



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 11:37 pm GMT

PDB ID : 6EQC  
EMDB ID : EMD-3821  
Title : Cryo-EM reconstruction of a complex of a binding protein and human adenovirus C5 hexon  
Authors : Schmid, M.; Ernst, P.; Honegger, A.; Suomalainen, M.; Zimmermann, M.; Braun, L.; Stauffer, S.; Thom, C.; Dreier, B.; Eibauer, M.; Kipar, A.; Vogel, V.; Greber, U.F.; Medalia, O.; Plueckthun, A.  
Deposited on : 2017-10-12  
Resolution : 7.40 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>.

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

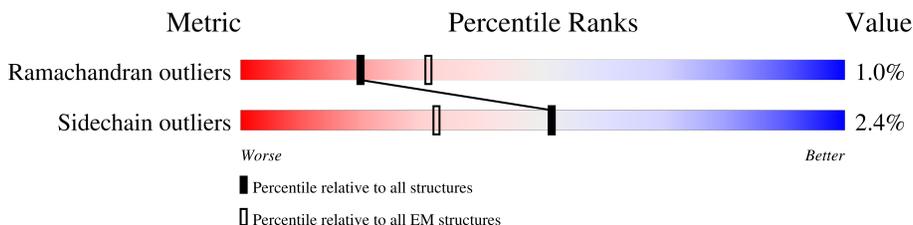
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 7.40 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	952	74% 20% . .
1	B	952	73% 21% . .
1	C	952	74% 19% . .
2	D	254	74% 14% . 8%
2	E	254	71% 19% . 8%
2	F	254	69% 21% . 8%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 53964 atoms, of which 26442 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 Hexon protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	921	14445	4686	7070	1250	1404	35	0	0
1	B	921	14445	4686	7070	1250	1404	35	0	0
1	C	921	14445	4686	7070	1250	1404	35	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	ALA	THR	conflict	UNP P04133
A	420	GLY	ILE	conflict	UNP P04133
A	422	ASN	THR	conflict	UNP P04133
A	423	SER	GLU	conflict	UNP P04133
A	425	TYR	LEU	conflict	UNP P04133
B	272	ALA	THR	conflict	UNP P04133
B	420	GLY	ILE	conflict	UNP P04133
B	422	ASN	THR	conflict	UNP P04133
B	423	SER	GLU	conflict	UNP P04133
B	425	TYR	LEU	conflict	UNP P04133
C	272	ALA	THR	conflict	UNP P04133
C	420	GLY	ILE	conflict	UNP P04133
C	422	ASN	THR	conflict	UNP P04133
C	423	SER	GLU	conflict	UNP P04133
C	425	TYR	LEU	conflict	UNP P04133

- Molecule 2 is a protein called scFv of 9C12 antibody.

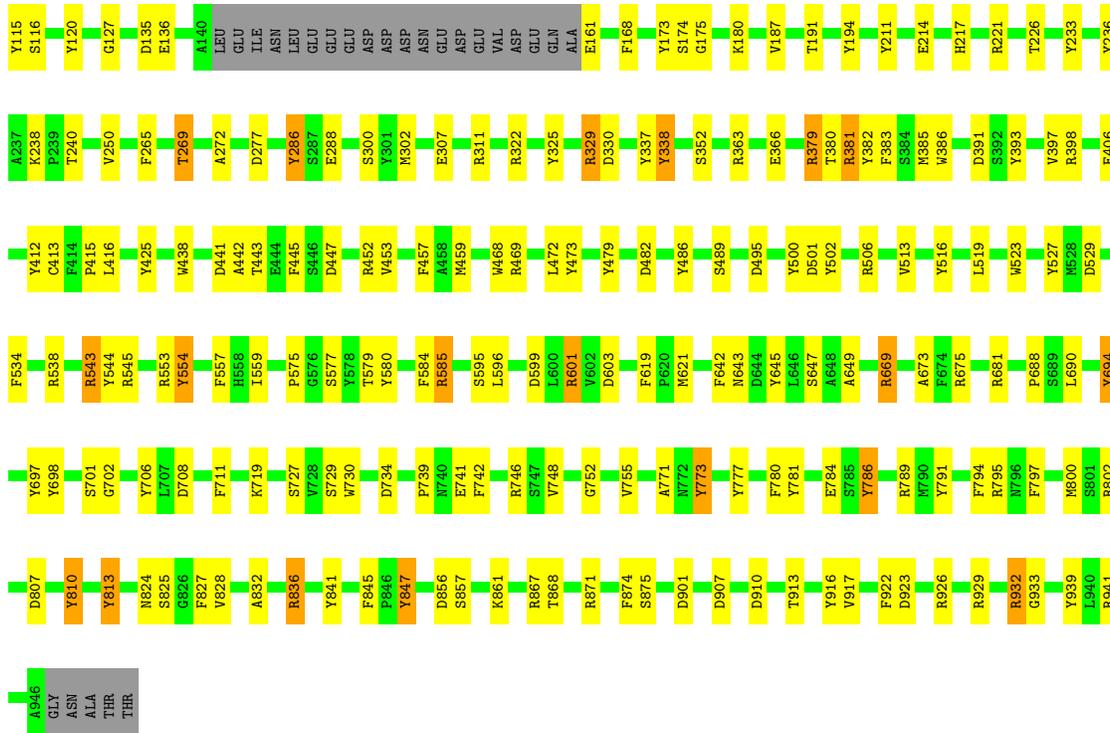
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	D	233	3543	1130	1744	306	356	7	0	0
2	E	233	3543	1130	1744	306	356	7	0	0

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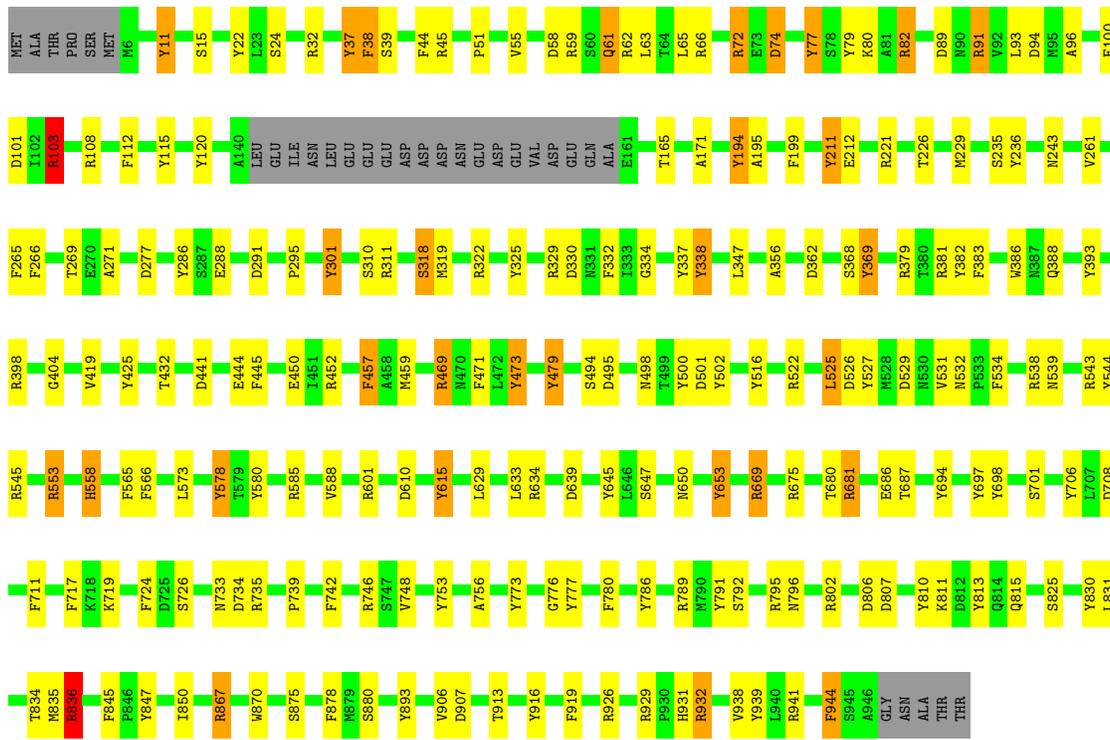
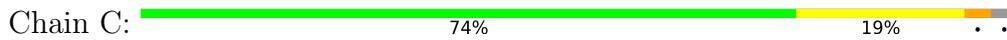
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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	F	233	3543	1130	1744	306	356	7	0	0

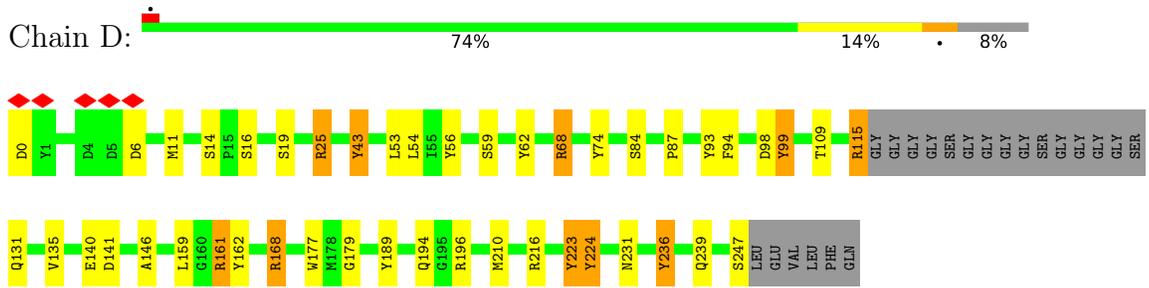




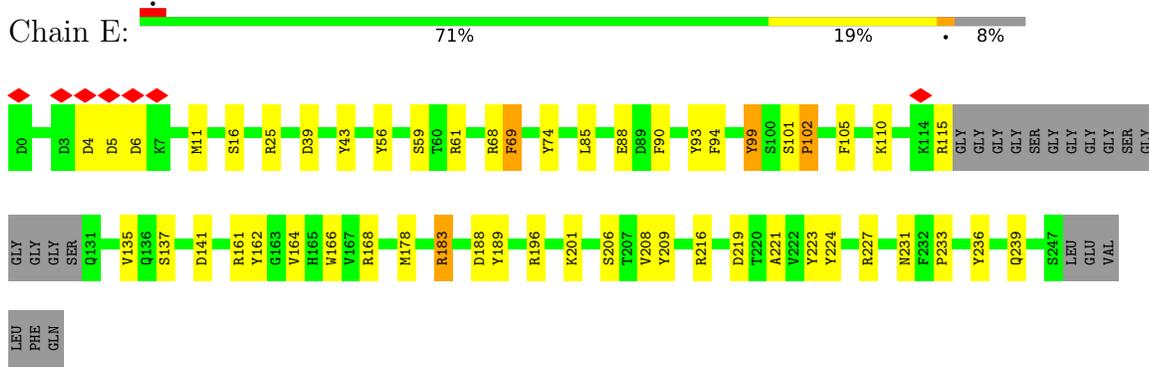
• Molecule 1: Hexon protein



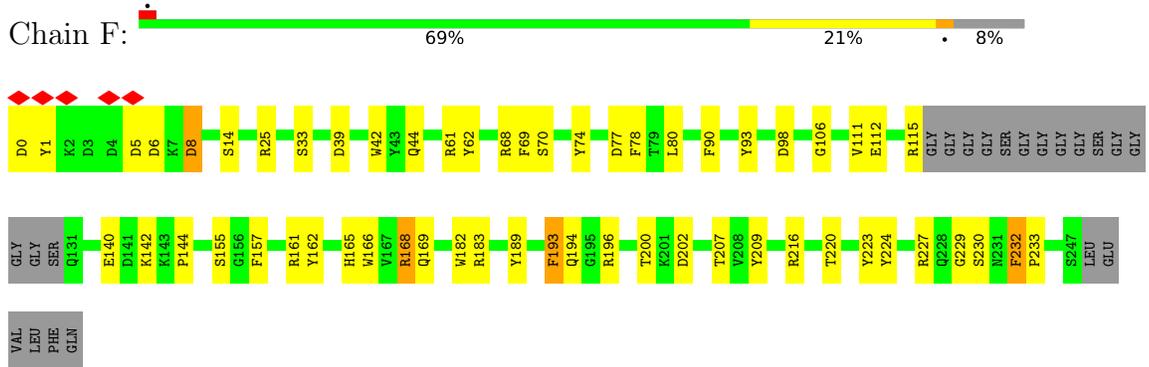
• Molecule 2: scFv of 9C12 antibody



• Molecule 2: scFv of 9C12 antibody



• Molecule 2: scFv of 9C12 antibody



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1880	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.0	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	0.080	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.014	Depositor
Map size ( $\text{\AA}$ )	1568.0, 1568.0, 1568.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.96, 1.96, 1.96	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	A	1.66	46/7574 (0.6%)	2.11	221/10299 (2.1%)
1	B	1.65	51/7574 (0.7%)	2.08	228/10299 (2.2%)
1	C	1.66	44/7574 (0.6%)	2.00	218/10299 (2.1%)
2	D	1.73	14/1839 (0.8%)	1.98	50/2490 (2.0%)
2	E	1.71	19/1839 (1.0%)	2.24	53/2490 (2.1%)
2	F	1.75	22/1839 (1.2%)	2.10	55/2490 (2.2%)
All	All	1.67	196/28239 (0.7%)	2.07	825/38367 (2.2%)

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	26
1	B	0	28
1	C	0	33
2	D	0	10
2	E	0	6
2	F	0	4
All	All	0	107

The worst 5 of 196 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	33	SER	CA-CB	8.58	1.65	1.52
1	A	186	GLY	CA-C	8.47	1.65	1.51
2	E	224	TYR	CB-CG	-8.27	1.39	1.51
1	B	21	GLU	CG-CD	7.95	1.63	1.51
1	C	653	TYR	CE2-CZ	7.74	1.48	1.38

The worst 5 of 825 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	ARG	NE-CZ-NH2	-27.23	106.68	120.30
2	E	196	ARG	NE-CZ-NH1	26.14	133.37	120.30
2	E	183	ARG	NE-CZ-NH2	-25.28	107.66	120.30
1	B	746	ARG	NE-CZ-NH1	23.92	132.26	120.30
2	F	168	ARG	NE-CZ-NH2	-23.38	108.61	120.30

There are no chirality outliers.

5 of 107 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	TYR	Sidechain
1	A	233	TYR	Sidechain
1	A	62	ARG	Sidechain
1	A	79	TYR	Sidechain
1	A	91	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	7375	7070	7068	0	0
1	B	7375	7070	7068	0	0
1	C	7375	7070	7068	0	0
2	D	1799	1744	1743	0	0
2	E	1799	1744	1743	0	0
2	F	1799	1744	1743	0	0
All	All	27522	26442	26433	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	917/952 (96%)	866 (94%)	43 (5%)	8 (1%)	17	57
1	B	917/952 (96%)	863 (94%)	47 (5%)	7 (1%)	19	60
1	C	917/952 (96%)	853 (93%)	51 (6%)	13 (1%)	11	46
2	D	229/254 (90%)	213 (93%)	15 (7%)	1 (0%)	34	72
2	E	229/254 (90%)	207 (90%)	18 (8%)	4 (2%)	9	42
2	F	229/254 (90%)	211 (92%)	16 (7%)	2 (1%)	17	57
All	All	3438/3618 (95%)	3213 (94%)	190 (6%)	35 (1%)	20	54

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	295	PRO
1	C	539	ASN
2	E	231	ASN
1	C	61	GLN
1	C	734	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	800/827 (97%)	780 (98%)	20 (2%)	47	68
1	B	800/827 (97%)	775 (97%)	25 (3%)	40	62
1	C	800/827 (97%)	778 (97%)	22 (3%)	43	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	197/206 (96%)	196 (100%)	1 (0%)	88	93
2	E	197/206 (96%)	195 (99%)	2 (1%)	76	86
2	F	197/206 (96%)	194 (98%)	3 (2%)	65	80
All	All	2991/3099 (96%)	2918 (98%)	73 (2%)	51	69

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	650	ASN
2	F	144	PRO
1	C	719	LYS
1	C	906	VAL
1	B	180	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

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

There are no chain breaks in this entry.

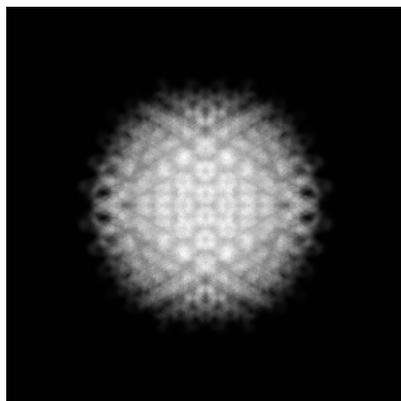
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3821. These allow visual inspection of the internal detail of the map and identification of artifacts.

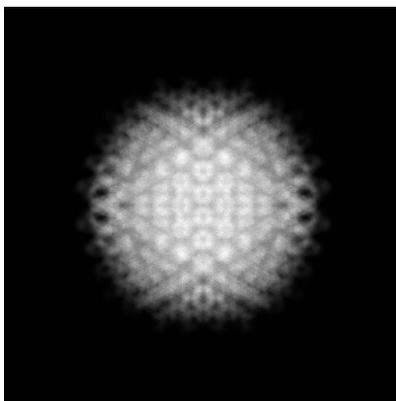
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

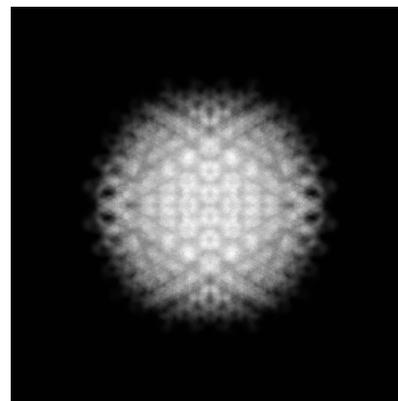
#### 6.1.1 Primary map



X

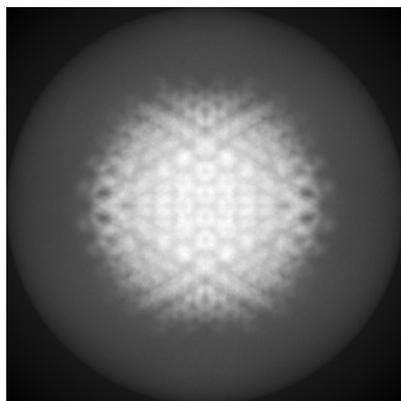


Y

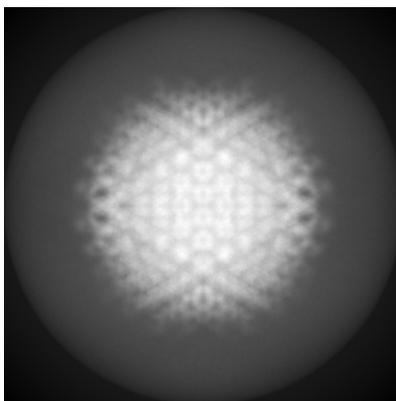


Z

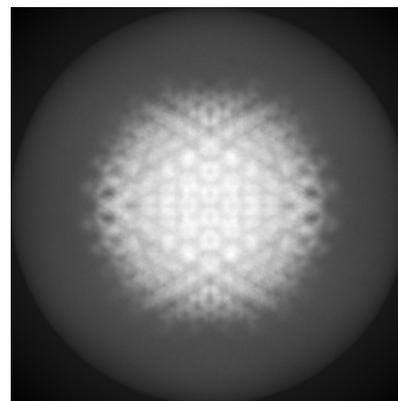
#### 6.1.2 Raw map



X



Y

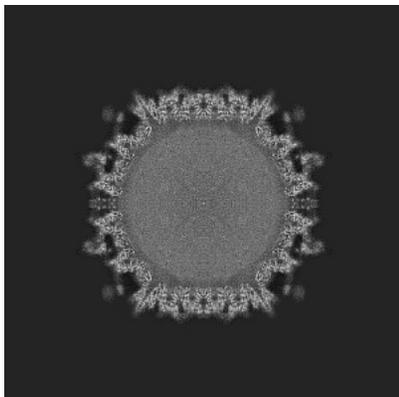


Z

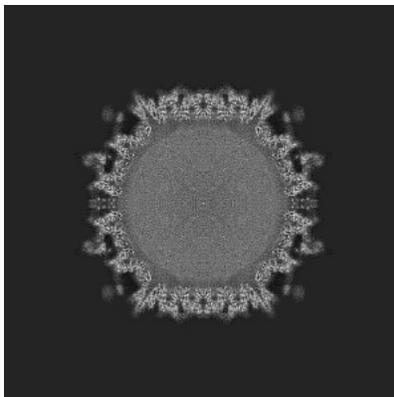
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

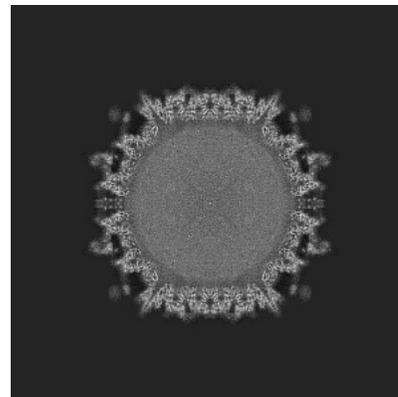
### 6.2.1 Primary map



X Index: 400

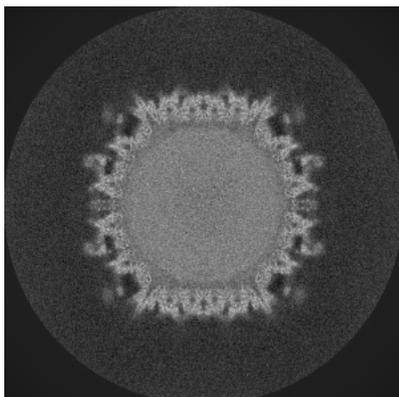


Y Index: 400

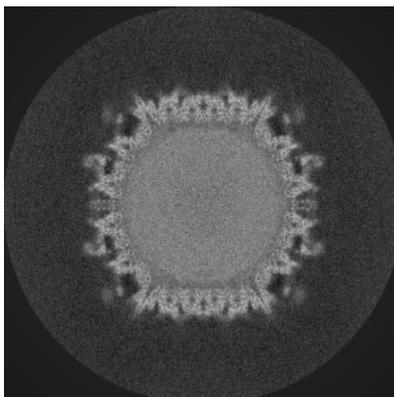


Z Index: 400

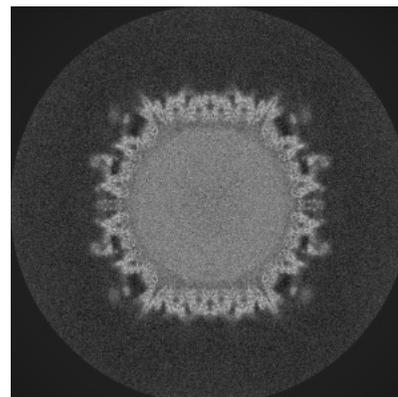
### 6.2.2 Raw map



X Index: 400



Y Index: 400

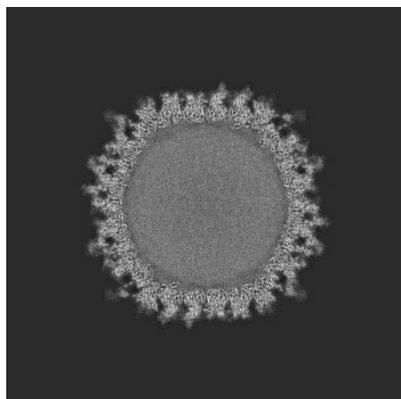


Z Index: 400

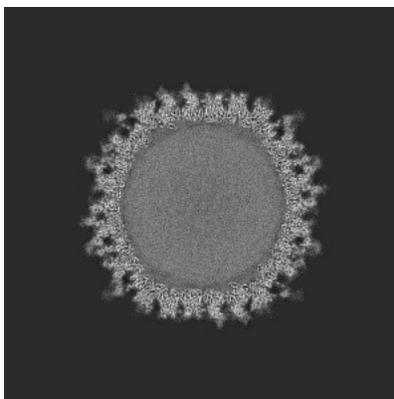
The images above show central slices of the map in three orthogonal directions.

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

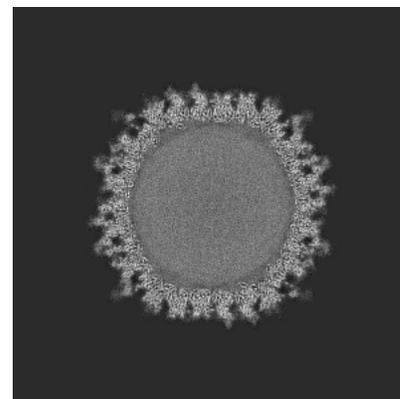
### 6.3.1 Primary map



X Index: 391

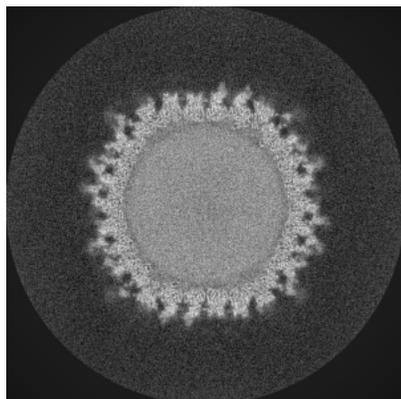


Y Index: 409

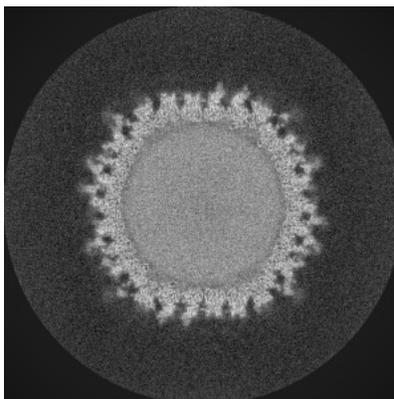


Z Index: 409

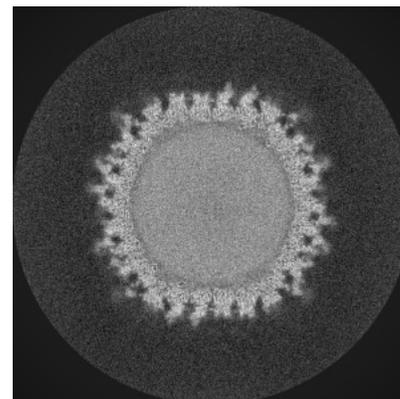
### 6.3.2 Raw map



X Index: 390



Y Index: 390

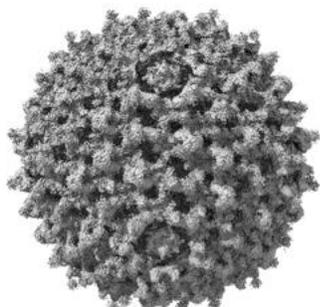


Z Index: 390

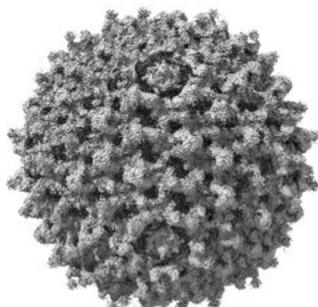
The images above show the largest variance slices of the map in three orthogonal directions.

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

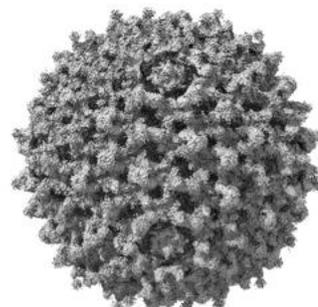
### 6.4.1 Primary map



X



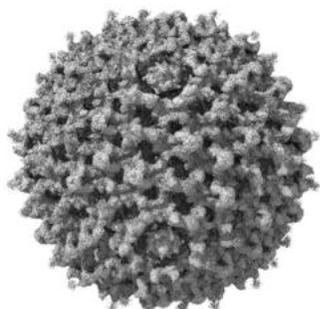
Y



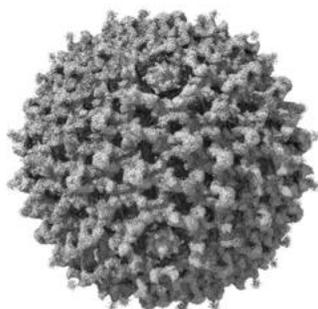
Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

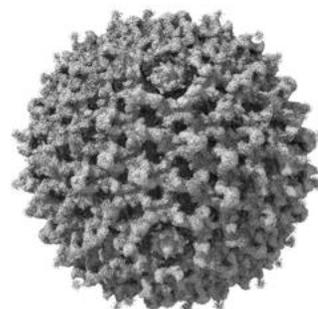
### 6.4.2 Raw map



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.

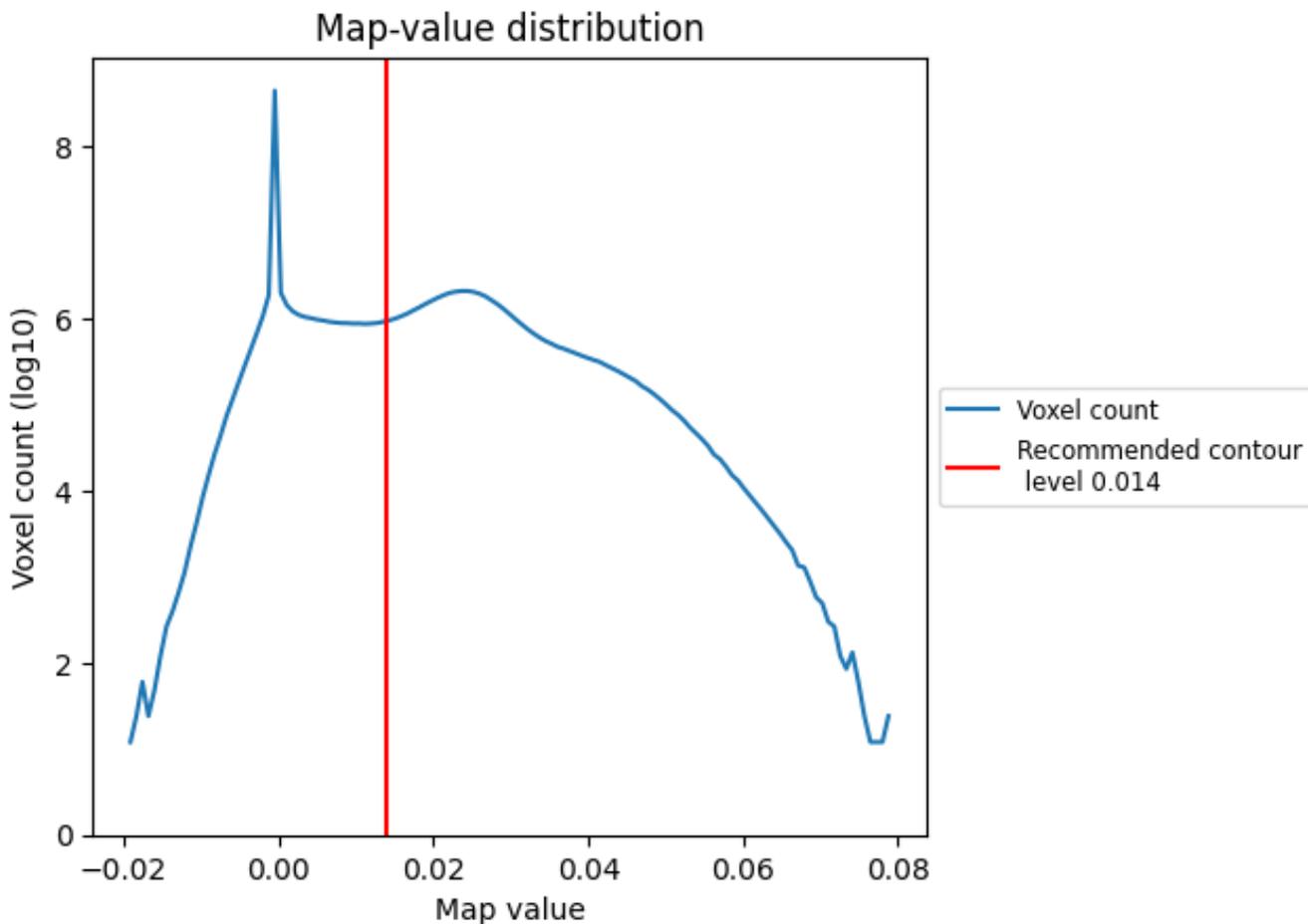
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

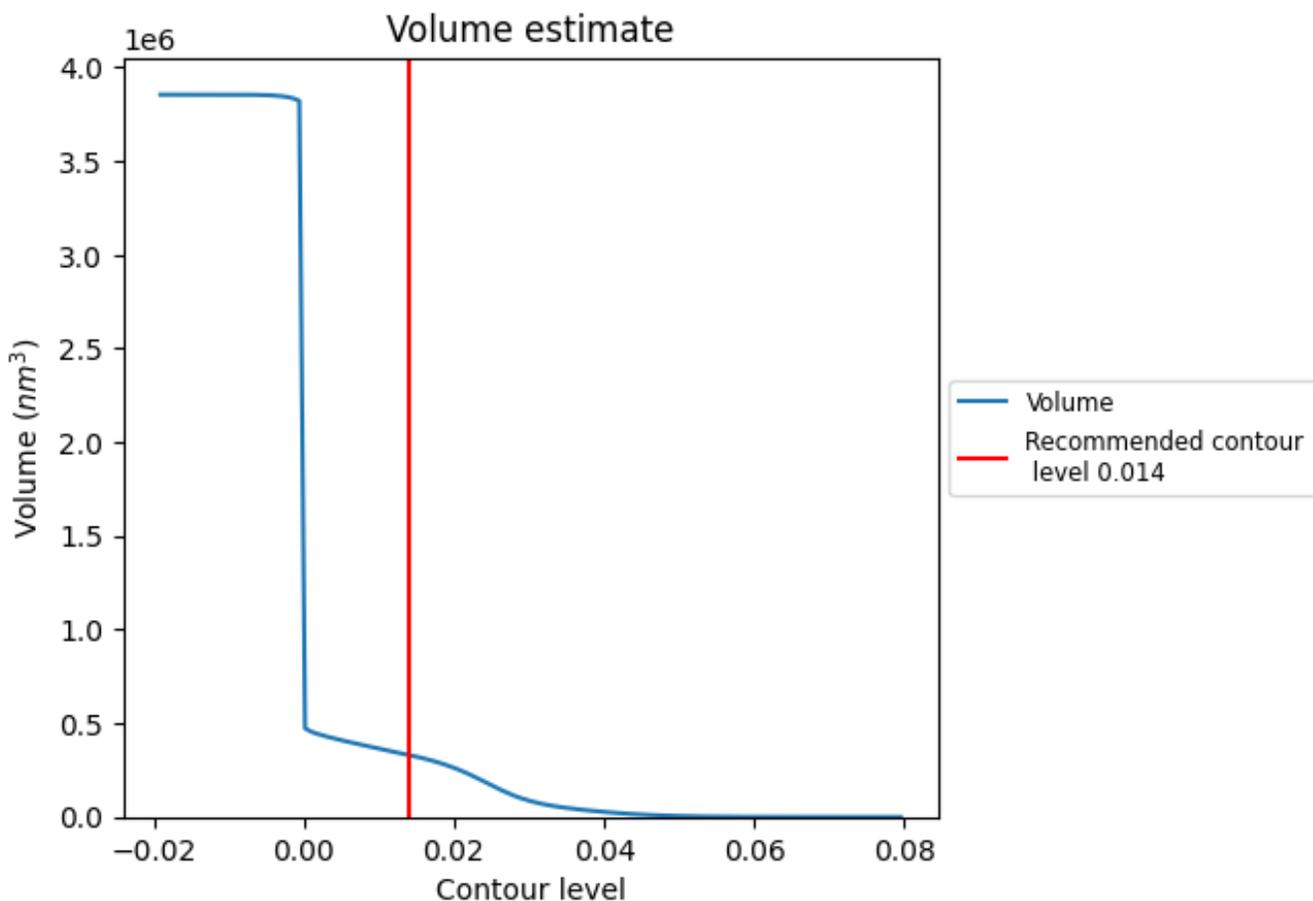
This section contains the results of statistical analysis of the map.

### 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.

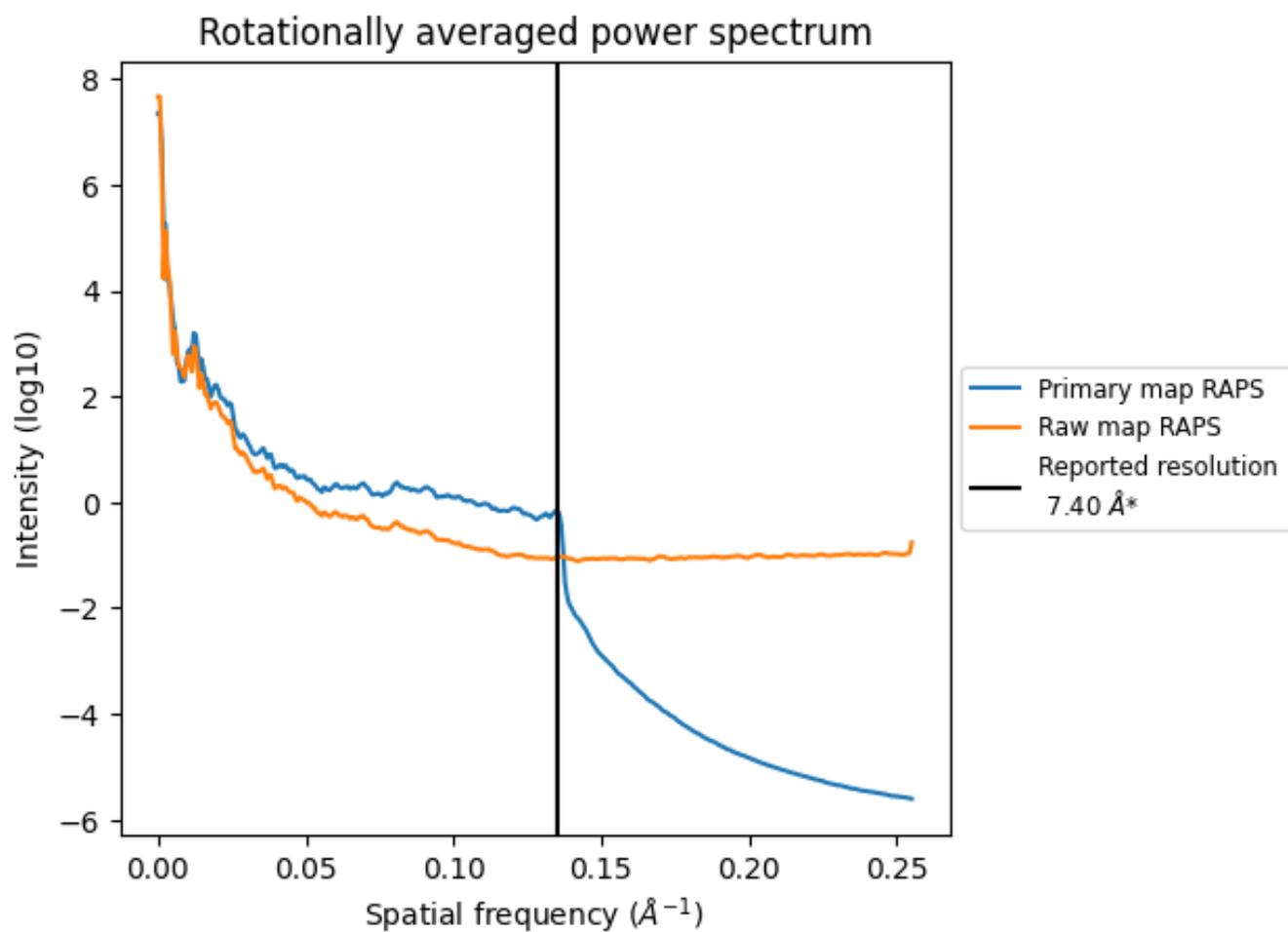
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 330949 nm<sup>3</sup>; this corresponds to an approximate mass of 298955 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

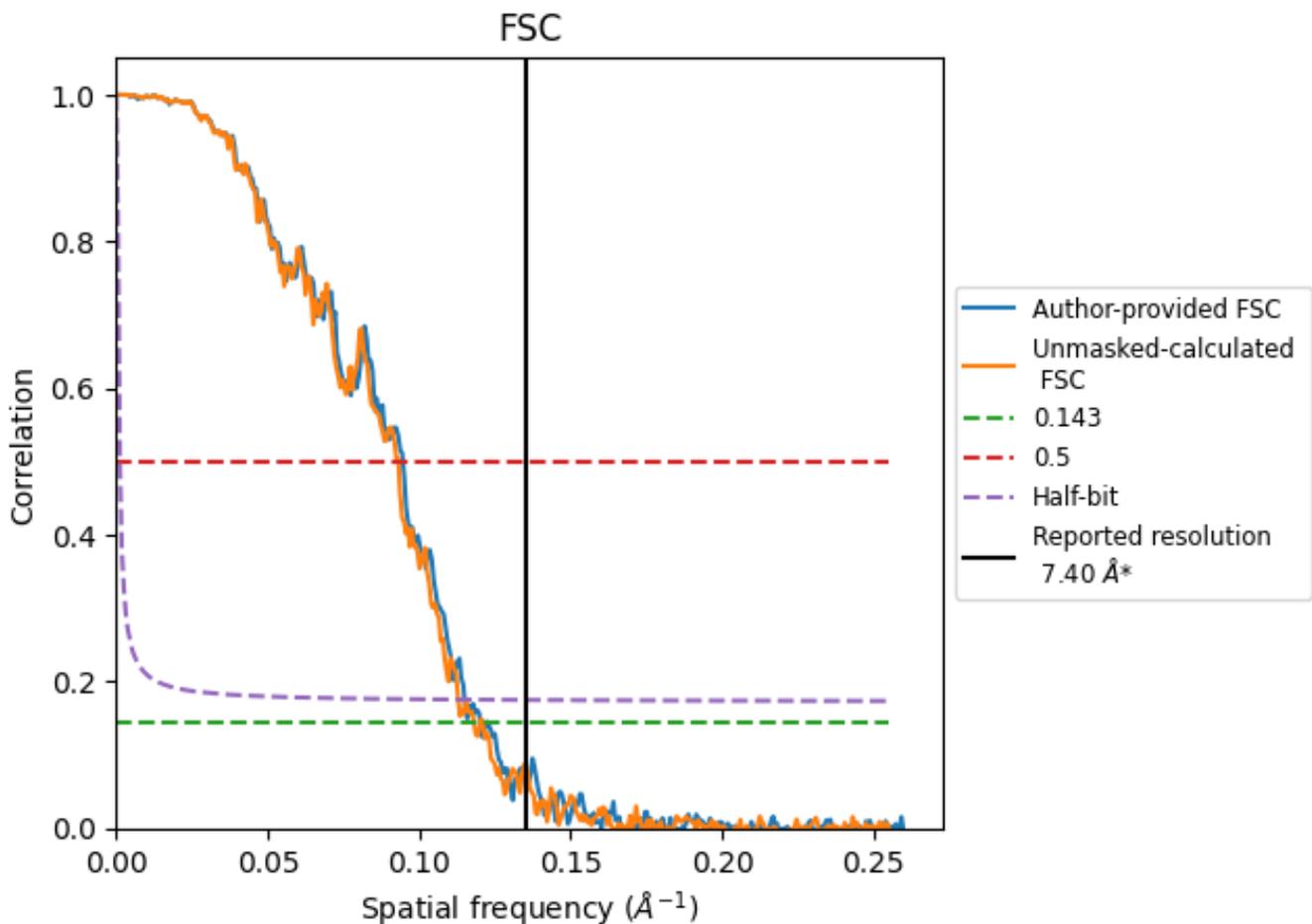


\*Reported resolution corresponds to spatial frequency of 0.135 Å<sup>-1</sup>

## 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 0.135 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	7.40	-	-
Author-provided FSC curve	8.32	10.57	8.70
Unmasked-calculated*	8.47	10.73	8.86

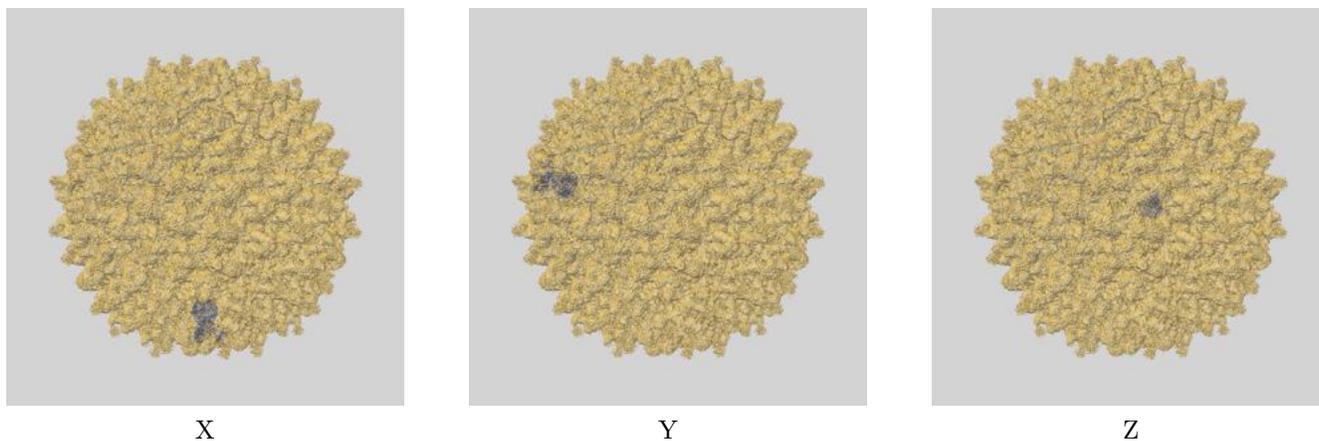
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.32 differs from the reported value 7.4 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.47 differs from the reported value 7.4 by more than 10 %

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

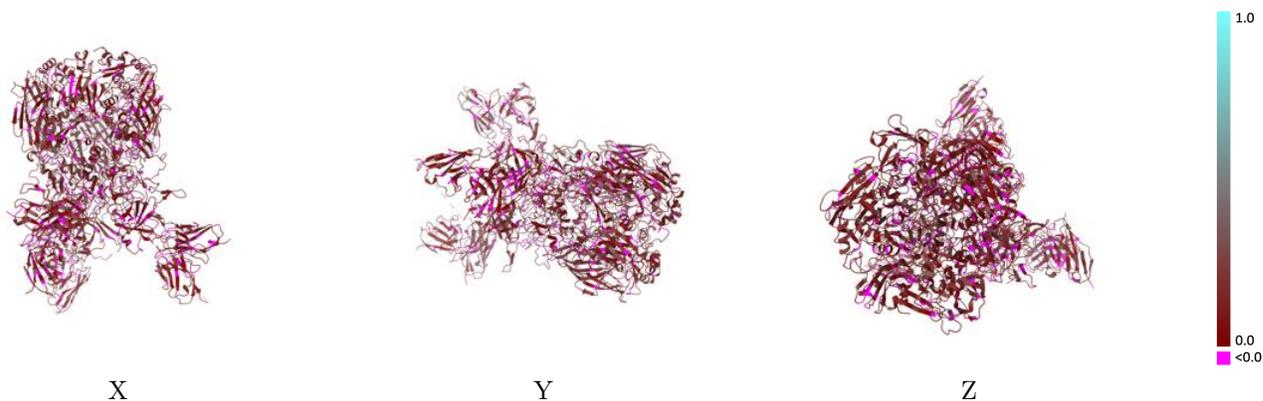
This section contains information regarding the fit between EMDB map EMD-3821 and PDB model 6EQC. Per-residue inclusion information can be found in section 3 on page 5.

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



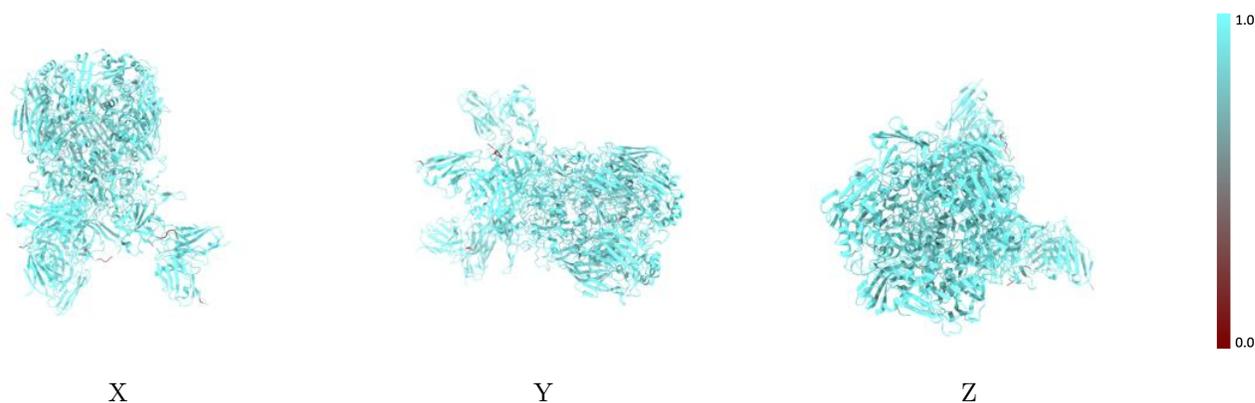
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



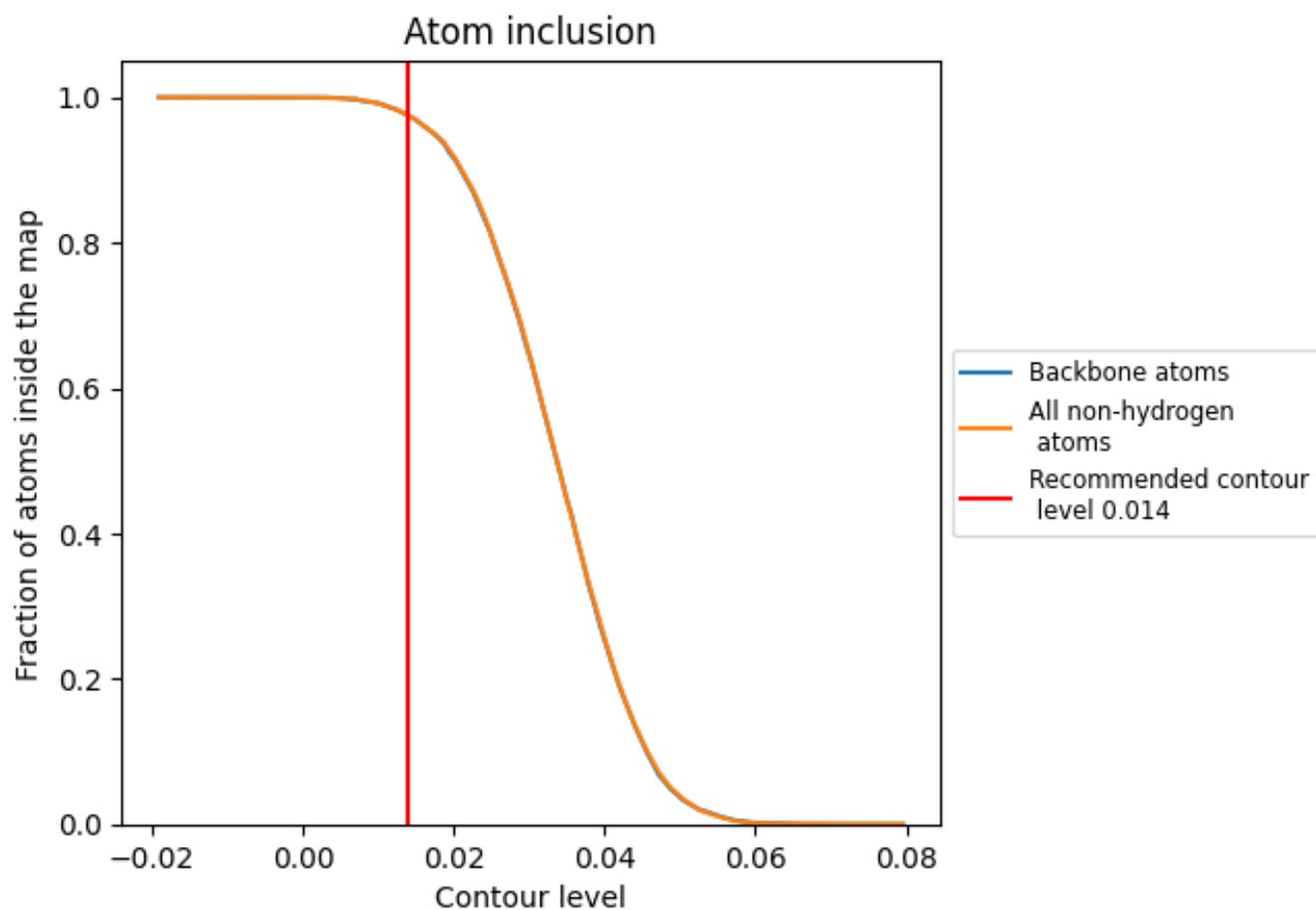
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 98% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9751	 0.1270
A	 0.9817	 0.1340
B	 0.9776	 0.1310
C	 0.9781	 0.1240
D	 0.9671	 0.1200
E	 0.9500	 0.1120
F	 0.9676	 0.1250

