



## wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 03:14 AM JST

PDB ID : 7E8F  
EMDB ID : EMD-31017  
Title : SARS-CoV-2 NTD in complex with N9 Fab  
Authors : Du, S.; Xiao, J.; Zhang, Z.  
Deposited on : 2021-03-01  
Resolution : 3.18 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.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

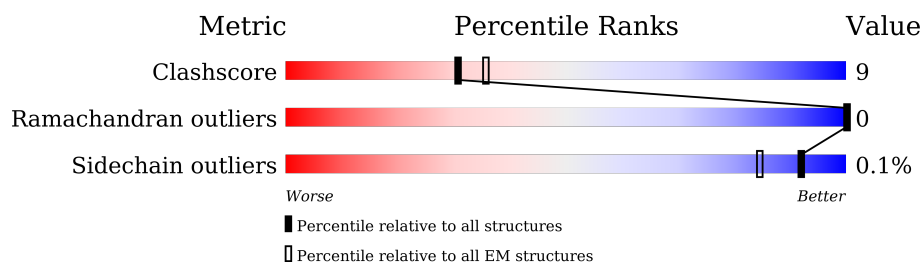
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.18 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	291	 9% 64% 24% 11%
2	H	230	 43% 11% 46%
3	L	212	 48% 50%
4	C	230	 44% 10% 46%
5	B	219	 40% 11% 49%
6	D	222	 5% 41% 12% 48%
7	E	214	 7% 42% 7% 50%
8	R	223	 6% 63% 22% 15%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8768 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 Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	258	Total	C	N	O	S	0	0
			2079	1351	341	382	5		

- Molecule 2 is a protein called N9 H.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	124	Total	C	N	O	S	0	0
			938	588	159	186	5		

- Molecule 3 is a protein called N9 L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	105	Total	C	N	O	S	0	0
			780	486	131	159	4		

- Molecule 4 is a protein called 368-2 H.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	124	Total	C	N	O	S	0	0
			944	593	165	182	4		

- Molecule 5 is a protein called 368-2 L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	112	Total	C	N	O	S	0	0
			852	537	143	168	4		

- Molecule 6 is a protein called 604 H.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	116	Total	C	N	O	S	0	0
			874	550	148	171	5		

- Molecule 7 is a protein called 604 L.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	106	Total	C	N	O	S	0	0
			803	506	132	163	2		

- Molecule 8 is a protein called Spike protein S1.

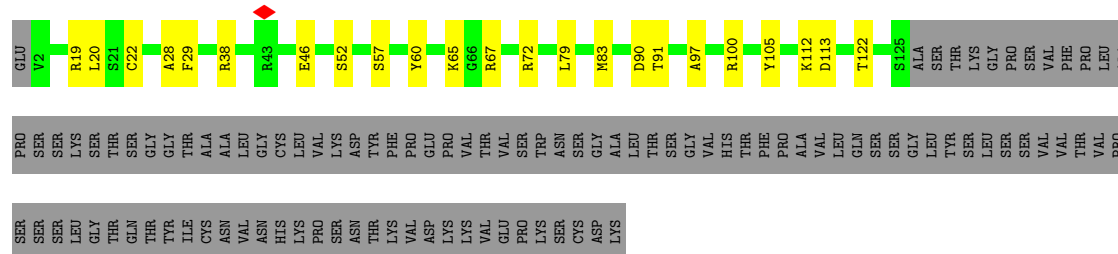
Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	189	Total	C	N	O	S	0	0
			1498	958	249	283	8		



VAL  
ALA  
PRO  
THR  
GLU  
CYS  
SER

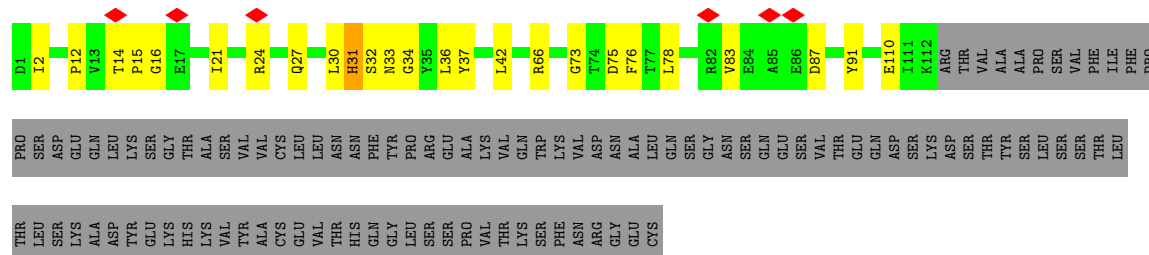
• Molecule 4: 368-2 H

Chain C: 44% 10% 46%



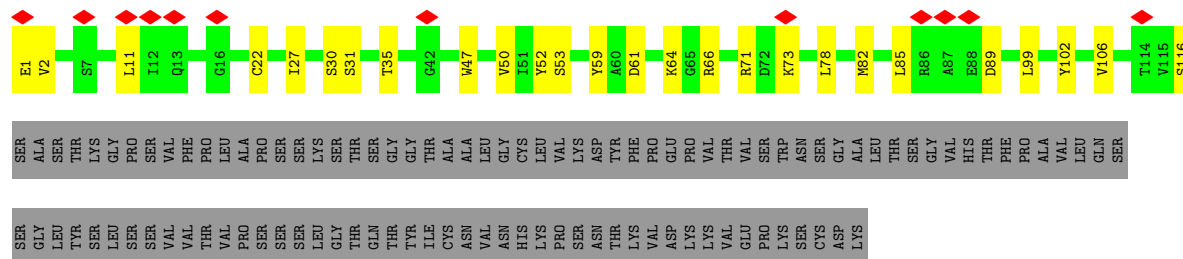
• Molecule 5: 368-2 L

Chain B: 40% 11% 49%



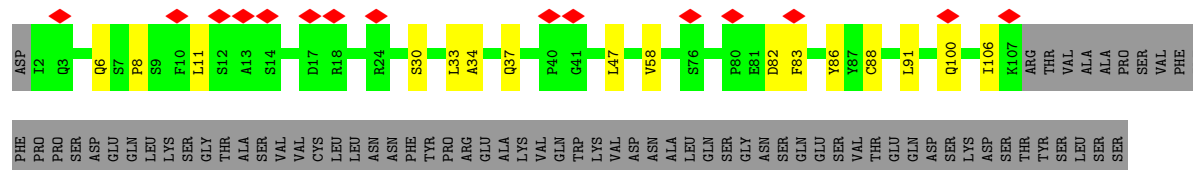
• Molecule 6: 604 H

Chain D: 5% 41% 12% 48%



• Molecule 7: 604 L

Chain E: 7% 42% 7% 50%



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

● Molecule 8: Spike protein S1



ARG	VAL	GLN	PRO	THR	GLU	SER	ILE	VAL	ARG	PHE	PRO	ASN	ILE	T333	N334	L335	C336	G339	E340	V341	F342	N343	F347	V350	W353	K356	R357	N360	C361	V362	N370	S371	A372	T376	F377	K378	C379	V382	S383	P384	T385	K386	D389	L390	C391	N394	V395
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R403	E406	K417	Y421	L425	D428	G431	C432	V433	I434	S438	M439	D442	S443	M448	Y449	M450	Y451	L455	F456	R457	L461	Y473	M481	Q493	Q498	Y505	R509	V512	F515	E516	LEU	HIS	ALA	PRO	A522	T523	V524	C525	G526
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PRO
LYS
LYS
SER
THR
ASN
LEU
VAL
LYS
ASN
LYS
CYS
VAL
ASN
PHE

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	304696	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 ( $e^-/\text{\AA}^2$ )	63.27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.195	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0359	Depositor
Map size ( $\text{\AA}$ )	168.32, 168.32, 168.32	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.052, 1.052, 1.052	Depositor



## 5 Model quality

### 5.1 Standard geometry

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	0.34	0/2138	0.52	1/2913 (0.0%)
2	H	0.33	0/959	0.48	0/1298
3	L	0.33	0/798	0.50	0/1087
4	C	0.33	0/965	0.50	0/1307
5	B	0.33	0/871	0.48	0/1183
6	D	0.32	0/891	0.47	0/1207
7	E	0.30	0/819	0.49	0/1112
8	R	0.36	0/1538	0.50	1/2090 (0.0%)
All	All	0.33	0/8979	0.50	2/12197 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
8	R	432	CYS	CA-CB-SG	6.38	125.49	114.00
1	A	166	CYS	CA-CB-SG	5.67	124.20	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	31	HIS	Peptide

## 5.2 Too-close contacts ⓘ

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	2079	0	2004	46	0
2	H	938	0	896	13	0
3	L	780	0	743	2	0
4	C	944	0	903	15	0
5	B	852	0	838	17	0
6	D	874	0	859	16	0
7	E	803	0	783	9	0
8	R	1498	0	1411	37	0
All	All	8768	0	8437	149	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 149 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)
8:R:379:CYS:HA	8:R:432:CYS:HB3	1.48	0.94
8:R:391:CYS:HA	8:R:525:CYS:HB3	1.58	0.85
5:B:2:ILE:HG12	5:B:27:GLN:HG3	1.60	0.82
7:E:83:PHE:HB3	7:E:106:ILE:HG12	1.62	0.81
1:A:131:CYS:HA	1:A:166:CYS:HB3	1.62	0.81

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	252/291 (87%)	208 (82%)	44 (18%)	0	100	100
2	H	122/230 (53%)	119 (98%)	3 (2%)	0	100	100
3	L	103/212 (49%)	99 (96%)	4 (4%)	0	100	100
4	C	122/230 (53%)	112 (92%)	10 (8%)	0	100	100
5	B	110/219 (50%)	102 (93%)	8 (7%)	0	100	100
6	D	114/222 (51%)	113 (99%)	1 (1%)	0	100	100
7	E	104/214 (49%)	98 (94%)	6 (6%)	0	100	100
8	R	185/223 (83%)	177 (96%)	8 (4%)	0	100	100
All	All	1112/1841 (60%)	1028 (92%)	84 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	230/261 (88%)	229 (100%)	1 (0%)	89	94
2	H	102/194 (53%)	102 (100%)	0	100	100
3	L	85/178 (48%)	85 (100%)	0	100	100
4	C	96/188 (51%)	96 (100%)	0	100	100
5	B	96/192 (50%)	96 (100%)	0	100	100
6	D	94/186 (50%)	94 (100%)	0	100	100
7	E	90/187 (48%)	90 (100%)	0	100	100
8	R	163/196 (83%)	163 (100%)	0	100	100
All	All	956/1582 (60%)	955 (100%)	1 (0%)	92	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN

### 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 [i](#)

There are no chain breaks in this entry.

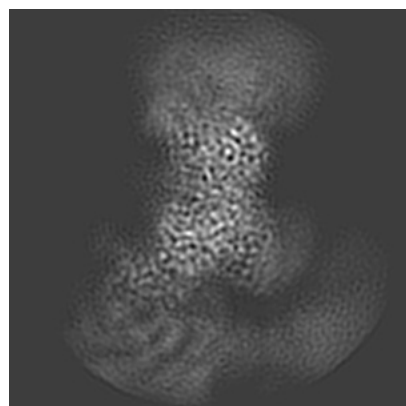
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31017. These allow visual inspection of the internal detail of the map and identification of artifacts.

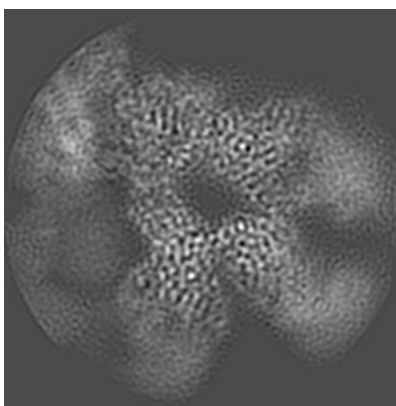
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

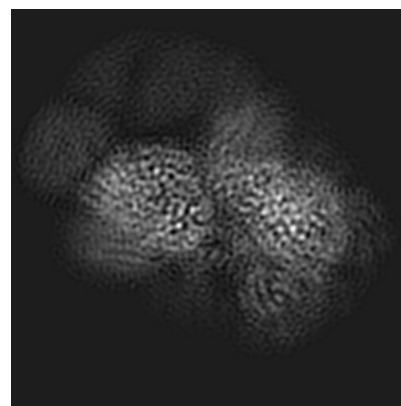
#### 6.1.1 Primary map



X

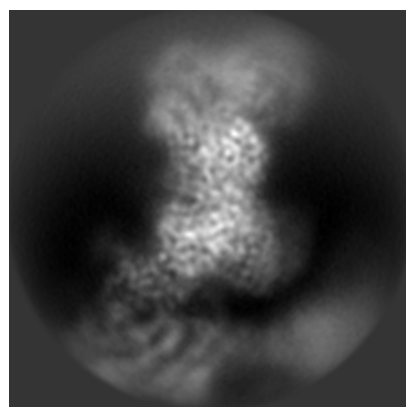


Y

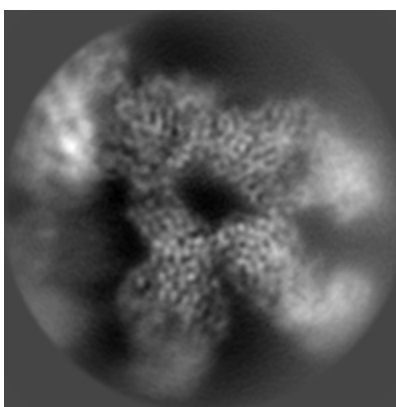


Z

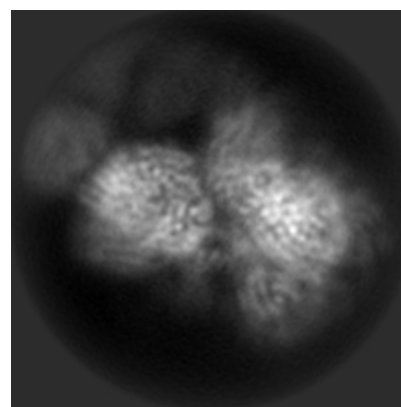
#### 6.1.2 Raw map



X



Y

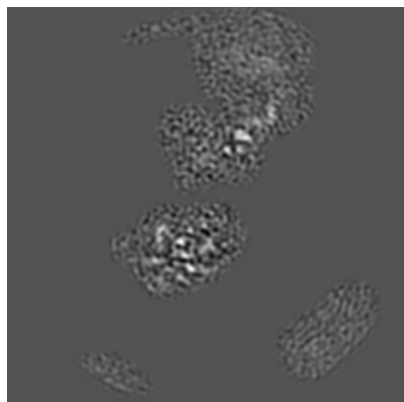


Z

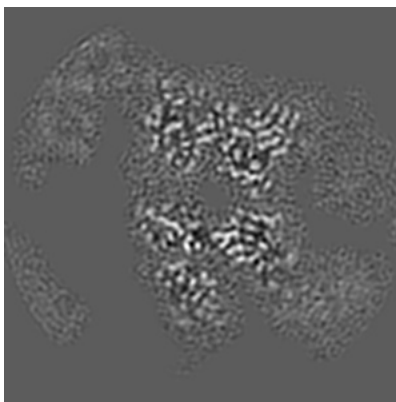
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

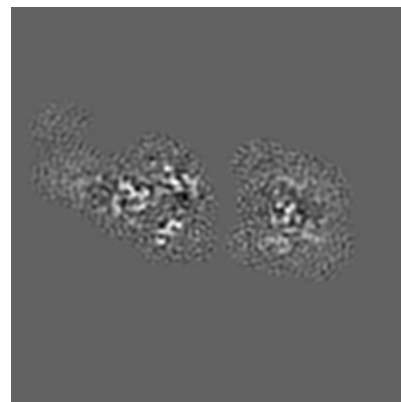
### 6.2.1 Primary map



X Index: 80

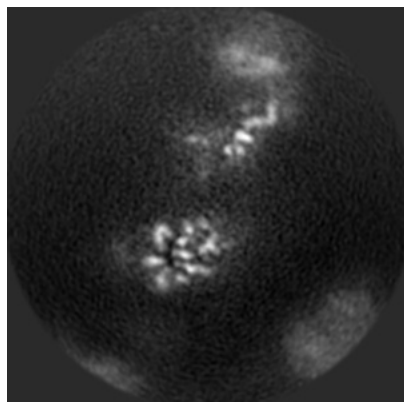


Y Index: 80

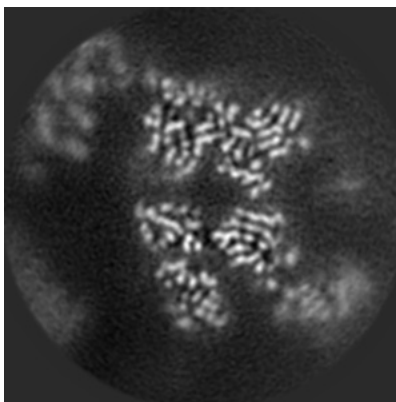


Z Index: 80

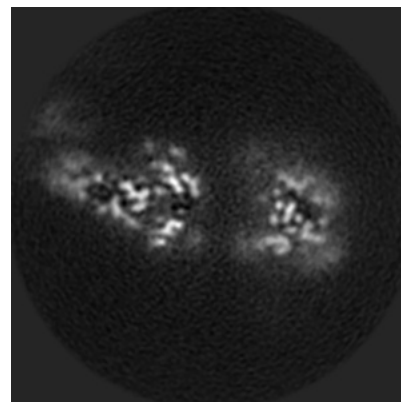
### 6.2.2 Raw map



X Index: 80



Y Index: 80

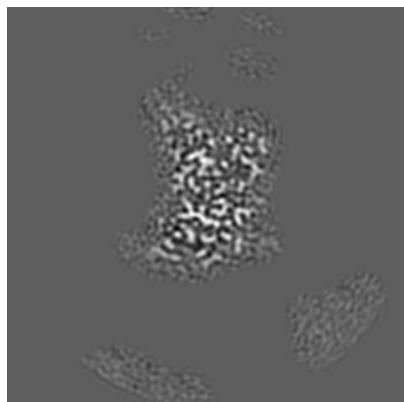


Z Index: 80

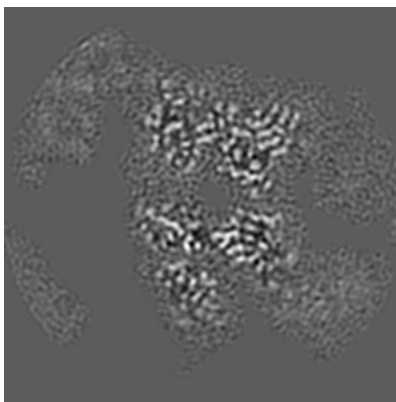
The images above show central slices of the map in three orthogonal directions.

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

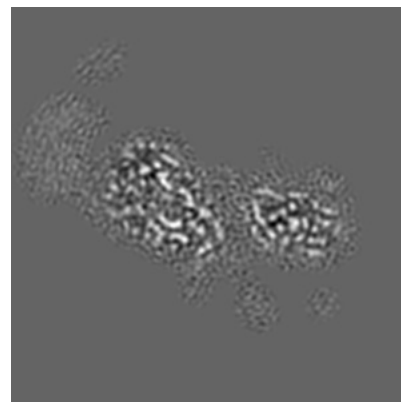
### 6.3.1 Primary map



X Index: 67

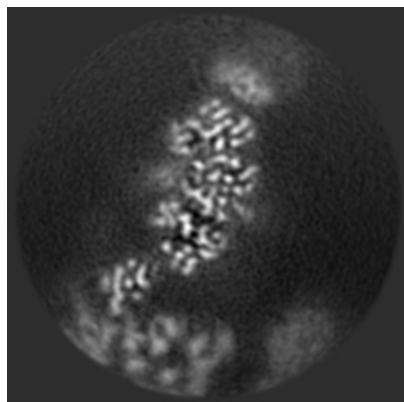


Y Index: 80

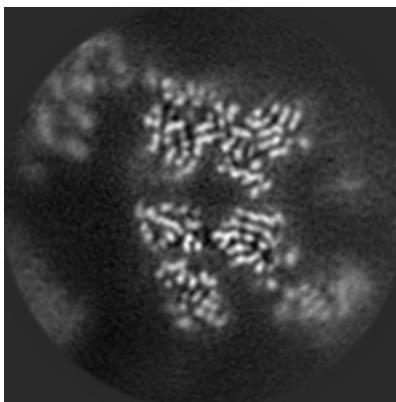


Z Index: 69

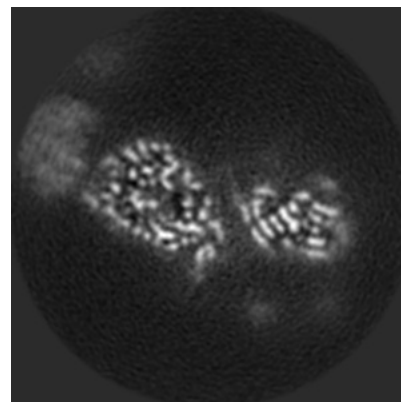
### 6.3.2 Raw map



X Index: 107



Y Index: 80



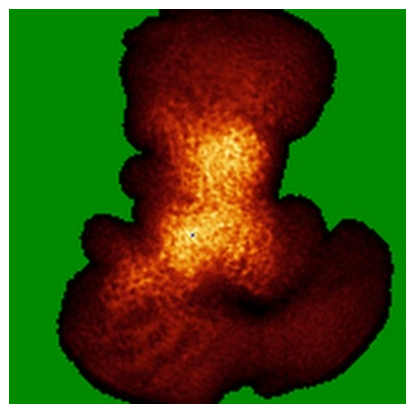
Z Index: 70

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

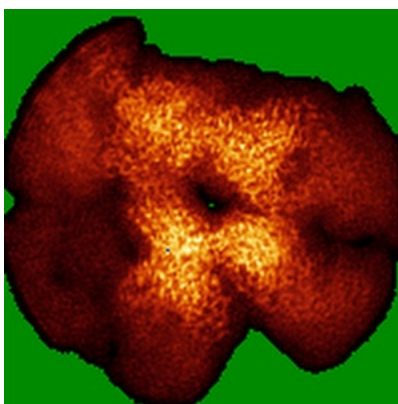


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

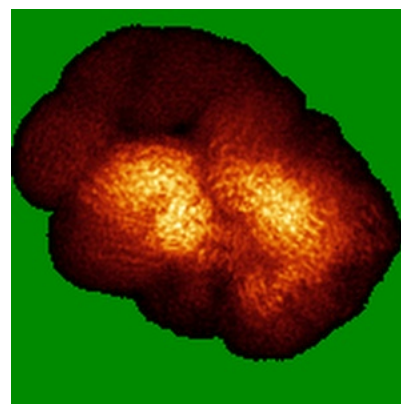
### 6.4.1 Primary map



X

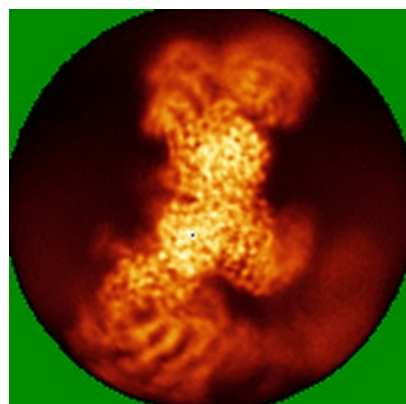


Y

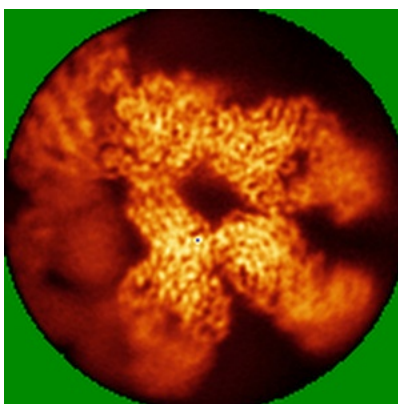


Z

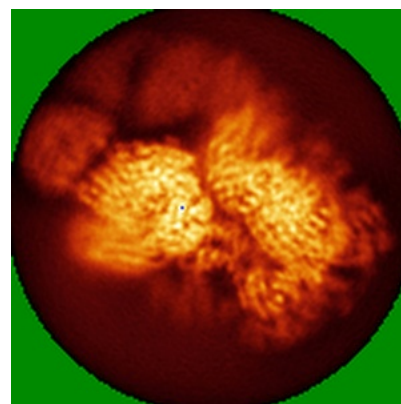
### 6.4.2 Raw map



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.



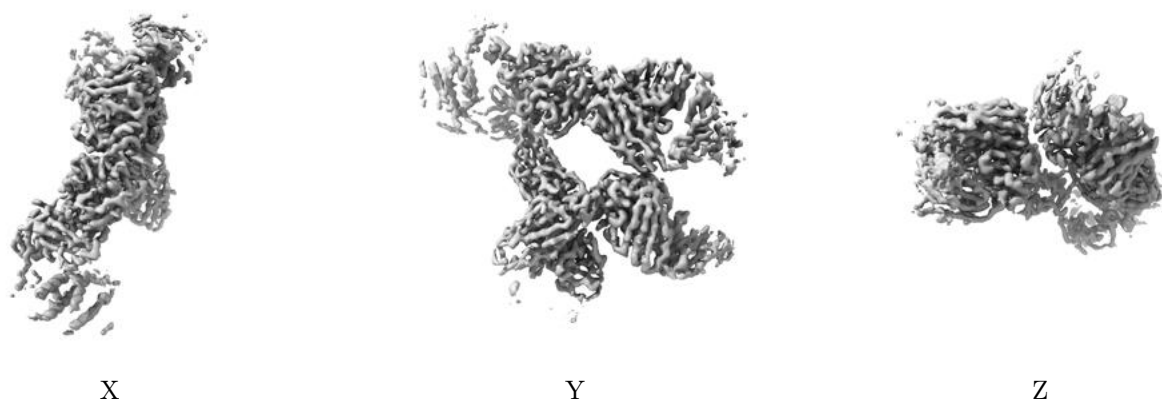
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0359. 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.

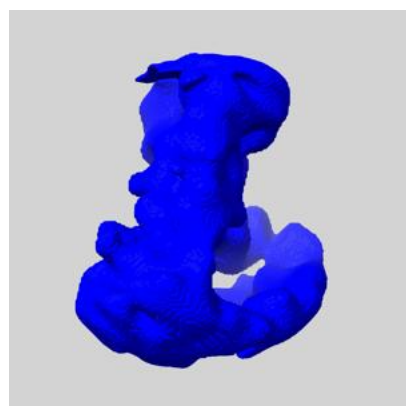
## 6.6 Mask visualisation [i](#)

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

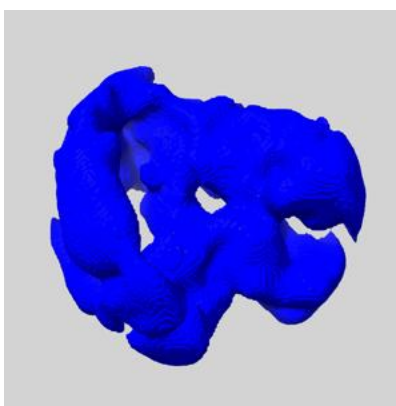
A mask typically either:

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

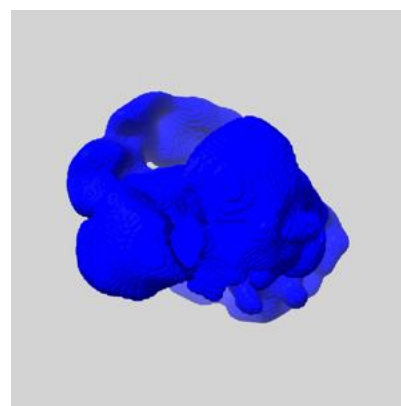
### 6.6.1 emd\_31017\_msk\_1.map [i](#)



X



Y

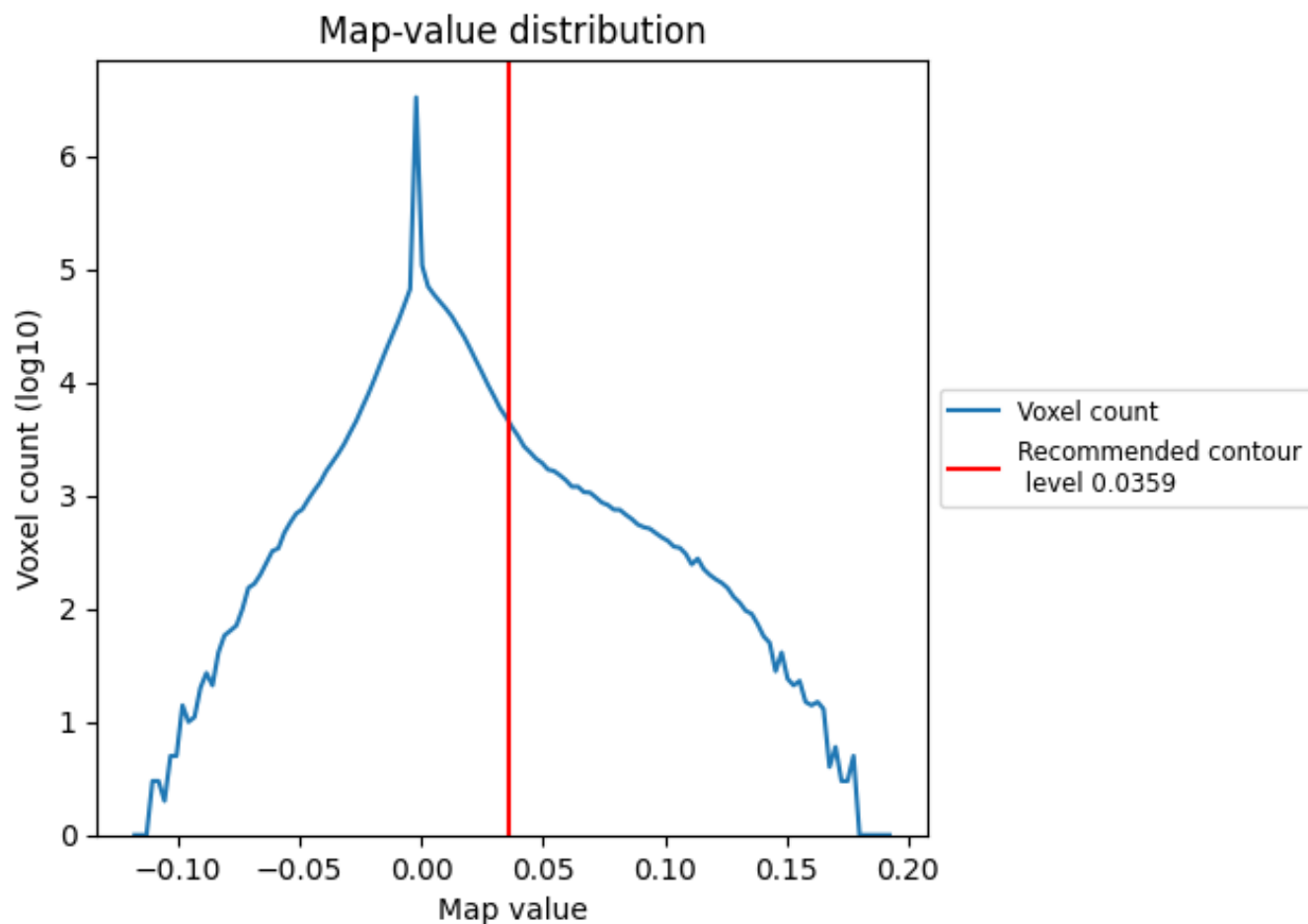


Z

## 7 Map analysis [i](#)

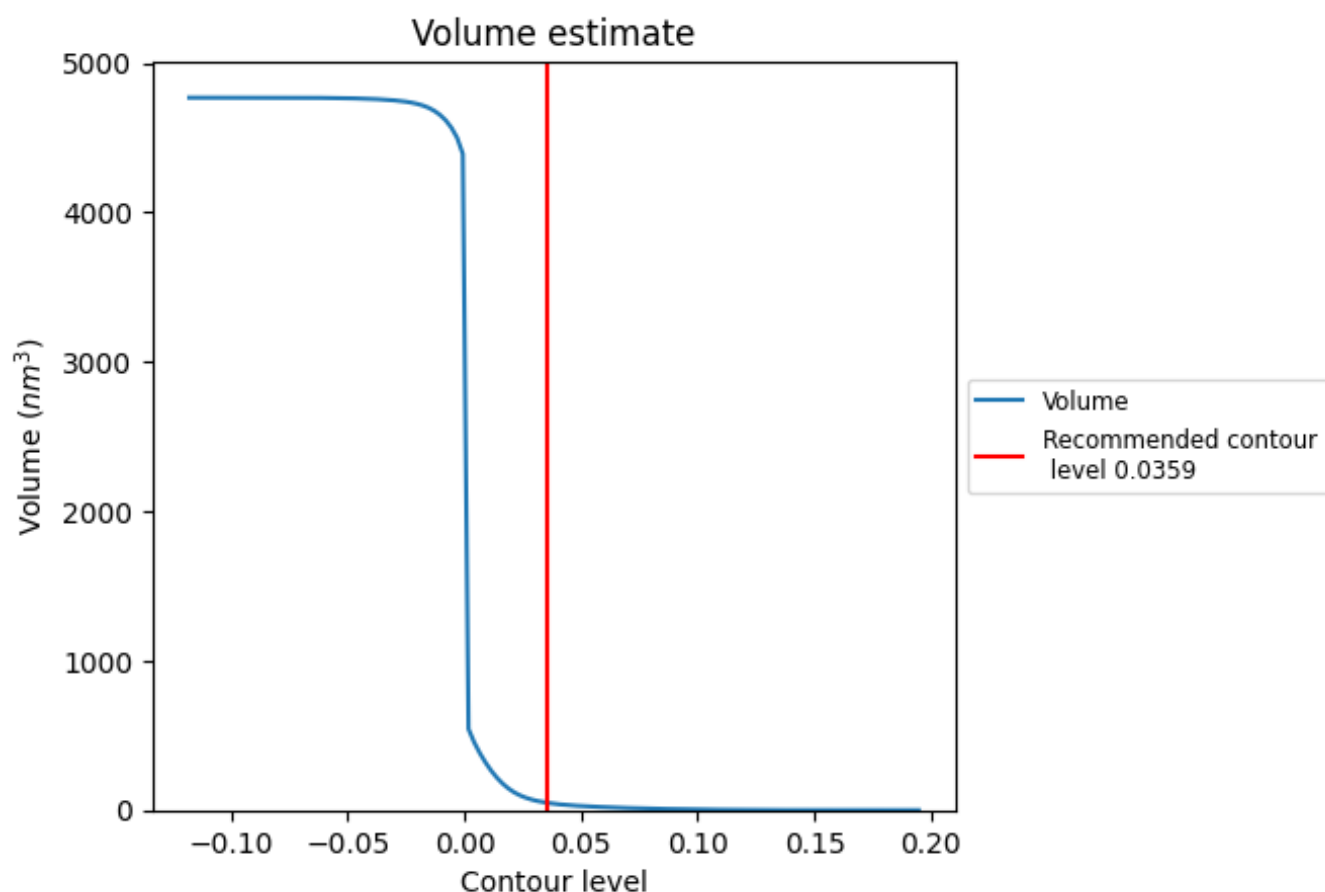
This section contains the results of statistical analysis of the map.

### 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.

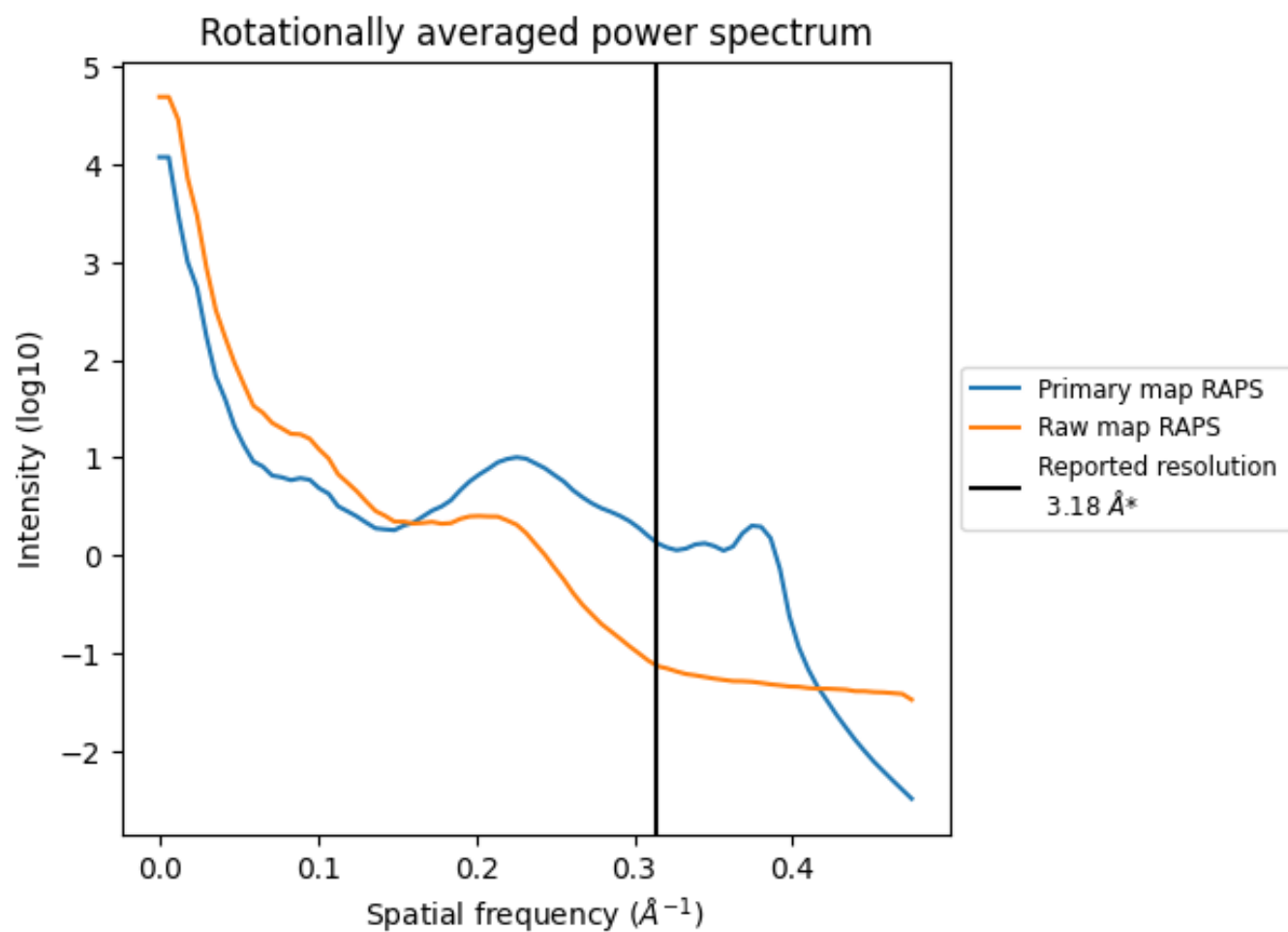
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 48 nm<sup>3</sup>; this corresponds to an approximate mass of 44 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 ⓘ

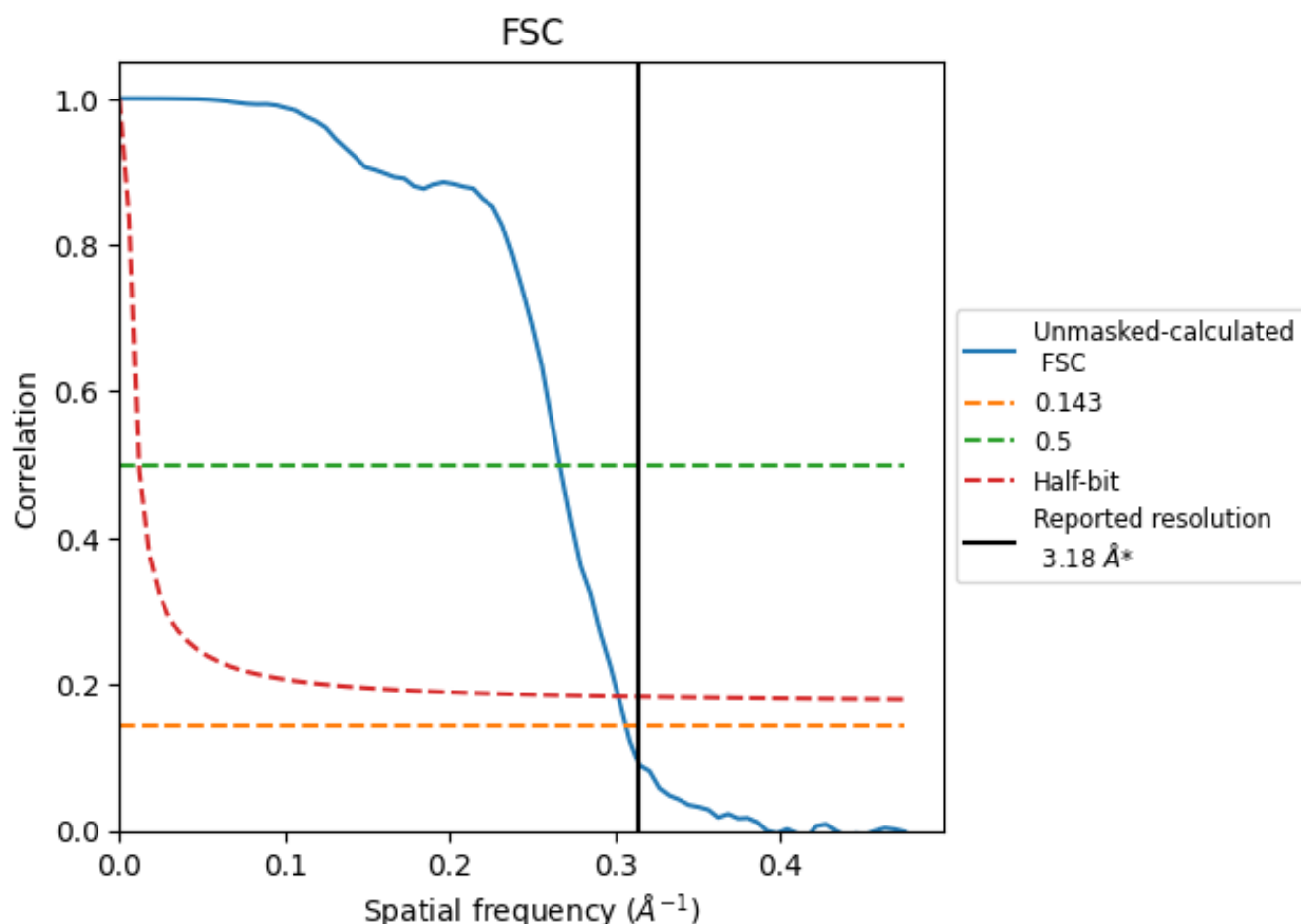


\*Reported resolution corresponds to spatial frequency of 0.314 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

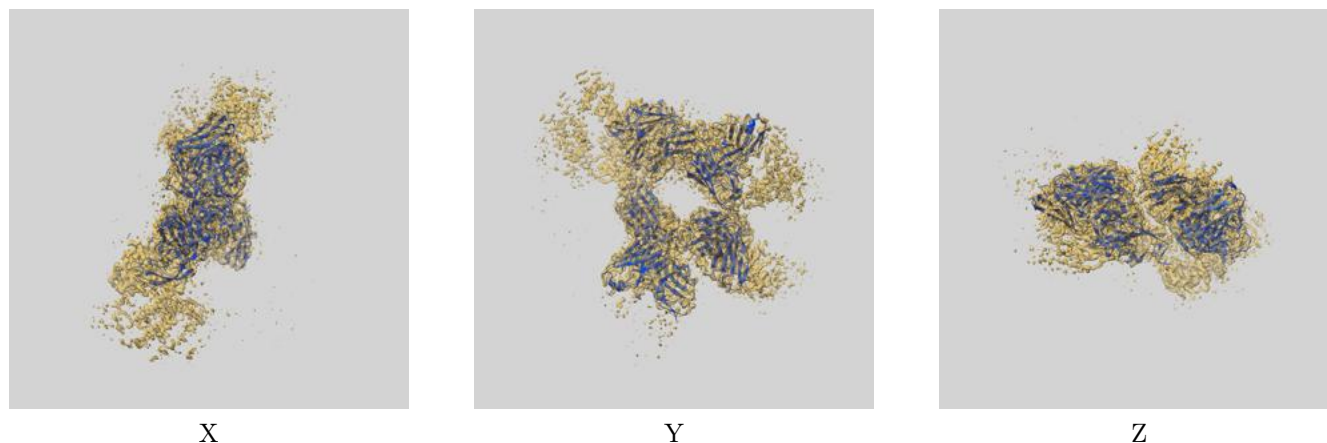
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.26	3.75	3.31

\*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-31017 and PDB model 7E8F. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

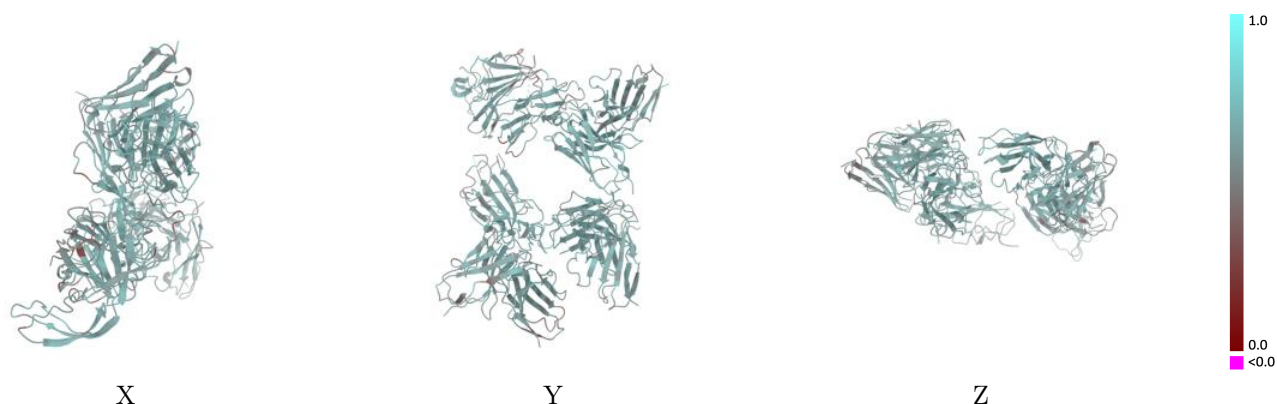
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0359 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.

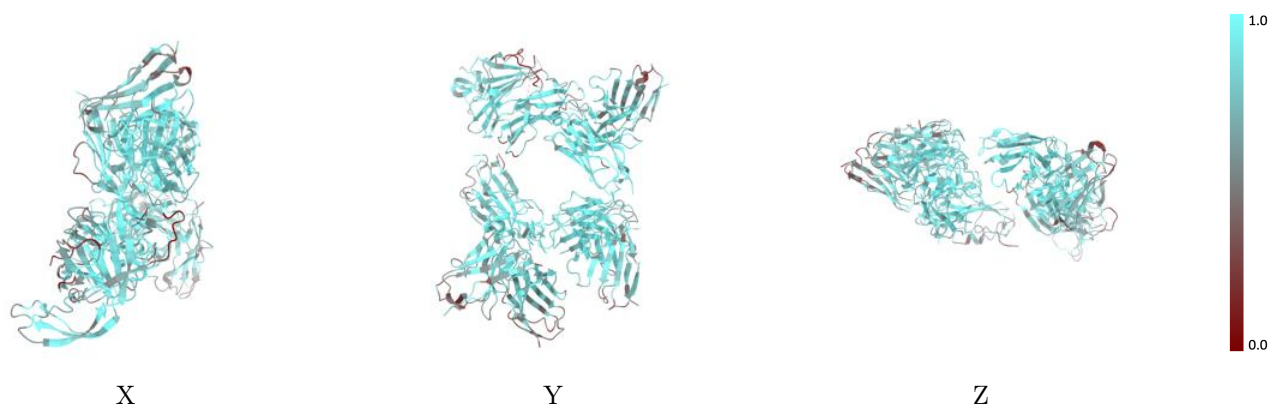


## 9.2 Q-score mapped to coordinate model [i](#)



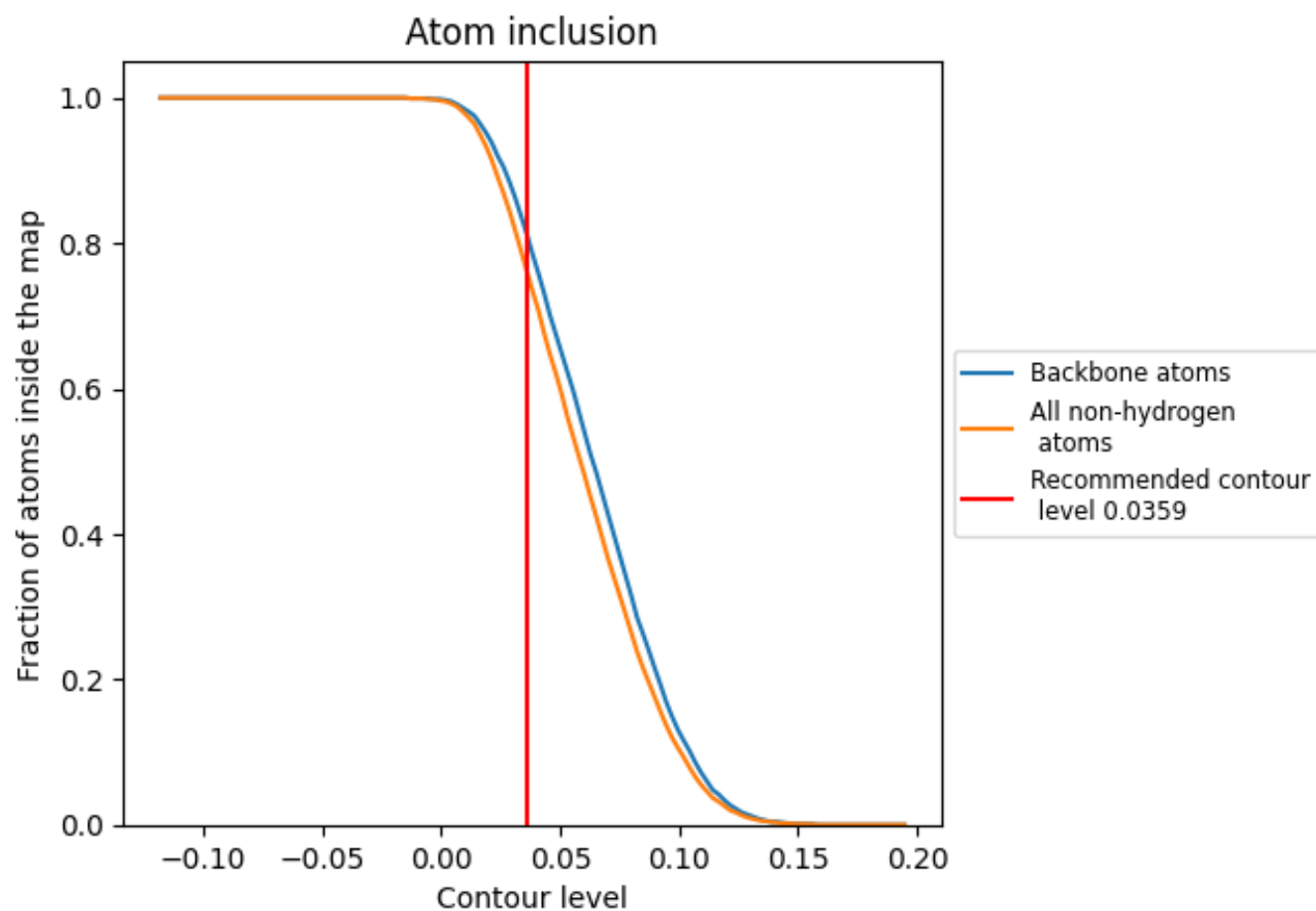
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0359).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 76% 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 (0.0359) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7640	<div></div> 0.5920
A	<div></div> 0.7310	<div></div> 0.5750
B	<div></div> 0.7620	<div></div> 0.5940
C	<div></div> 0.8480	<div></div> 0.6160
D	<div></div> 0.7180	<div></div> 0.5850
E	<div></div> 0.6860	<div></div> 0.5680
H	<div></div> 0.8640	<div></div> 0.6290
L	<div></div> 0.7220	<div></div> 0.5840
R	<div></div> 0.7860	<div></div> 0.5980

1.0

0.0

<0.0