



## wwPDB EM Validation Summary Report ⓘ

Jan 15, 2025 – 09:47 am GMT

PDB ID : 8QEP  
EMDB ID : EMD-18375  
Title : RNA polymerase II bound to Alu RNA right arm  
Authors : Tluckova, K.; Bernecky, C.  
Deposited on : 2023-09-01  
Resolution : 2.50 Å(reported)  
Based on initial model : 5OIK

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>.

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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

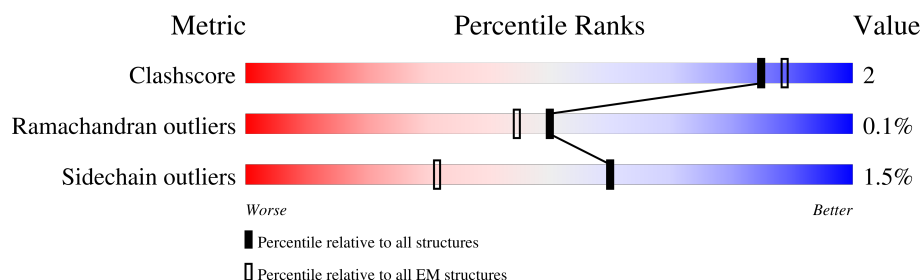
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 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.



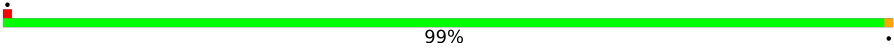
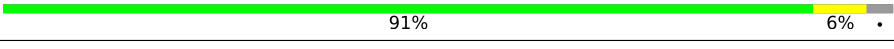

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	1970	
2	B	1174	
3	C	275	
4	E	210	
5	F	127	
6	G	172	
7	H	150	
8	I	125	

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Mol	Chain	Length	Quality of chain
9	J	67	 99%
10	K	117	 91%6%
11	L	58	 72%5%22%

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 25480 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1060	Total	C	N	O	S	0	0
			8440	5317	1488	1589	46		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1035	Total	C	N	O	S	0	0
			8290	5260	1446	1532	52		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	259	Total	C	N	O	S	0	0
			2079	1305	357	411	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	82	Total	C	N	O	S	0	0
			658	418	113	122	5		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	41	Total	C	N	O	0	0
			326	218	55	53		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	117	Total	C	N	O	S	0	0
			950	587	169	183	11		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	67	Total	C	N	O	S	0	0
			534	345	90	93	6		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	114	Total	C	N	O	S	0	0
			912	588	151	172	1		

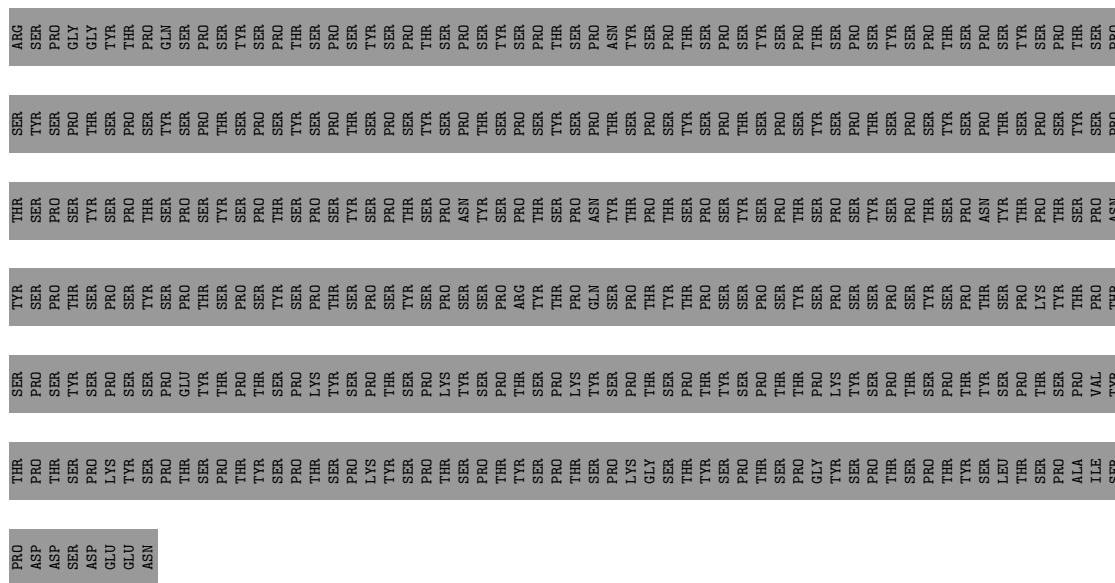
- Molecule 11 is a protein called RNA polymerase II, I and III subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	45	Total	C	N	O	S	0	0
			380	236	73	65	6		

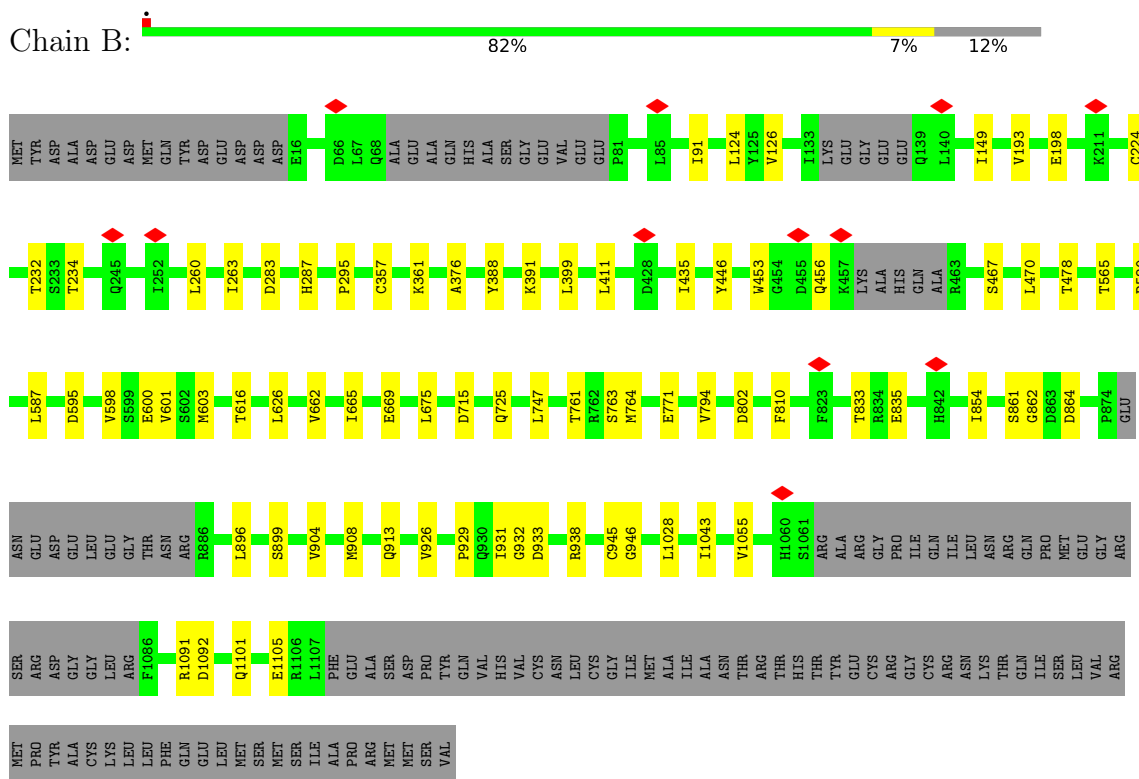
- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	I	2	Total	Zn	0
			2	2	
12	J	1	Total	Zn	0
			1	1	
12	L	1	Total	Zn	0
			1	1	

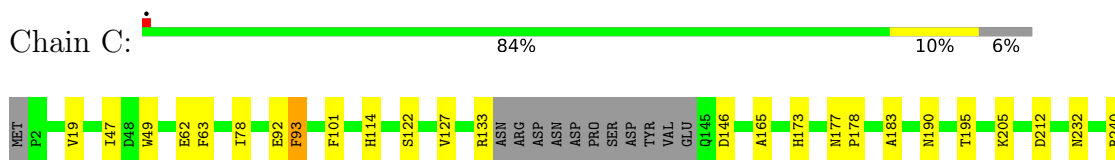


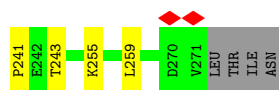


- Molecule 2: DNA-directed RNA polymerase subunit beta



- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

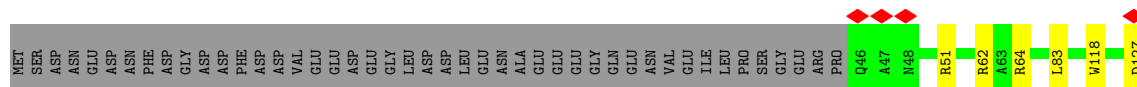




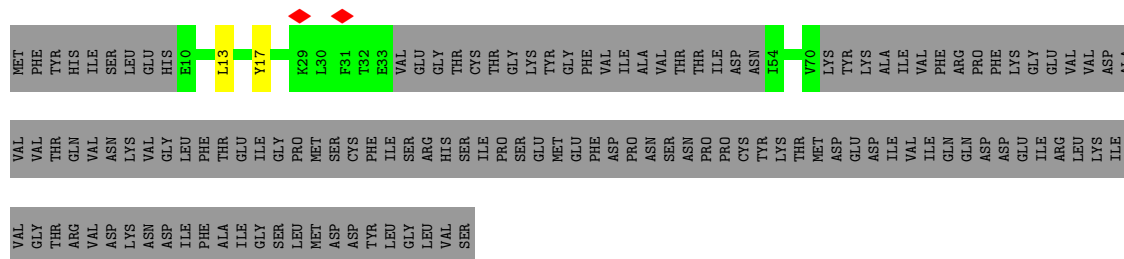
- Molecule 4: DNA-directed RNA polymerase II subunit E



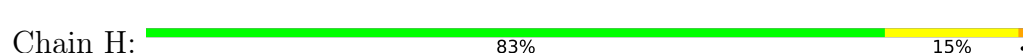
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



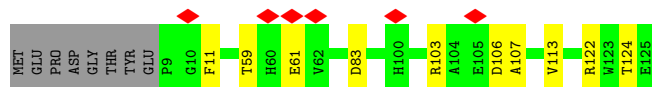
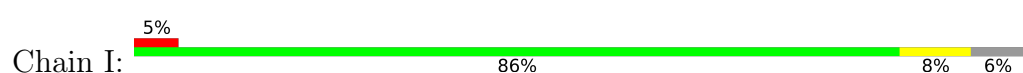
- Molecule 6: DNA-directed RNA polymerase subunit



- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC3



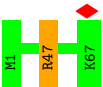
- Molecule 8: DNA-directed RNA polymerase II subunit RPB9



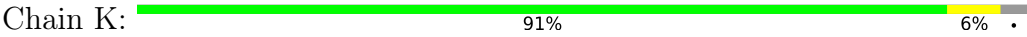
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC5



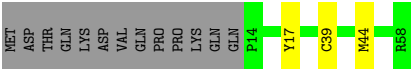




- Molecule 10: DNA-directed RNA polymerase II subunit RPB11-a



- Molecule 11: RNA polymerase II, I and III subunit K



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	875265	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	427.52, 427.52, 427.52	wwPDB
Map dimensions	428, 428, 428	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9988785, 0.9988785, 0.9988785	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/8594	0.54	0/11617
2	B	0.25	0/8456	0.54	0/11415
3	C	0.25	0/2122	0.56	0/2883
4	E	0.25	0/1752	0.53	0/2366
5	F	0.24	0/668	0.54	0/901
6	G	0.25	0/334	0.53	0/452
7	H	0.26	0/1207	0.56	0/1628
8	I	0.27	0/973	0.54	0/1316
9	J	0.26	0/543	0.54	0/730
10	K	0.24	0/931	0.49	0/1261
11	L	0.28	0/386	0.68	0/511
All	All	0.25	0/25966	0.54	0/35080

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
1	A	0	2
2	B	0	1
9	J	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	483	ARG	Sidechain
1	A	932	ARG	Sidechain
2	B	1091	ARG	Sidechain
9	J	47	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8440	0	8483	37	0
2	B	8290	0	8326	40	0
3	C	2079	0	2032	14	0
4	E	1721	0	1737	4	0
5	F	658	0	684	3	0
6	G	326	0	339	1	0
7	H	1186	0	1147	11	0
8	I	950	0	879	5	0
9	J	534	0	553	0	0
10	K	912	0	930	5	0
11	L	380	0	386	1	0
12	I	2	0	0	0	0
12	J	1	0	0	0	0
12	L	1	0	0	0	0
All	All	25480	0	25496	108	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 2.

The worst 5 of 108 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)
3:C:205:LYS:NZ	3:C:212:ASP:O	2.16	0.78
7:H:58:LEU:HD11	7:H:143:LEU:HD11	1.78	0.65
2:B:411:LEU:HD11	2:B:435:ILE:HG23	1.80	0.63
11:L:17:TYR:HB3	11:L:44:MET:HB3	1.82	0.62
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.83	0.59

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	A	1052/1970 (53%)	1020 (97%)	32 (3%)	0	100	100
2	B	1023/1174 (87%)	984 (96%)	38 (4%)	1 (0%)	48	69
3	C	255/275 (93%)	247 (97%)	8 (3%)	0	100	100
4	E	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
5	F	80/127 (63%)	77 (96%)	3 (4%)	0	100	100
6	G	37/172 (22%)	34 (92%)	3 (8%)	0	100	100
7	H	146/150 (97%)	140 (96%)	5 (3%)	1 (1%)	19	35
8	I	115/125 (92%)	111 (96%)	4 (4%)	0	100	100
9	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
10	K	112/117 (96%)	107 (96%)	5 (4%)	0	100	100
11	L	43/58 (74%)	37 (86%)	6 (14%)	0	100	100
All	All	3135/4445 (70%)	3022 (96%)	111 (4%)	2 (0%)	50	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	595	ASP
7	H	72	ASP

### 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	
1	A	942/1749 (54%)	926 (98%)	16 (2%)	56	79
2	B	909/1027 (88%)	901 (99%)	8 (1%)	75	90
3	C	236/252 (94%)	229 (97%)	7 (3%)	36	63
4	E	191/192 (100%)	190 (100%)	1 (0%)	86	95
5	F	71/111 (64%)	69 (97%)	2 (3%)	38	65
6	G	35/153 (23%)	35 (100%)	0	100	100
7	H	129/131 (98%)	127 (98%)	2 (2%)	58	80
8	I	105/112 (94%)	103 (98%)	2 (2%)	52	77
9	J	56/56 (100%)	55 (98%)	1 (2%)	54	78
10	K	103/106 (97%)	102 (99%)	1 (1%)	73	88
11	L	42/55 (76%)	41 (98%)	1 (2%)	44	70
All	All	2819/3944 (72%)	2778 (98%)	41 (2%)	60	82

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	127	VAL
7	H	18	GLU
3	C	133	ARG
5	F	83	LEU
8	I	124	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1021	HIS
8	I	50	ASN
2	B	1025	ASN
10	K	69	HIS
7	H	126	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

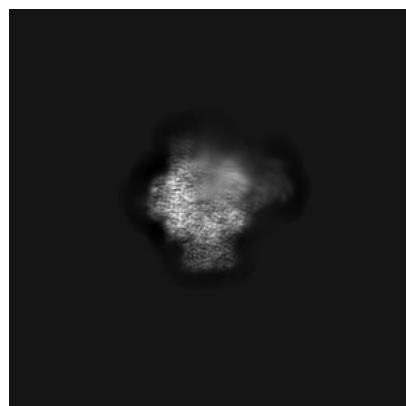
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18375. These allow visual inspection of the internal detail of the map and identification of artifacts.

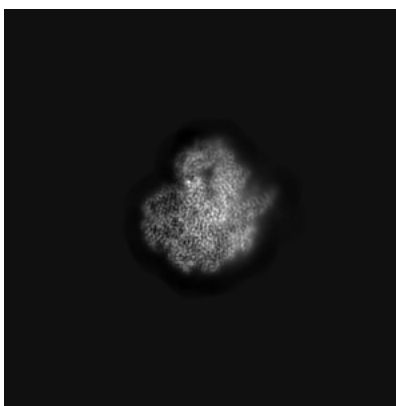
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

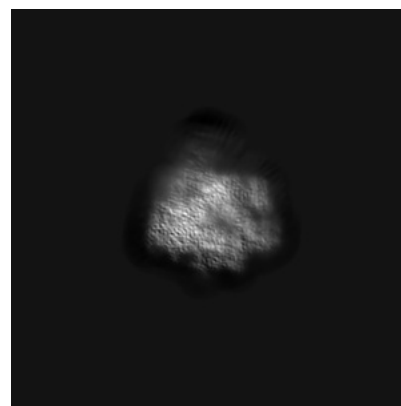
#### 6.1.1 Primary map



X

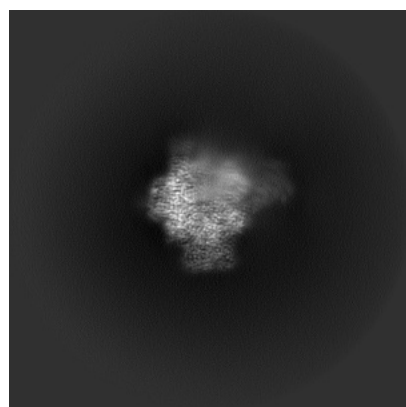


Y

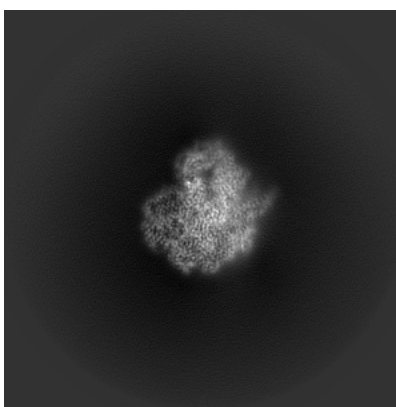


Z

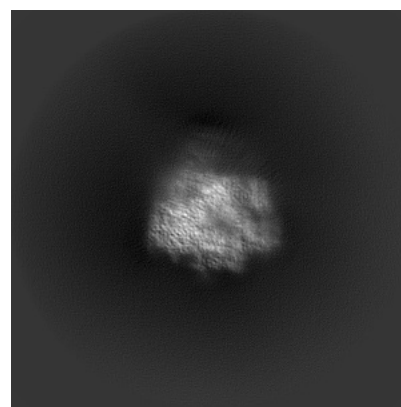
#### 6.1.2 Raw map



X



Y



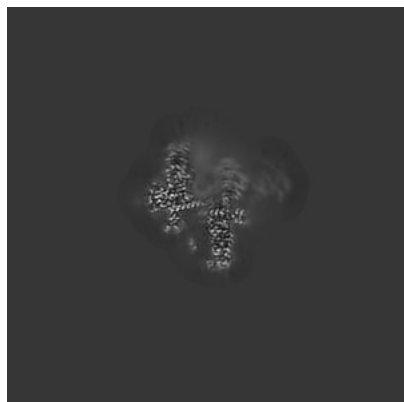
Z

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

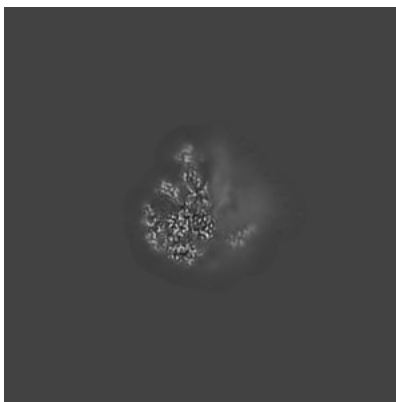


## 6.2 Central slices [i](#)

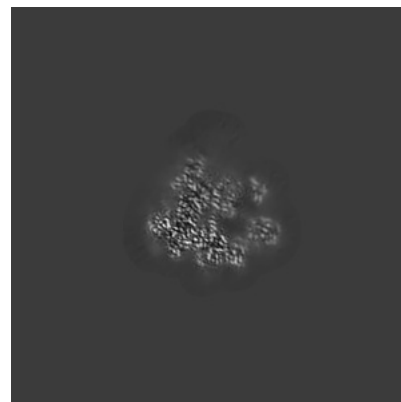
### 6.2.1 Primary map



X Index: 214

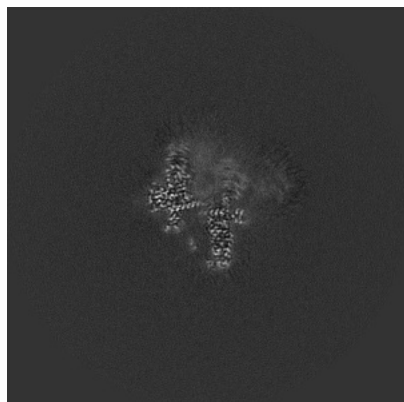


Y Index: 214

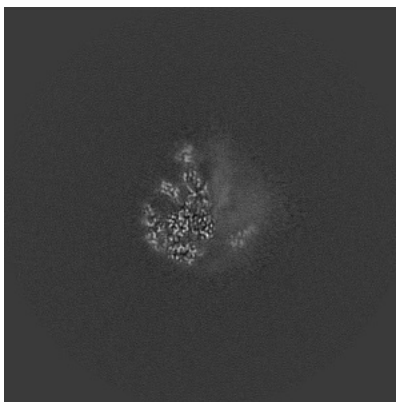


Z Index: 214

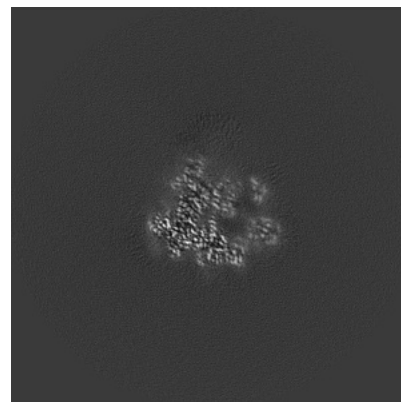
### 6.2.2 Raw map



X Index: 214



Y Index: 214

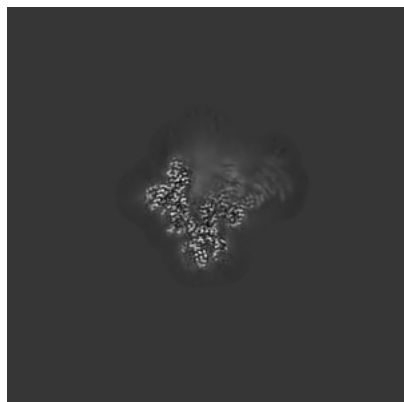


Z Index: 214

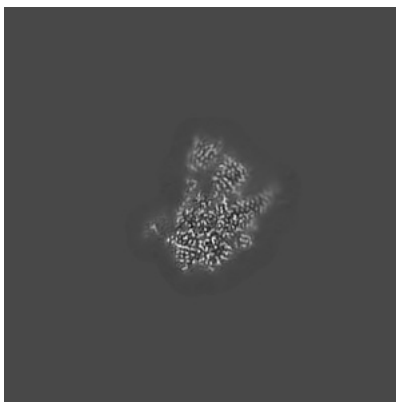
The images above show central slices of the map in three orthogonal directions.

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

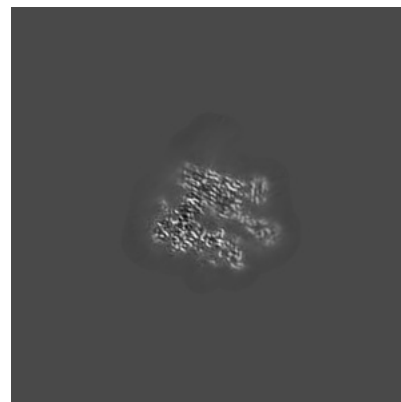
### 6.3.1 Primary map



X Index: 202

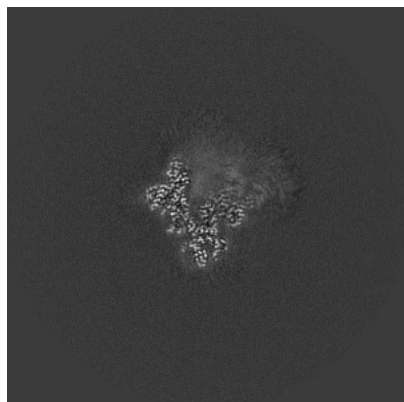


Y Index: 185

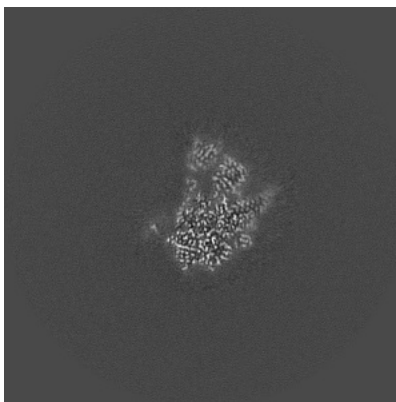


Z Index: 208

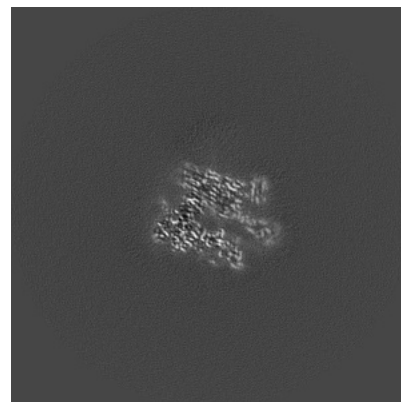
### 6.3.2 Raw map



X Index: 202



Y Index: 185

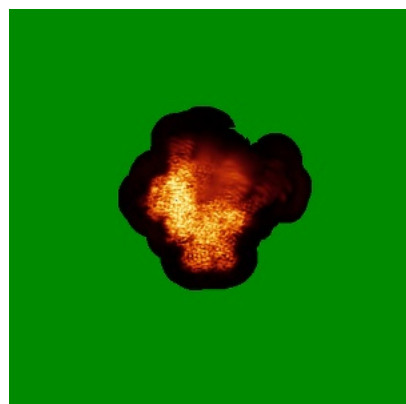


Z Index: 208

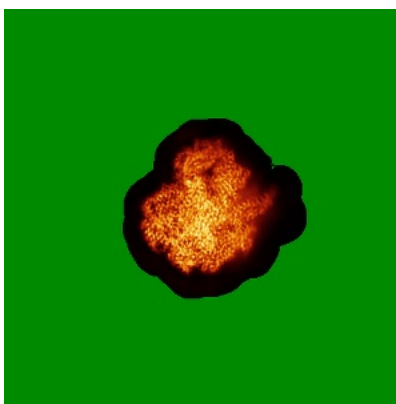
The images above show the largest variance slices of the map in three orthogonal directions.

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

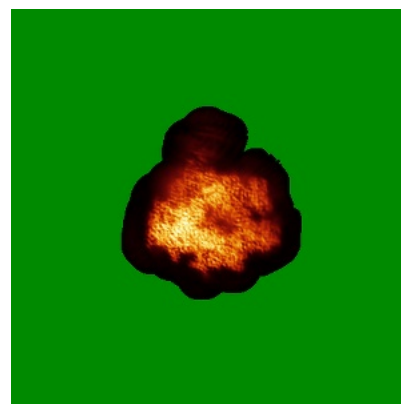
### 6.4.1 Primary map



X



Y

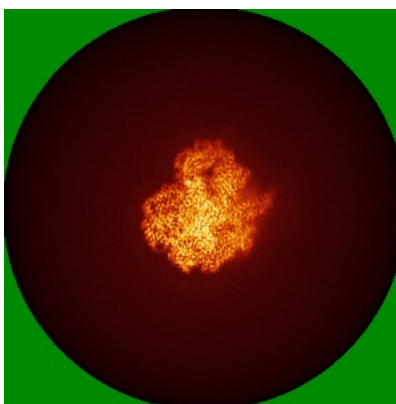


Z

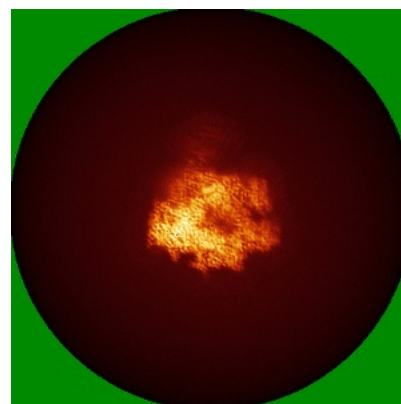
### 6.4.2 Raw map



X



Y



Z

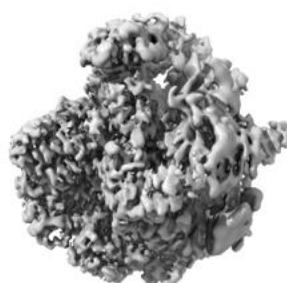
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

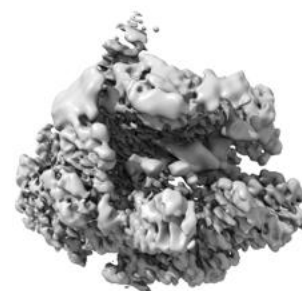
### 6.5.1 Primary map



X



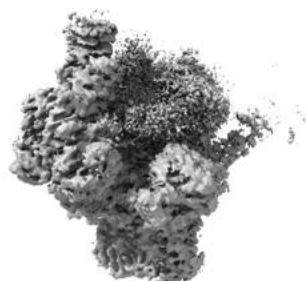
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. 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



X



Y



Z

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.

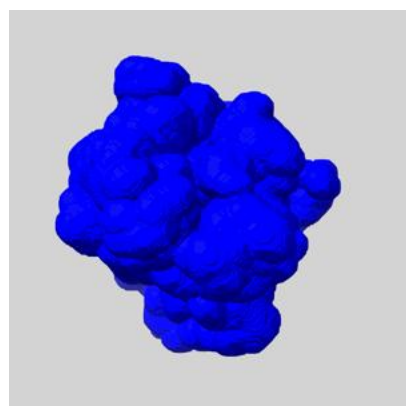
## 6.6 Mask visualisation [i](#)

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

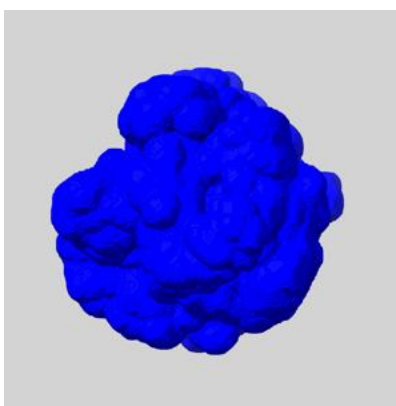
A mask typically either:

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

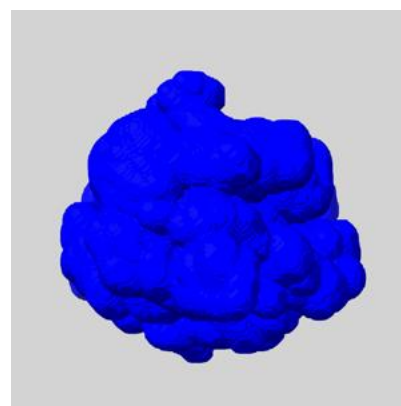
### 6.6.1 emd\_18375\_msk\_1.map [i](#)



X



Y

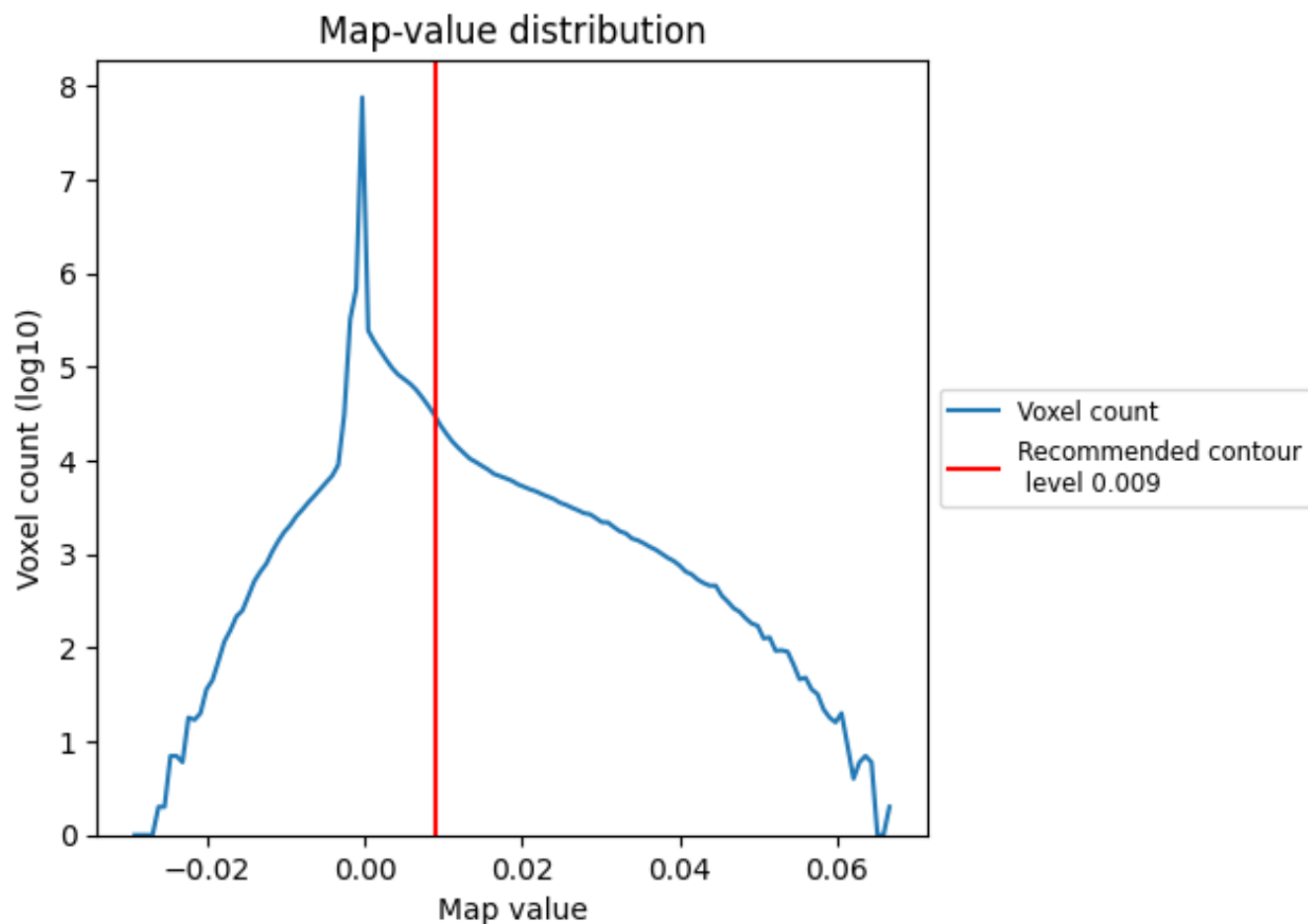


Z

## 7 Map analysis [i](#)

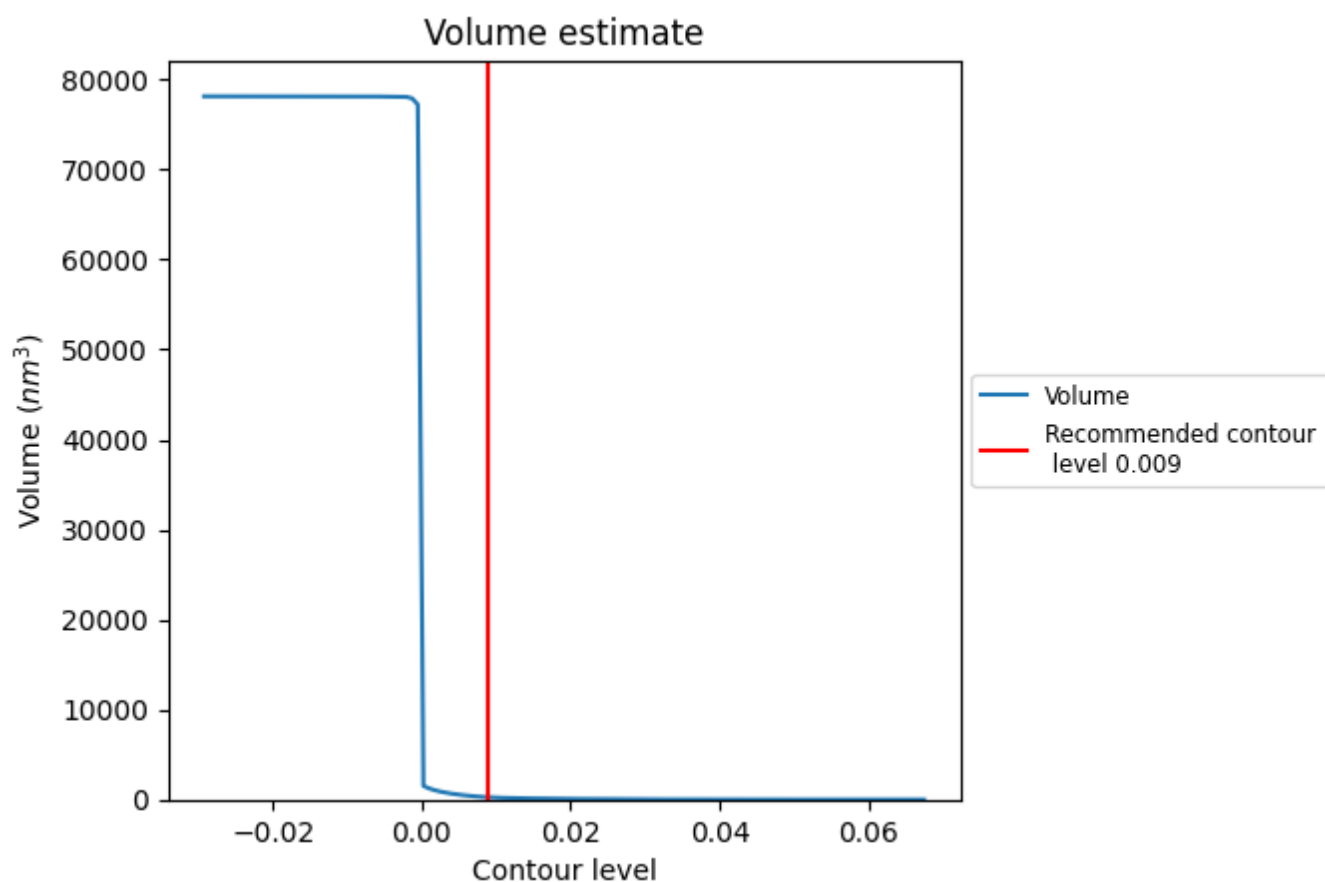
This section contains the results of statistical analysis of the map.

### 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.

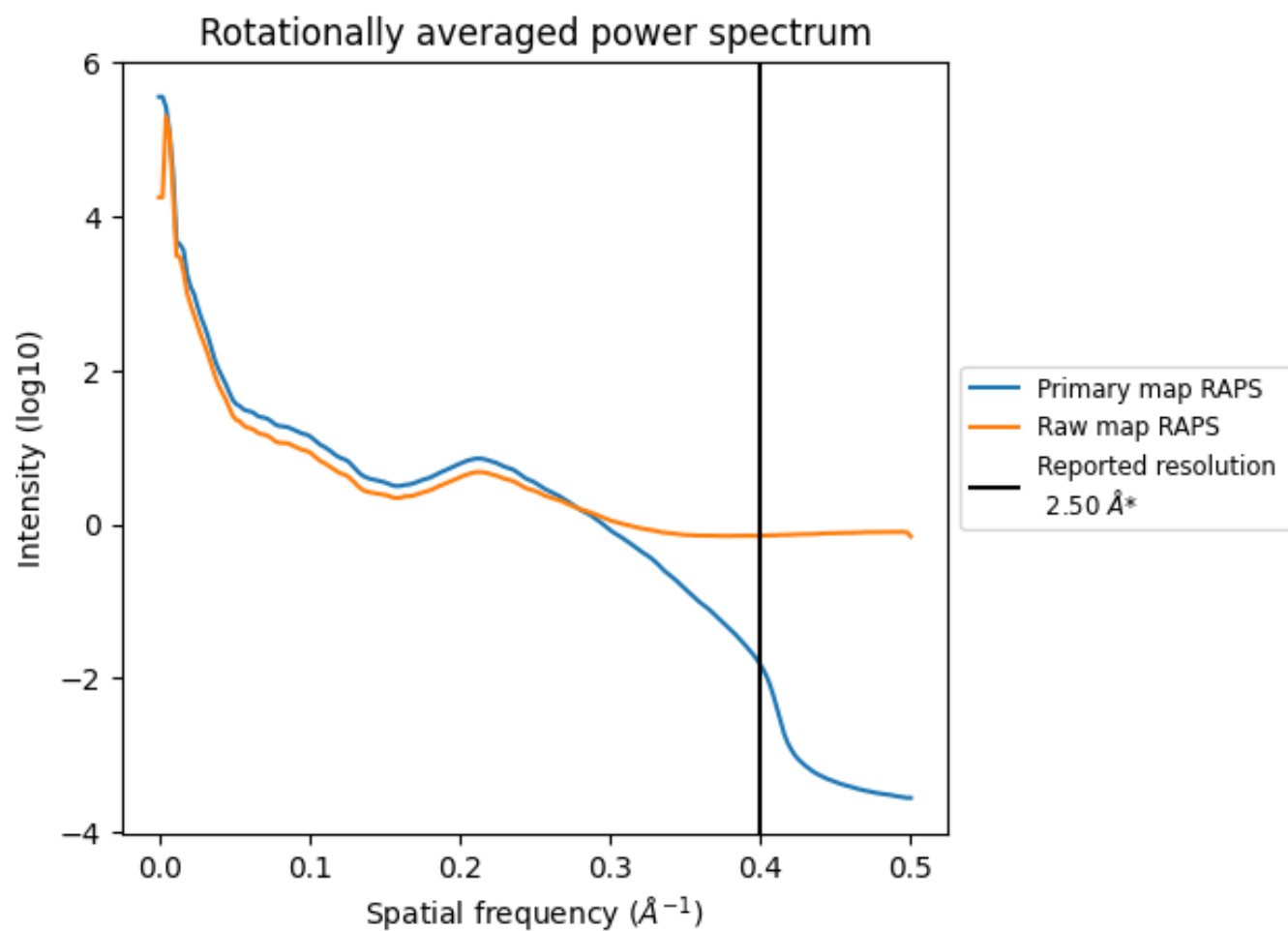
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 251  $\text{nm}^3$ ; this corresponds to an approximate mass of 227 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 ⓘ



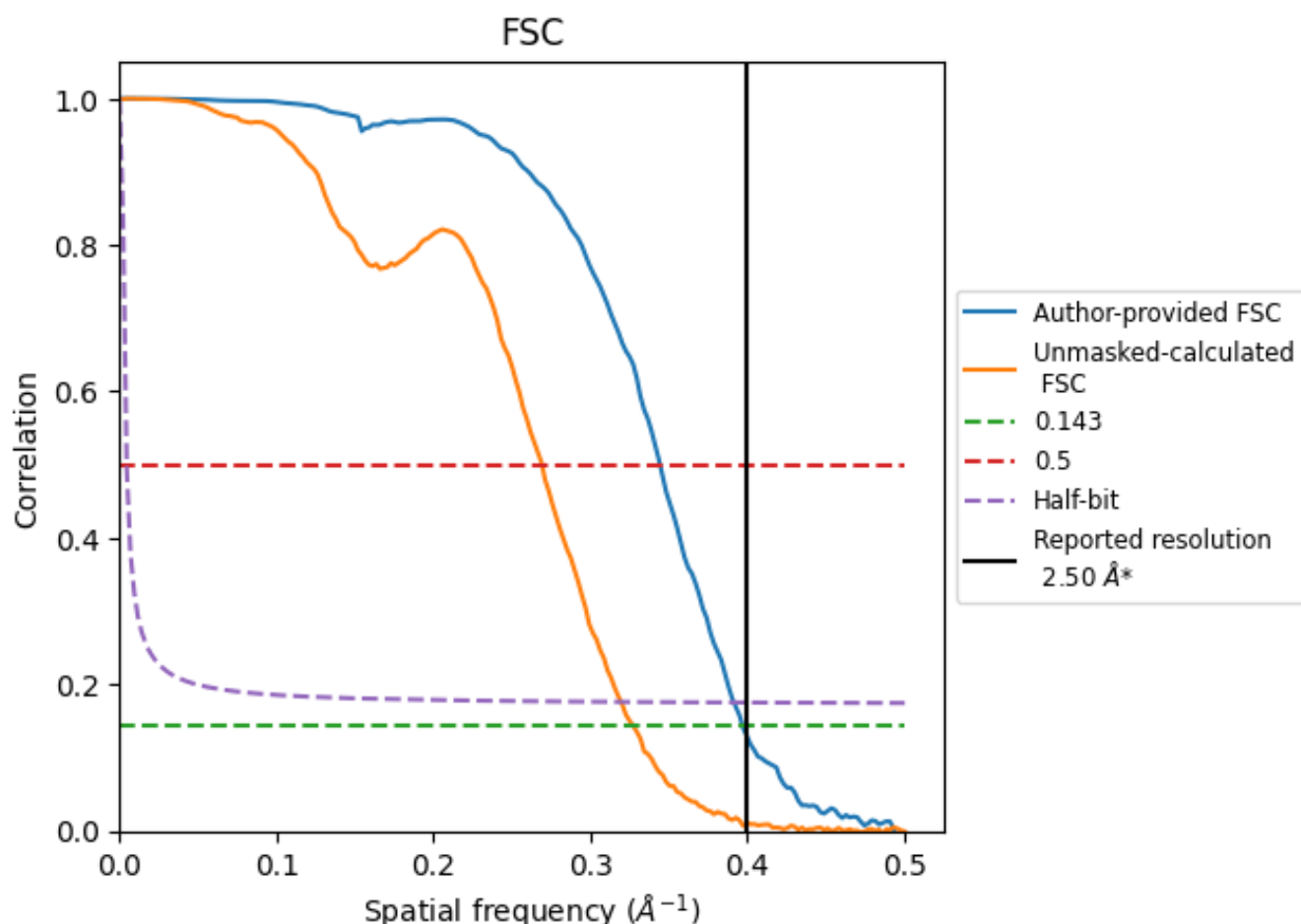
\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>



## 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 0.400 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

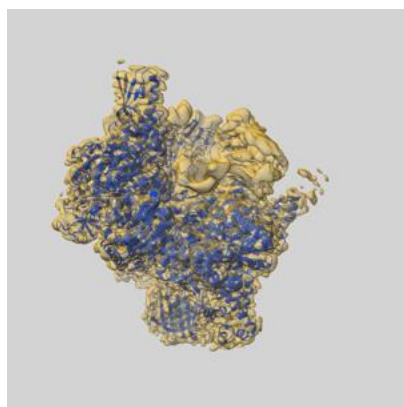
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.52	2.90	2.55
Unmasked-calculated*	3.05	3.71	3.13

\*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 3.05 differs from the reported value 2.5 by more than 10 %

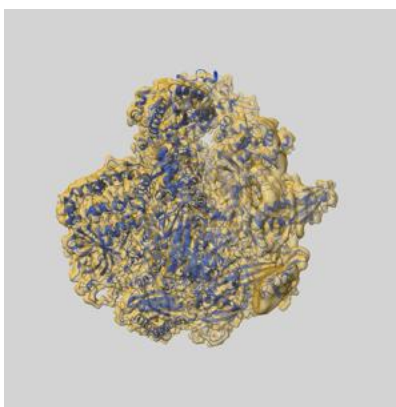
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18375 and PDB model 8QEP. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

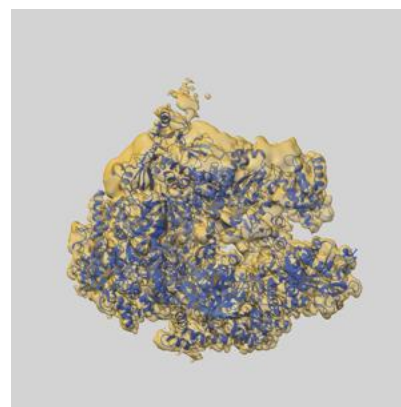
### 9.1 Map-model overlay [i](#)



X



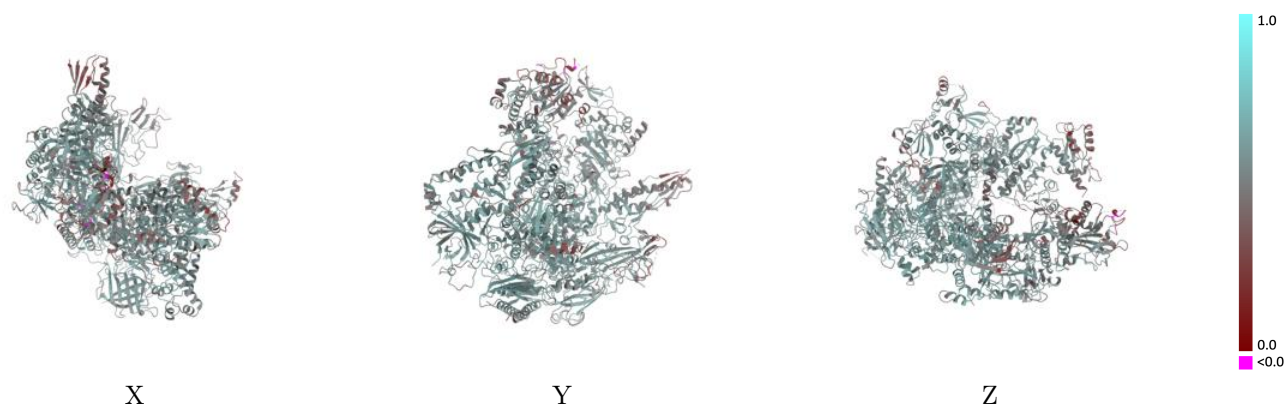
Y



Z

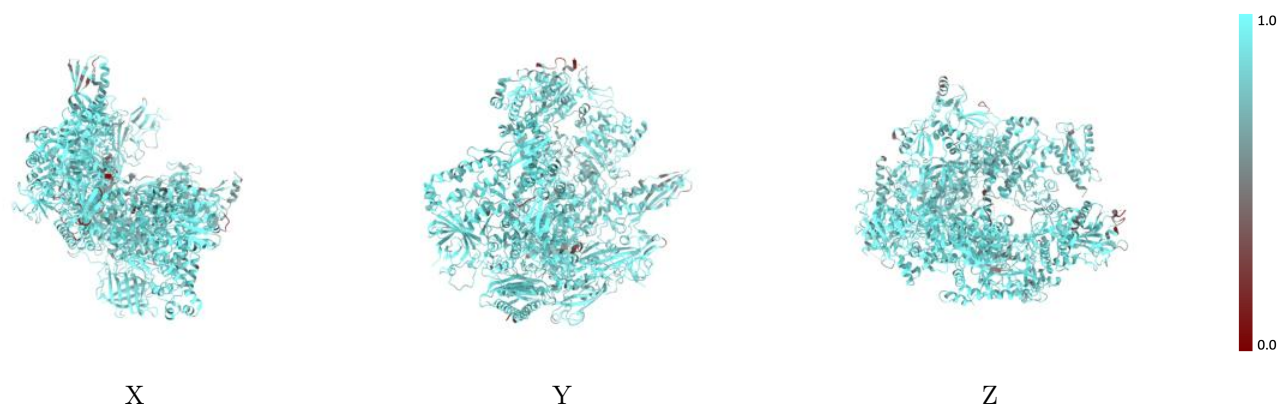
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



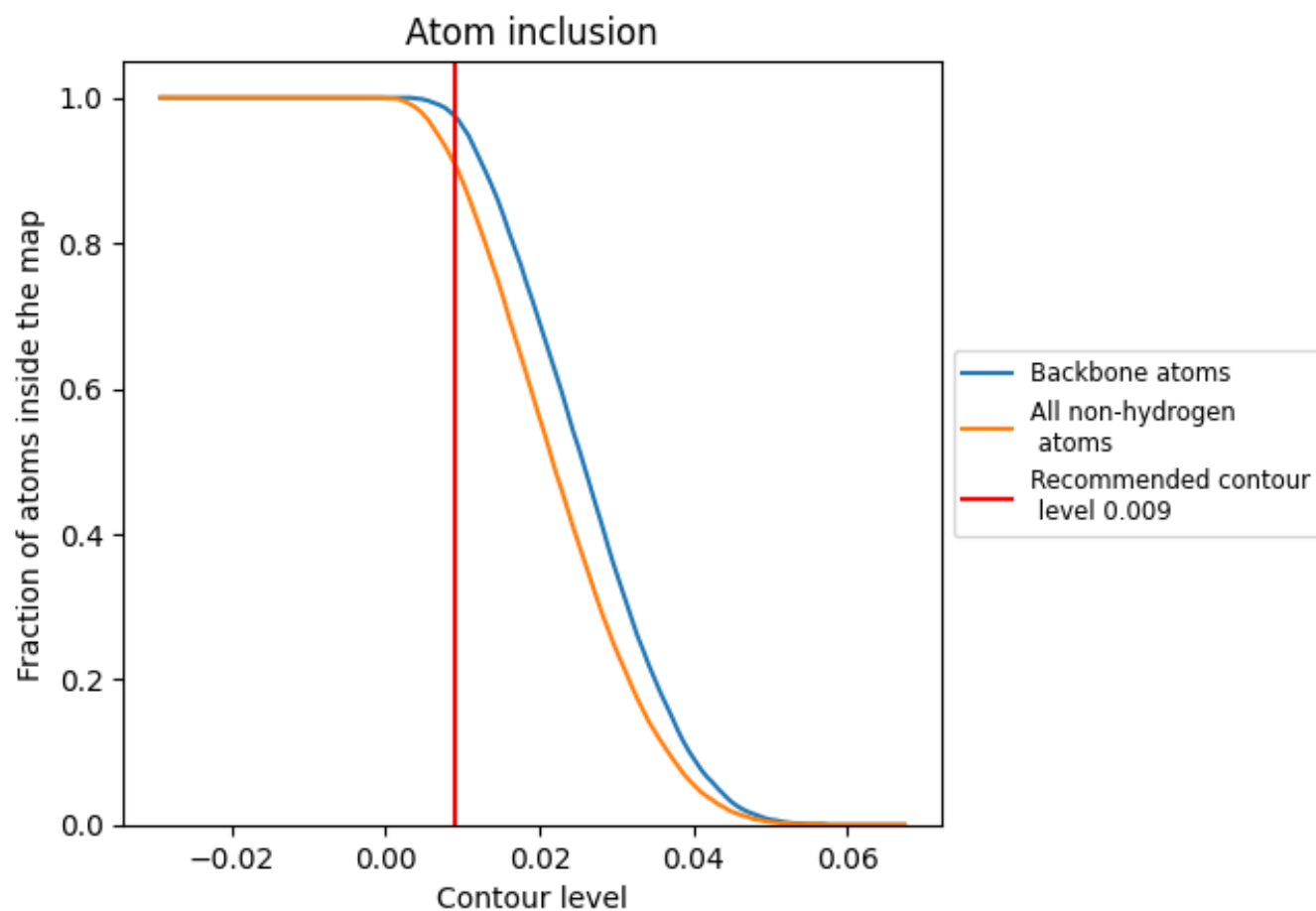
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9090	<div></div> 0.5500
A	<div></div> 0.9070	<div></div> 0.5480
B	<div></div> 0.9200	<div></div> 0.5550
C	<div></div> 0.9290	<div></div> 0.5770
E	<div></div> 0.8740	<div></div> 0.5020
F	<div></div> 0.8940	<div></div> 0.5410
G	<div></div> 0.7440	<div></div> 0.4580
H	<div></div> 0.9340	<div></div> 0.5640
I	<div></div> 0.8550	<div></div> 0.5010
J	<div></div> 0.9310	<div></div> 0.6130
K	<div></div> 0.9240	<div></div> 0.5820
L	<div></div> 0.9090	<div></div> 0.5280

1.0

0.0

<0.0