



## wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:41 AM UTC

PDB ID : 5GAP / pdb\_00005gap  
EMDB ID : EMD-8014  
Title : Body region of the U4/U6.U5 tri-snRNP  
Authors : Nguyen, T.H.D.; Galej, W.P.; Oubridge, C.; Bai, X.C.; Newman, A.; Scheres, S.; Nagai, K.  
Deposited on : 2015-12-15  
Resolution : 3.60 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](mailto: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:

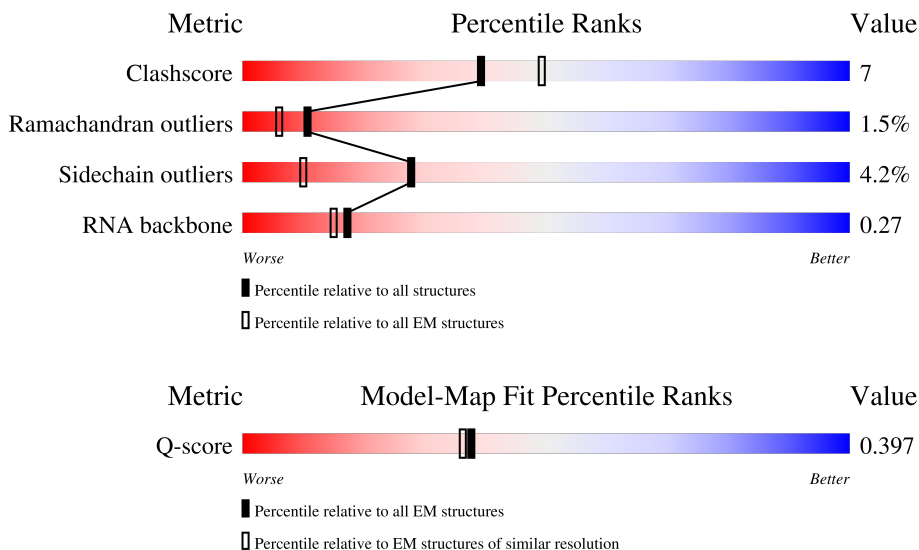
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.60 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.



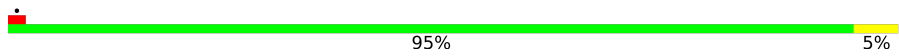
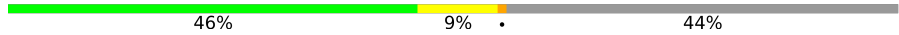






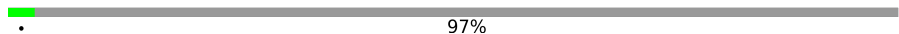
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 ( 3.10 - 4.10 )

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  $\geq 3$ , 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	V	67	
2	W	112	
3	U	214	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	x	82	 95% 5%
5	A	2413	 46% 9% 44%
6	H	465	 58% 17% 23%
7	J	899	 64% 15% 19%
8	D	143	 74% 20% 6%
9	F	494	 63% 18% 16%
10	G	469	 58% 9% 32%
11	K	126	 68% 26% 6%
12	B	2163	 97%

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 31576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U4 snRNA, 5' region, nucleotides 1-67.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	V	67	1426	637	247	475	67	0	0

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	W	56	1190	533	210	391	56	0	0

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	U	20	414	186	64	144	20	0	0

- Molecule 4 is a protein called unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	x	82	410	246	82	82	0	0

- Molecule 5 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	1349	11066	7094	1901	2031	40	0	0

- Molecule 6 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	357	2789	1743	501	532	13	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	J	729	5822	3726	992	1079	25	0	0

- Molecule 8 is a protein called Spliceosomal protein DIB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	140	1151	728	200	212	11	0	0

- Molecule 9 is a protein called Pre-mRNA-processing factor 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	415	3218	2052	575	580	11	0	0

- Molecule 10 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	318	2632	1659	469	488	16	0	0

- Molecule 11 is a protein called 13 kDa ribonucleoprotein-associated protein.

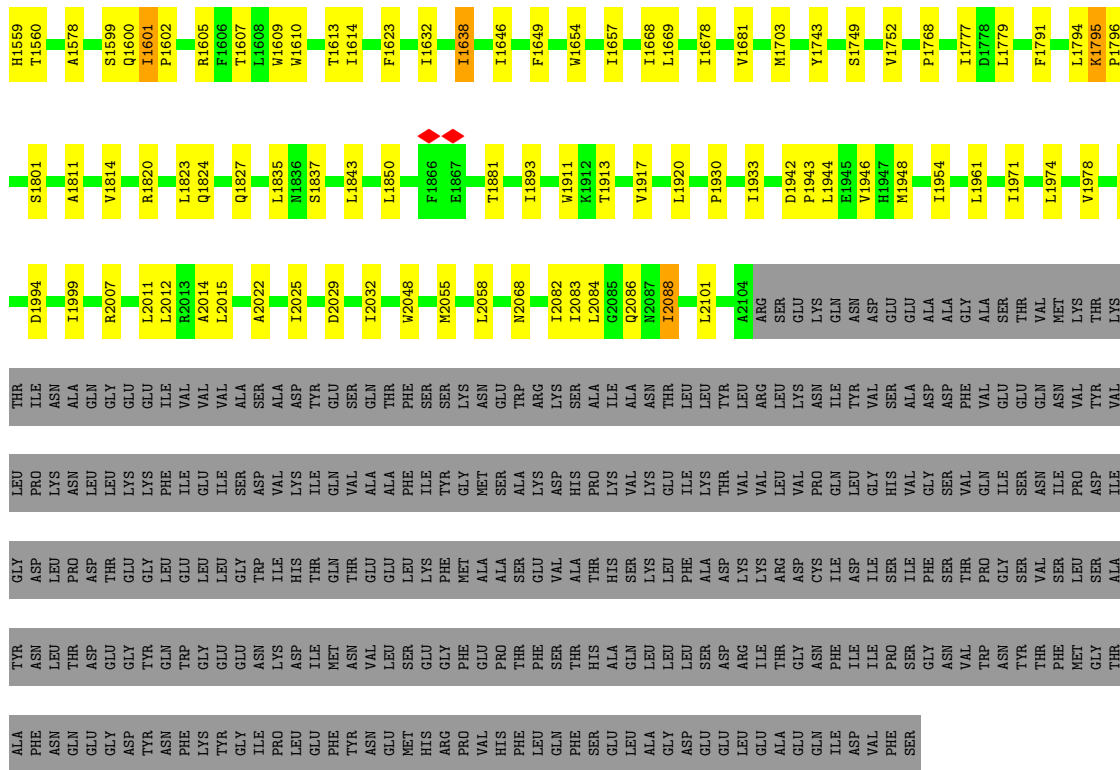
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	124	936	597	161	174	4	0	0

- Molecule 12 is a protein called Pre-mRNA-splicing helicase BRR2.

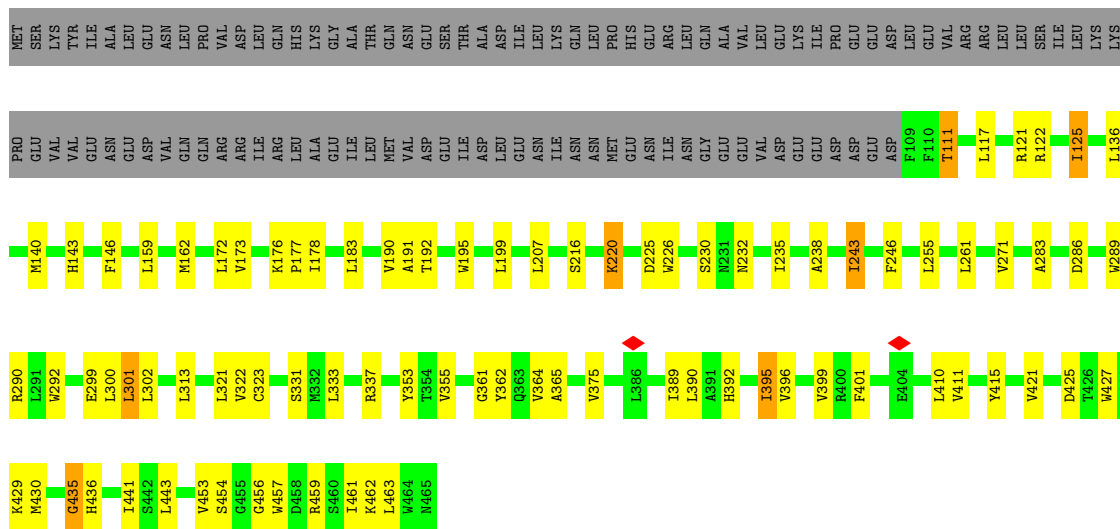
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	B	71	522	326	89	106	1	0	0



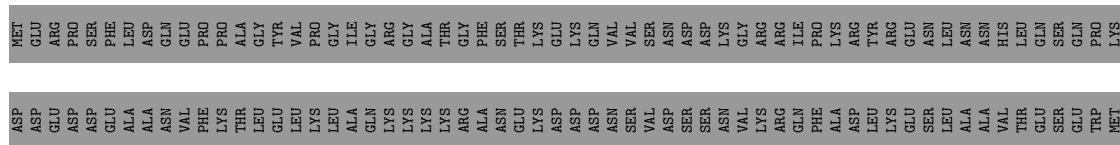




● Molecule 6: U4/U6 small nuclear ribonucleoprotein PRP4



● Molecule 7: Pre-mRNA-splicing factor 6











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140155	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 ( $e^-/\text{\AA}^2$ )	38	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.326	Depositor
Minimum map value	-0.232	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	543.39996, 543.39996, 543.39996	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.43, 1.43, 1.43	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	V	0.41	0/1593	0.88	5/2480 (0.2%)
2	W	0.41	0/1328	0.94	8/2061 (0.4%)
3	U	0.40	0/459	0.77	1/710 (0.1%)
5	A	0.54	1/11327 (0.0%)	1.04	14/15348 (0.1%)
6	H	0.51	0/2845	0.93	3/3843 (0.1%)
7	J	0.57	0/5934	1.21	8/8039 (0.1%)
8	D	0.56	0/1172	1.06	2/1578 (0.1%)
9	F	0.58	0/3273	1.19	9/4413 (0.2%)
10	G	0.54	0/2687	0.99	3/3611 (0.1%)
11	K	0.61	0/949	1.18	1/1292 (0.1%)
12	B	0.61	0/529	1.13	0/716
All	All	0.54	1/32096 (0.0%)	1.07	54/44091 (0.1%)

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
5	A	0	3
9	F	0	1
12	B	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1369	ASN	CA-C	-5.24	1.46	1.52

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	95	C	C4'-C3'-O3'	8.08	121.52	109.40

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	49	A	C2'-C3'-O3'	7.76	121.14	109.50
7	J	239	THR	N-CA-C	7.75	120.62	111.71
5	A	1369	ASN	CA-C-O	-7.45	112.66	120.55
1	V	17	A	C2'-C3'-O3'	7.36	124.74	113.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1278	VAL	Peptide
5	A	1994	ASP	Peptide
5	A	979	SER	Peptide
12	B	423	ILE	Peptide
9	F	154	SER	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	V	1426	0	716	22	0
2	W	1190	0	603	14	0
3	U	414	0	213	4	0
4	x	410	0	89	3	0
5	A	11066	0	11078	149	0
6	H	2789	0	2725	56	0
7	J	5822	0	5792	110	0
8	D	1151	0	1138	19	0
9	F	3218	0	3297	55	0
10	G	2632	0	2599	28	0
11	K	936	0	987	25	0
12	B	522	0	506	6	0
All	All	31576	0	29743	443	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 443 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:A:1275:MET:HE3	5:A:1281:ASN:CG	1.83	1.02
5:A:1578:ALA:HB1	5:A:1602:PRO:HB3	1.40	1.02
5:A:1275:MET:HE3	5:A:1281:ASN:ND2	1.86	0.91
9:F:112:MET:HE2	9:F:203:ILE:HD12	1.61	0.82
10:G:272:VAL:HG12	10:G:280:VAL:HG21	1.59	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	
5	A	1343/2413 (56%)	1226 (91%)	104 (8%)	13 (1%)	12	45
6	H	355/465 (76%)	301 (85%)	48 (14%)	6 (2%)	7	35
7	J	719/899 (80%)	650 (90%)	56 (8%)	13 (2%)	6	34
8	D	138/143 (96%)	126 (91%)	11 (8%)	1 (1%)	18	51
9	F	413/494 (84%)	364 (88%)	38 (9%)	11 (3%)	4	27
10	G	316/469 (67%)	283 (90%)	32 (10%)	1 (0%)	36	65
11	K	122/126 (97%)	111 (91%)	9 (7%)	2 (2%)	7	36
12	B	69/2163 (3%)	57 (83%)	8 (12%)	4 (6%)	1	13
All	All	3475/7172 (48%)	3118 (90%)	306 (9%)	51 (2%)	11	37

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	1093	LYS
5	A	1278	VAL
5	A	2088	ILE
6	H	362	TYR
7	J	479	GLU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	A	1216/2182 (56%)	1194 (98%)	22 (2%)	51 68
6	H	305/410 (74%)	288 (94%)	17 (6%)	19 47
7	J	627/813 (77%)	600 (96%)	27 (4%)	26 52
8	D	129/132 (98%)	119 (92%)	10 (8%)	11 38
9	F	346/445 (78%)	316 (91%)	30 (9%)	9 34
10	G	289/436 (66%)	281 (97%)	8 (3%)	38 60
11	K	102/104 (98%)	89 (87%)	13 (13%)	4 22
12	B	56/1955 (3%)	53 (95%)	3 (5%)	20 47
All	All	3070/6477 (47%)	2940 (96%)	130 (4%)	28 53

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	17	THR
11	K	53	ILE
7	J	498	GLN
7	J	460	THR
11	K	69	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
7	J	673	GLN
9	F	171	GLN
7	J	733	ASN
7	J	795	GLN
9	F	240	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	V	66/67 (98%)	30 (45%)	6 (9%)
2	W	54/112 (48%)	20 (37%)	9 (16%)
3	U	19/214 (8%)	8 (42%)	1 (5%)
All	All	139/393 (35%)	58 (41%)	16 (11%)

5 of 58 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	V	2	U
1	V	11	A
1	V	18	A
1	V	19	U
1	V	20	A

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	W	84	C
2	W	83	A
2	W	45	A
2	W	75	A
2	W	32	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	x	1
5	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	62:UNK	C	101:UNK	N	54.04
1	A	1860:VAL	C	1861:THR	N	4.50

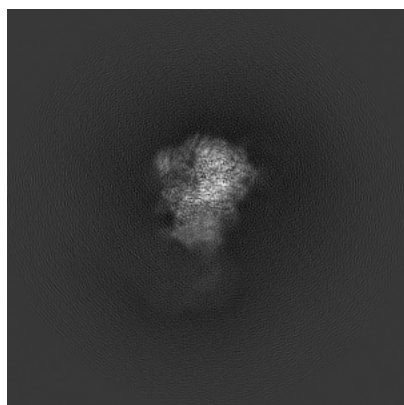
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8014. These allow visual inspection of the internal detail of the map and identification of artifacts.

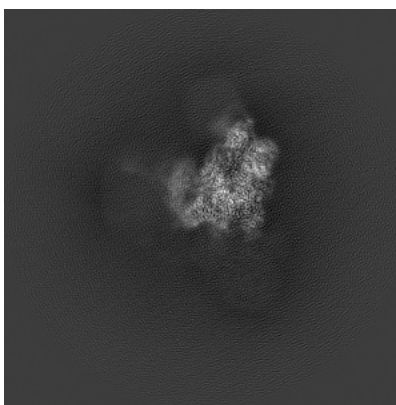
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

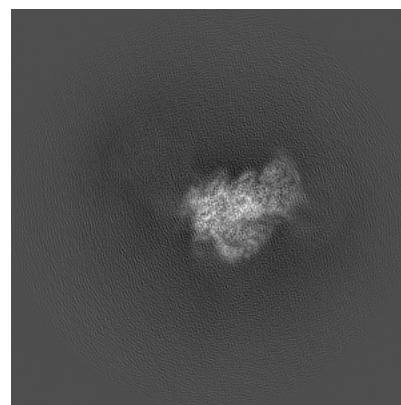
#### 6.1.1 Primary map



X



Y

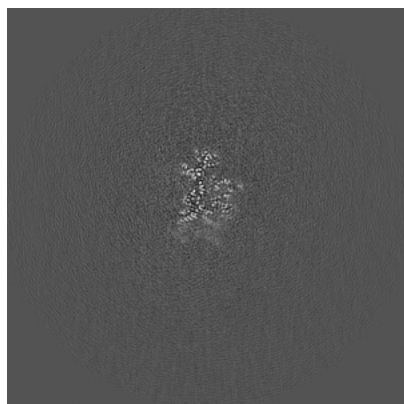


Z

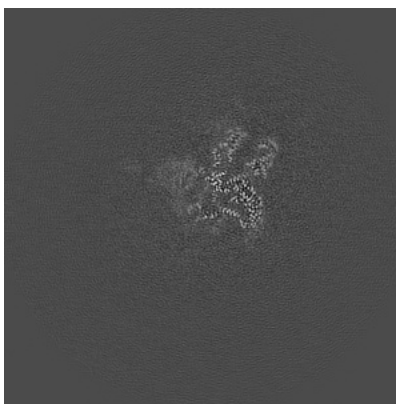
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

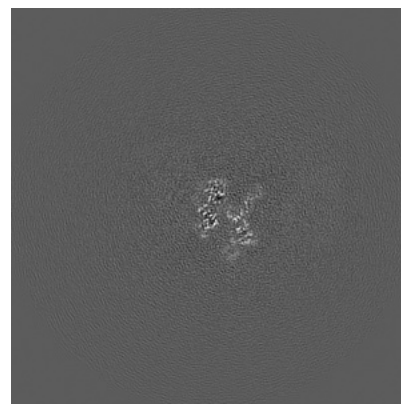
#### 6.2.1 Primary map



X Index: 190



Y Index: 190

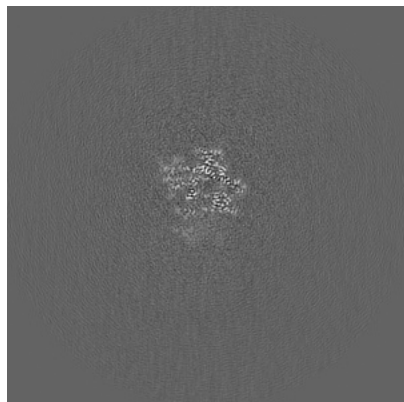


Z Index: 190

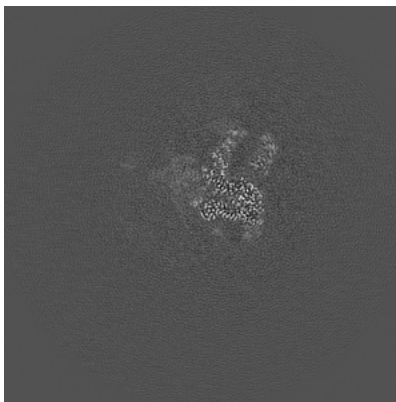
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

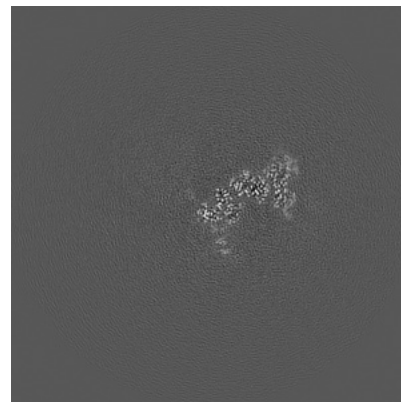
### 6.3.1 Primary map



X Index: 197



Y Index: 186

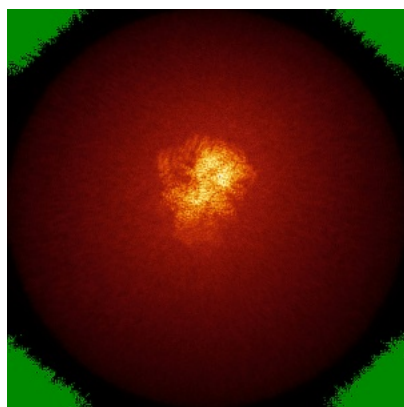


Z Index: 221

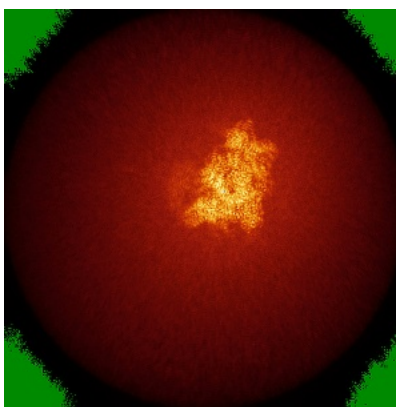
The images above show the largest variance slices of the map in three orthogonal directions.

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

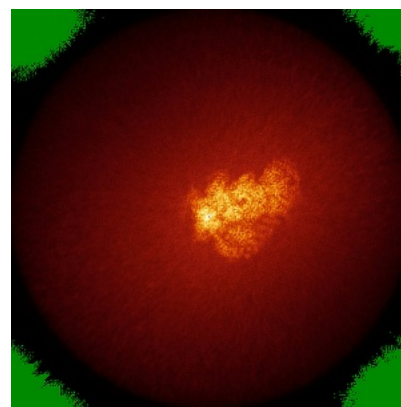
### 6.4.1 Primary map



X



Y

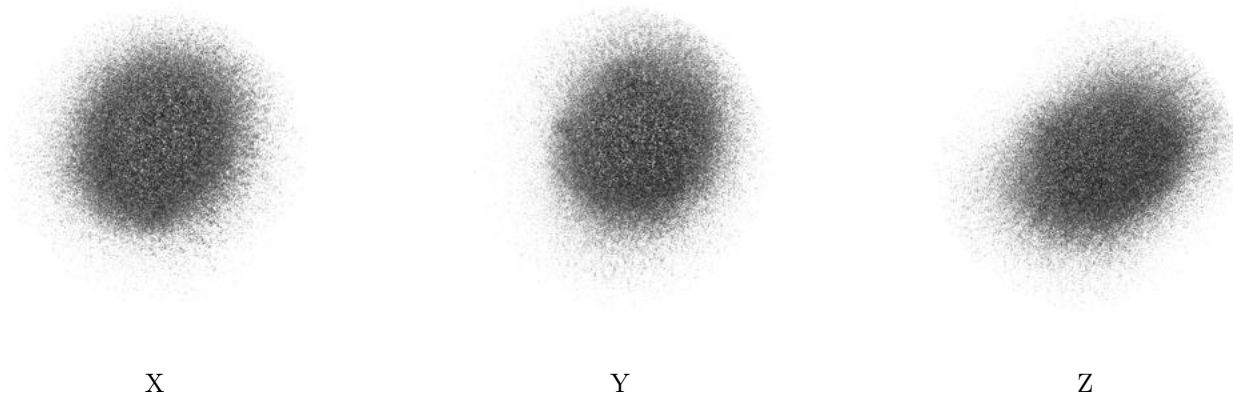


Z

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.

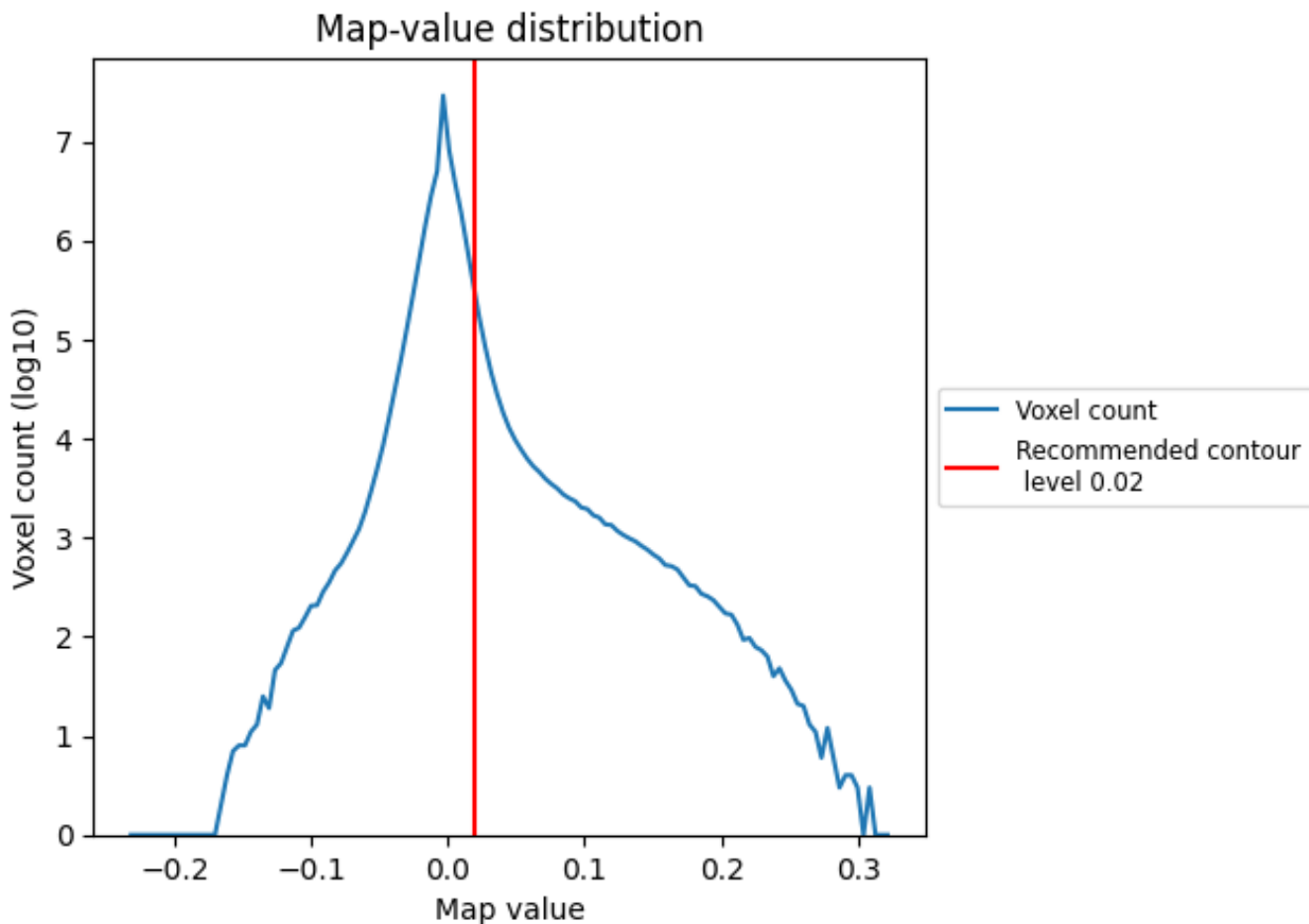
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

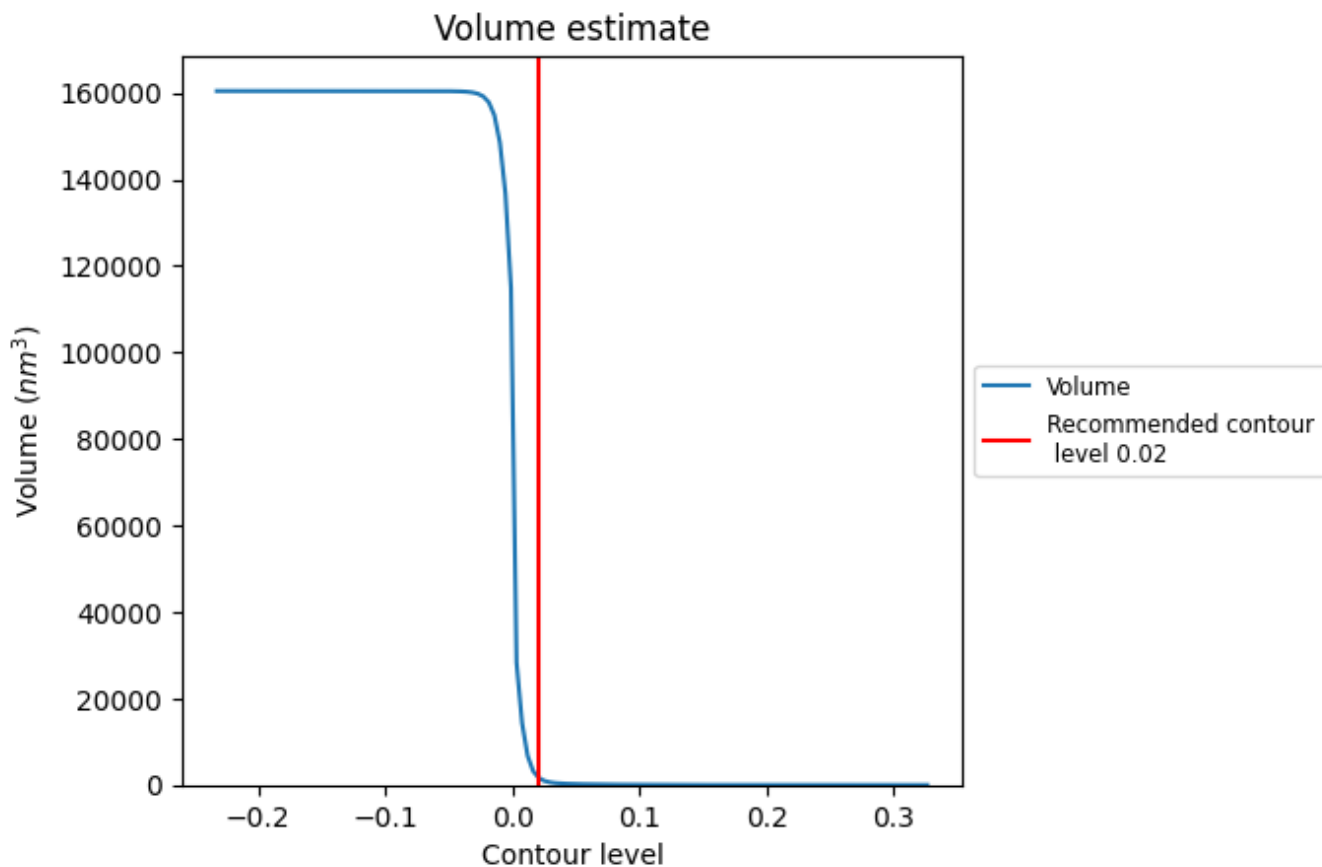
This section contains the results of statistical analysis of the map.

### 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.

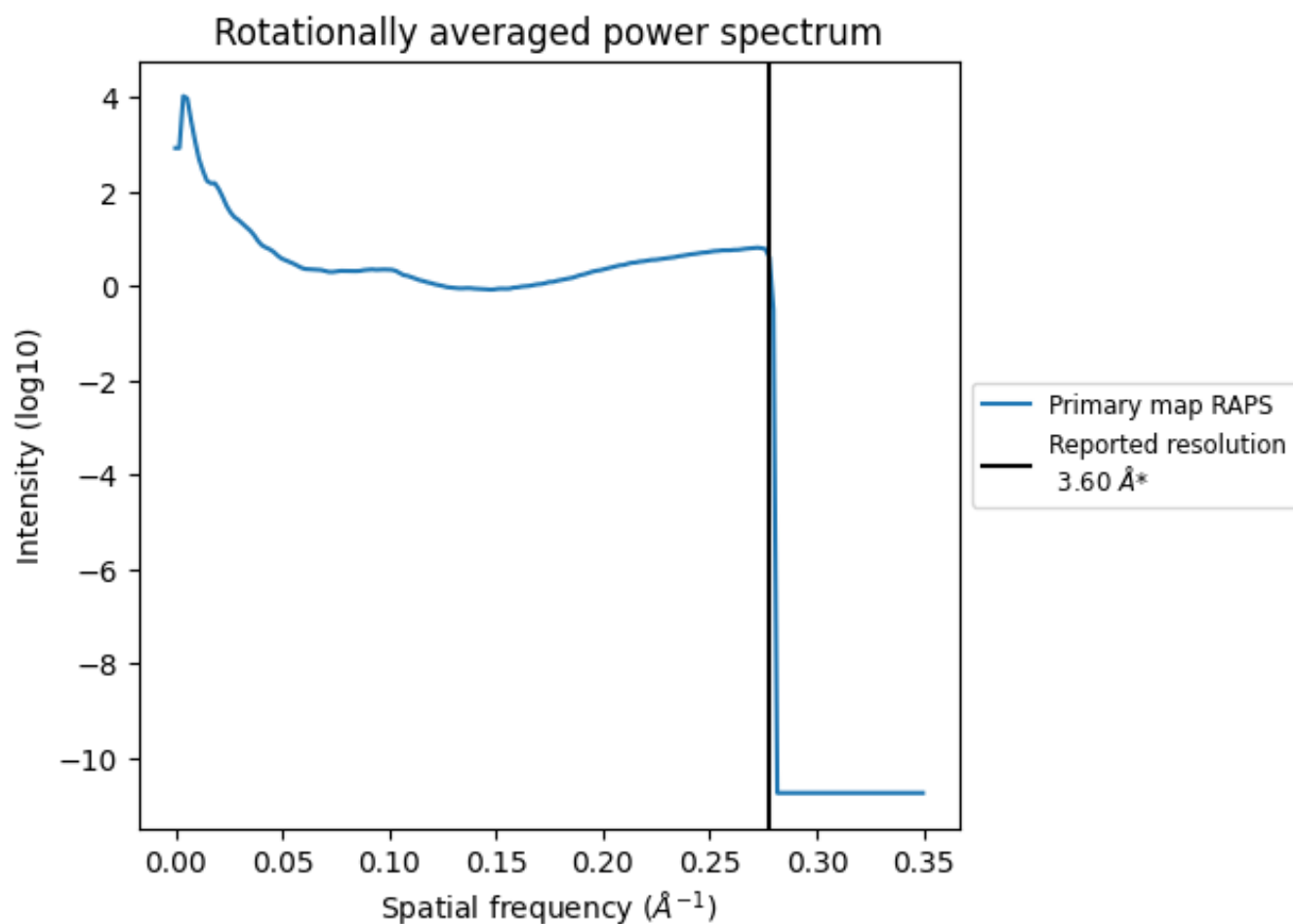
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1921  $\text{nm}^3$ ; this corresponds to an approximate mass of 1735 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [\(i\)](#)

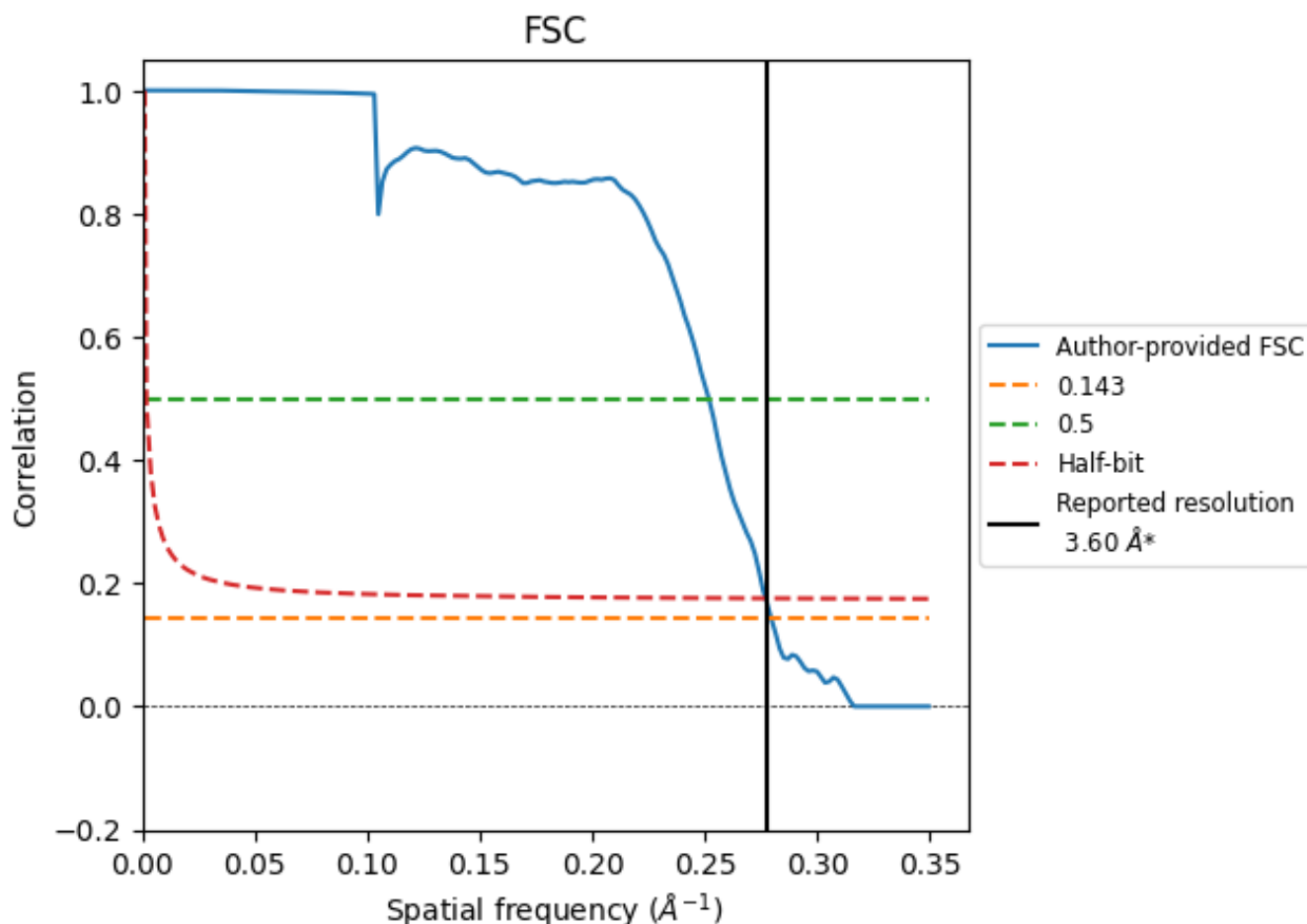


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 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 0.278  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

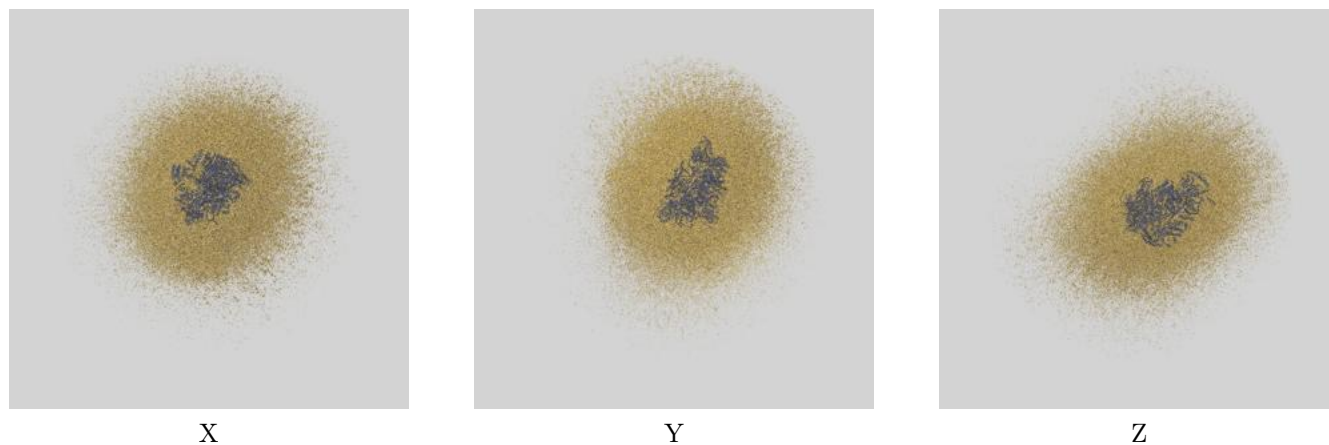
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	3.97	3.61
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

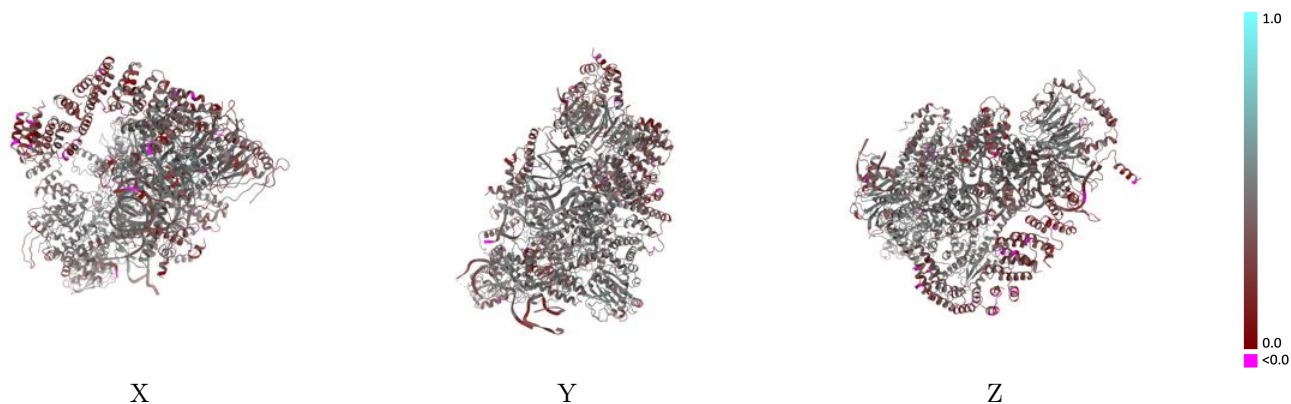
This section contains information regarding the fit between EMDB map EMD-8014 and PDB model 5GAP. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



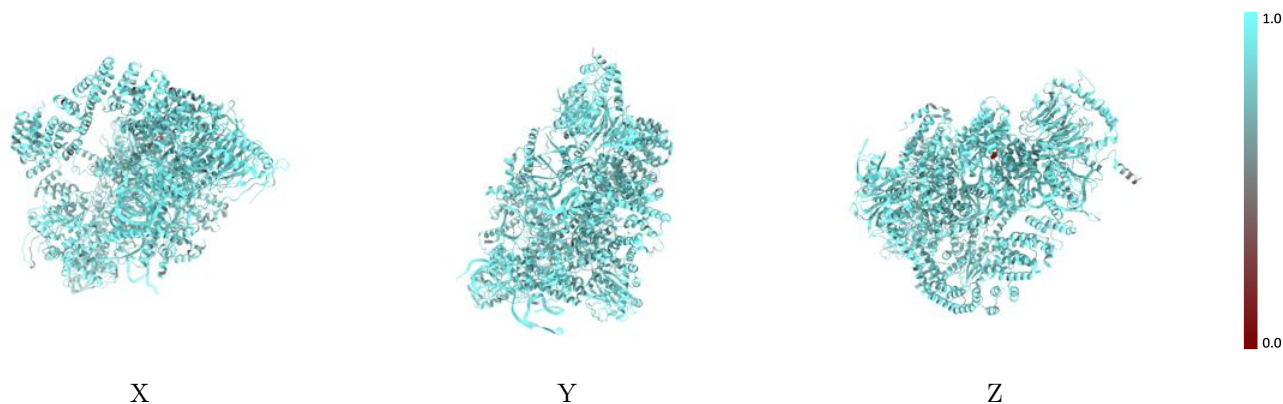
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



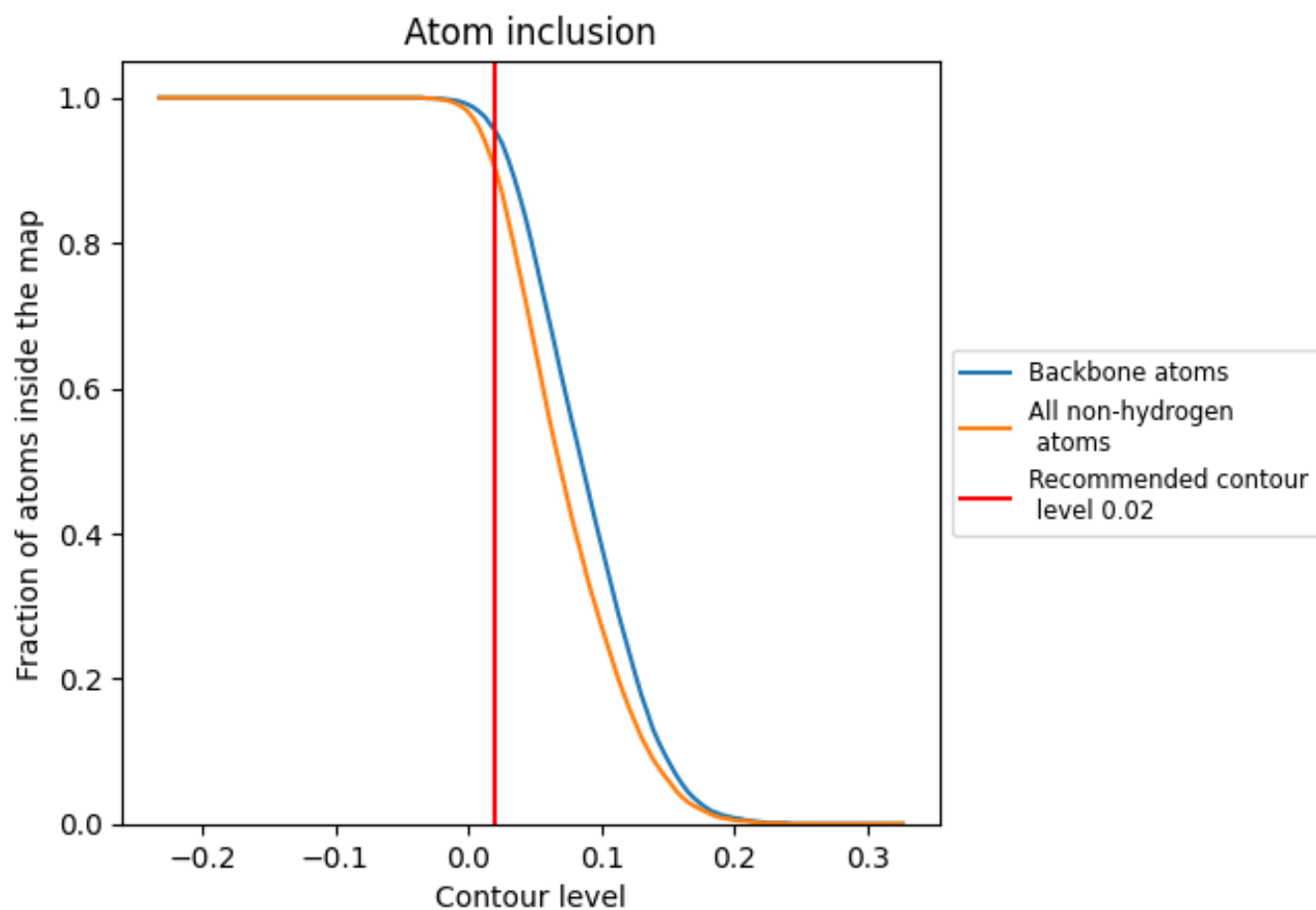
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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	 0.9020	 0.3970
A	 0.9040	 0.4340
B	 0.8190	 0.3180
D	 0.8950	 0.4260
F	 0.8990	 0.4110
G	 0.8870	 0.3770
H	 0.8950	 0.4080
J	 0.8810	 0.3130
K	 0.9130	 0.4670
U	 0.9250	 0.2810
V	 0.9670	 0.4390
W	 0.9640	 0.3760
x	 0.9390	 0.4020

