16



- Molecule 13: Small ribosomal subunit protein uS17

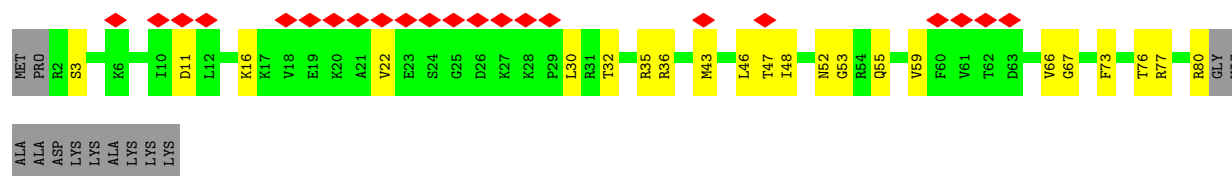


- Molecule 14: Small ribosomal subunit protein bS18



- Molecule 15: Small ribosomal subunit protein uS19





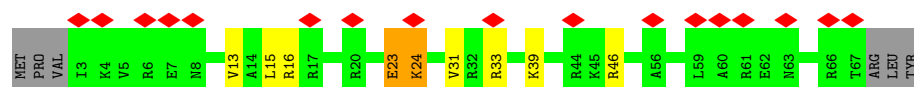
- Molecule 16: Small ribosomal subunit protein bS20

Chain AS: 90% 8%



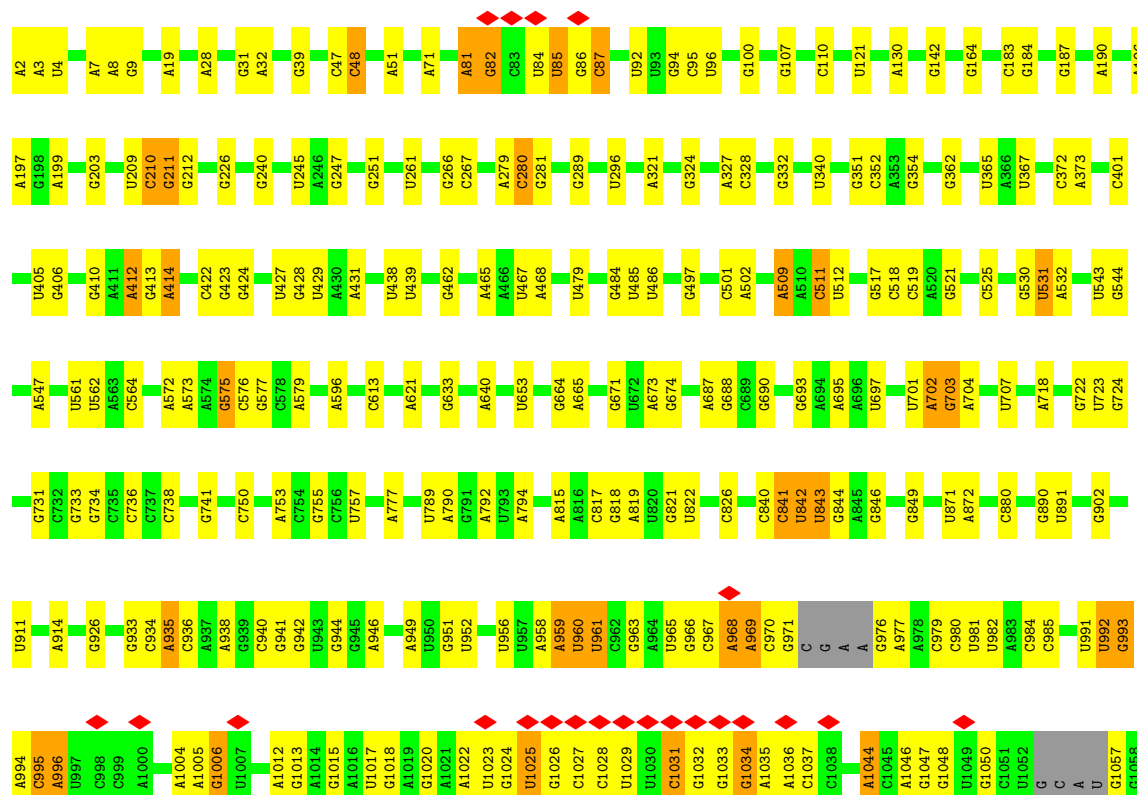
- Molecule 17: Small ribosomal subunit protein bS21

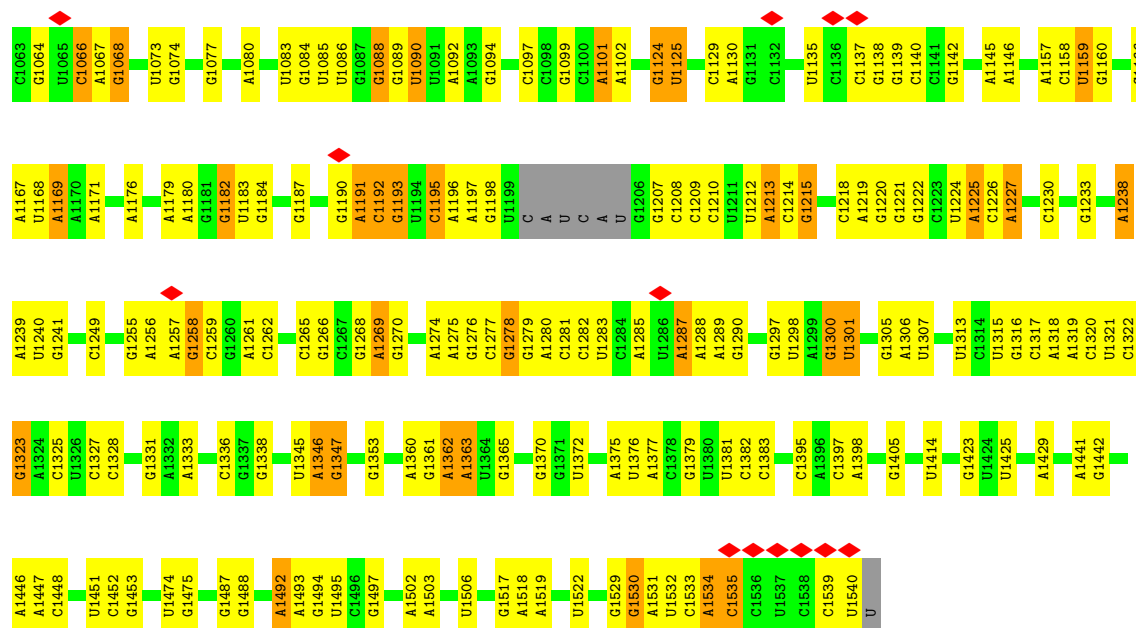
Chain AT: 24% 79% 10% 8%



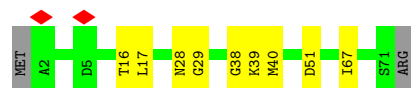
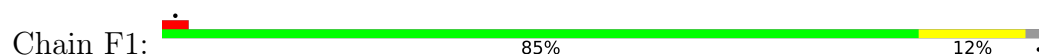
- Molecule 18: 16S Ribosomal RNA

Chain D1: 70% 25%

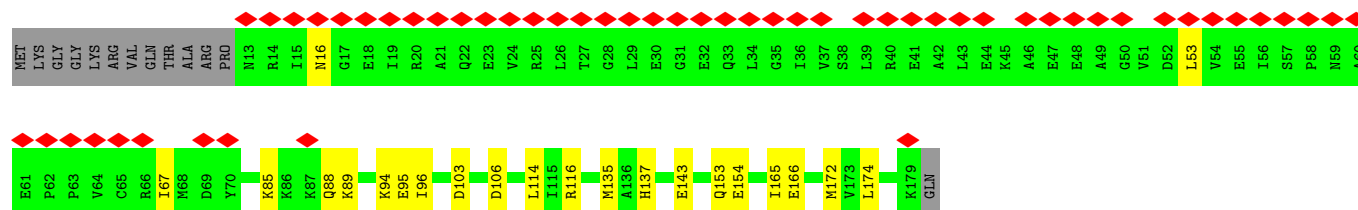
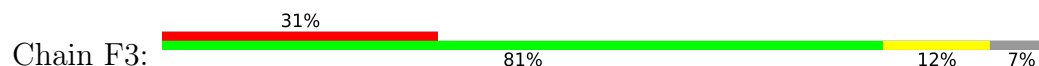




- Molecule 19: Translation initiation factor IF-1



- Molecule 20: Translation initiation factor IF-3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39565	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	18.790	Depositor
Minimum map value	-4.492	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.707	Depositor
Recommended contour level	3	Depositor
Map size (\AA)	400.32, 400.32, 400.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.834, 0.834, 0.834	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	AA	0.14	0/1787	0.35	0/2408
2	AC	0.17	0/1665	0.37	0/2227
3	AD	0.18	0/1169	0.41	0/1573
4	AE	0.19	0/835	0.40	0/1128
5	AF	0.15	0/1195	0.35	0/1602
6	AG	0.18	0/989	0.36	0/1326
7	AH	0.16	0/892	0.42	0/1191
8	AJ	0.15	0/885	0.35	0/1195
9	AK	0.18	0/969	0.41	0/1300
10	AL	0.13	0/731	0.32	0/973
11	AN	0.16	0/722	0.38	0/964
12	AO	0.17	0/659	0.32	0/884
13	AP	0.16	0/657	0.35	0/881
14	AQ	0.18	0/544	0.41	0/731
15	AR	0.14	0/652	0.33	0/877
16	AS	0.16	0/671	0.35	0/888
17	AT	0.22	0/550	0.60	2/728 (0.3%)
18	D1	0.17	0/36629	0.28	0/57135
19	F1	0.14	0/564	0.34	0/759
20	F3	0.12	0/1354	0.29	0/1806
All	All	0.17	0/54119	0.31	2/80576 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AT	23	GLU	CA-C-N	5.51	132.07	121.54
17	AT	23	GLU	C-N-CA	5.51	132.07	121.54

There are no chirality outliers.

There are no planarity outliers.

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	AA	1756	0	1787	17	0
2	AC	1643	0	1710	28	0
3	AD	1156	0	1199	26	0
4	AE	817	0	808	16	0
5	AF	1181	0	1240	25	0
6	AG	979	0	1034	15	0
7	AH	882	0	909	16	0
8	AJ	869	0	878	13	0
9	AK	955	0	1019	16	0
10	AL	724	0	775	16	0
11	AN	714	0	737	8	0
12	AO	649	0	666	7	0
13	AP	648	0	691	7	0
14	AQ	535	0	552	5	0
15	AR	637	0	665	18	0
16	AS	665	0	714	7	0
17	AT	544	0	579	8	0
18	D1	32716	0	16470	196	0
19	F1	557	0	573	8	0
20	F3	1340	0	1402	18	0
All	All	49967	0	34408	396	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 396 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)
18:D1:1495:U:O2'	20:F3:106:ASP:OD2	1.93	0.87
12:AO:75:ILE:O	12:AO:80:LYS:NZ	2.12	0.83
18:D1:1006:G:O6	18:D1:1023:U:O2	1.98	0.81
18:D1:1015:G:HO2'	18:D1:1218:C:HO2'	1.22	0.80
6:AG:47:ASP:OD1	6:AG:61:THR:OG1	2.00	0.79

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	223/241 (92%)	211 (95%)	12 (5%)	0	100	100
2	AC	203/206 (98%)	185 (91%)	18 (9%)	0	100	100
3	AD	155/167 (93%)	134 (86%)	20 (13%)	1 (1%)	21	51
4	AE	98/135 (73%)	82 (84%)	16 (16%)	0	100	100
5	AF	149/179 (83%)	136 (91%)	13 (9%)	0	100	100
6	AG	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
7	AH	109/130 (84%)	91 (84%)	18 (16%)	0	100	100
8	AJ	114/129 (88%)	97 (85%)	17 (15%)	0	100	100
9	AK	121/124 (98%)	98 (81%)	23 (19%)	0	100	100
10	AL	88/118 (75%)	81 (92%)	7 (8%)	0	100	100
11	AN	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	34
12	AO	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
13	AP	78/84 (93%)	67 (86%)	11 (14%)	0	100	100
14	AQ	63/75 (84%)	58 (92%)	5 (8%)	0	100	100
15	AR	77/92 (84%)	67 (87%)	10 (13%)	0	100	100
16	AS	83/87 (95%)	79 (95%)	4 (5%)	0	100	100
17	AT	63/71 (89%)	44 (70%)	18 (29%)	1 (2%)	7	27
19	F1	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
20	F3	165/180 (92%)	149 (90%)	16 (10%)	0	100	100
All	All	2150/2391 (90%)	1921 (89%)	226 (10%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	122	VAL
11	AN	46	LYS

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Mol	Chain	Res	Type
17	AT	24	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	186/199 (94%)	186 (100%)	0	100	100
2	AC	172/173 (99%)	172 (100%)	0	100	100
3	AD	119/126 (94%)	119 (100%)	0	100	100
4	AE	87/116 (75%)	87 (100%)	0	100	100
5	AF	124/147 (84%)	124 (100%)	0	100	100
6	AG	104/105 (99%)	104 (100%)	0	100	100
7	AH	91/107 (85%)	91 (100%)	0	100	100
8	AJ	89/99 (90%)	89 (100%)	0	100	100
9	AK	103/104 (99%)	103 (100%)	0	100	100
10	AL	75/96 (78%)	75 (100%)	0	100	100
11	AN	76/77 (99%)	76 (100%)	0	100	100
12	AO	65/65 (100%)	65 (100%)	0	100	100
13	AP	74/78 (95%)	74 (100%)	0	100	100
14	AQ	56/65 (86%)	56 (100%)	0	100	100
15	AR	70/79 (89%)	70 (100%)	0	100	100
16	AS	65/66 (98%)	65 (100%)	0	100	100
17	AT	55/61 (90%)	55 (100%)	0	100	100
19	F1	63/65 (97%)	63 (100%)	0	100	100
20	F3	146/156 (94%)	146 (100%)	0	100	100
All	All	1820/1984 (92%)	1820 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
12	AO	59	HIS
20	F3	33	GLN
20	F3	84	GLN
3	AD	11	GLN
2	AC	35	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	D1	1521/1540 (98%)	263 (17%)	12 (0%)

5 of 263 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	D1	4	U
18	D1	7	A
18	D1	8	A
18	D1	9	G
18	D1	32	A

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	D1	1025	U
18	D1	1190	G
18	D1	1534	A
18	D1	1300	G
18	D1	871	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

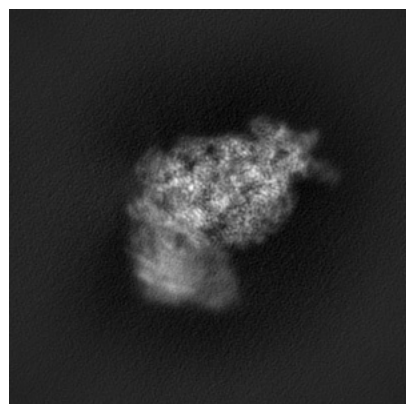
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55173. These allow visual inspection of the internal detail of the map and identification of artifacts.

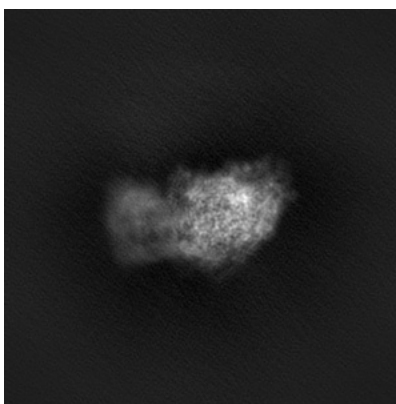
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

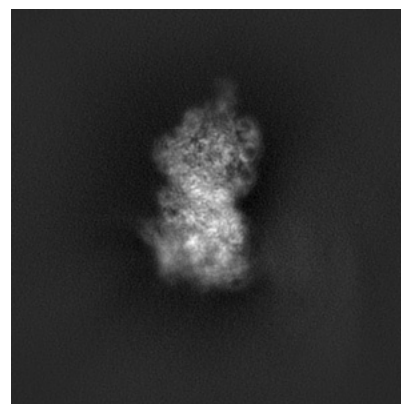
6.1.1 Primary map



X

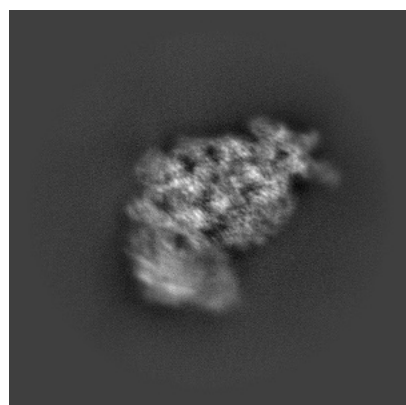


Y

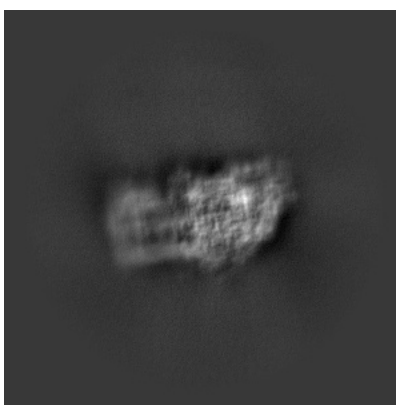


Z

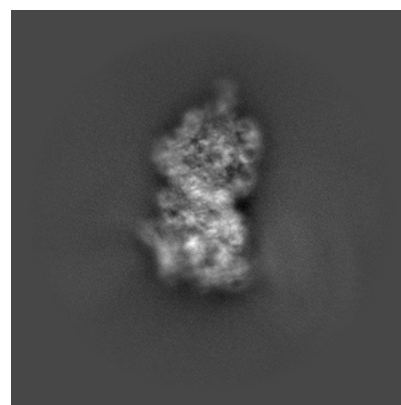
6.1.2 Raw map



X



Y

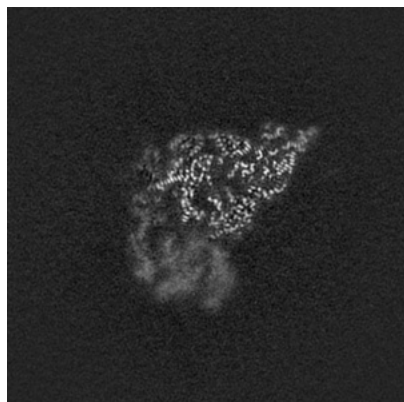


Z

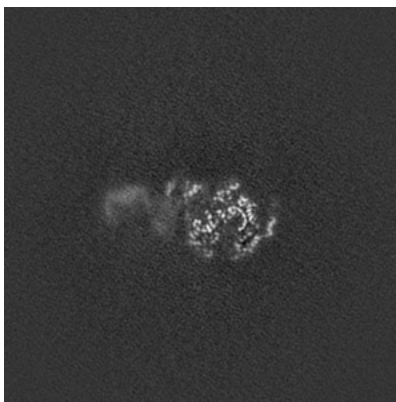
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

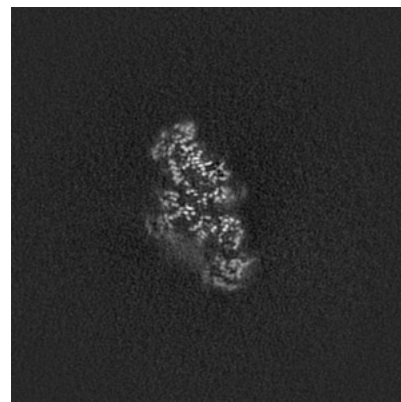
6.2.1 Primary map



X Index: 240

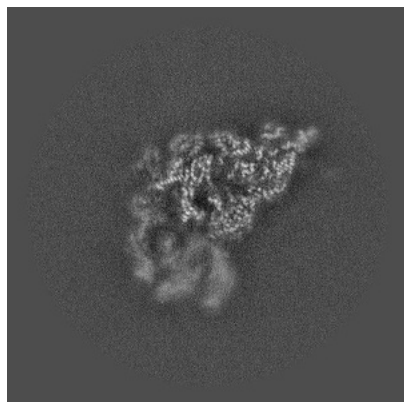


Y Index: 240

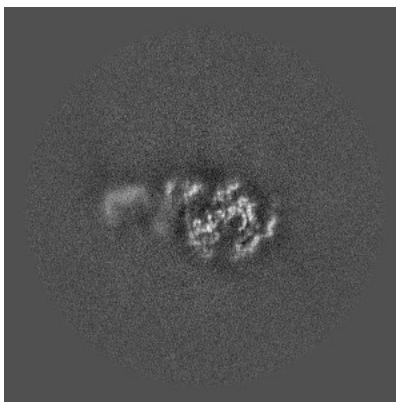


Z Index: 240

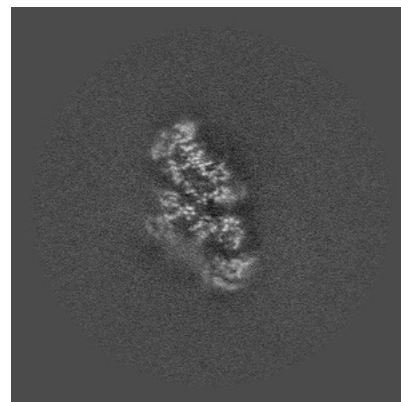
6.2.2 Raw map



X Index: 240



Y Index: 240

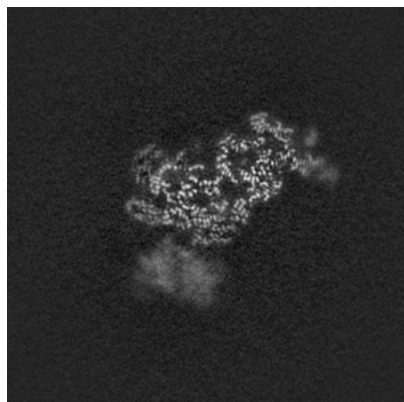


Z Index: 240

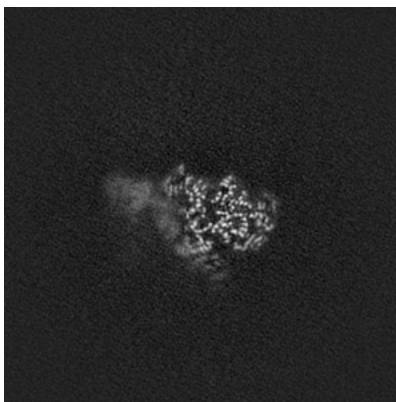
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 256

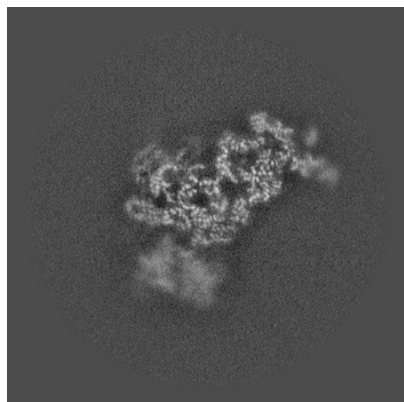


Y Index: 226

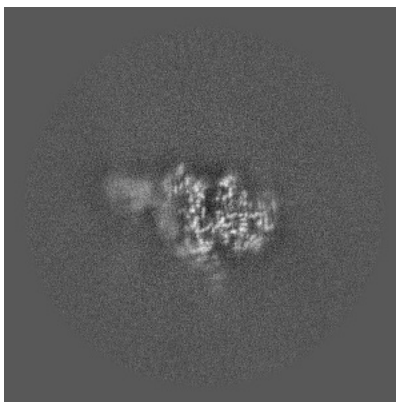


Z Index: 289

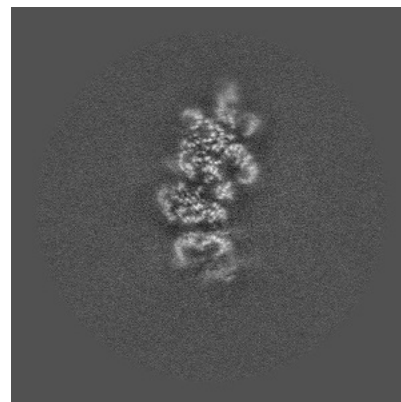
6.3.2 Raw map



X Index: 256



Y Index: 227

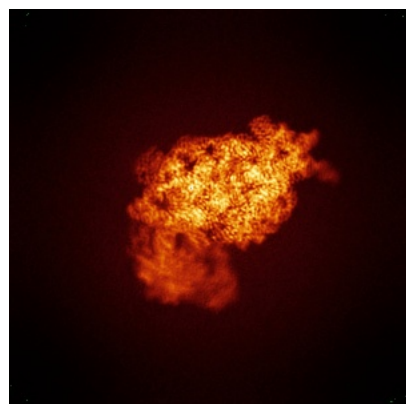


Z Index: 289

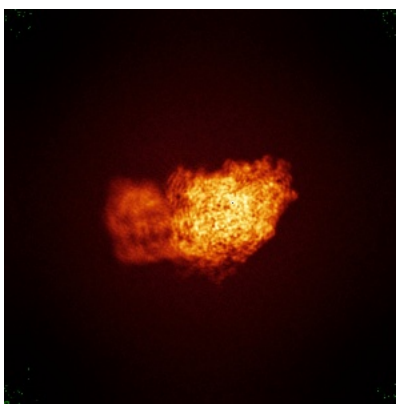
The images above show the largest variance slices of the map in three orthogonal directions.

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

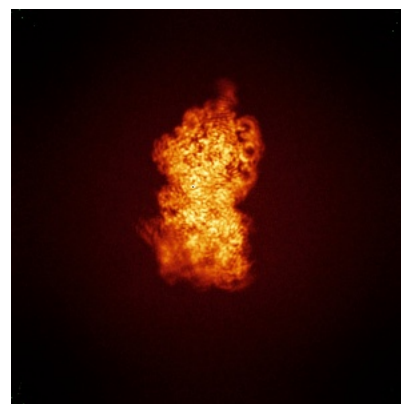
6.4.1 Primary map



X

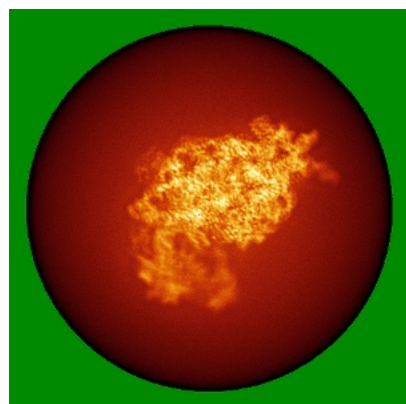


Y

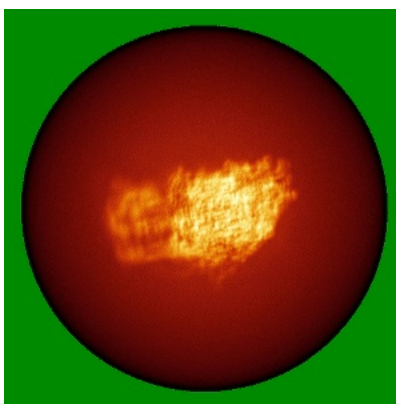


Z

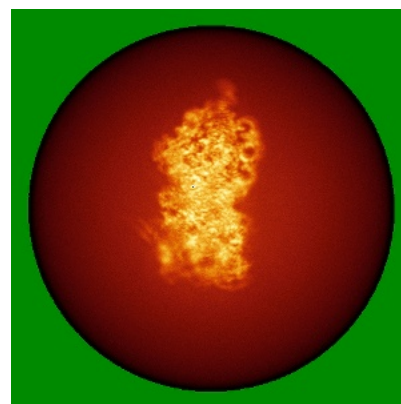
6.4.2 Raw map



X



Y

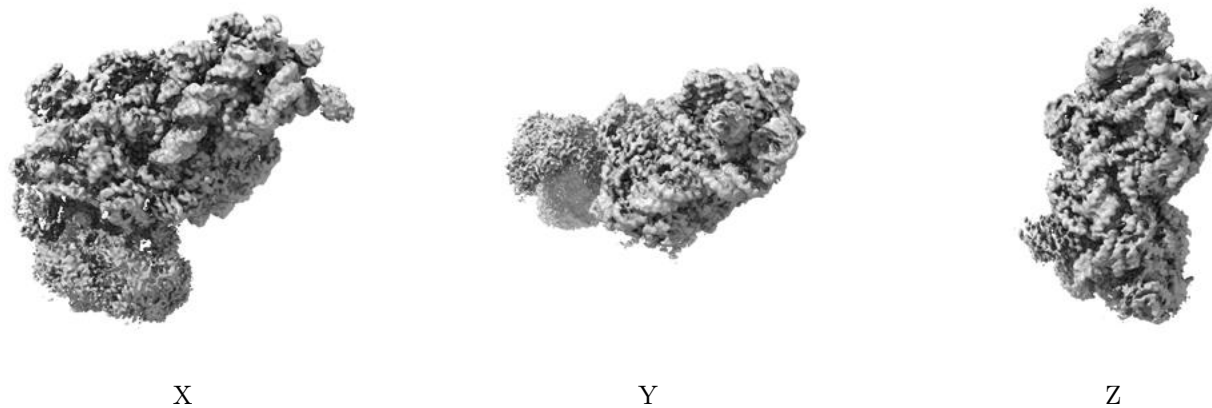


Z

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

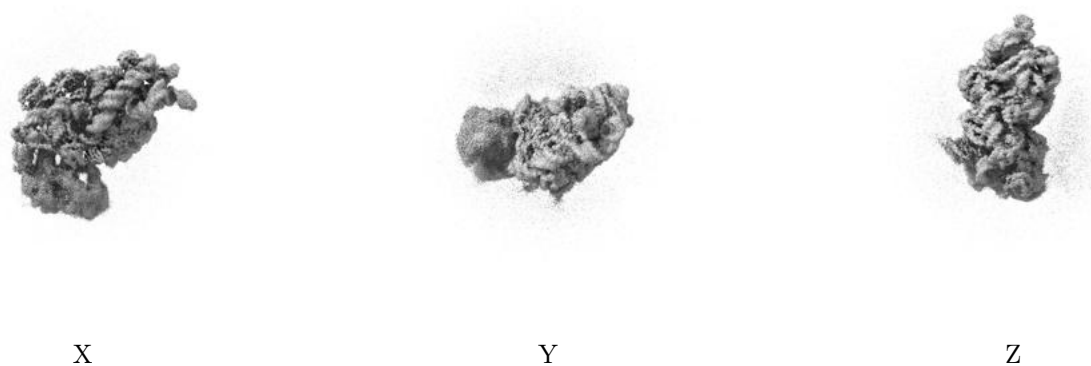
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

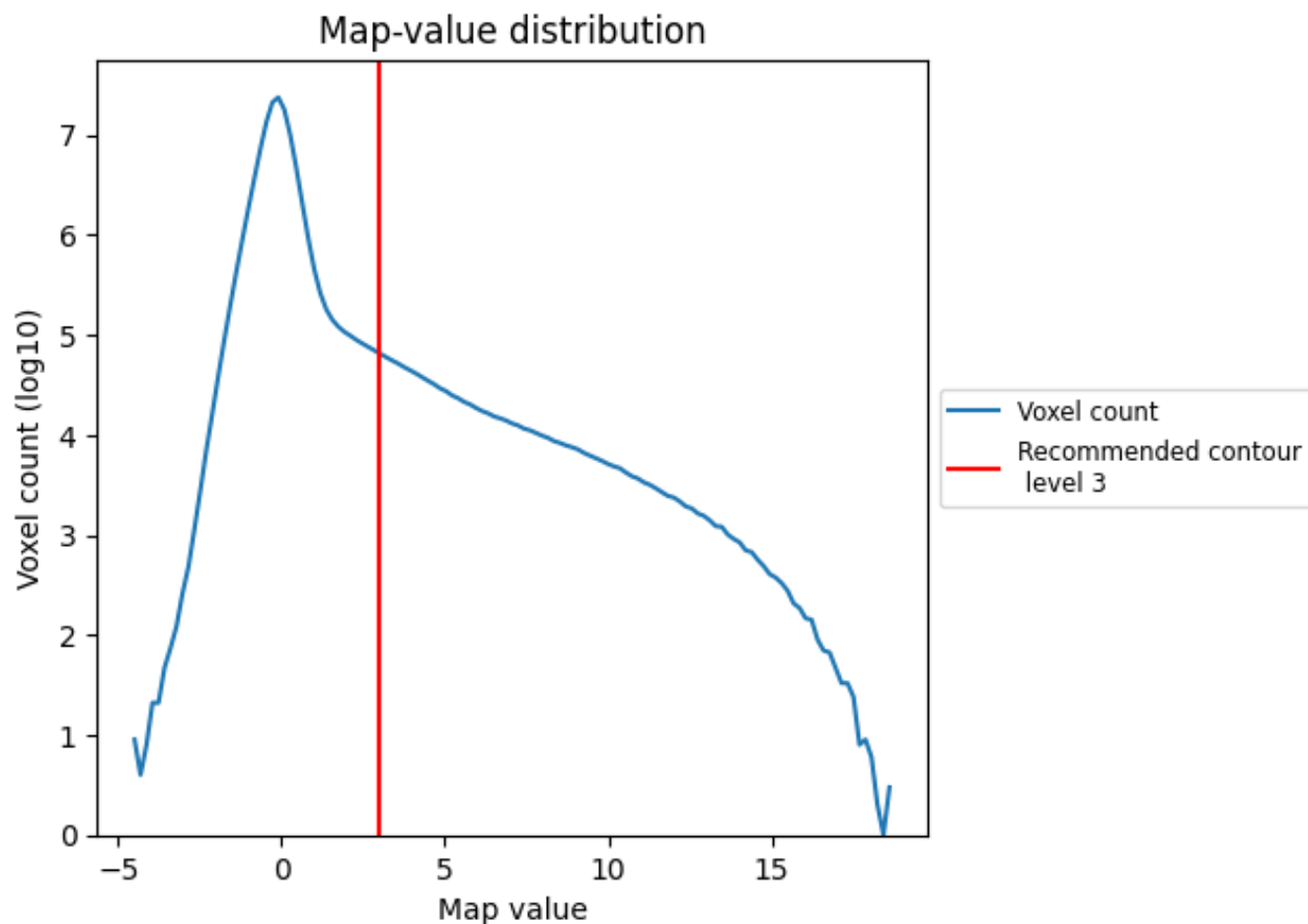
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

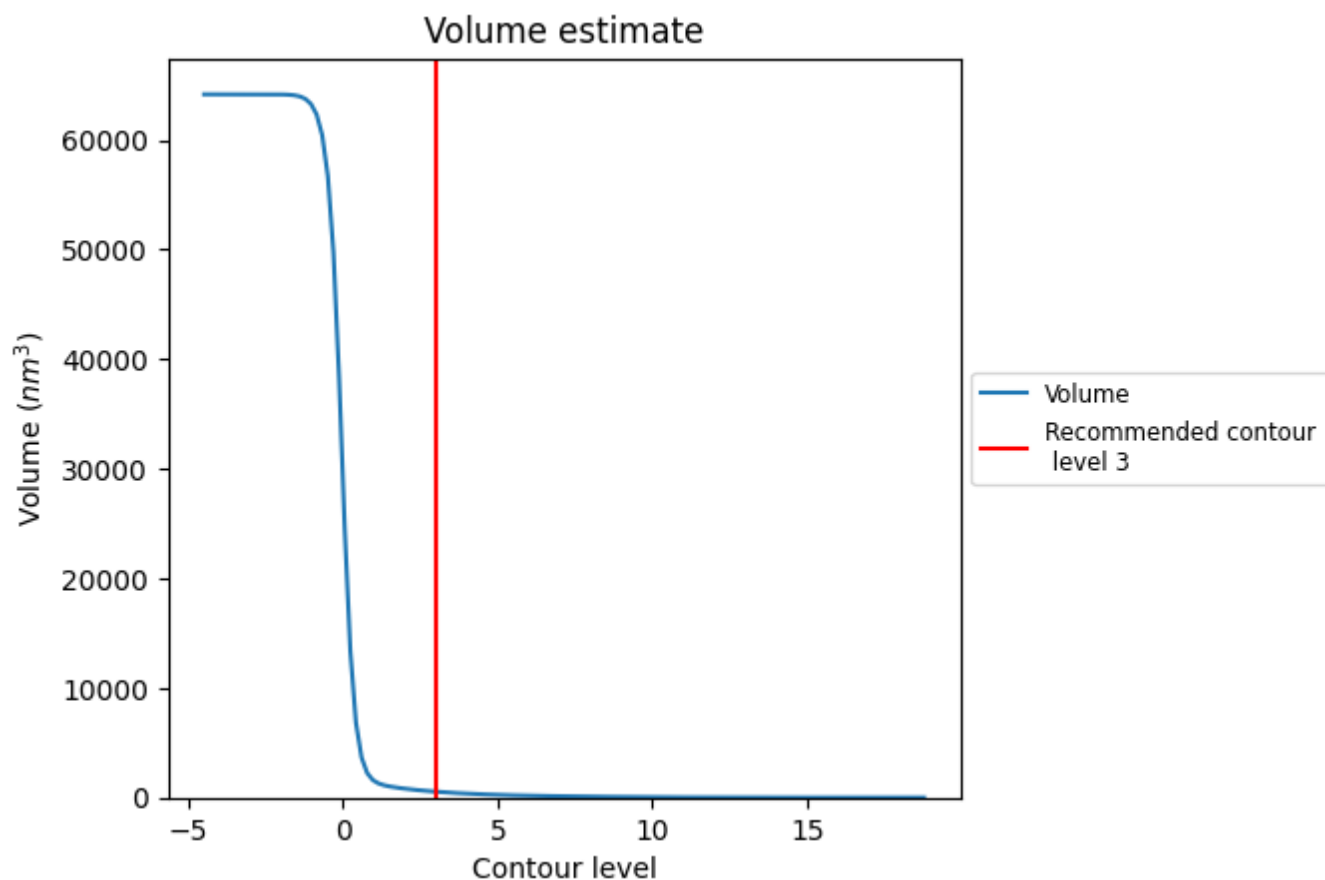
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

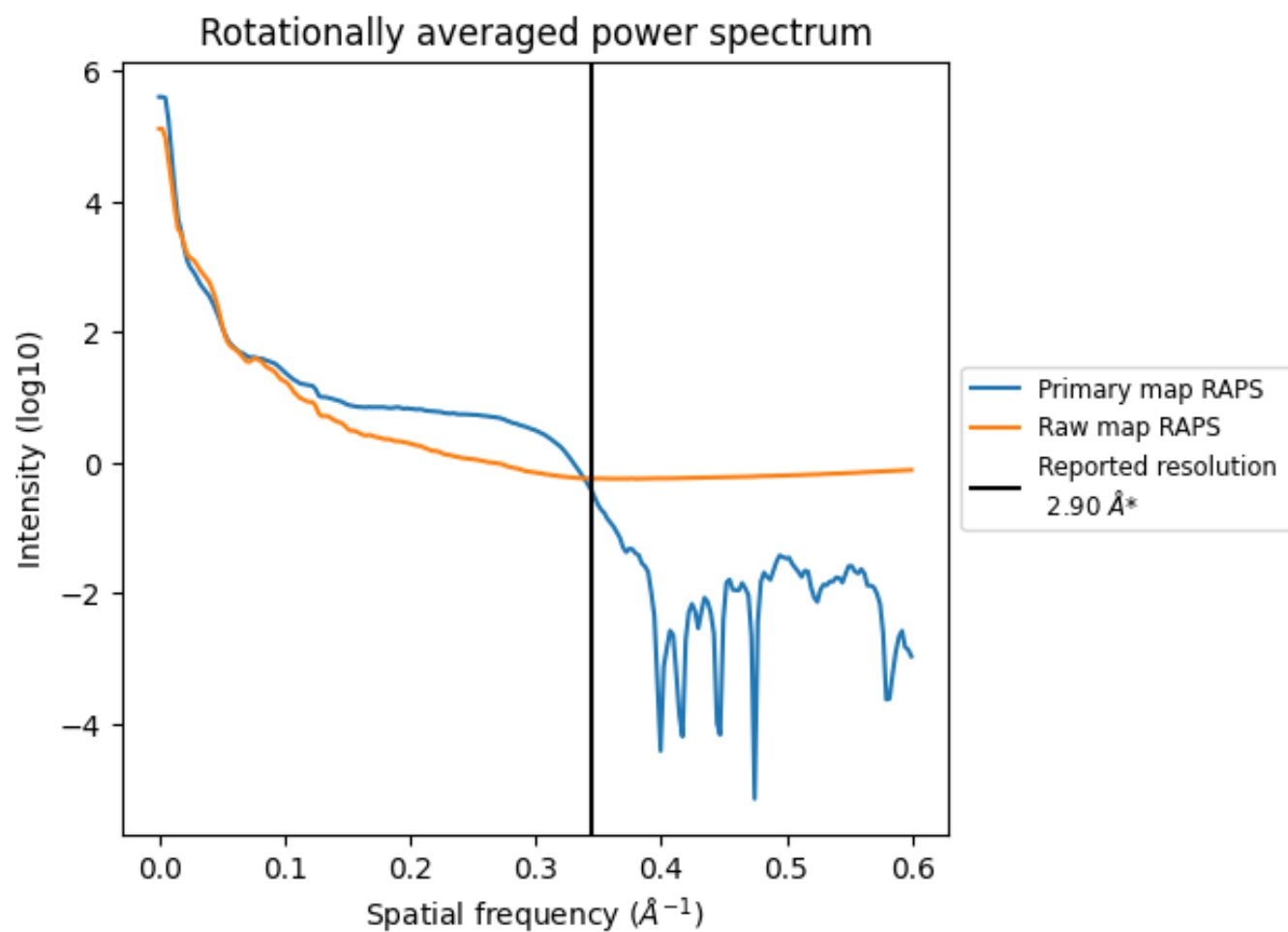
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 537 nm³; this corresponds to an approximate mass of 485 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 ⓘ

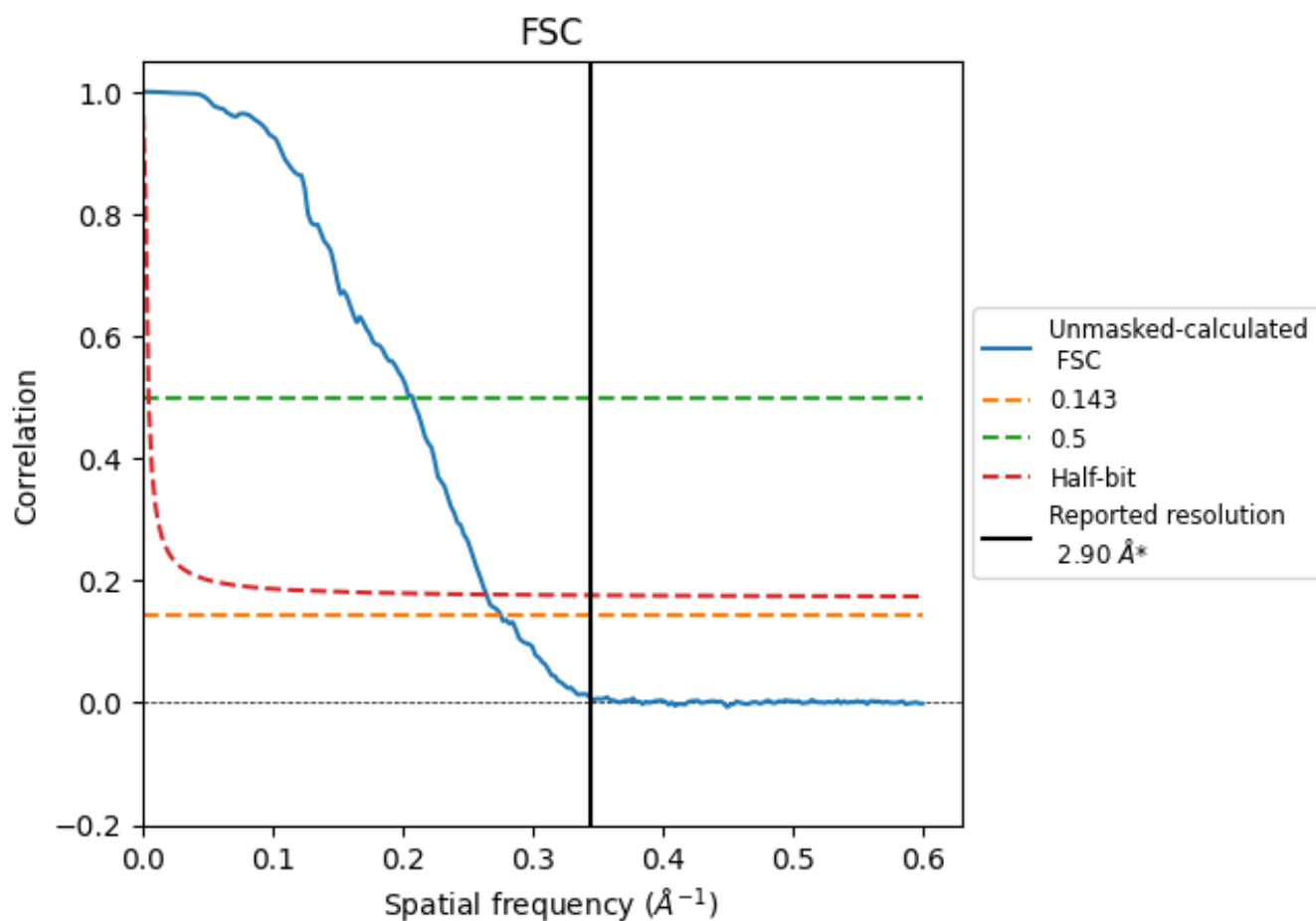


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

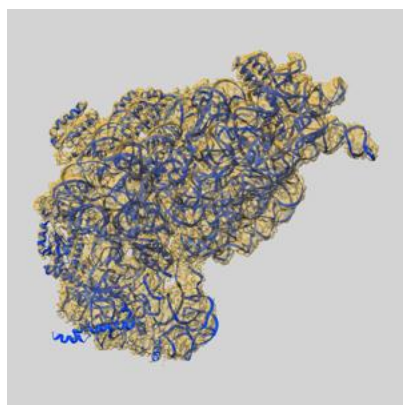
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.63	4.82	3.78

*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 3.63 differs from the reported value 2.9 by more than 10 %

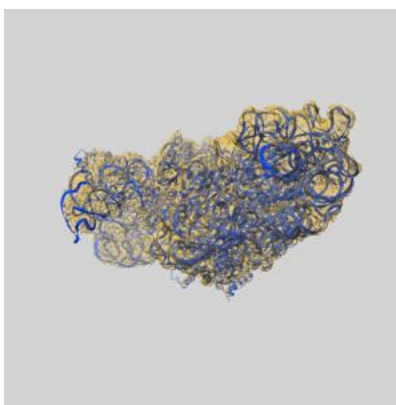
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55173 and PDB model 9SS1. Per-residue inclusion information can be found in section 3 on page 7.

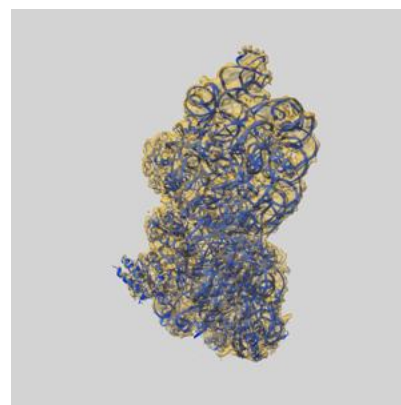
9.1 Map-model overlay [i](#)



X



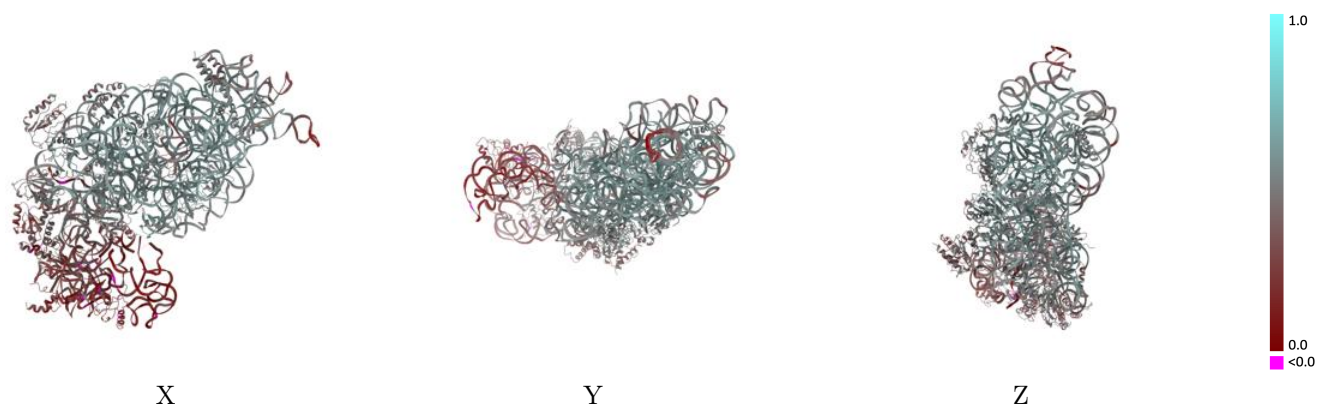
Y



Z

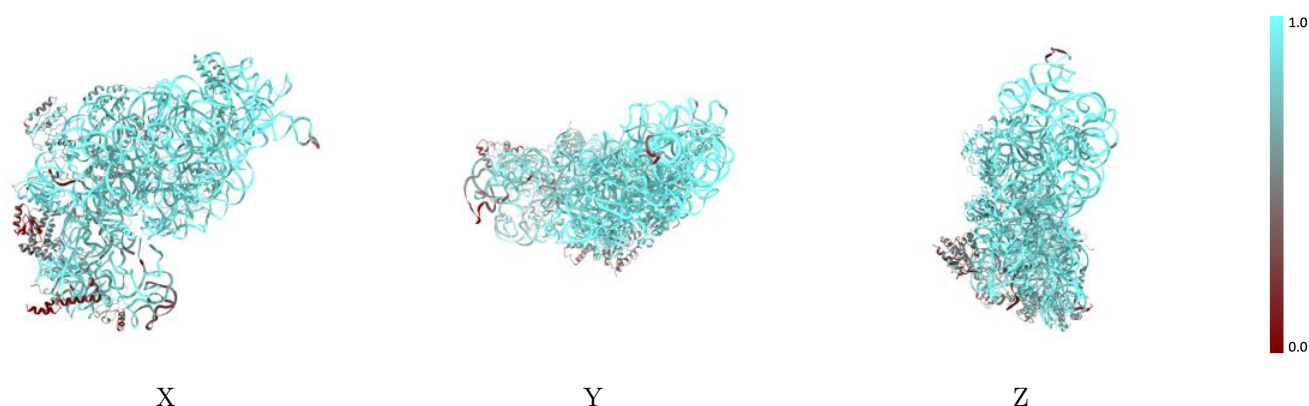
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



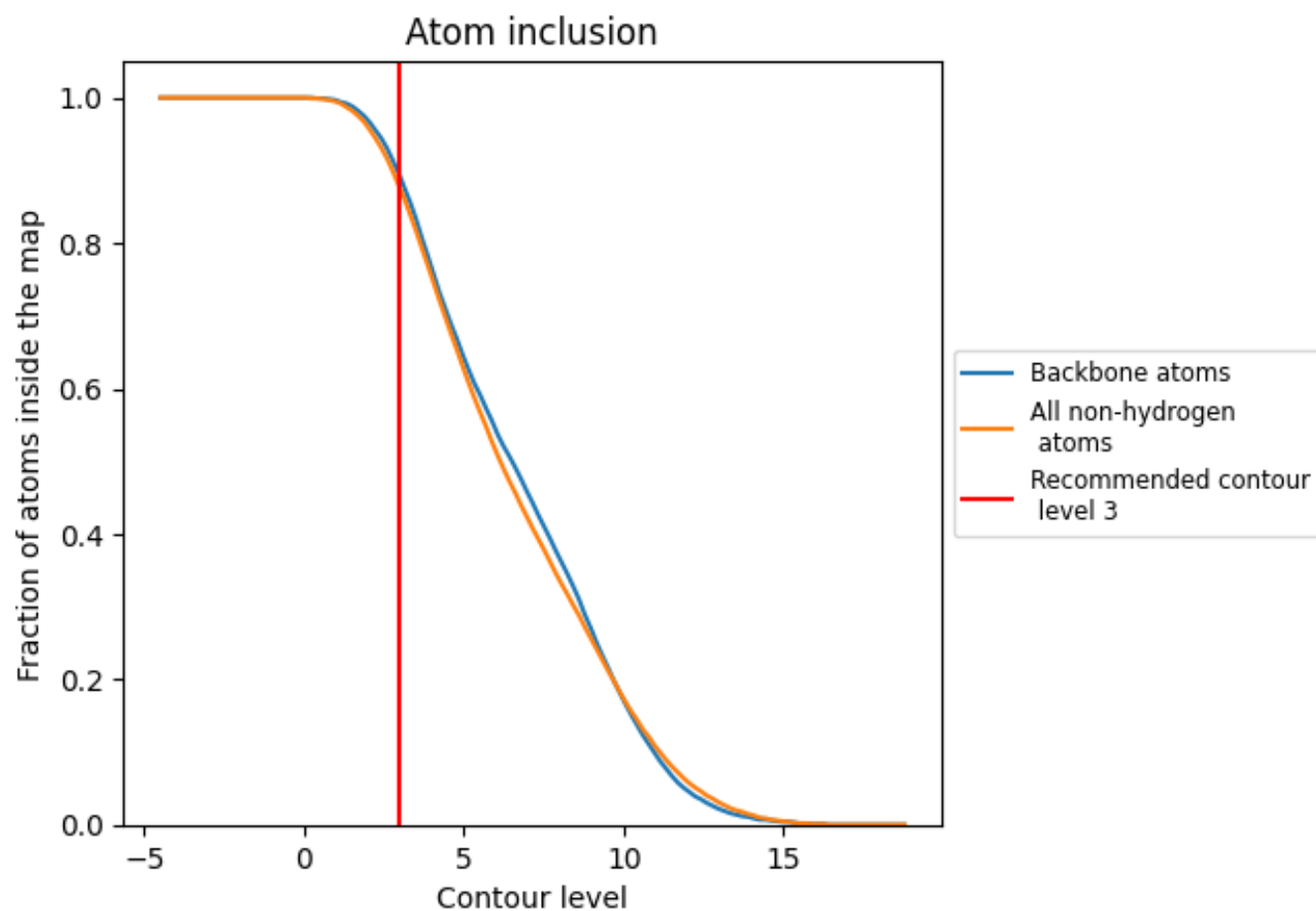
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).











































9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8750	 0.4450
AA	 0.4350	 0.3930
AC	 0.9230	 0.4910
AD	 0.9350	 0.4990
AE	 0.6820	 0.4100
AF	 0.6460	 0.3640
AG	 0.9340	 0.5320
AH	 0.6600	 0.2990
AJ	 0.9290	 0.4590
AK	 0.9510	 0.5450
AL	 0.1960	 0.1820
AN	 0.8220	 0.4590
AO	 0.9310	 0.5430
AP	 0.9590	 0.5450
AQ	 0.6870	 0.4480
AR	 0.5990	 0.2160
AS	 0.9260	 0.5050
AT	 0.5420	 0.3240
D1	 0.9420	 0.4530
F1	 0.8970	 0.5240
F3	 0.6250	 0.3940

