



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 07:21 am GMT

PDB ID : 8QK3
EMDB ID : EMD-18455
Title : Human Adenovirus type 11 fiber knob in complex with its cell receptors, Desmoglein-2 and CD46
Authors : Effantin, G.
Deposited on : 2023-09-14
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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) : 2.39

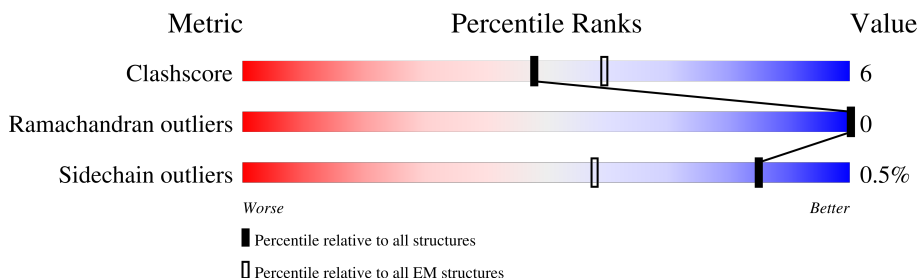
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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 ≥ 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	325	
1	B	325	
1	C	325	
2	E	392	
3	D	1118	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7535 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 Fiber protein.

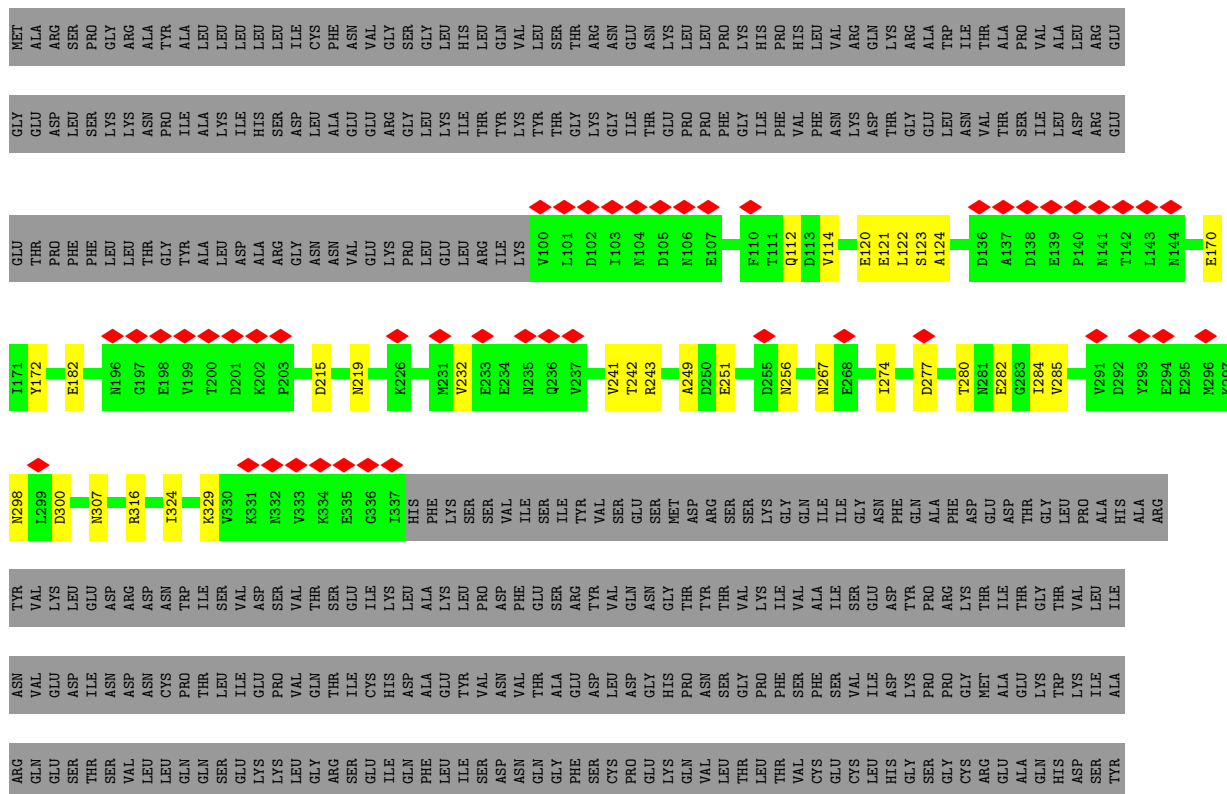
Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	197	Total	C	N	O	S	0	0
			1548	971	258	310	9		
1	A	197	Total	C	N	O	S	0	0
			1548	971	258	310	9		
1	C	197	Total	C	N	O	S	0	0
			1548	971	258	310	9		

- Molecule 2 is a protein called Membrane cofactor protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	126	Total	C	N	O	S	0	0
			1018	659	160	189	10		

- Molecule 3 is a protein called Desmoglein-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	238	Total	C	N	O	S	0	0
			1873	1182	307	381	3		



PHE	GLY	TYR	THR	ASN	GLU	ARG	VAL	VAL
	GLY	PRO	GLU	GLY	ASN	ALA	VAL	GLY
GLY	GLN	ALA	GLU	LYS	HIS	THR	VAL	VAL
GLU	PRO	ALA	SER	ILE	THR	GLN	SER	SER
SER	LEU	THR	SER	GLN	LYS	THR	LEU	ALA
GLY	ALA	LEU	SER	ARG	ASP	GLY	PRO	ALA
HIS	MET	VAL	ARG	GLN	CYS	ALA	VAL	ILE
SER	ASN	ASP	GLN	LYS	LEU	THR	ASP	ALA
ASN	PRO	GLN	ALA	PRO	LEU	GLY	ASN	LEU
SER	ILE	PRO	GLN	ALA	VAL	ALA	GLY	MET
THR	ALA	TYR	LYS	THR	TYR	ILE	GLY	ILE
ILE	VAL	ALA	VAL	GLU	SER	MET	SER	LEU
THR	GLY	ASN	ALA	THR	GLN	THR	VAL	ALA
THR	GLN	GLY	THR	SER	GLU	THR	VAL	LEU
SER	ASN	GLY	PRO	MET	ASN	GLU	GLY	GLY
SER	VAL	THR	LEU	ASN	THR	THR	ARG	LEU
THR	THR	VAL	PRO	THR	GLU	THR	ASN	LEU
ARG	VAL	VAL	ASP	ALA	SER	LYS	ASN	LEU
VAL	VAL	VAL	PRO	SER	LEU	THR	GLY	LEU
THR	GLU	THR	MET	HIS	ASN	ALA	GLY	VAL
LYS	ARG	GLU	ALA	SER	ALA	ARG	GLY	PRO
HIS	VAL	ARG	SER	LEU	SER	ALA	MET	LEU
SER	LEU	VAL	ARG	CYS	ILE	THR	ALA	LEU
THR	ALA	ILE	ASN	GLU	GLY	GLY	LYS	LEU
VAL	PRO	GLN	VAL	GLN	CYS	ALA	GLU	LEU
GLN	ALA	PRO	ILE	THR	CYS	SER	ALA	MET
HIS	SER	HIS	ALA	MET	SER	ARG	THR	CYS
SER	THR	GLY	THR	VAL	PHE	ASP	MET	HIS
TYR	LEU	GLY	GLU	ASN	ILE	MET	LYS	CYS
SER	GLN	GLY	THR	SER	GLY	ALA	GLY	GLY
SER	ASN	SER	SER	GLU	GLU	ALA	SER	LYS
	TYR	ASN	TYR	ASN	GLU	ALA	SER	ALA
	GLN	LEU	THR	TYR	ASP	ALA	ALA	LYS
	ILE	GLY	GLY	SER	ASP	ALA	SER	GLY
	PRO	GLY	SER	SER	ARG	ALA	PHE	PHE
	THR	THR	THR	GLY	PHE	VAL	VAL	THR
	GLU	GLN	MET	SER	LEU	ALA	LYS	PRO
	ASN	HIS	PRO	SER	ASP	LEU	GLY	ILE
	ASN	LEU	PRO	PHE	ASP	ASN	GLN	PRO
	MET	GLN	THR	PRO	LEU	GLU	HIS	GLY
	THR	ASP	THR	VAL	GLY	GLU	THR	THR
	ALA	VAL	THR	PRO	LEU	PHE	MET	ILE
	ARG	PRO	ILE	LYS	LYS	LEU	GLU	ILE
	ASN	TYR	LEU	SER	PHE	ARG	GLU	MET
	ASN	VAL	GLY	LEU	LYS	ASN	MET	LEU
	THR	MET	PRO	GLN	THR	TYR	ASP	HIS
	VAL	VAL	SER	GLU	LEU	PHE	PRO	LEU
	SER	ARG	GLN	ALA	THR	THR	GLY	TRP
	GLY	GLU	GLU	ASN	GLU	ASP	TRP	ASN
	ALA	ARG	GLN	ALA	VAL	LYS	GLU	ASN
	GLY	GLU	SER	GLU	CYS	ALA	GLU	GLY
	VAL	SER	LEU	LYS	LEU	ALA	HIS	GLY
	PRO	PHE	ILE	VAL	GLY	THR	ARG	ALA
	PRO	LEU	THR	THR	GLN	TYR	SER	PRO
	LEU	ALA	THR	GLN	ILE	GLU	LEU	PRO
	PRO	PRO	GLU	GLU	ILE	THR	GLU	GLY
	ASP	SER	ARG	ILE	ASP	ASP	SER	LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	180510	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	210.0, 210.0, 210.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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	0.27	0/1581	0.52	0/2156
1	B	0.28	0/1581	0.50	0/2156
1	C	0.27	0/1581	0.50	0/2156
2	E	0.29	0/1052	0.48	0/1432
3	D	0.26	0/1905	0.48	0/2591
All	All	0.27	0/7700	0.50	0/10491

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	1548	0	1487	22	0
1	B	1548	0	1487	19	0
1	C	1548	0	1487	20	0
2	E	1018	0	966	15	0
3	D	1873	0	1843	20	0
All	All	7535	0	7270	84	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 6.

The worst 5 of 84 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)
2:E:65:CYS:SG	2:E:107:CYS:SG	1.38	1.37
2:E:65:CYS:CB	2:E:107:CYS:SG	2.44	1.06
3:D:170:GLU:OE1	3:D:172:TYR:OH	1.91	0.87
3:D:120:GLU:O	3:D:123:SER:OG	1.93	0.86
1:A:233:LYS:NZ	1:A:288:TYR:OH	2.14	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	
1	A	195/325 (60%)	192 (98%)	3 (2%)	0	100	100
1	B	195/325 (60%)	184 (94%)	11 (6%)	0	100	100
1	C	195/325 (60%)	186 (95%)	9 (5%)	0	100	100
2	E	124/392 (32%)	123 (99%)	1 (1%)	0	100	100
3	D	236/1118 (21%)	231 (98%)	5 (2%)	0	100	100
All	All	945/2485 (38%)	916 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	175/285 (61%)	173 (99%)	2 (1%)	70	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	175/285 (61%)	174 (99%)	1 (1%)	84	92
1	C	175/285 (61%)	174 (99%)	1 (1%)	84	92
2	E	110/346 (32%)	110 (100%)	0	100	100
3	D	213/966 (22%)	213 (100%)	0	100	100
All	All	848/2167 (39%)	844 (100%)	4 (0%)	85	93

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

Mol	Chain	Res	Type
1	B	135	TRP
1	A	135	TRP
1	A	182	PHE
1	C	135	TRP

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 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

There are no chain breaks in this entry.

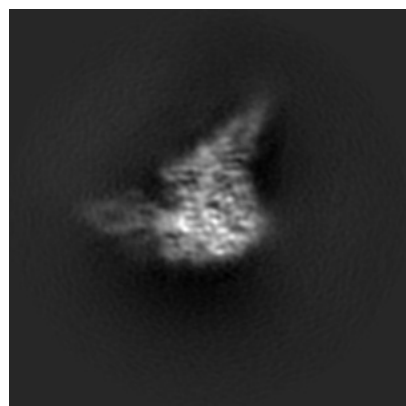
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18455. These allow visual inspection of the internal detail of the map and identification of artifacts.

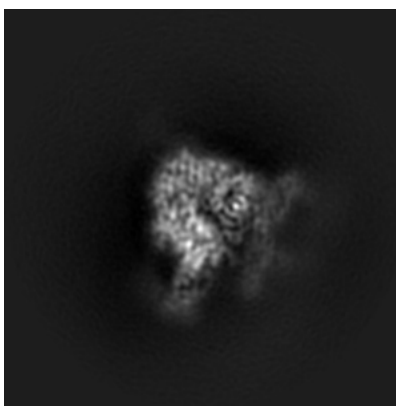
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

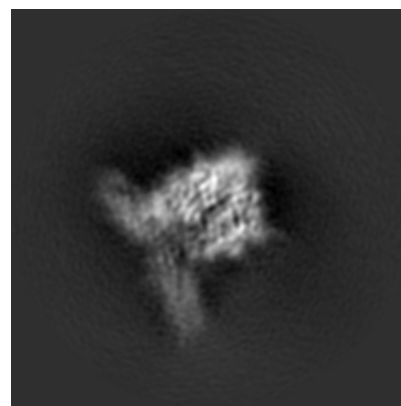
6.1.1 Primary map



X

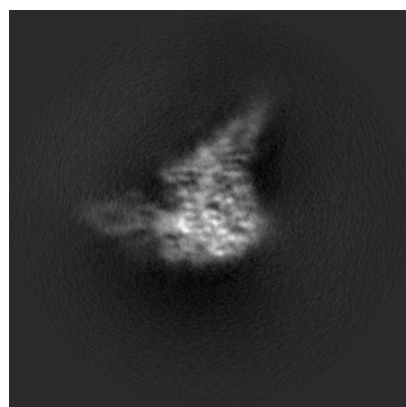


Y

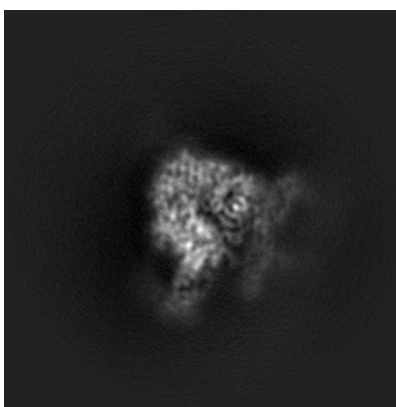


Z

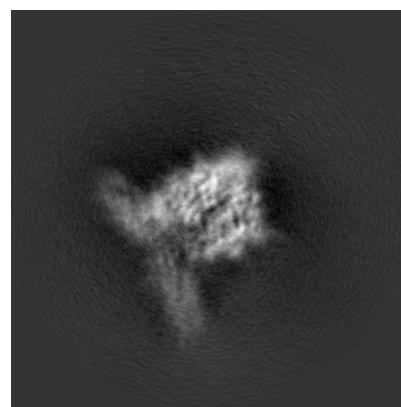
6.1.2 Raw map



X



Y

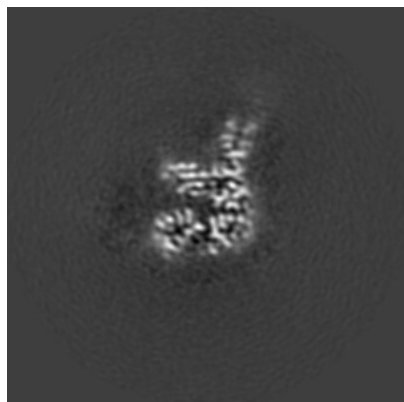


Z

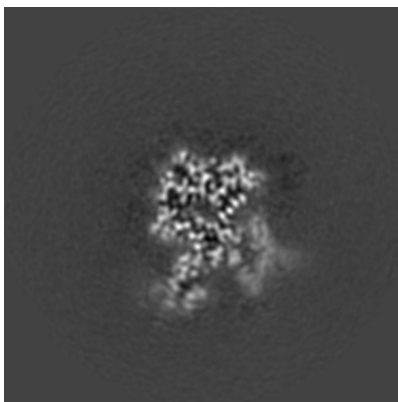
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

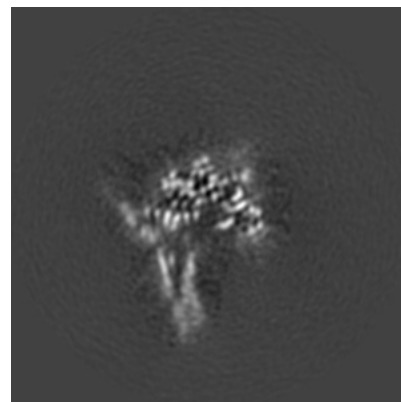
6.2.1 Primary map



X Index: 125

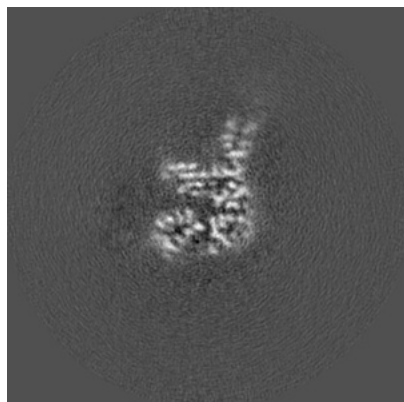


Y Index: 125

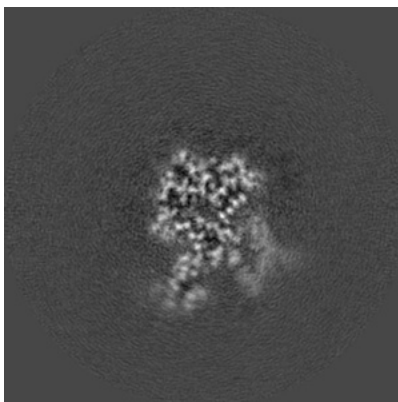


Z Index: 125

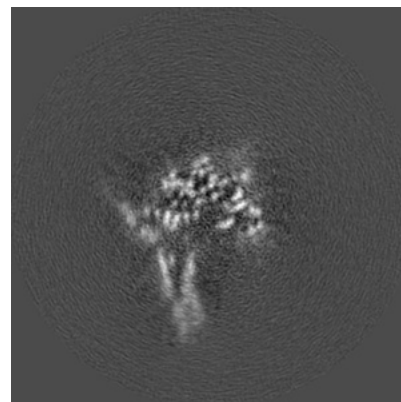
6.2.2 Raw map



X Index: 125



Y Index: 125

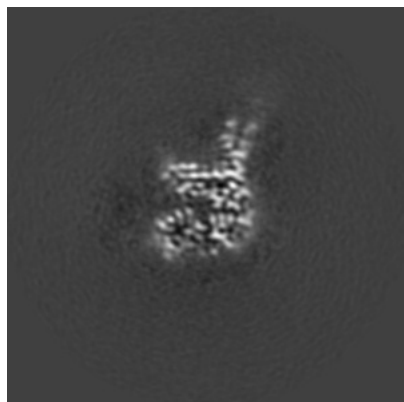


Z Index: 125

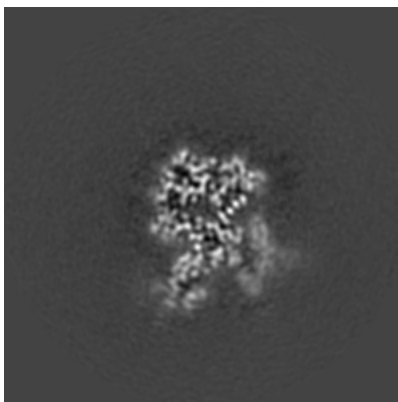
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

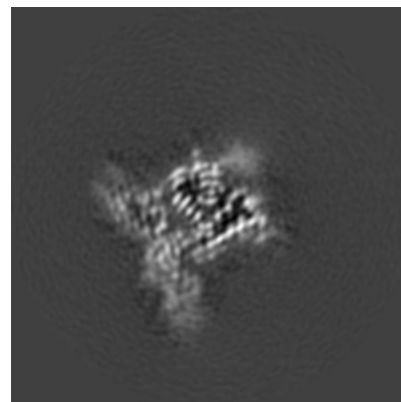
6.3.1 Primary map



X Index: 126

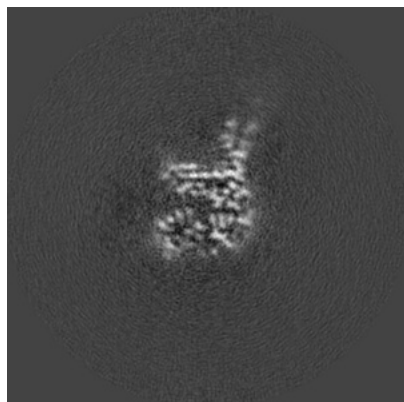


Y Index: 124

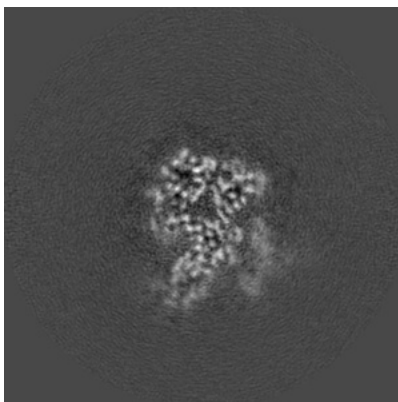


Z Index: 116

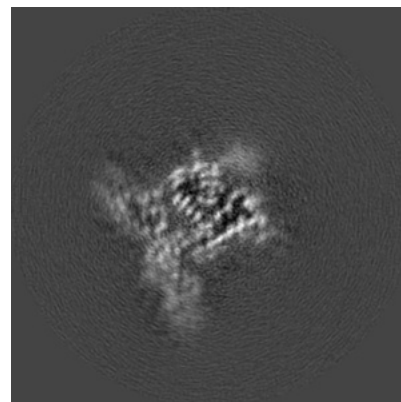
6.3.2 Raw map



X Index: 126



Y Index: 122



Z Index: 116

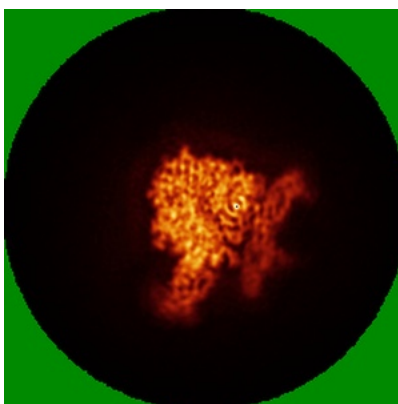
The images above show the largest variance slices of the map in three orthogonal directions.

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

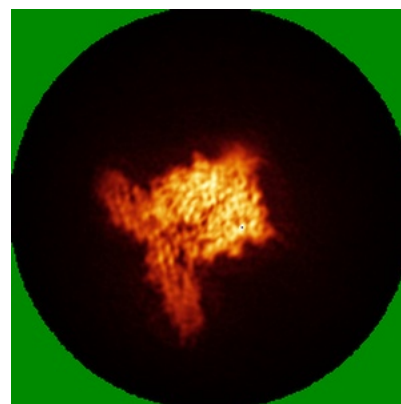
6.4.1 Primary map



X



Y

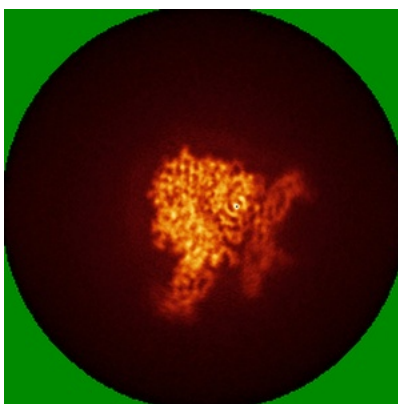


Z

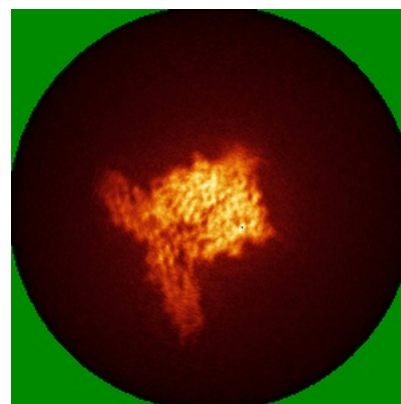
6.4.2 Raw map



X



Y

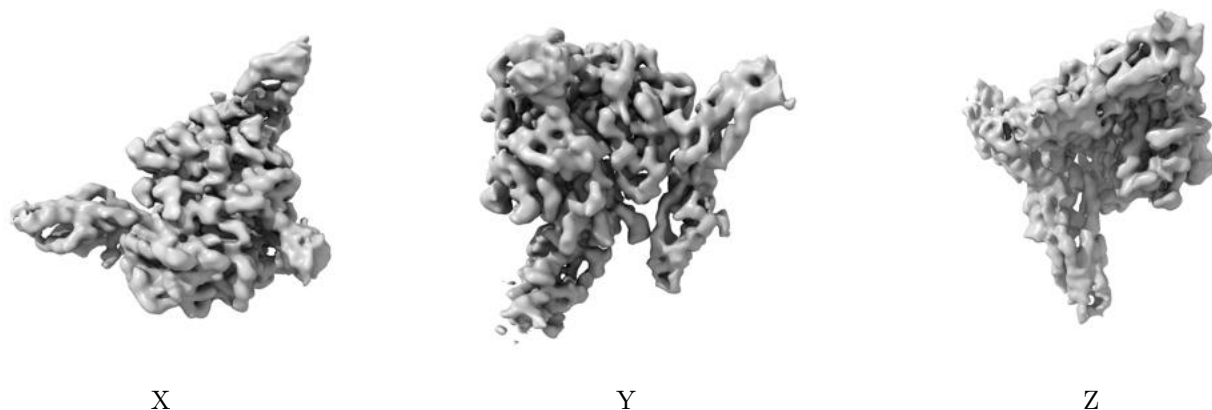


Z

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

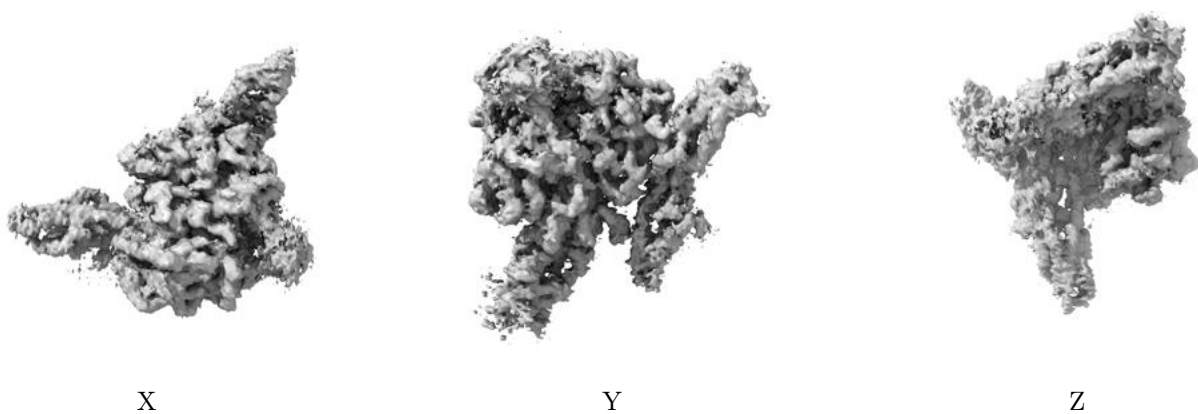
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

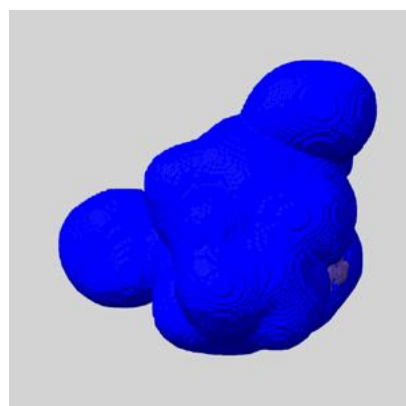
6.6 Mask visualisation [i](#)

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

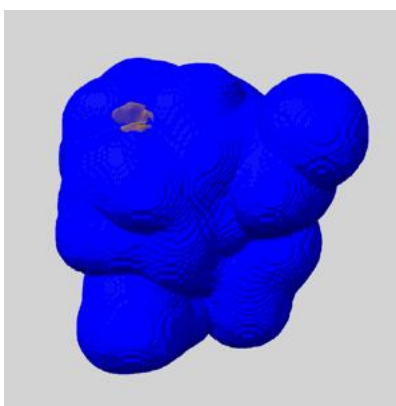
A mask typically either:

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

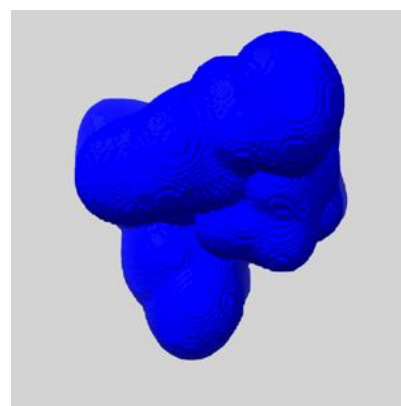
6.6.1 emd_18455_msk_1.map [i](#)



X



Y

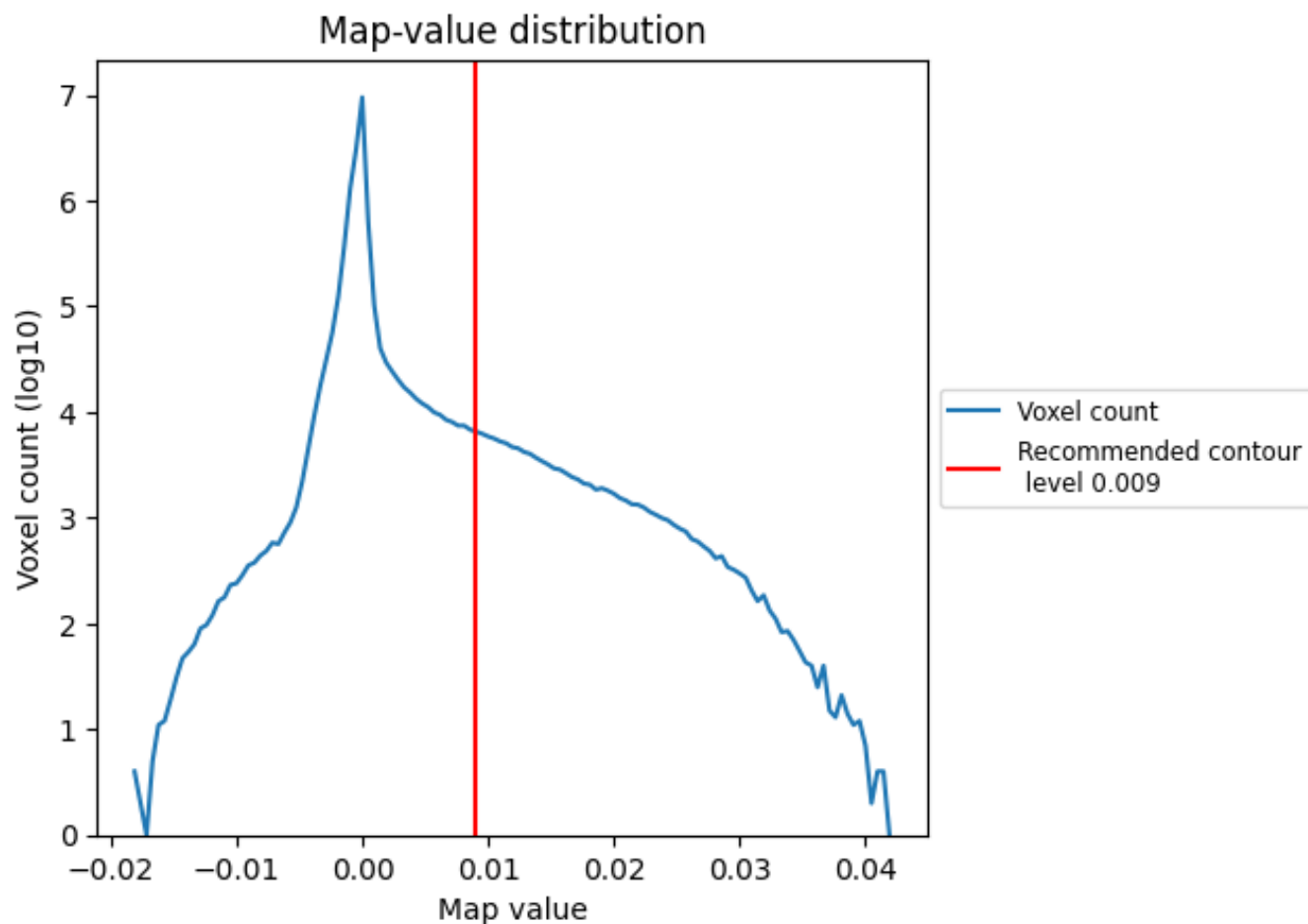


Z

7 Map analysis [i](#)

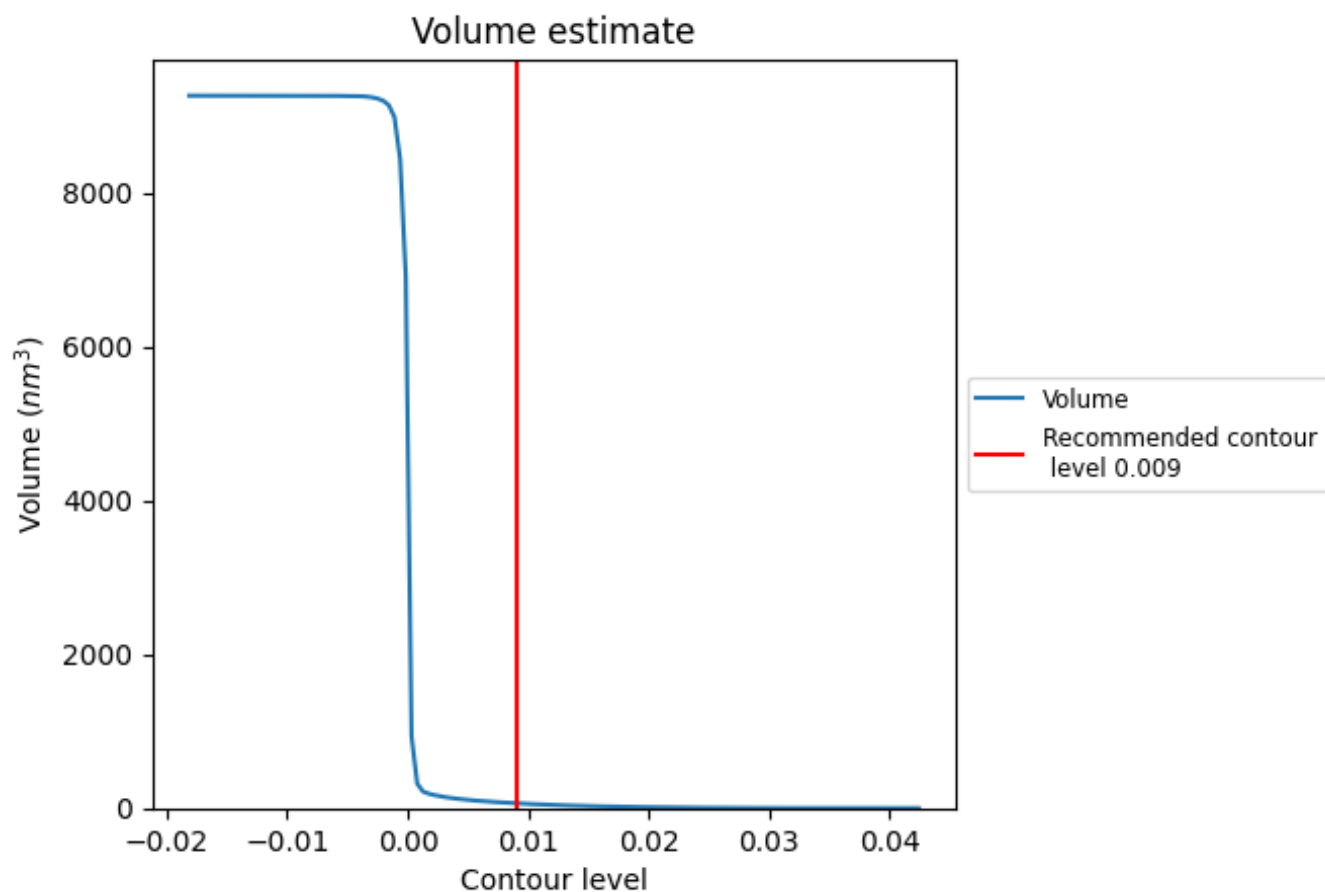
This section contains the results of statistical analysis of the map.

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.

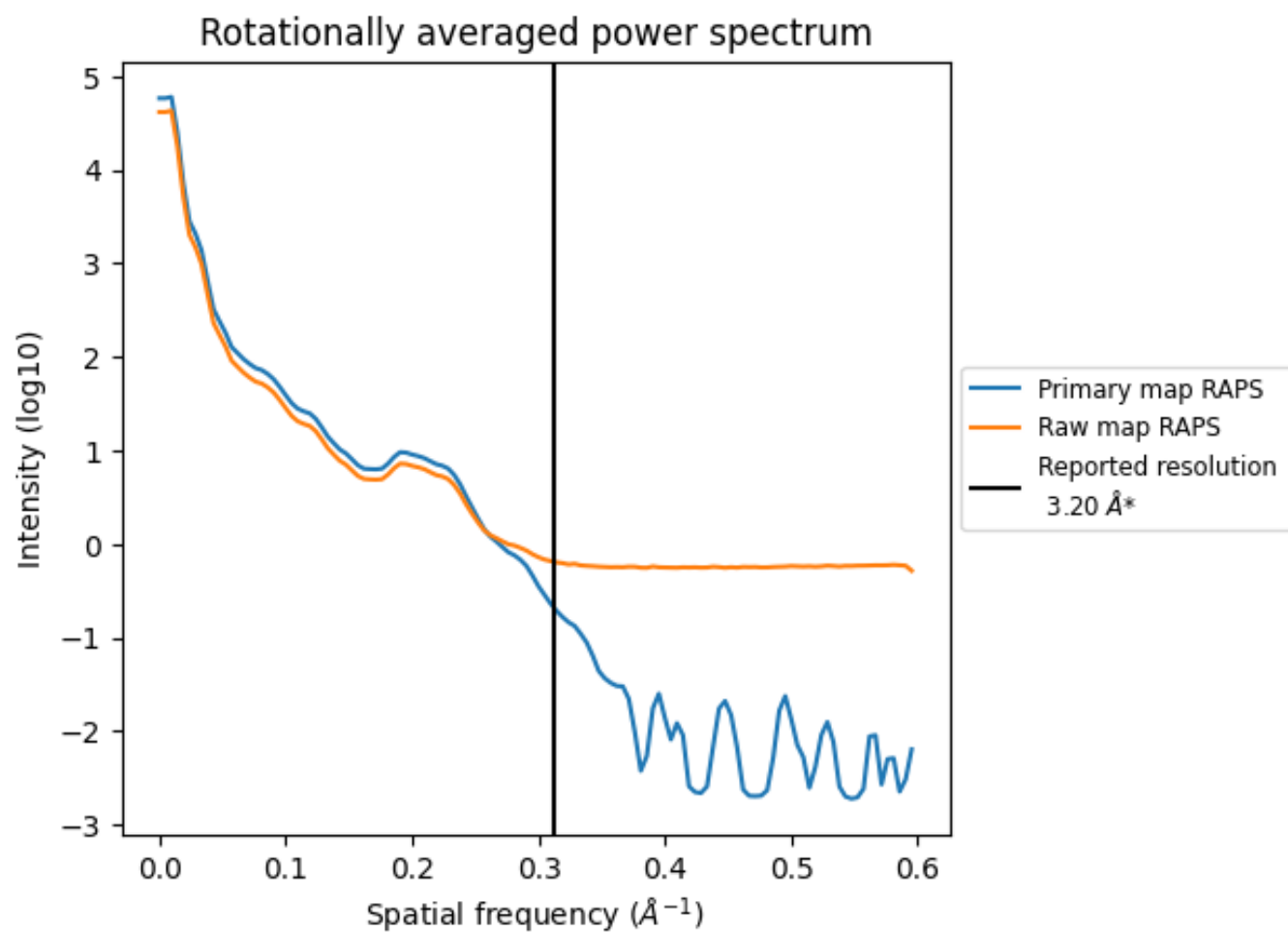
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 63 nm³; this corresponds to an approximate mass of 57 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 ⓘ

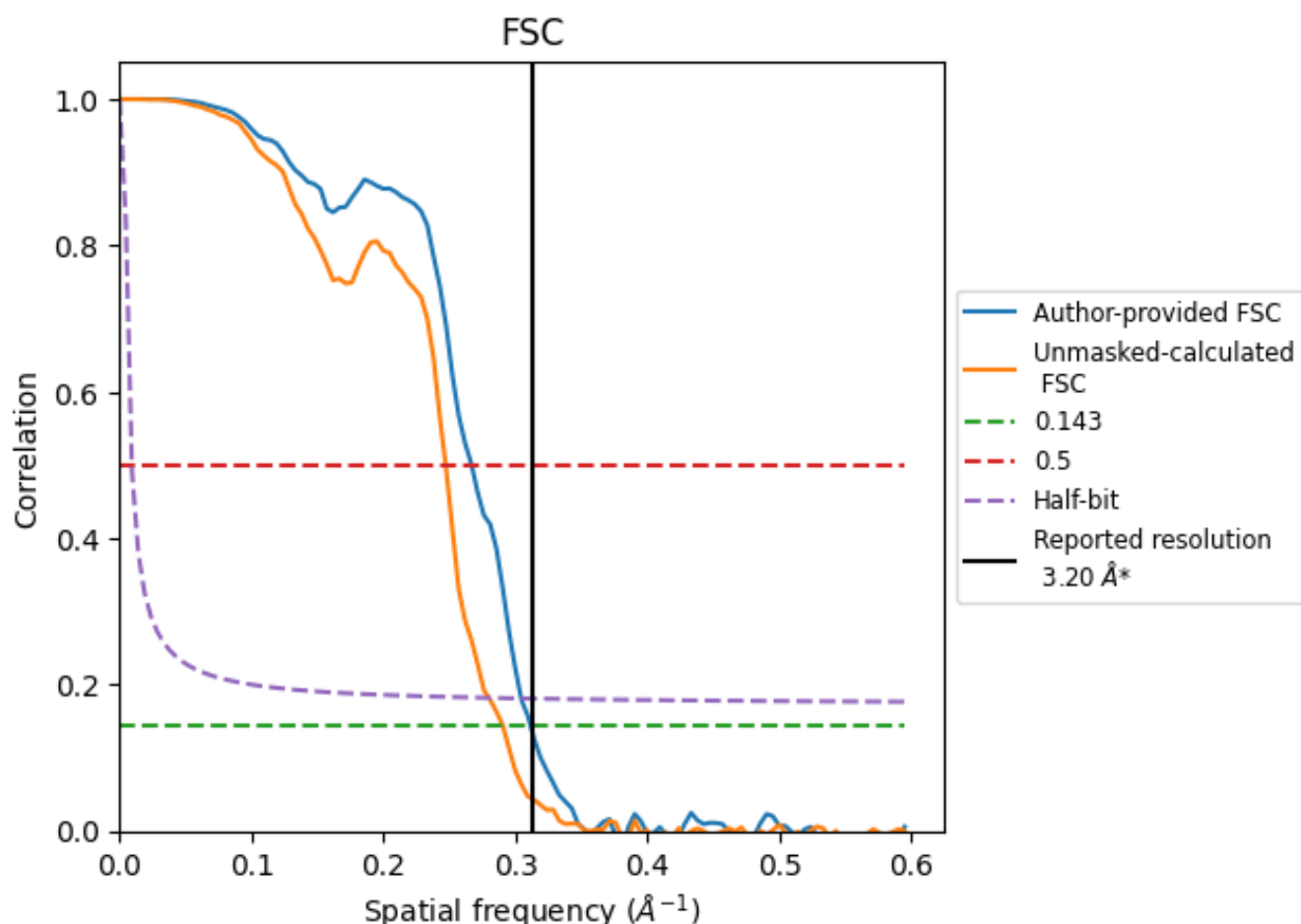


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	3.75	3.28
Unmasked-calculated*	3.44	4.04	3.57

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

9 Map-model fit [i](#)

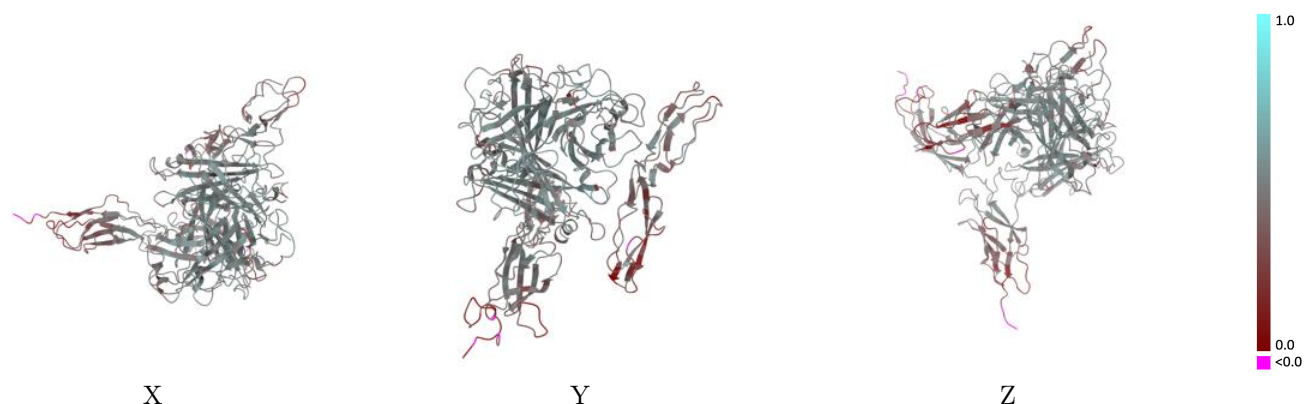
This section contains information regarding the fit between EMDB map EMD-18455 and PDB model 8QK3. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



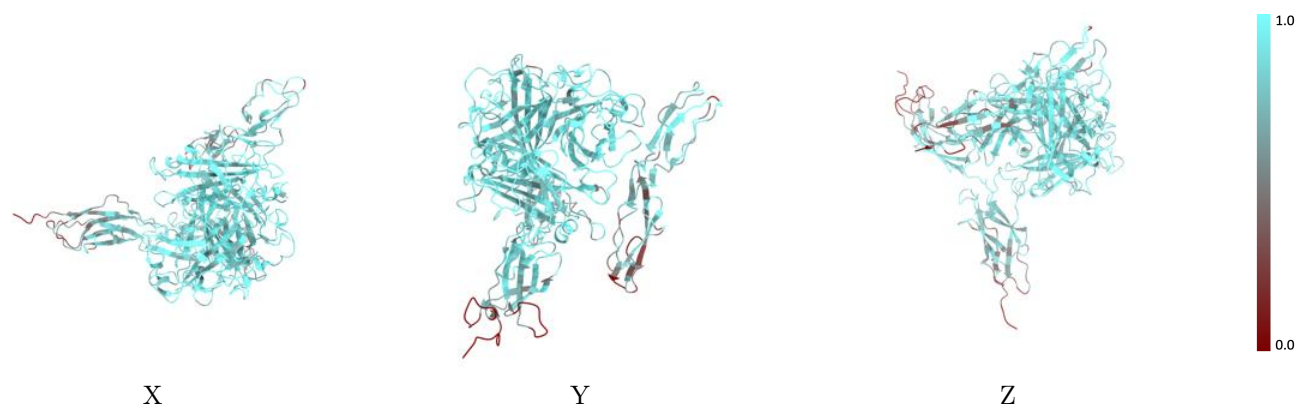
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



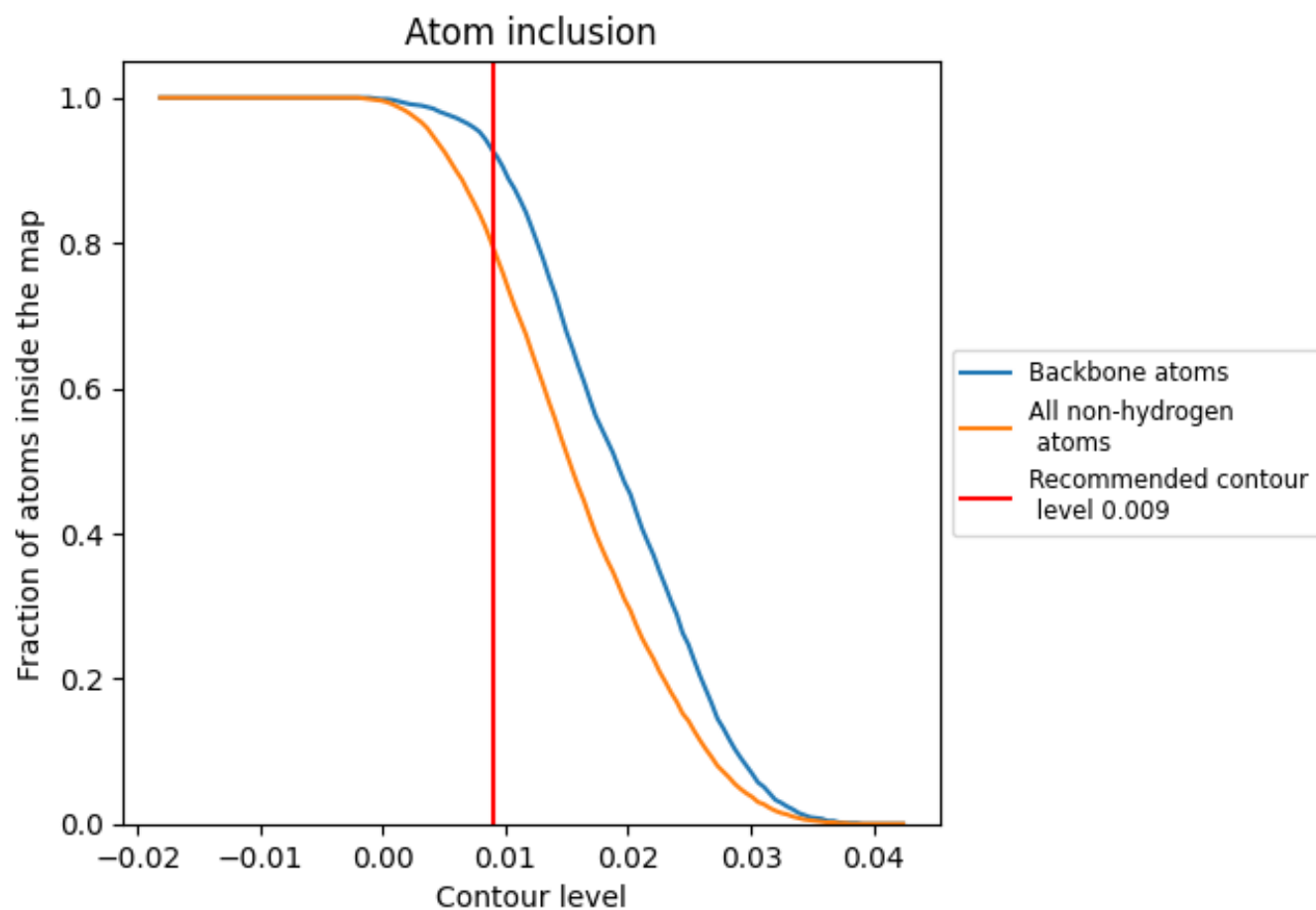
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 79% 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> 0.7940	<div></div> 0.4460
A	<div></div> 0.8780	<div></div> 0.4980
B	<div></div> 0.8770	<div></div> 0.4900
C	<div></div> 0.8940	<div></div> 0.5030
D	<div></div> 0.6390	<div></div> 0.3570
E	<div></div> 0.6740	<div></div> 0.3790

