



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 06:52 PM UTC

PDB ID : 7OQC / pdb_00007oqc
EMDB ID : EMD-13029
Title : The U1 part of *Saccharomyces cerevisiae* spliceosomal pre-A complex (delta BS-A ACT1)
Authors : Zhang, Z.; Rigo, N.; Dybkov, O.; Fourmann, J.; Will, C.L.; Kumar, V.; Urlaub, H.; Stark, H.; Luehrmann, R.
Deposited on : 2021-06-03
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

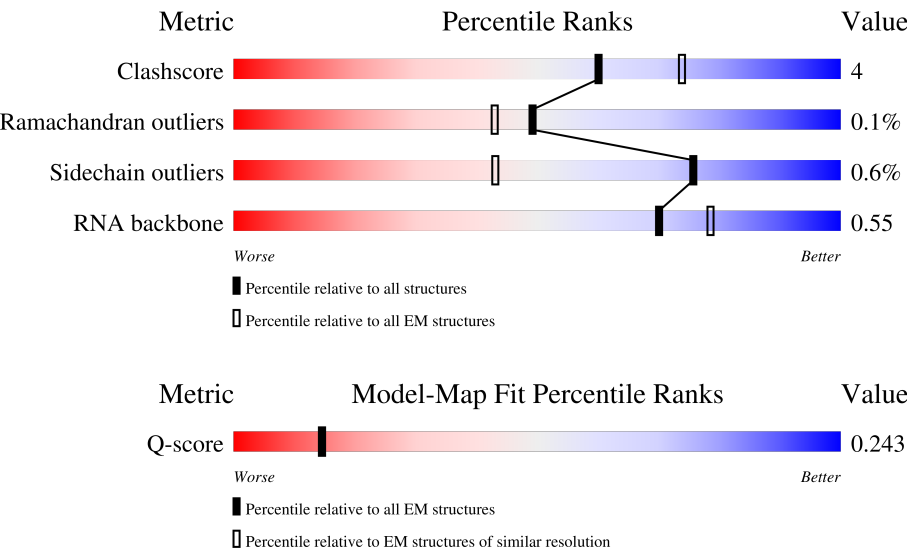
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	F	523	
2	I	371	
3	E	544	

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Mol	Chain	Length	Quality of chain
4	J	620	
5	1	568	
6	G	492	
7	A	298	
8	C	231	
9	b	196	
10	d	101	
11	e	94	
12	f	86	
13	g	77	
14	h	146	
15	i	110	
16	H	261	
17	D	629	
18	B	300	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 35050 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 Protein NAM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	267	Total	C	N	O	S	0	0
			1758	1091	316	341	10		

- Molecule 2 is a RNA chain called ACT1 pre-mRNA (delta BS-A),ACT1 pre-mRNA (delta BS-A),ACT1 pre-mRNA (delta BS-A),ACT1 pre-mRNA (delta BS-A),ACT1 pre-mRNA (delta BS-A),ACT1 pre-mRNA (delta BS-A),ACT1 pre-mRNA (delta BS-A),ACT1 pre-mRNA (delta BS-A),ACT1 pre-mRNA (delta BS-A).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	63	Total	C	N	O	P	0	0
			847	359	33	392	63		

- Molecule 3 is a protein called U1 small nuclear ribonucleoprotein component PRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	544	Total	C	N	O	S	0	0
			4561	2990	723	828	20		

- Molecule 4 is a protein called U1 small nuclear ribonucleoprotein component SNU71.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	105	Total	C	N	O	S	0	0
			687	427	127	132	1		

- Molecule 5 is a RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	558	Total	C	N	O	P	0	0
			11822	5287	2003	3974	558		

- Molecule 6 is a protein called 56 kDa U1 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	239	Total	C	N	O	S	0	0
			1954	1267	321	354	12		

- Molecule 7 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	132	Total	C	N	O	S	0	0
			1058	674	193	187	4		

- Molecule 8 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	195	Total	C	N	O	S	0	0
			1570	976	301	288	5		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	121	Total	C	N	O	S	0	0
			972	613	183	173	3		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	93	Total	C	N	O	S	0	0
			714	453	125	133	3		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e	77	Total	C	N	O	S	0	0
			600	395	96	106	3		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	73	Total	C	N	O	S	0	0
			585	376	102	106	1		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	g	72	Total	C	N	O	S	0	0
			556	352	97	105	2		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	h	107	Total	C	N	O	S	0	0
			771	487	138	143	3		

- Molecule 15 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	i	99	Total	C	N	O	S	0	0
			805	514	148	139	4		

- Molecule 16 is a protein called Protein LUC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	192	Total	C	N	O	S	0	0
			1201	740	226	228	7		

- Molecule 17 is a protein called Pre-mRNA-processing factor 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	576	Total	C	N	O	S	0	0
			3530	2204	642	680	4		

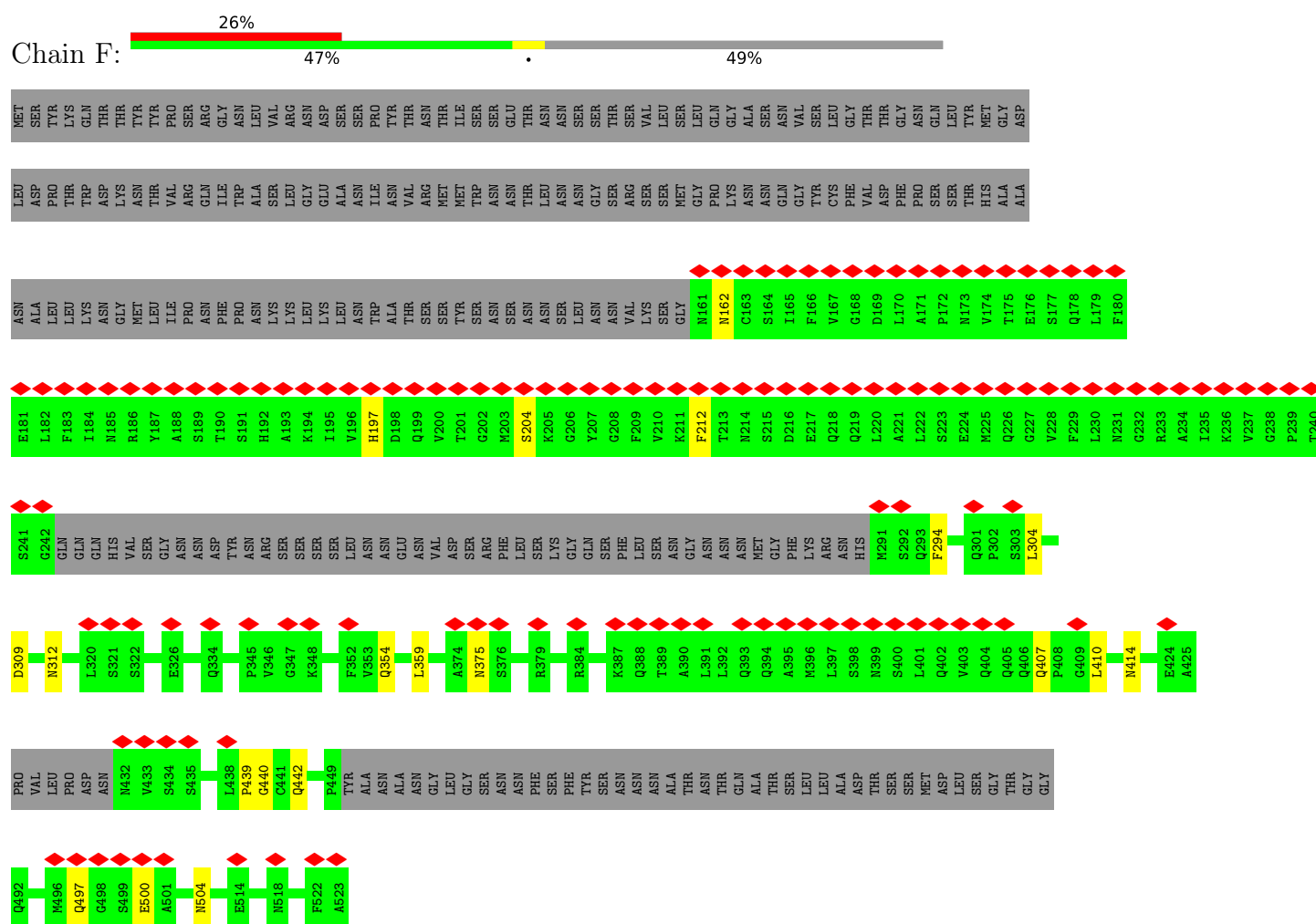
- Molecule 18 is a protein called U1 small nuclear ribonucleoprotein 70 kDa homolog.

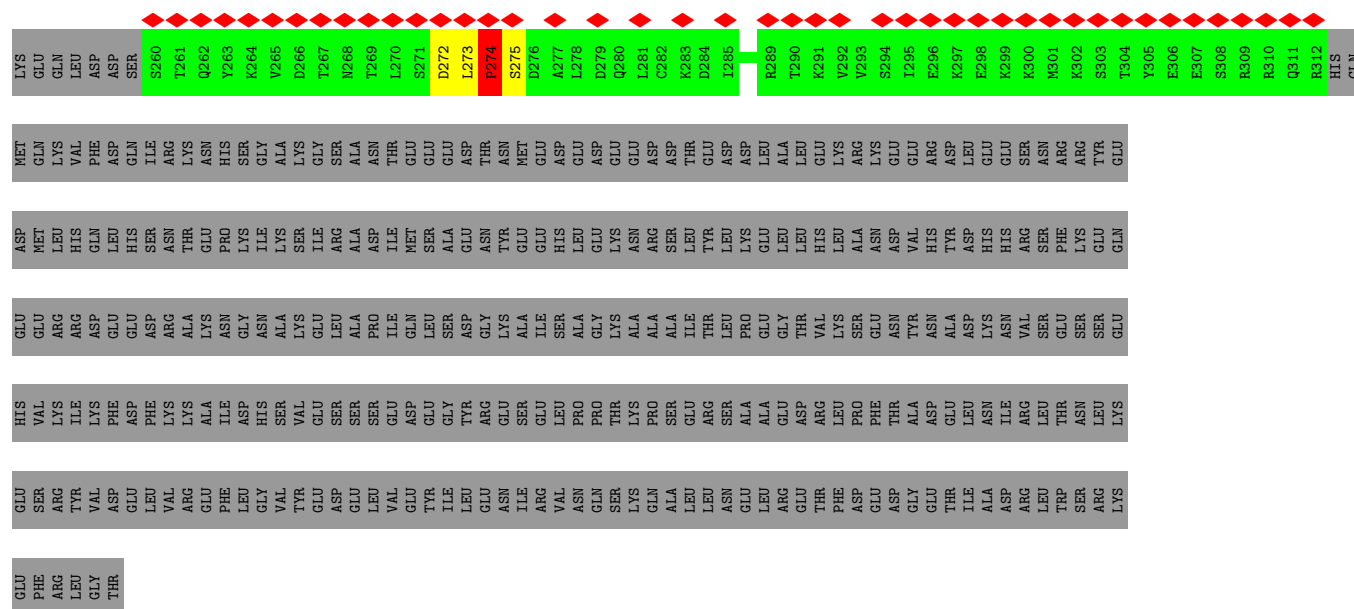
Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	186	Total	C	N	O		0	0
			1059	647	206	206			

3 Residue-property plots

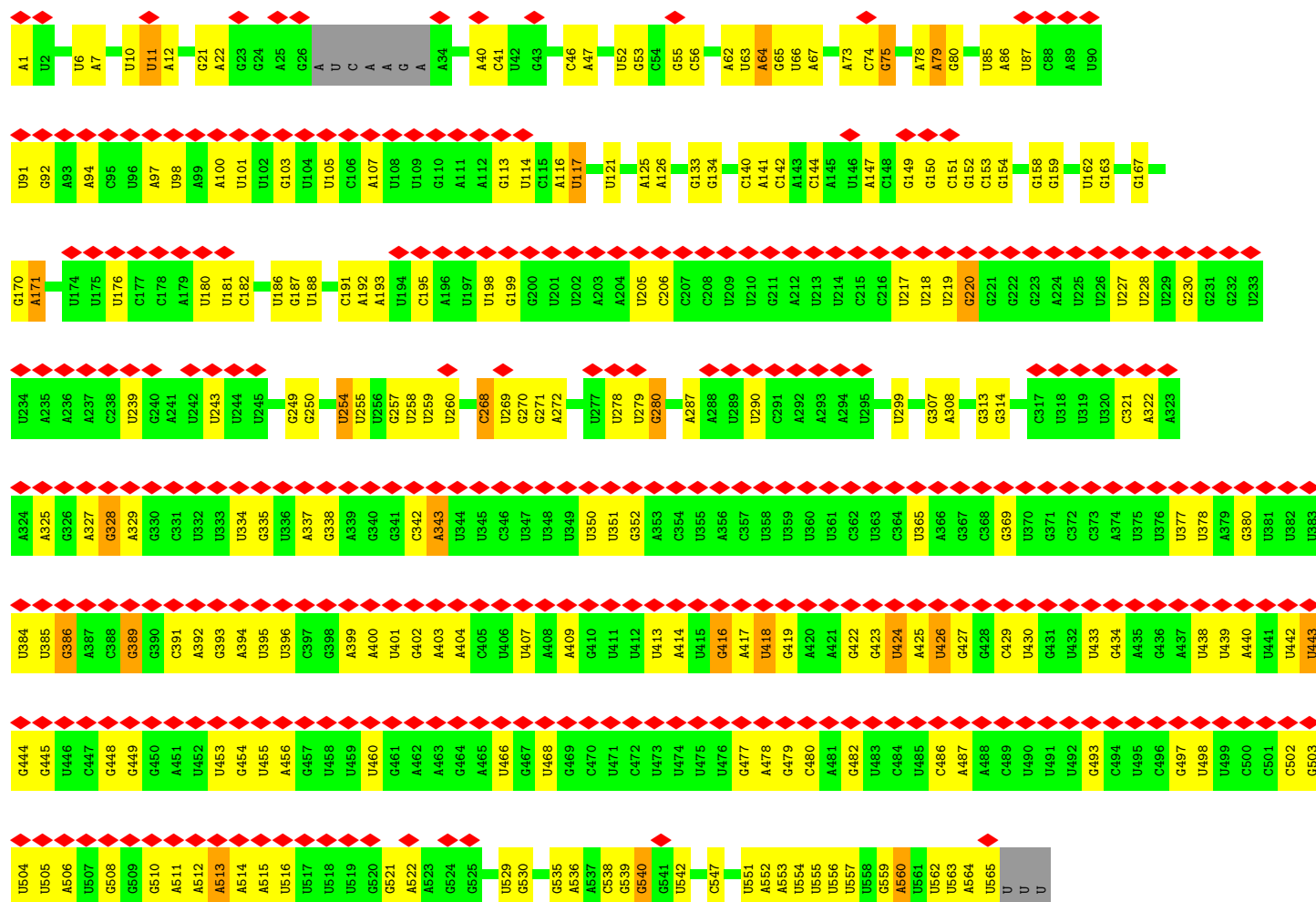
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Protein NAM8

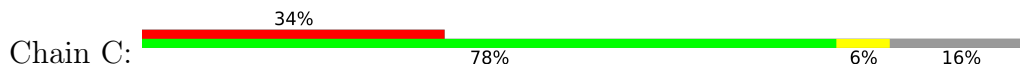
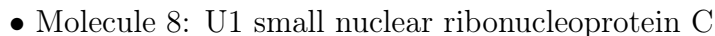
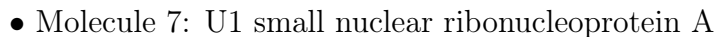


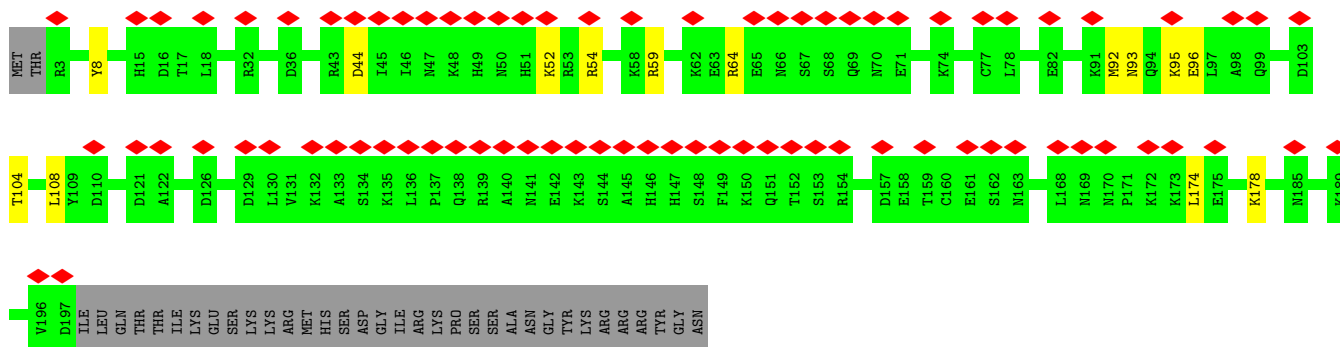


- Molecule 5: U1 snRNA

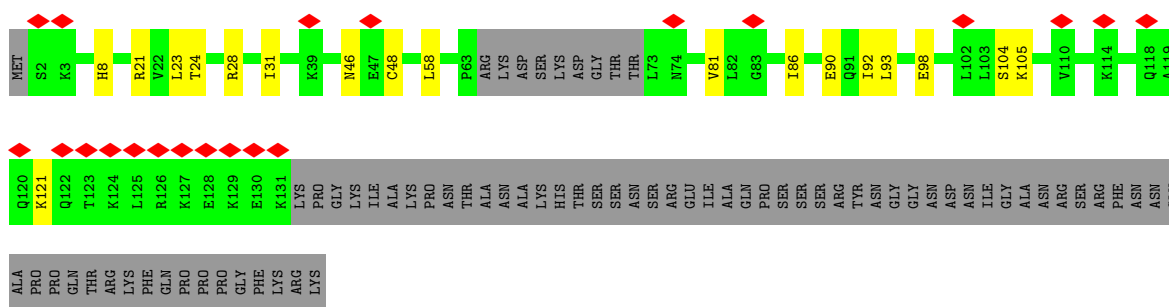


- Chain G:

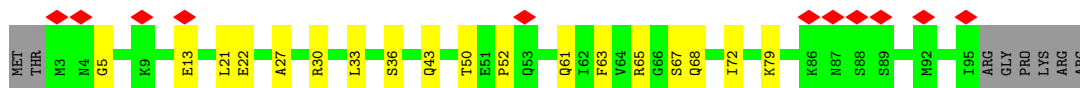
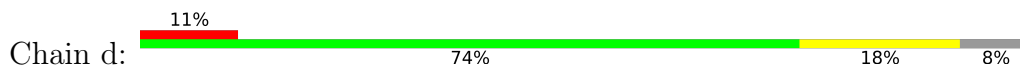




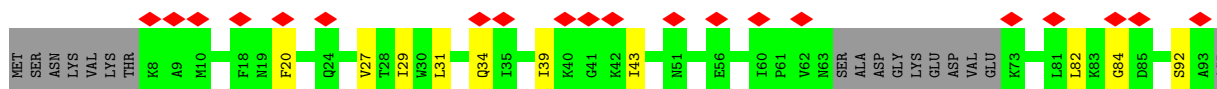
- Molecule 9: Small nuclear ribonucleoprotein-associated protein B



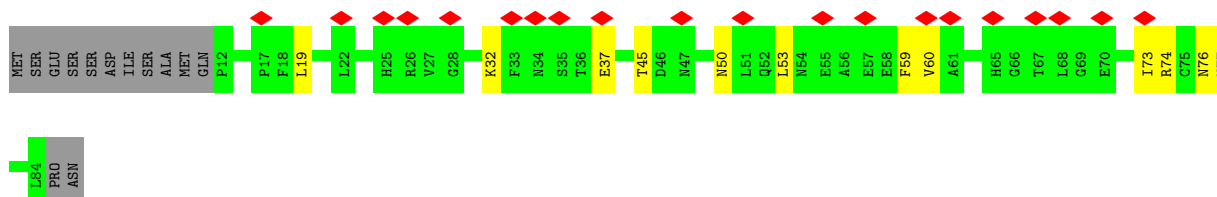
- Molecule 10: Small nuclear ribonucleoprotein Sm D3



- Molecule 11: Small nuclear ribonucleoprotein E

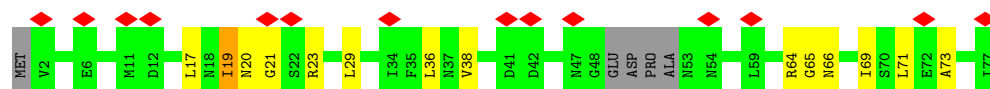


- Molecule 12: Small nuclear ribonucleoprotein F



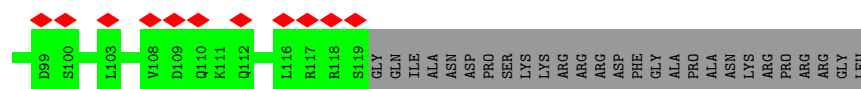
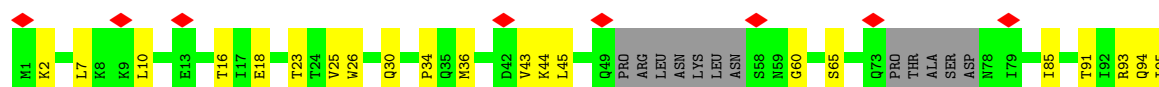
- Molecule 13: Small nuclear ribonucleoprotein G

Chain g: 18% 75% 17% 6%



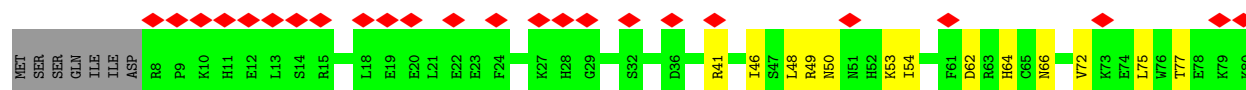
- Molecule 14: Small nuclear ribonucleoprotein Sm D1

Chain h: 13% 59% 14% 27%



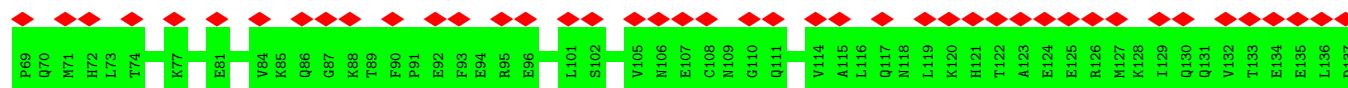
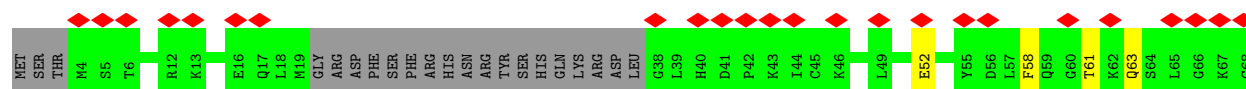
- Molecule 15: Small nuclear ribonucleoprotein Sm D2

Chain i: 25% 71% 19% 10%

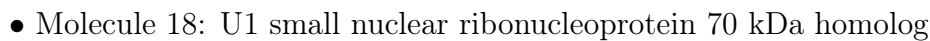


- Molecule 16: Protein LUC7

Chain H: 49% 71% 26%



Chain D:



Chain B:



THR
PRO
THR
ALA
ALA
VAL
THR
SER
VAL
TYR
LYS
SER
ARG
ASN
SER
ARG
THR
ARG
GLU
SER
GLN
PRO
ALA
PRO
LYS
GLU
ALA
PRO
ASP
TYR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217460	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.188	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.042	Depositor
Map size (Å)	464.0, 464.0, 464.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

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	F	0.17	0/1784	0.49	0/2436
2	I	0.12	0/234	0.25	0/362
3	E	0.18	0/4676	0.45	0/6320
4	J	0.24	0/695	0.67	1/948 (0.1%)
5	1	0.29	1/13201 (0.0%)	0.34	2/20553 (0.0%)
6	G	0.18	0/1996	0.48	0/2682
7	A	0.17	0/1072	0.56	0/1437
8	C	0.18	0/1601	0.48	0/2154
9	b	0.19	0/978	0.56	0/1306
10	d	0.23	0/726	0.60	2/984 (0.2%)
11	e	0.20	0/610	0.56	0/826
12	f	0.21	0/597	0.55	0/807
13	g	0.15	0/559	0.55	2/751 (0.3%)
14	h	0.16	0/776	0.45	0/1053
15	i	0.17	0/818	0.49	0/1099
16	H	0.13	0/1212	0.36	0/1652
17	D	0.17	0/3570	0.40	0/4924
18	B	0.16	0/1071	0.45	0/1482
All	All	0.22	1/36176 (0.0%)	0.43	7/51776 (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
7	A	0	1
13	g	0	1
18	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	325	A	O3'-P	-27.08	1.20	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	274	PRO	CA-N-CD	-8.88	99.56	112.00
5	1	442	U	OP2-P-O3'	-8.61	82.18	108.00
5	1	442	U	OP1-P-O3'	-8.59	82.24	108.00
10	d	5	GLY	CA-C-N	6.01	124.02	120.24
10	d	5	GLY	C-N-CA	6.01	124.02	120.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	12	ARG	Peptide
18	B	176	ILE	Peptide
13	g	20	ASN	Peptide

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	F	1758	0	1443	14	0
2	I	847	0	532	11	0
3	E	4561	0	4549	45	0
4	J	687	0	534	12	0
5	1	11822	0	5940	96	0
6	G	1954	0	1961	23	0
7	A	1058	0	1118	10	0
8	C	1570	0	1555	11	0
9	b	972	0	1048	14	0
10	d	714	0	738	16	0
11	e	600	0	634	6	0
12	f	585	0	587	8	0
13	g	556	0	583	9	0
14	h	771	0	751	15	0
15	i	805	0	834	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	H	1201	0	902	4	0
17	D	3530	0	2469	25	0
18	B	1059	0	651	10	0
All	All	35050	0	26829	275	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 4.

The worst 5 of 275 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)
5:1:384:U:H3	5:1:434:G:H1	1.01	0.97
5:1:380:G:H1	5:1:438:U:H3	1.07	0.96
4:J:272:ASP:C	4:J:274:PRO:HD3	1.97	0.88
4:J:273:LEU:N	4:J:274:PRO:HD3	1.89	0.87
5:1:389:G:H1	5:1:430:U:H3	0.86	0.85

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	F	259/523 (50%)	251 (97%)	8 (3%)	0	100	100
3	E	542/544 (100%)	521 (96%)	21 (4%)	0	100	100
4	J	101/620 (16%)	92 (91%)	8 (8%)	1 (1%)	12	46
6	G	235/492 (48%)	222 (94%)	13 (6%)	0	100	100
7	A	126/298 (42%)	116 (92%)	10 (8%)	0	100	100
8	C	193/231 (84%)	183 (95%)	10 (5%)	0	100	100
9	b	117/196 (60%)	110 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	d	91/101 (90%)	87 (96%)	4 (4%)	0	100	100
11	e	73/94 (78%)	67 (92%)	5 (7%)	1 (1%)	9	39
12	f	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
13	g	68/77 (88%)	62 (91%)	5 (7%)	1 (2%)	8	39
14	h	101/146 (69%)	98 (97%)	3 (3%)	0	100	100
15	i	95/110 (86%)	91 (96%)	4 (4%)	0	100	100
16	H	186/261 (71%)	180 (97%)	6 (3%)	0	100	100
17	D	570/629 (91%)	554 (97%)	16 (3%)	0	100	100
18	B	182/300 (61%)	169 (93%)	13 (7%)	0	100	100
All	All	3010/4708 (64%)	2872 (95%)	135 (4%)	3 (0%)	49	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	274	PRO
11	e	34	GLN
13	g	21	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	
1	F	138/451 (31%)	137 (99%)	1 (1%)	76	79
3	E	508/519 (98%)	502 (99%)	6 (1%)	63	73
4	J	49/568 (9%)	49 (100%)	0	100	100
6	G	218/448 (49%)	218 (100%)	0	100	100
7	A	117/273 (43%)	117 (100%)	0	100	100
8	C	171/214 (80%)	171 (100%)	0	100	100
9	b	108/176 (61%)	108 (100%)	0	100	100
10	d	81/89 (91%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	e	68/83 (82%)	68 (100%)	0	100	100
12	f	65/77 (84%)	64 (98%)	1 (2%)	57	70
13	g	62/66 (94%)	62 (100%)	0	100	100
14	h	75/129 (58%)	75 (100%)	0	100	100
15	i	90/103 (87%)	89 (99%)	1 (1%)	65	74
16	H	72/234 (31%)	72 (100%)	0	100	100
17	D	193/603 (32%)	190 (98%)	3 (2%)	55	69
18	B	40/265 (15%)	40 (100%)	0	100	100
All	All	2055/4298 (48%)	2043 (99%)	12 (1%)	76	80

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	f	60	VAL
15	i	103	VAL
17	D	610	LYS
17	D	608	LEU
3	E	416	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
10	d	68	GLN
16	H	63	GLN
12	f	76	ASN
14	h	78	ASN
17	D	466	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	9/371 (2%)	0	0
5	1	556/568 (97%)	117 (21%)	9 (1%)
All	All	565/939 (60%)	117 (20%)	9 (1%)

5 of 117 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	1	11	U
5	1	12	A
5	1	40	A
5	1	41	C
5	1	55	G

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	1	399	A
5	1	505	U
5	1	151	C
5	1	152	G
5	1	258	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	2
5	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	8:C	O3'	103:N	P	54.06
1	I	128:N	O3'	130:N	P	17.87
1	1	325:A	O3'	326:G	P	1.20

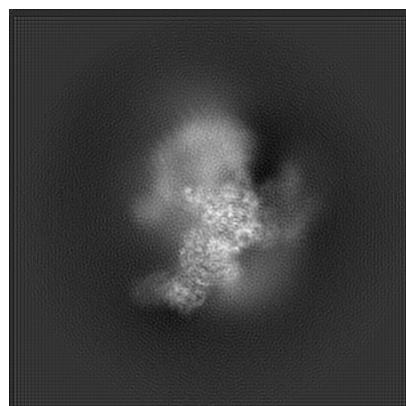
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13029. These allow visual inspection of the internal detail of the map and identification of artifacts.

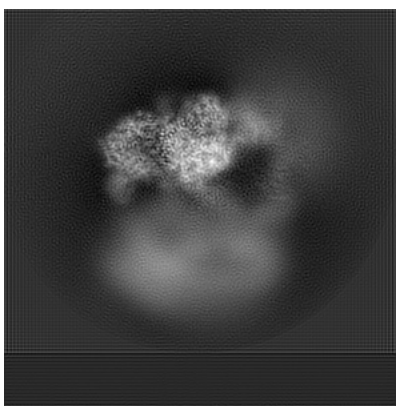
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

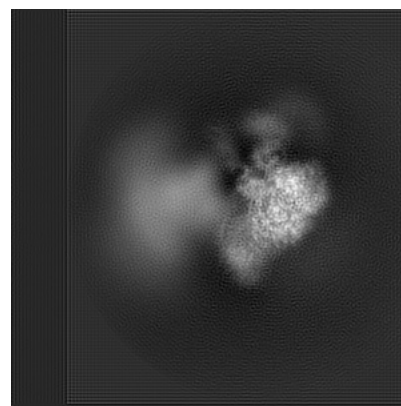
6.1.1 Primary map



X

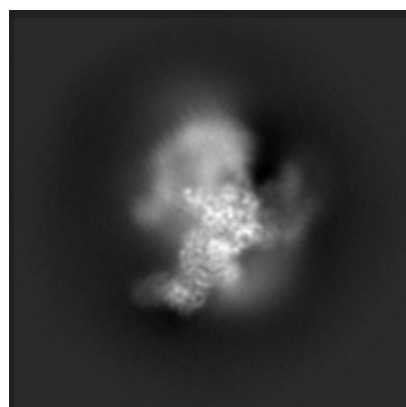


Y

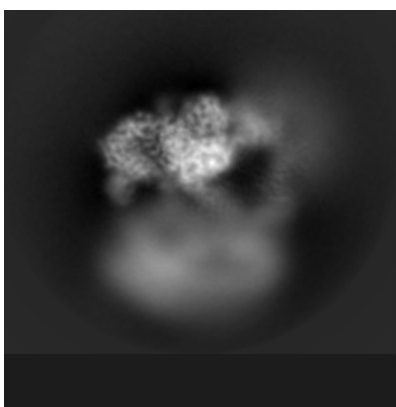


Z

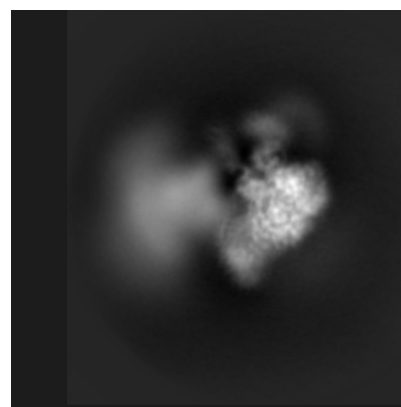
6.1.2 Raw map



X



Y

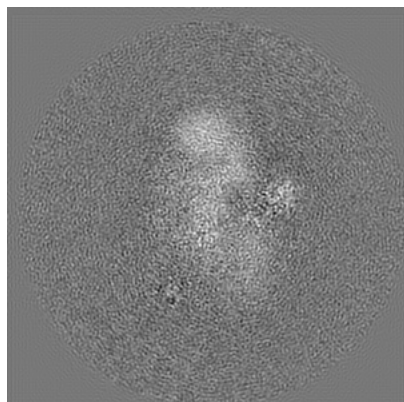


Z

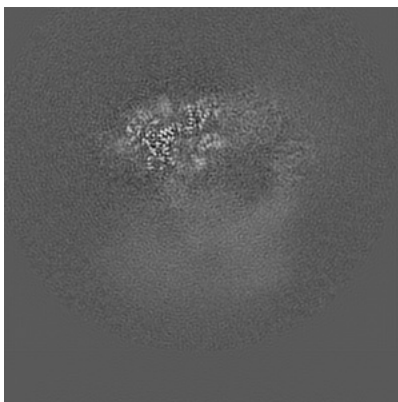
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

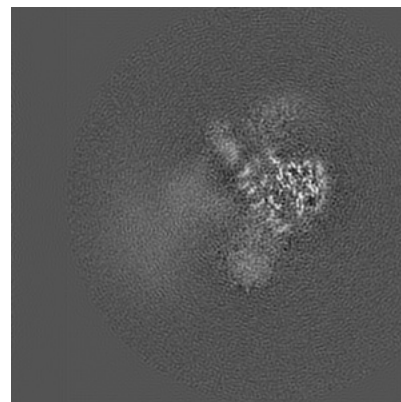
6.2.1 Primary map



X Index: 200

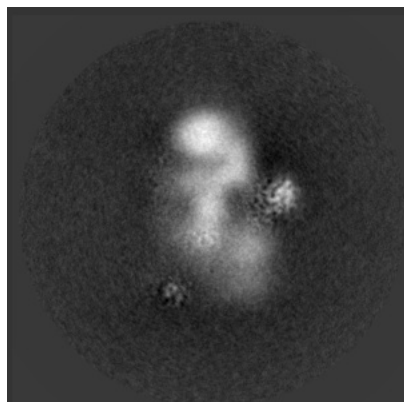


Y Index: 200

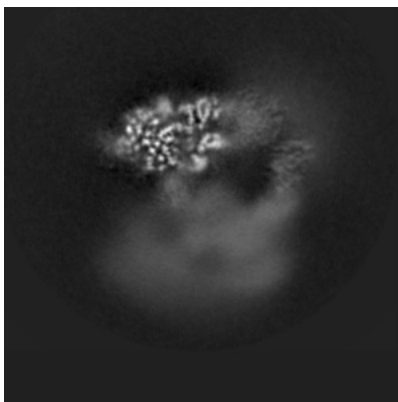


Z Index: 200

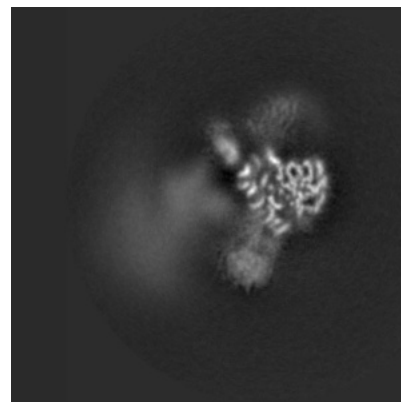
6.2.2 Raw map



X Index: 200



Y Index: 200

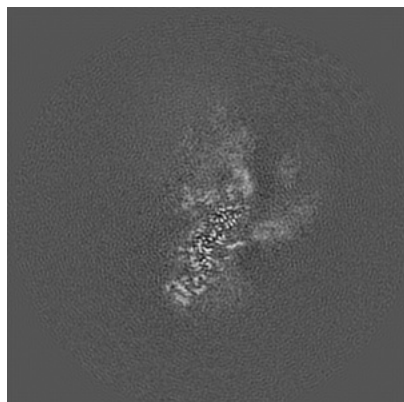


Z Index: 200

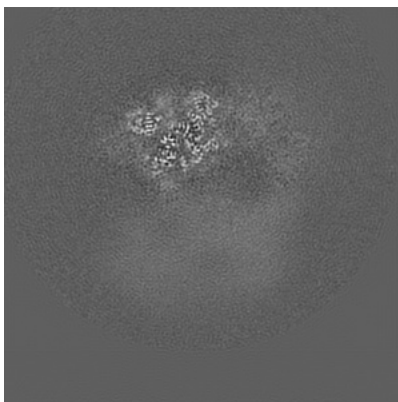
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

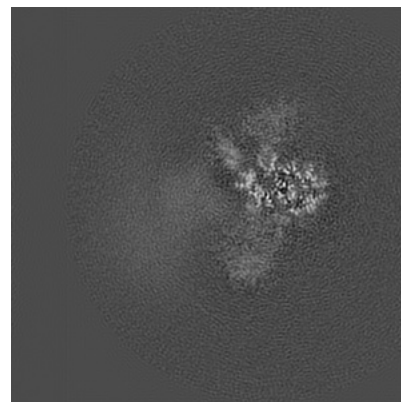
6.3.1 Primary map



X Index: 271

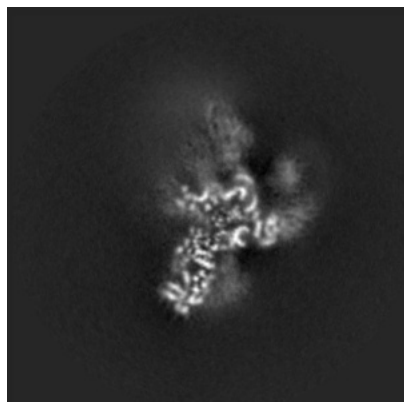


Y Index: 209

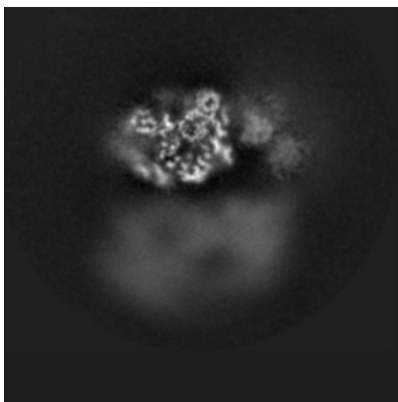


Z Index: 194

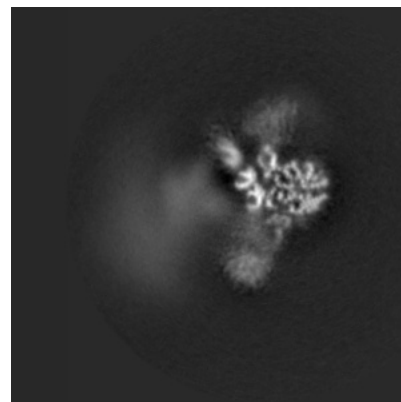
6.3.2 Raw map



X Index: 265



Y Index: 220

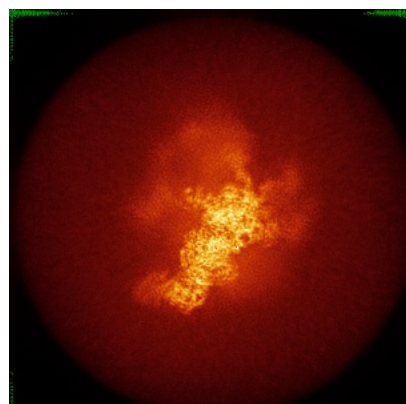


Z Index: 195

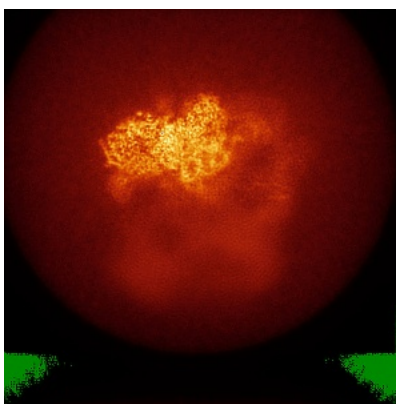
The images above show the largest variance slices of the map in three orthogonal directions.

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

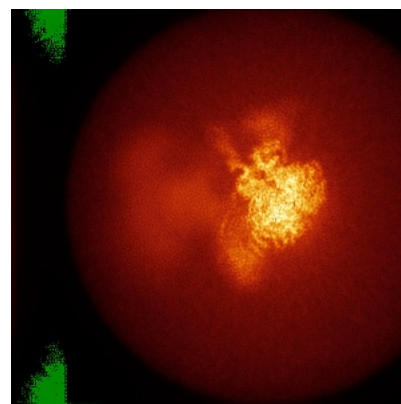
6.4.1 Primary map



X



Y

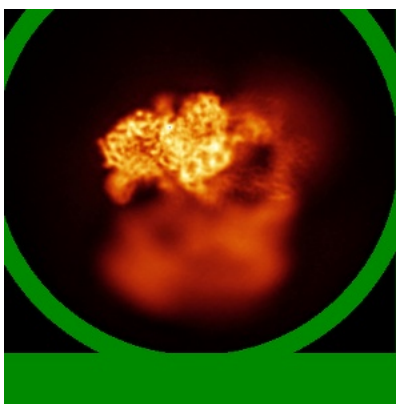


Z

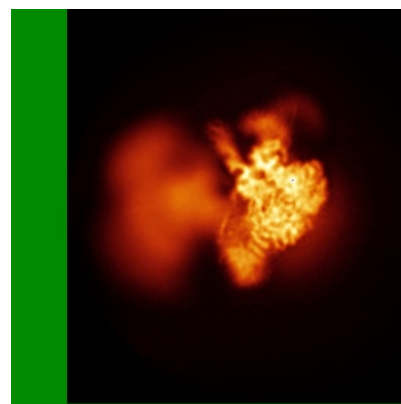
6.4.2 Raw map



X



Y

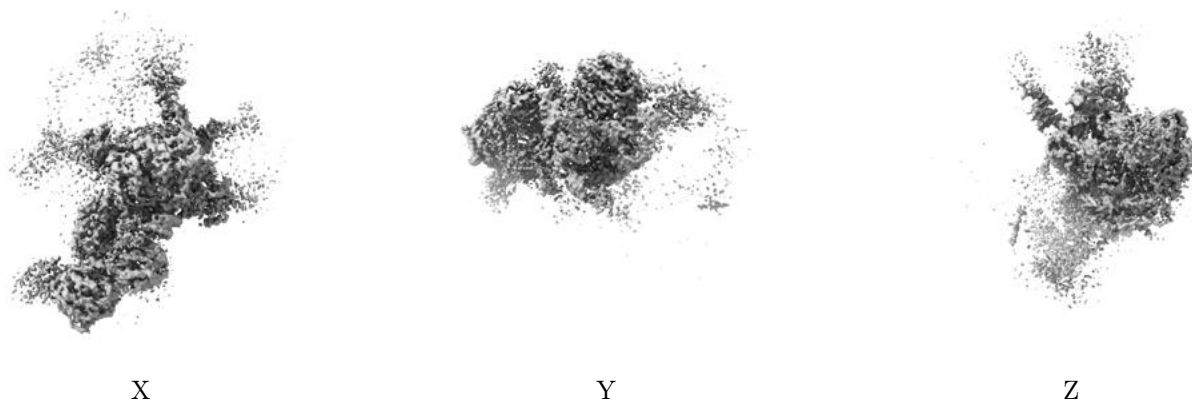


Z

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 0.042. 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.

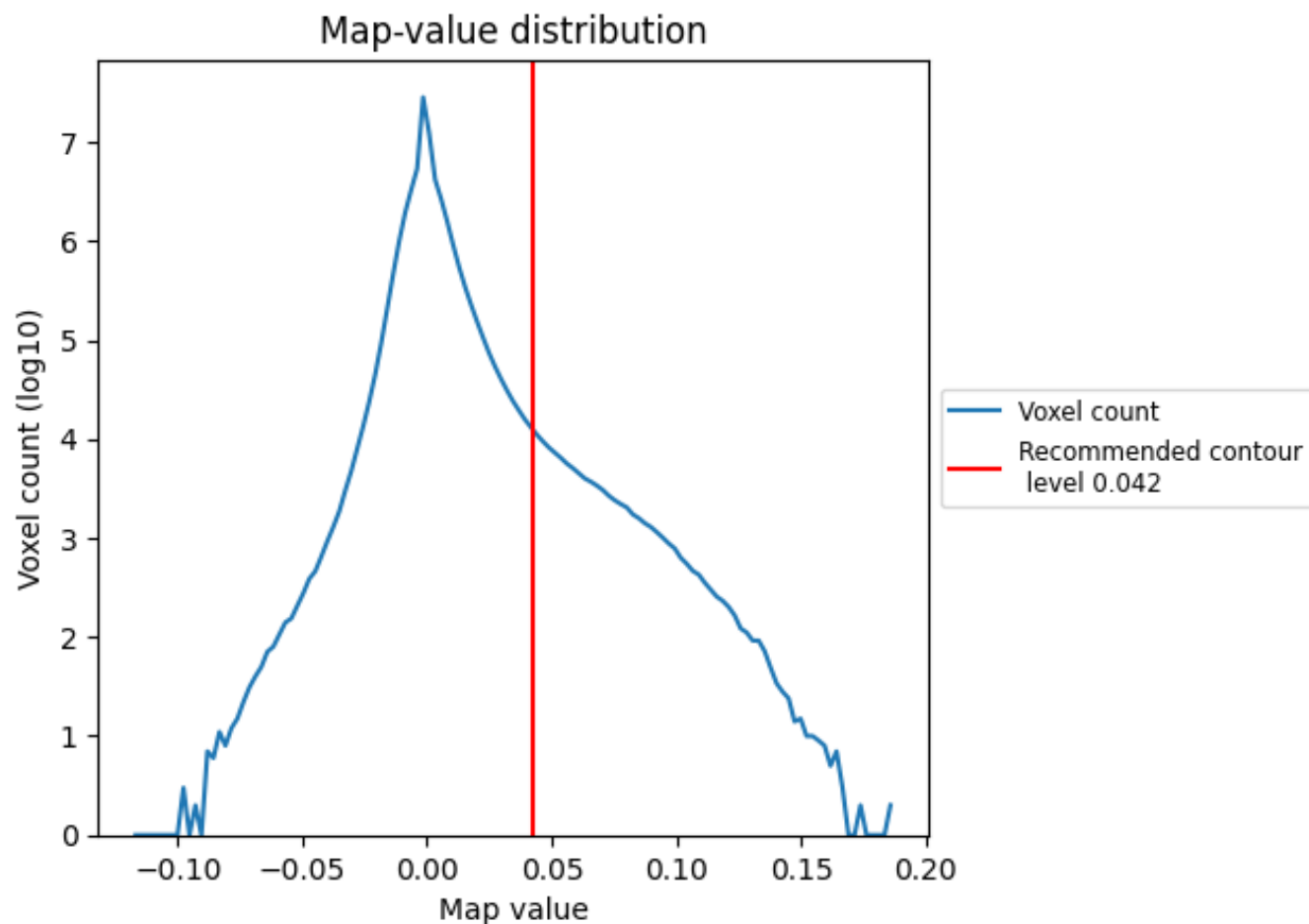
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

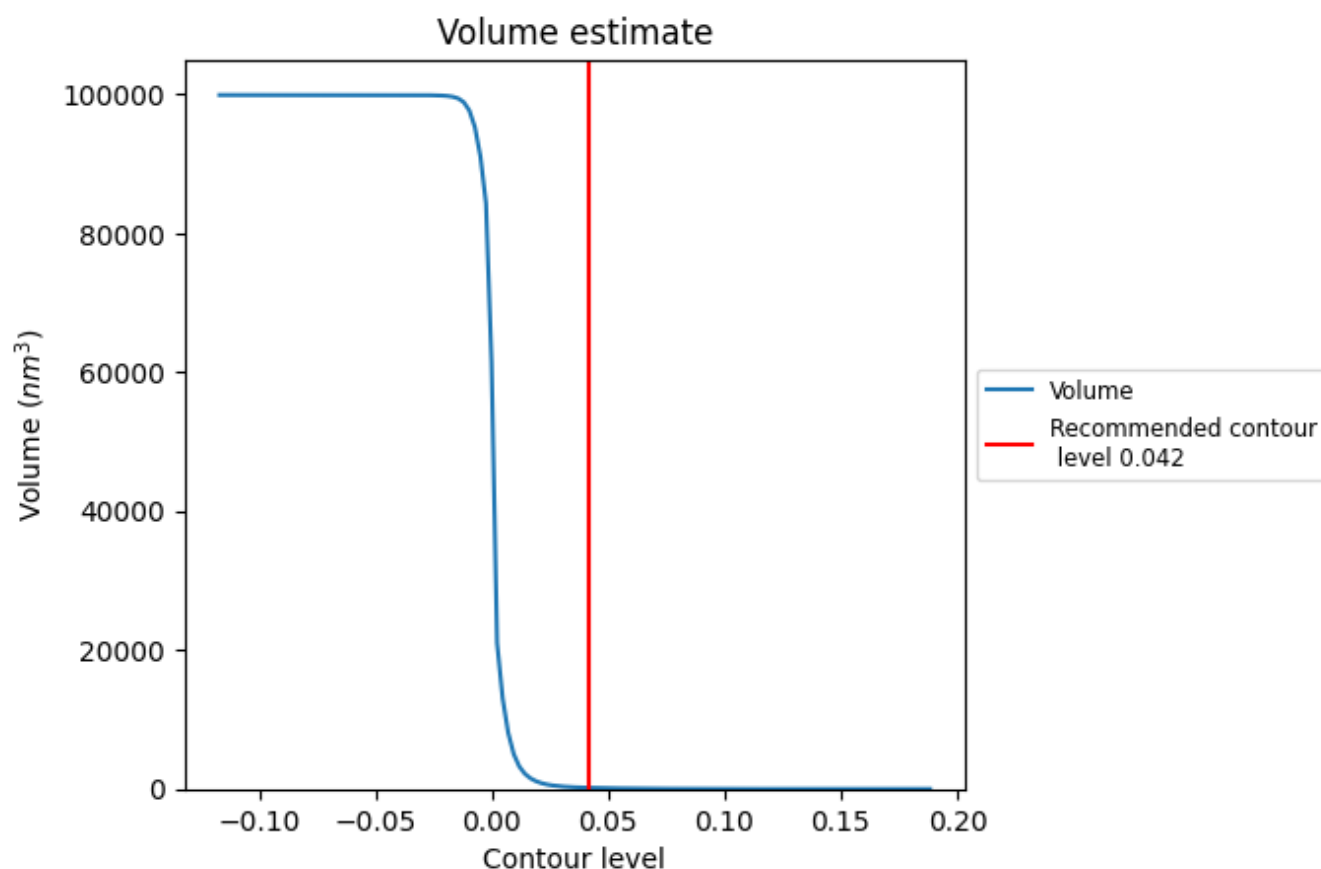
This section contains the results of statistical analysis of the map.

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.

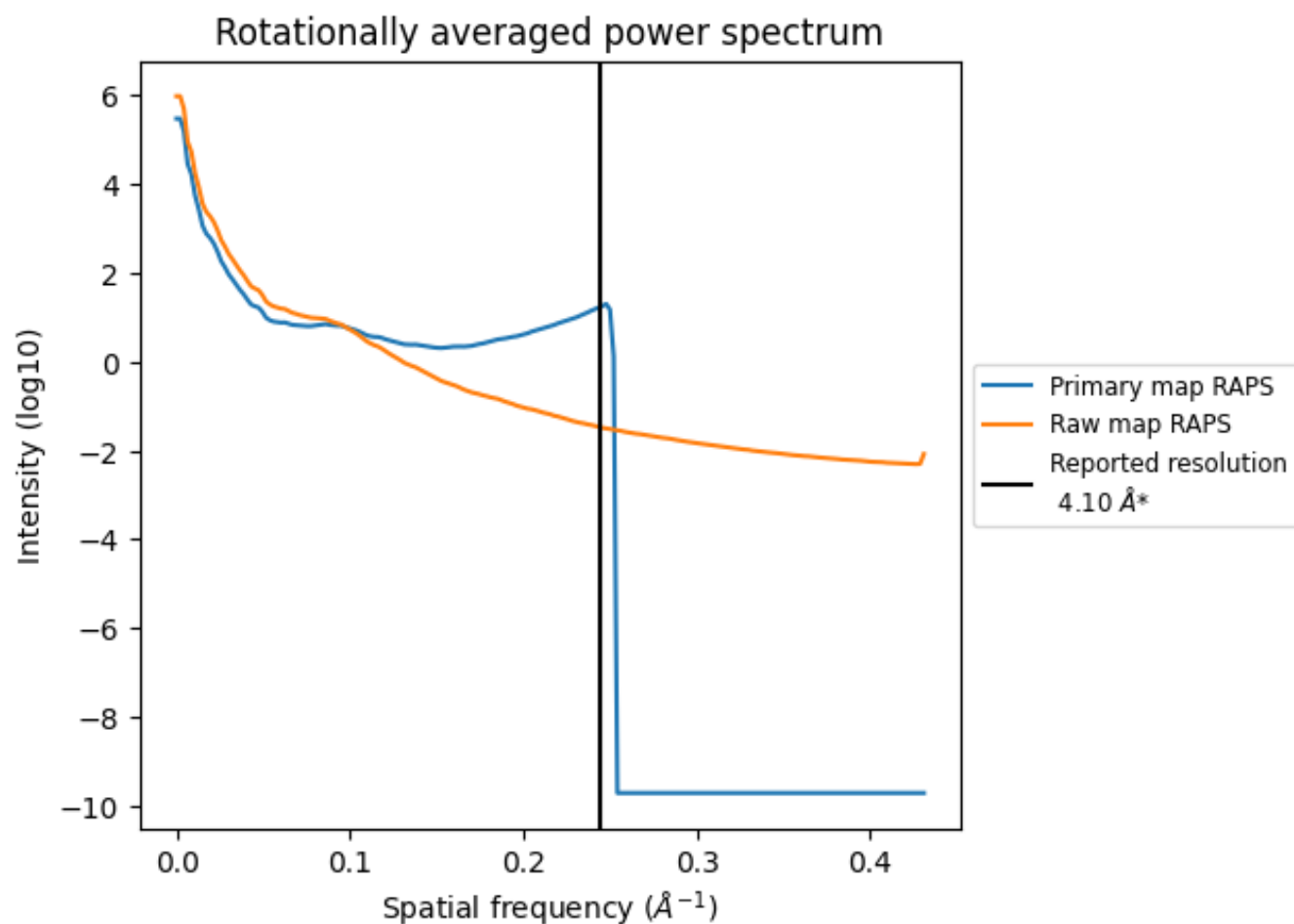
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm³; this corresponds to an approximate mass of 151 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 ⓘ

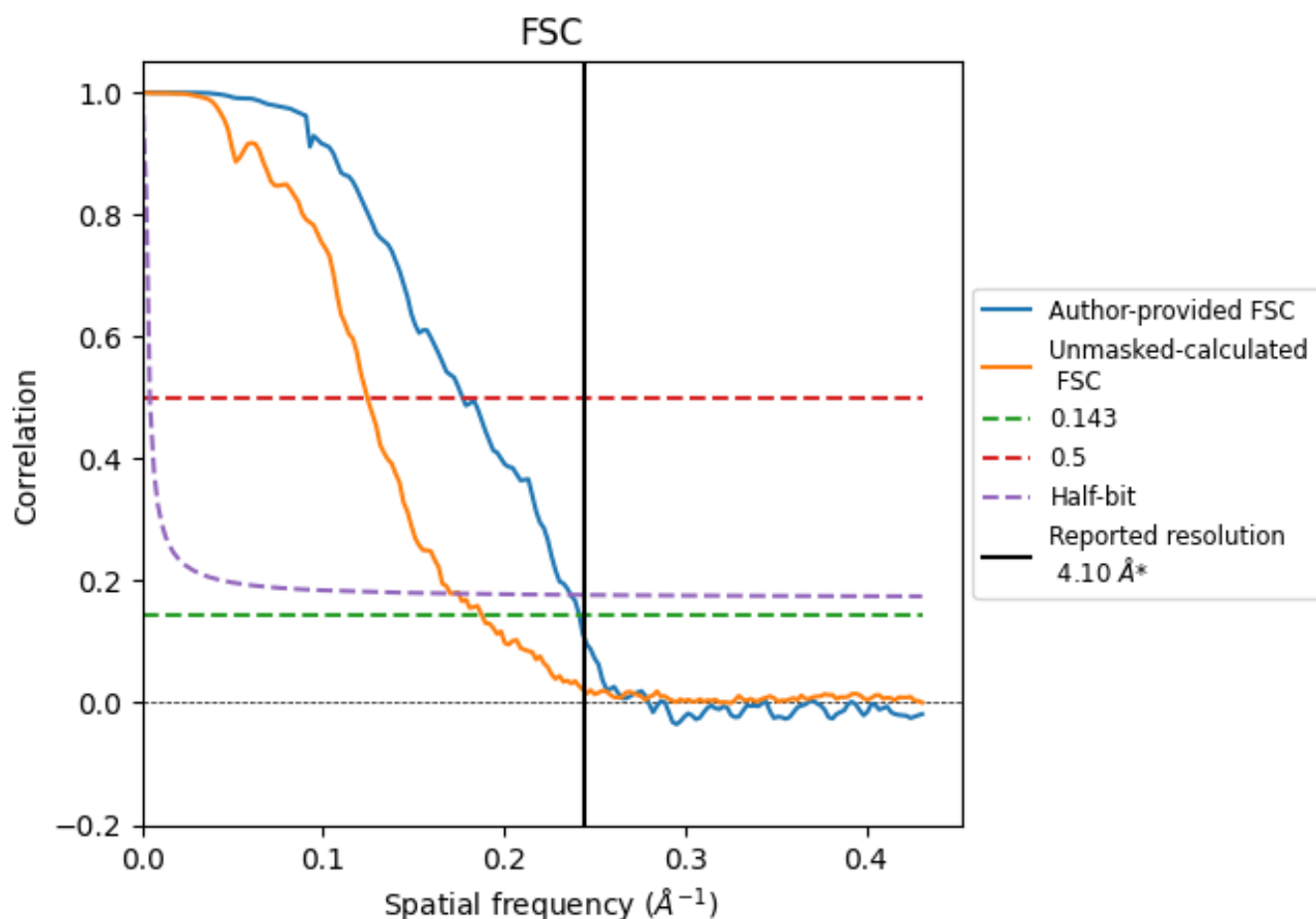


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

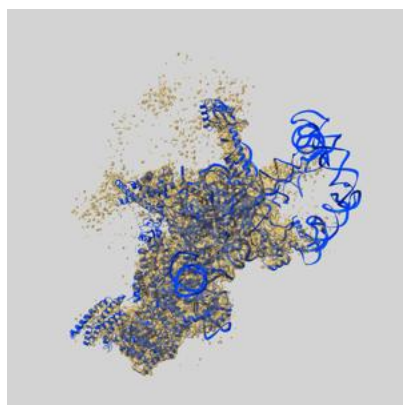
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.14	5.65	4.22
Unmasked-calculated*	5.33	8.04	5.72

*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 5.33 differs from the reported value 4.1 by more than 10 %

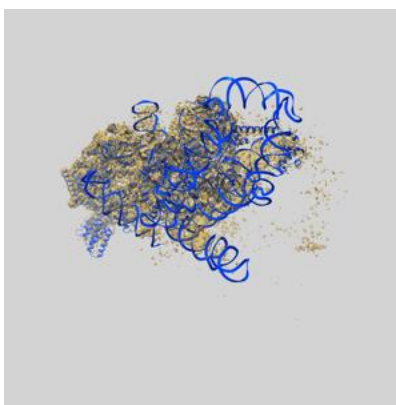
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13029 and PDB model 7OQC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

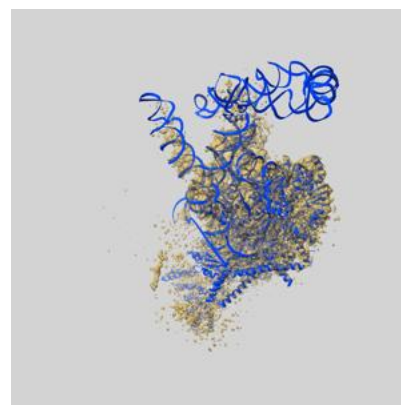
9.1 Map-model overlay [i](#)



X



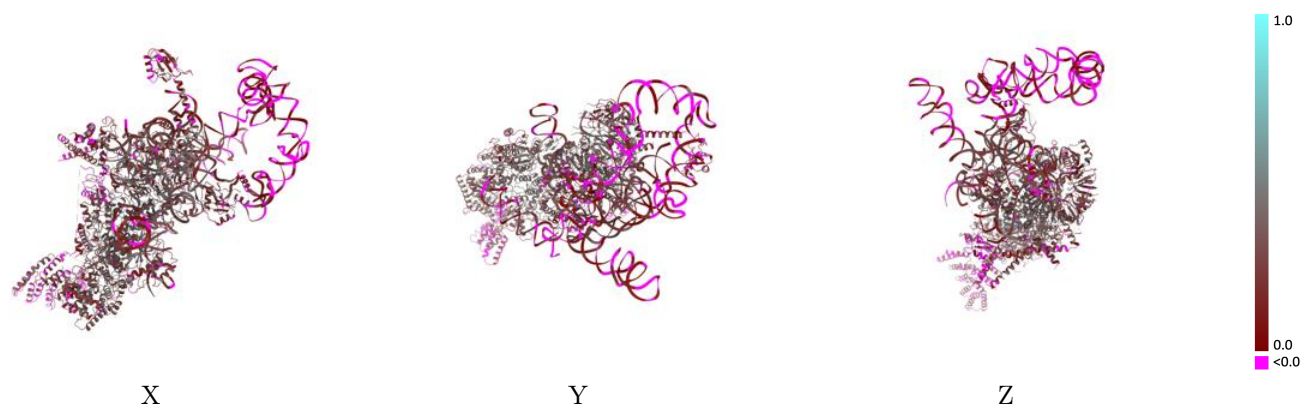
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.042 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](#)



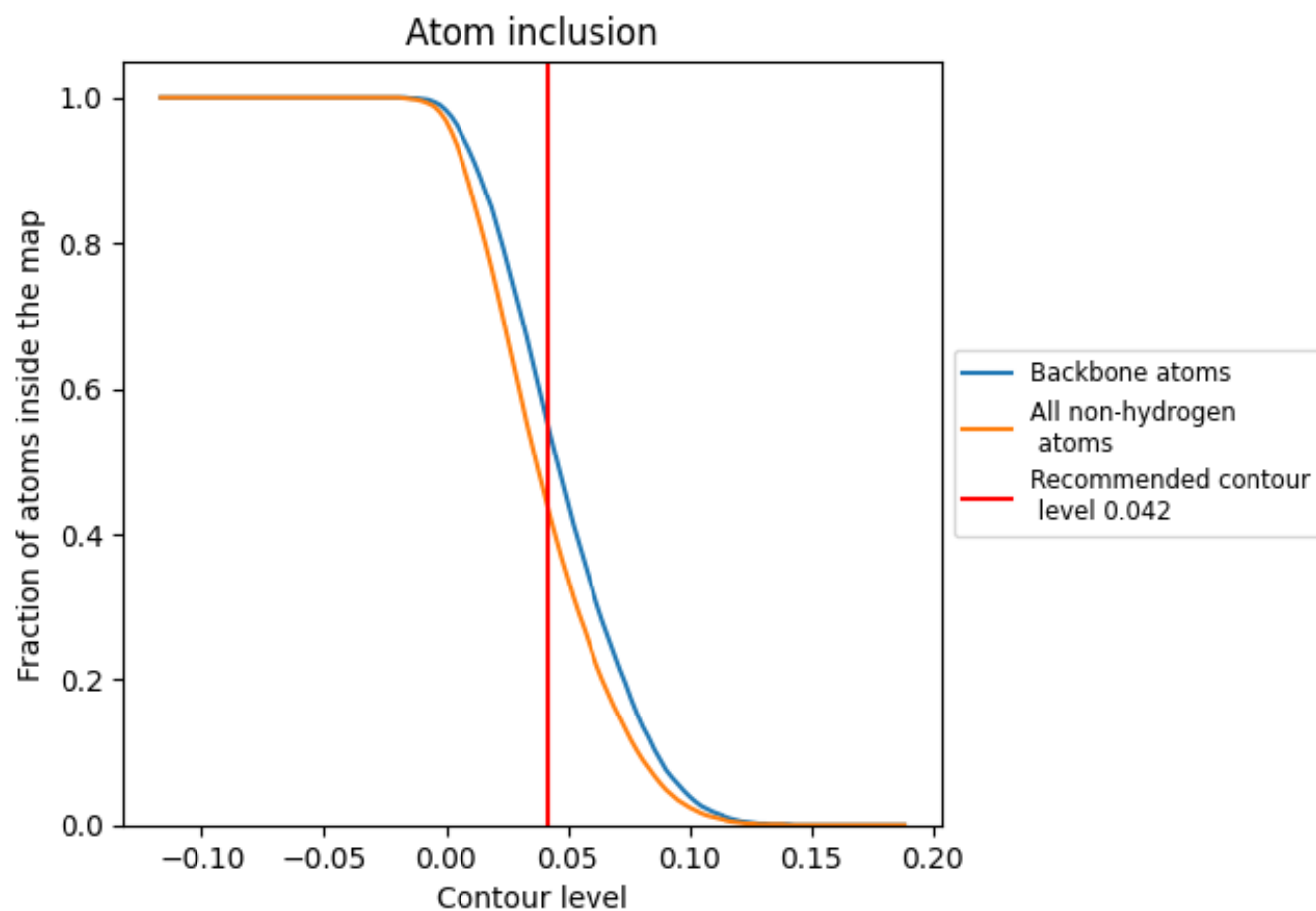
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.042).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 44% 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 (0.042) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4350	 0.2430
1	 0.3370	 0.1520
A	 0.3840	 0.2010
B	 0.3390	 0.2140
C	 0.4780	 0.3240
D	 0.4530	 0.2540
E	 0.6250	 0.3490
F	 0.4080	 0.2600
G	 0.5300	 0.3060
H	 0.3370	 0.2090
I	 0.2140	 0.1160
J	 0.3210	 0.2680
b	 0.5400	 0.3570
d	 0.5930	 0.3800
e	 0.5210	 0.2950
f	 0.5330	 0.2600
g	 0.5550	 0.3740
h	 0.5980	 0.3720
i	 0.5300	 0.2970

