



## wwPDB EM Validation Summary Report ⓘ

Dec 6, 2020 – 07:46 am GMT

PDB ID : 6YYS  
EMDB ID : EMD-11004  
Title : Structure of Mycobacterium smegmatis HelD protein in complex with RNA polymerase core - State II, primary channel engaged and active site interfering  
Authors : Kouba, T.; Koval, T.; Krasny, L.; Dohnalek, J.  
Deposited on : 2020-05-05  
Resolution : 3.08 Å (reported)  
Based on initial models : 6VSX, 6F6W

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

EMDB validation analysis : 0.0.0.dev61  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.15.1



## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 27930 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	224	Total	C	N	O	S	0	0
			1700	1070	293	334	3		
1	B	233	Total	C	N	O	S	0	0
			1771	1112	305	351	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1089	Total	C	N	O	S	0	0
			8433	5276	1476	1646	35		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1278	Total	C	N	O	S	0	0
			9983	6249	1809	1884	41		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	83	Total	C	N	O	0	0
			646	411	108	127		

- Molecule 5 is a protein called RNA polymerase-associated transcription factor HelD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	690	Total	C	N	O	S	0	0
			5394	3364	972	1042	16		

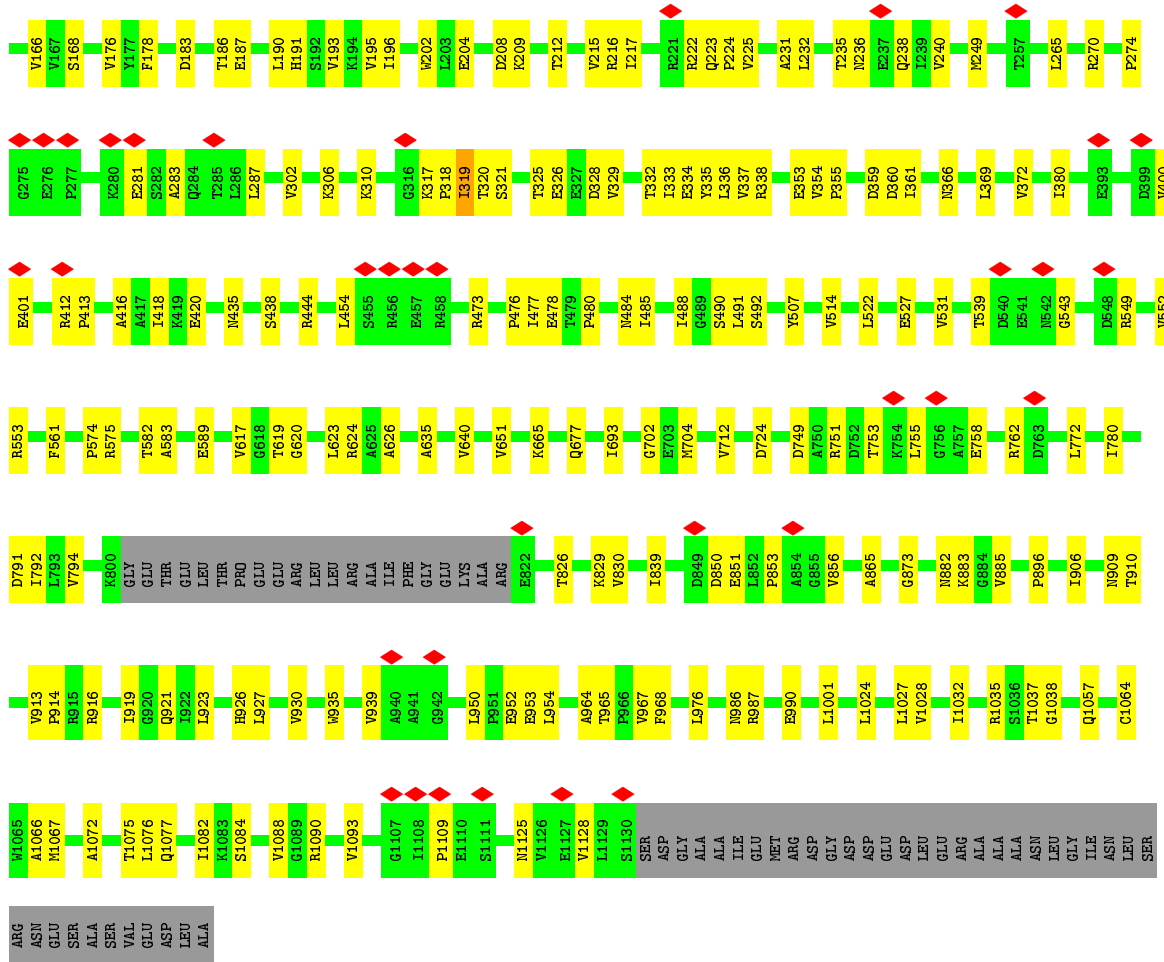
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	D	2	Total 2	Zn 2	0

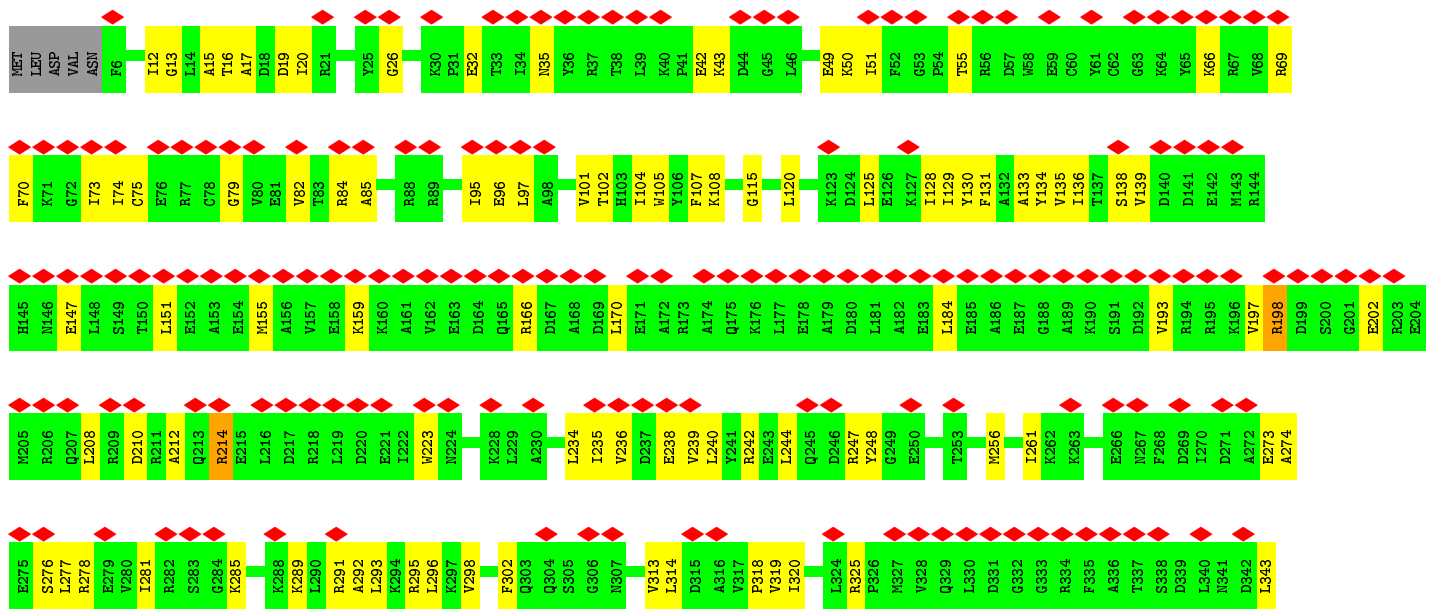
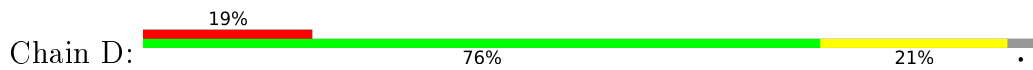
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total 1	Mg 1	0





● Molecule 3: DNA-directed RNA polymerase subunit beta'





A717	V641	V648	V349	V350	V351	R352	A353	V354	A355	R356	I357	G358	R359	G360	W361	L362	T363	R364	D365	D366	K367	R368	A369	M373	R374	A375	D376	V377	V378	L381	E382	D383	H384	E385	Q386	F387	L391	D392	A393	L394	W395	P396	I397	L398	T399	P400	E401	D402	V403	L404	A405	T409	S410	H411	L414	R415
LEU	S642	E643	E644	A645	G646	R647	E648	G649	T650	S651	V652	I654	P657	D658	V659	P660	G661	T662	V663	P664	P665	S666	E667	T668	K669	G670	L671	E672	L677	V678	V679	E680	R683	I684	D687	G688	P689	R690	A693	V697	T703	Q704	R705	L706	D712	A713	L714	F715	Q716							
ALA	LEU	GLY	LEU	ALA	GLU	GLY	ASP	ALA	ALA	THR	VAL	GLU	GLN	ARG	THR	SER	ALA	D440	E441	L442	L446	G447	R448	M449	K450	A451	A452	D453	E454	Y466	D482	D483	E484	D485	H486	L487	L488	A489	I493	R501	D506	R513	R518	T521	H524	D528	E529	E532								
L541	R544	C545	P546	T551	Y582	S586	V587	M588	Y589	R590	A593	E594	I595	W596	A597	V598	A599	A604	E605	F606	A607	P608	D609	A610	T611	P612	P613	D614	S615	V616	R617	A618	C619	G620	V621	A622	P623	W624	A625	R626	Q627	V628	T629	D630	D631	D632	I633	A634	S635	A636	I637	A638				
A419	E421	C422	W423	R425	A426	D427	G428	E429	V433	V436	D440	E441	L442	L446	G447	R448	M449	K450	A451	A452	D453	E454	Y466	D482	D483	E484	D485	H486	L487	L488	A489	I493	R501	D506	R513	R518	T521	H524	D528	E529	E532															



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	173500	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.728	Depositor
Minimum map value	-0.227	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	299.19598, 299.19598, 299.19598	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8310999, 0.8310999, 0.8310999	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.32	0/1726	0.50	0/2348
1	B	0.30	0/1798	0.49	0/2446
2	C	0.32	0/8583	0.49	0/11632
3	D	0.29	0/10145	0.48	0/13709
4	E	0.29	0/659	0.48	0/897
5	H	0.28	0/5498	0.46	0/7476
All	All	0.30	0/28409	0.48	0/38508

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1700	0	1742	21	0
1	B	1771	0	1803	36	0
2	C	8433	0	8377	154	0
3	D	9983	0	10103	210	0
4	E	646	0	642	15	0
5	H	5394	0	5269	108	0
6	D	2	0	0	0	0

*Continued on next page...*

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
All	All	27930	0	27936	510	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 9.

The worst 5 of 510 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:D:599:TYR:OH	3:D:608:GLU:OE1	1.93	0.84
3:D:125:LEU:HD11	3:D:261:ILE:HD11	1.56	0.84
2:C:910:THR:HG23	3:D:730:VAL:HG23	1.65	0.78
1:A:210:SER:OG	1:B:229:SER:O	2.00	0.76
2:C:623:LEU:HD12	2:C:702:GLY:O	1.86	0.75

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	222/350 (63%)	212 (96%)	10 (4%)	0	100	100
1	B	231/350 (66%)	214 (93%)	17 (7%)	0	100	100
2	C	1085/1169 (93%)	994 (92%)	90 (8%)	1 (0%)	51	82
3	D	1276/1317 (97%)	1172 (92%)	104 (8%)	0	100	100
4	E	81/107 (76%)	71 (88%)	10 (12%)	0	100	100
5	H	686/736 (93%)	601 (88%)	85 (12%)	0	100	100
All	All	3581/4029 (89%)	3264 (91%)	316 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	319	ILE

### 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	191/297 (64%)	191 (100%)	0	100	100
1	B	199/297 (67%)	199 (100%)	0	100	100
2	C	921/984 (94%)	921 (100%)	0	100	100
3	D	1062/1095 (97%)	1058 (100%)	4 (0%)	91	95
4	E	69/86 (80%)	69 (100%)	0	100	100
5	H	553/583 (95%)	553 (100%)	0	100	100
All	All	2995/3342 (90%)	2991 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	69	ARG
3	D	198	ARG
3	D	214	ARG
3	D	604	LYS

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

Mol	Chain	Res	Type
3	D	494	HIS
3	D	505	HIS
4	E	85	GLN
3	D	349	ASN
3	D	1092	HIS

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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.

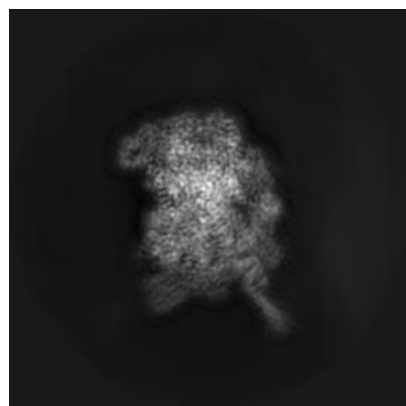
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11004. These allow visual inspection of the internal detail of the map and identification of artifacts.

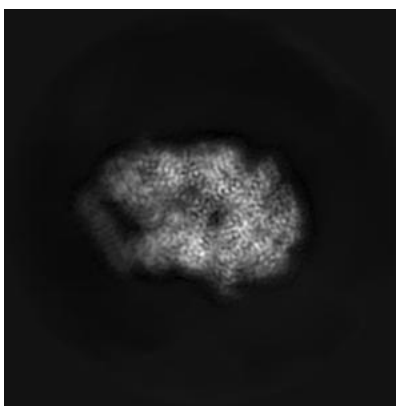
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

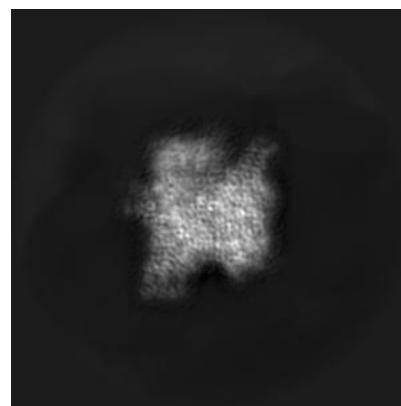
#### 6.1.1 Primary map



X

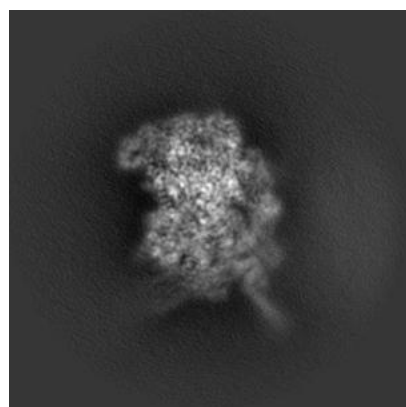


Y

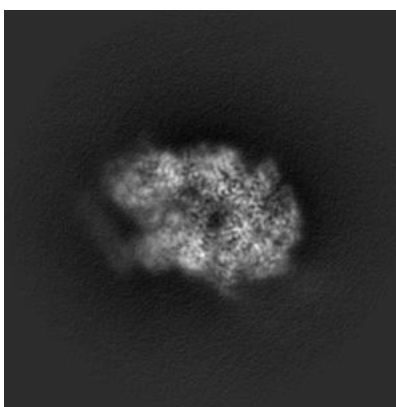


Z

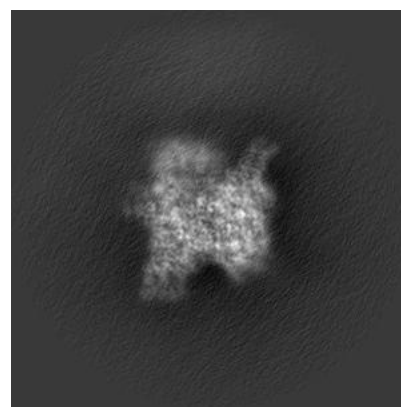
#### 6.1.2 Raw map



X



Y

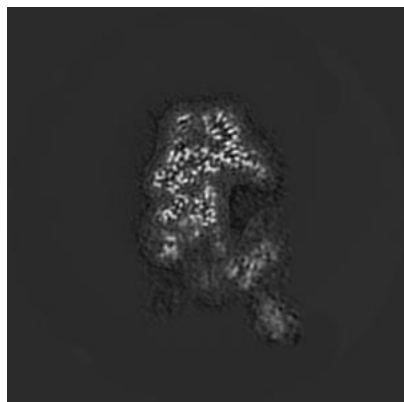


Z

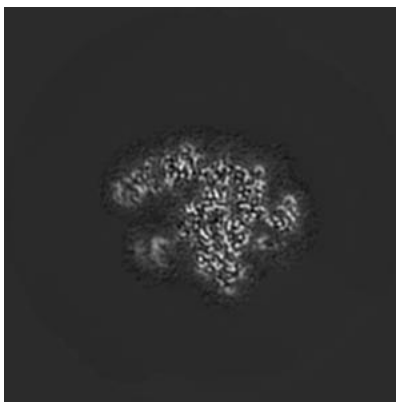
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

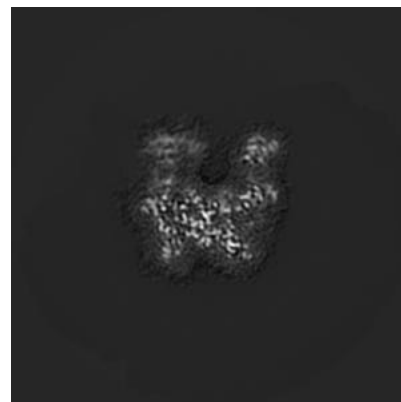
### 6.2.1 Primary map



X Index: 180

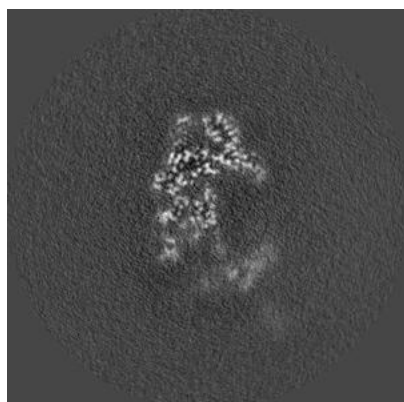


Y Index: 180

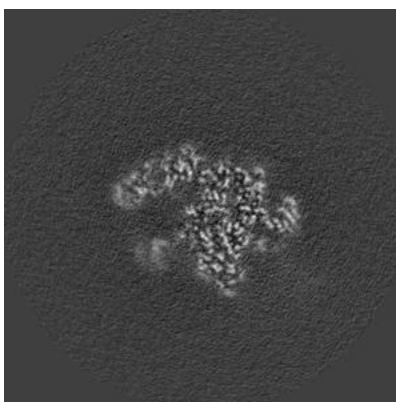


Z Index: 180

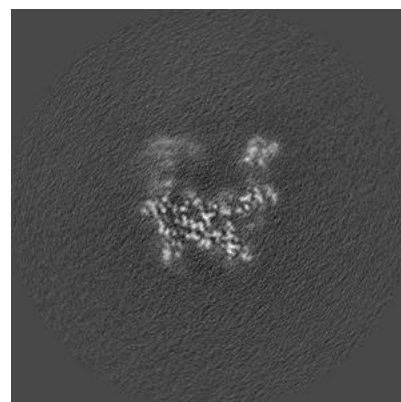
### 6.2.2 Raw map



X Index: 180



Y Index: 180

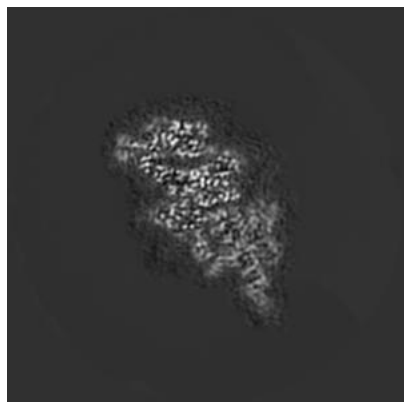


Z Index: 180

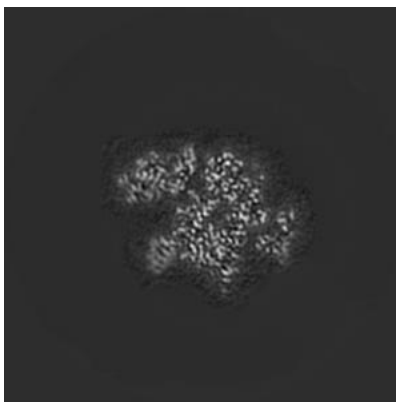
The images above show central slices of the map in three orthogonal directions.

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

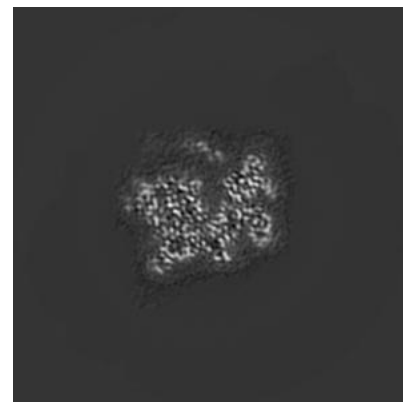
### 6.3.1 Primary map



X Index: 146

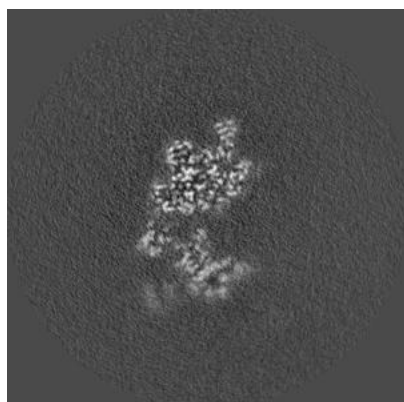


Y Index: 173

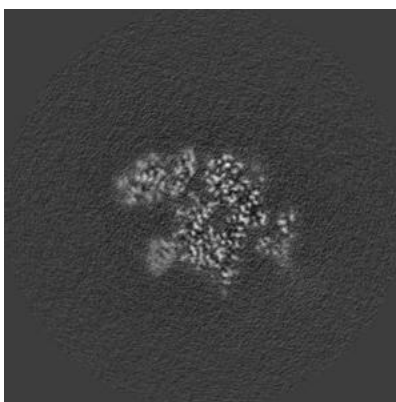


Z Index: 204

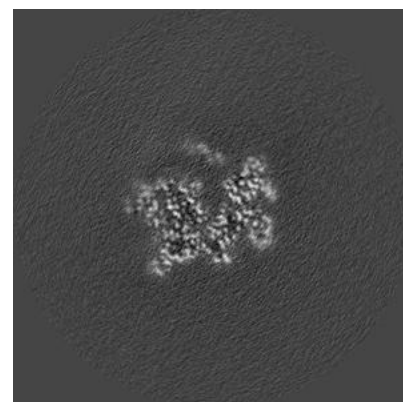
### 6.3.2 Raw map



X Index: 196



Y Index: 173



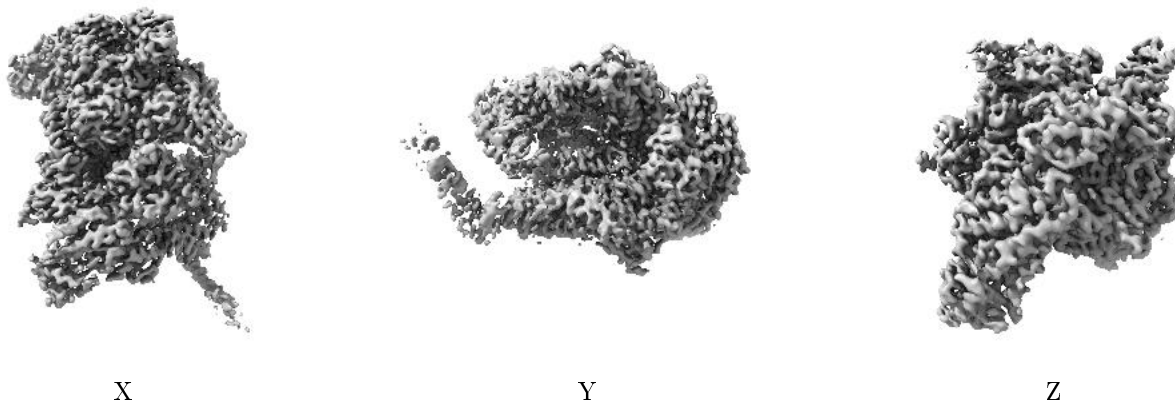
Z Index: 204

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



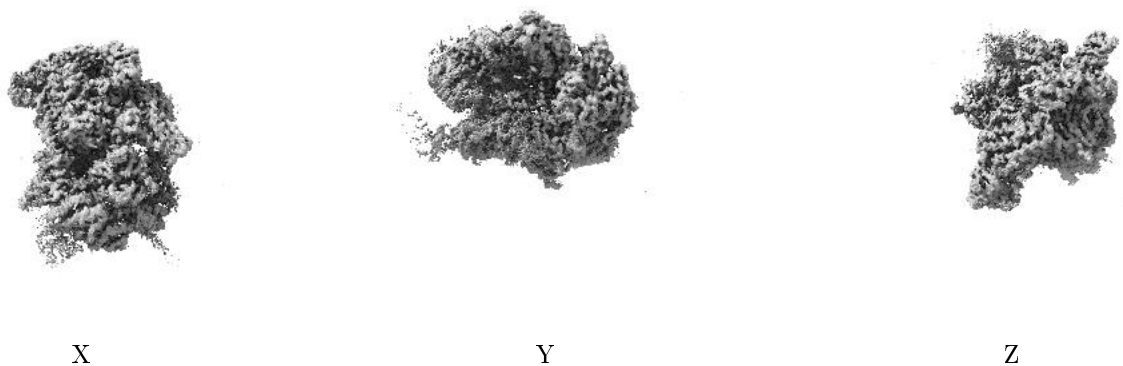
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.17. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

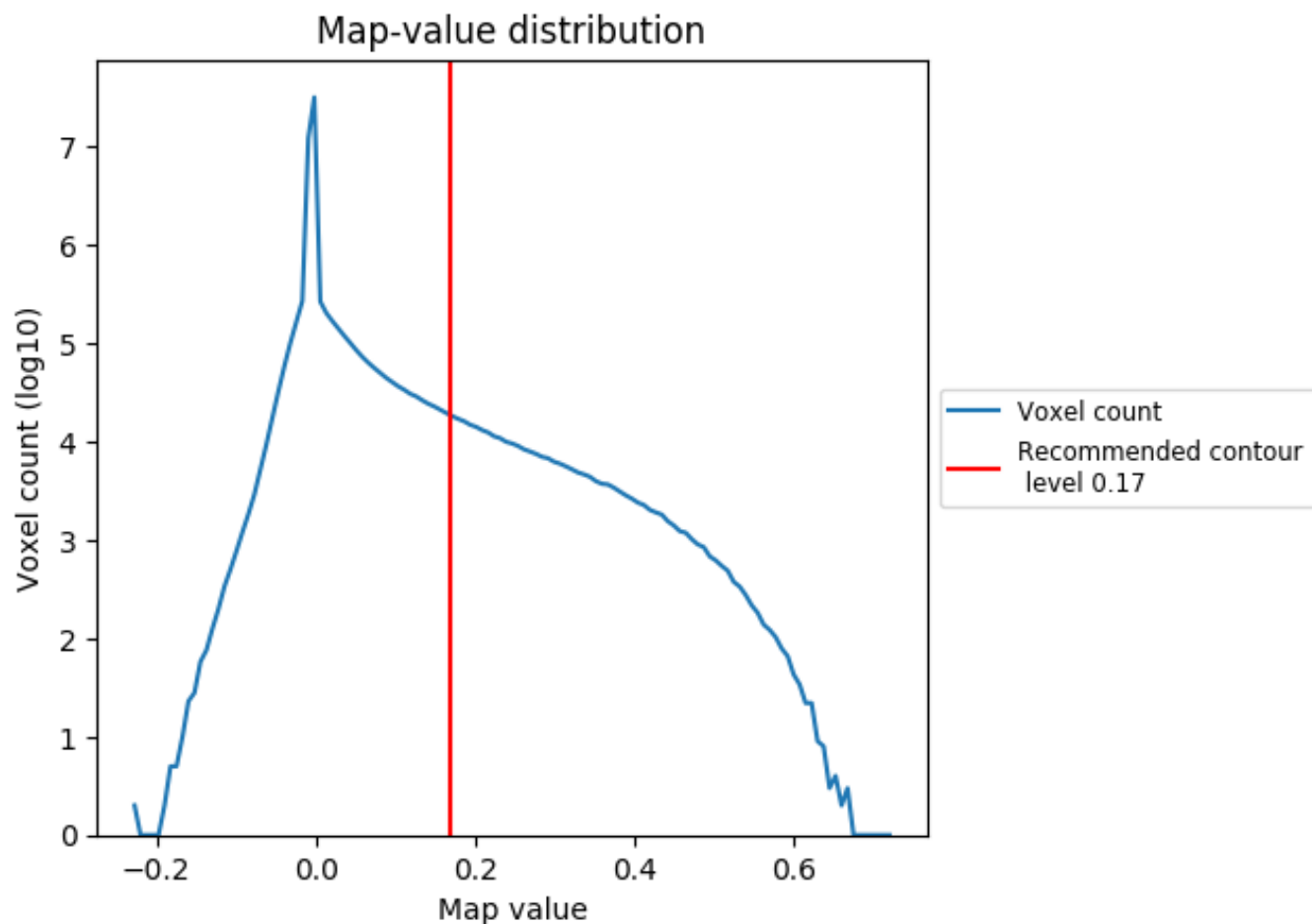
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

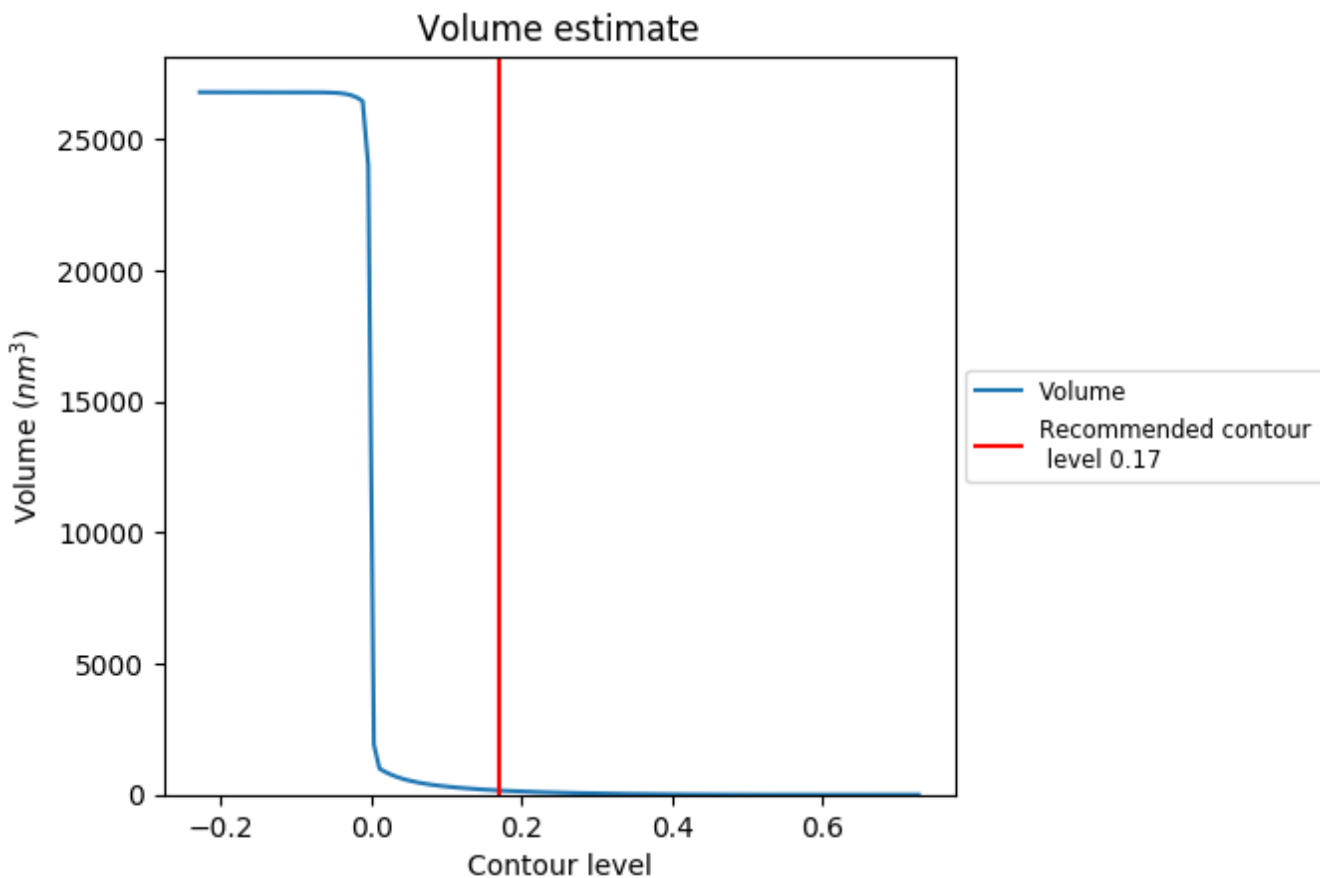
This section contains the results of statistical analysis of the map.

### 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.

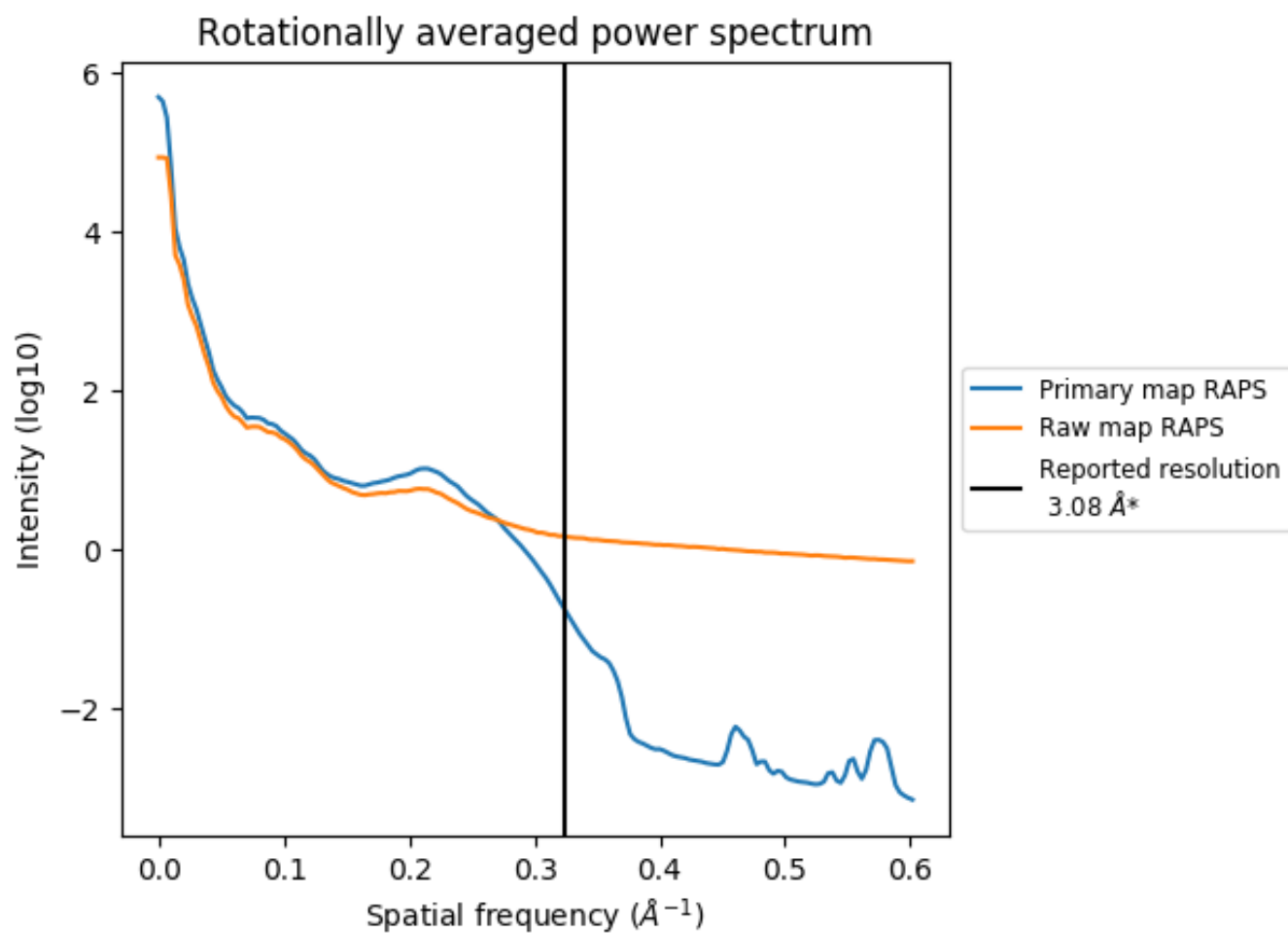
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 161 nm<sup>3</sup>; this corresponds to an approximate mass of 146 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

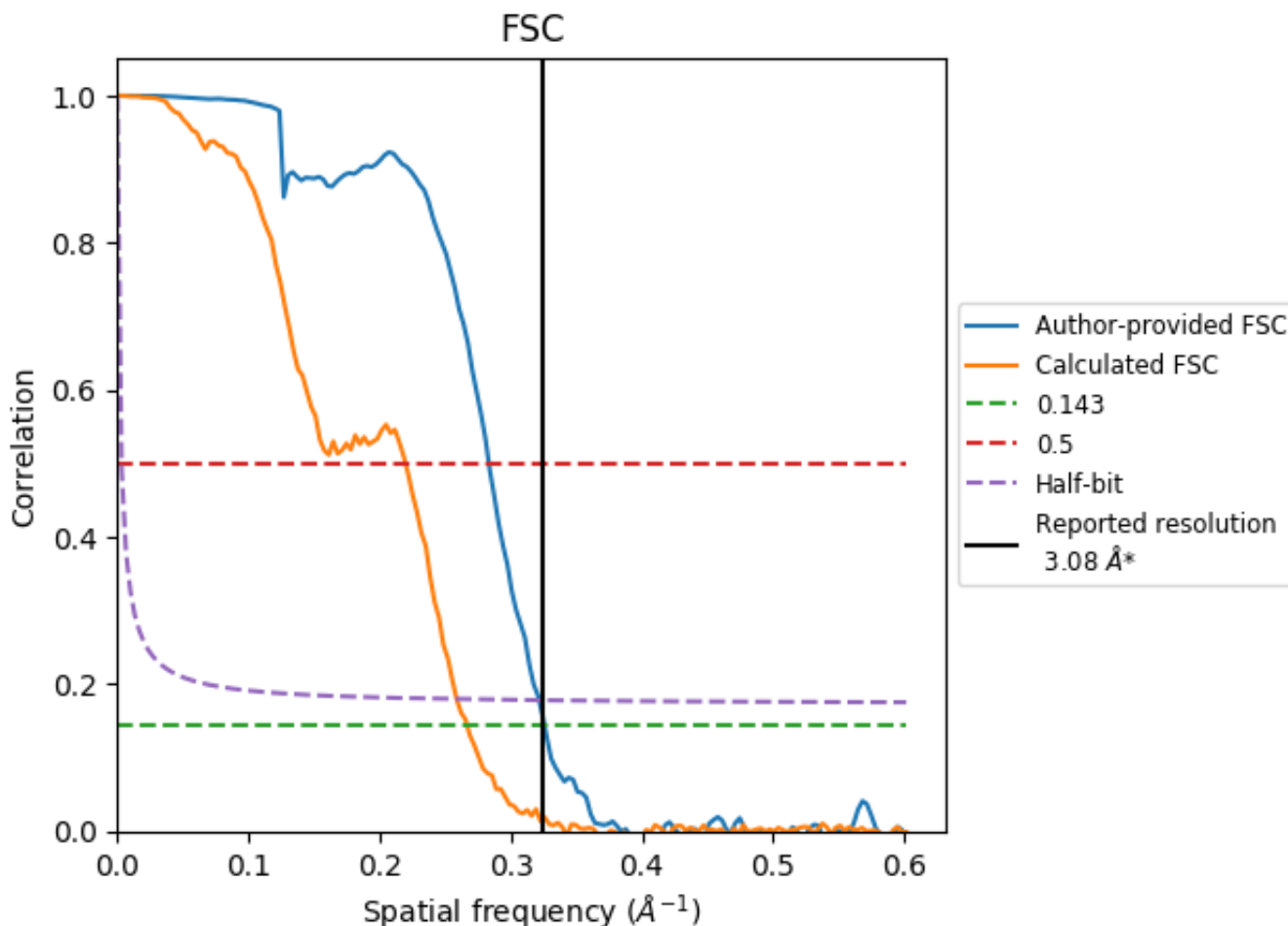


\*Reported resolution corresponds to spatial frequency of 0.325 Å<sup>-1</sup>

## 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 0.325 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

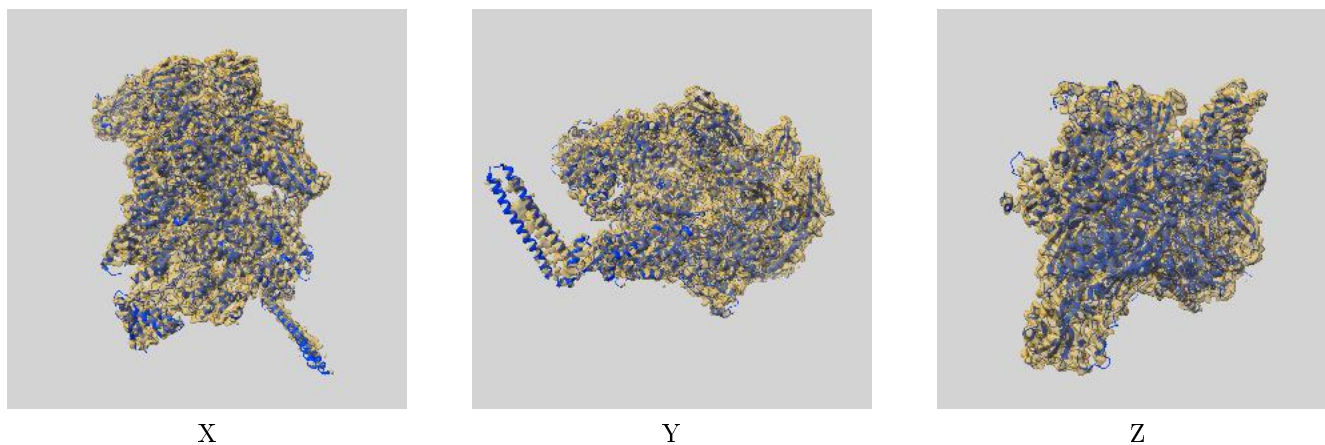
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.10	3.57	3.14
Calculated*	3.80	4.62	3.92

\*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 3.80 differs from the reported value 3.08 by more than 10 %

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

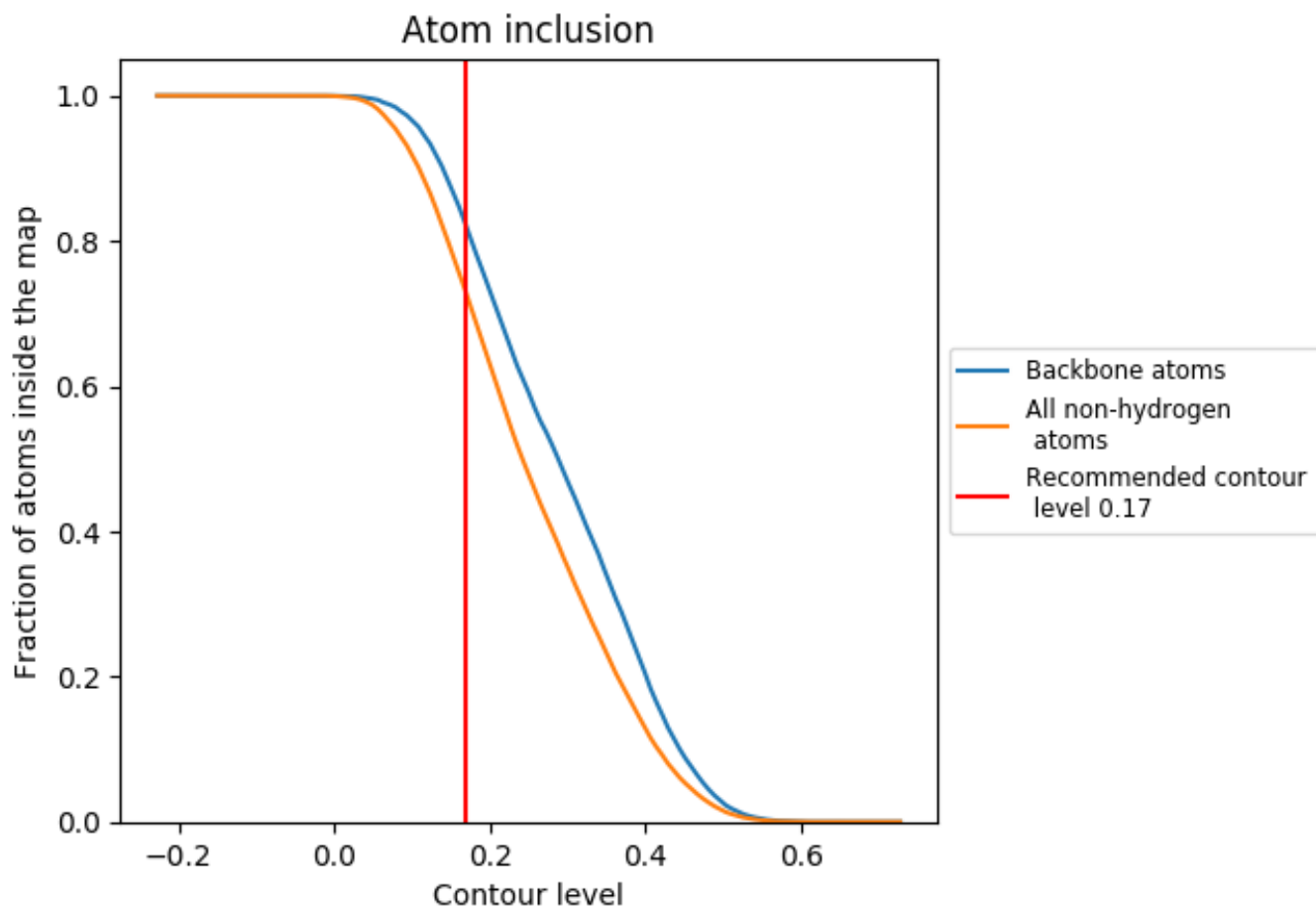
This section contains information regarding the fit between EMDB map EMD-11004 and PDB model 6YYS. Per-residue inclusion information can be found in section 3 on page 5.

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



The images above show the 3D surface view of the map at the recommended contour level 0.17 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 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.