



## wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 10:16 PM EDT

PDB ID : 6PZT  
EMDB ID : EMD-20537  
Title : cryo-EM structure of human NKCC1  
Authors : Cao, E.; Wang, Q.; Yang, X.  
Deposited on : 2019-08-01  
Resolution : 3.46 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

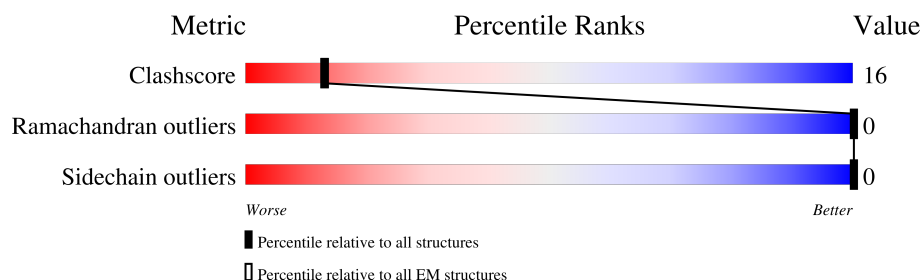
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.46 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	1212	
1	B	1212	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6062 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 Solute carrier family 12 member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	466	Total	C	N	O	S	0	0
			3031	1957	513	549	12		
1	A	466	Total	C	N	O	S	0	0
			3031	1957	513	549	12		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	289	ASN	LYS	engineered mutation	UNP P55011
B	351	ARG	GLY	engineered mutation	UNP P55011
A	289	ASN	LYS	engineered mutation	UNP P55011
A	351	ARG	GLY	engineered mutation	UNP P55011



[illegible]

- Molecule 1: Solute carrier family 12 member 2

Chain A:  27% 11% 62%

GLY	ASN	E670	Y533	Y583	I311	PRO	GLU	GLU	GLU	PRO
LEU	TRP	E670	Y533	V384	V312	SER	GLY	ALA	ALA	ALA
MET	TRP	E670	Y533	V385	V312	LEU	SER	SER	SER	ALA
CYS	GLY	E673	G541	G386	G315	ALA	SER	GLY	ALA	ALA
ILE	SER	I674	S542	F387	A315	GLU	LEU	GLY	GLY	PRO
GLY	SER	I674	S542	A388	G316	LEU	HIS	SER	ASP	THR
HIS	THR	I678	V645	E589	G316	LEU	SER	GLY	GLY	ALA
VAL	GLN	I681	R546	T390	S320	ASP	GLY	PRO	PRO	PRO
HIS	ALA	F681	G550	V392	I324	GLU	GLY	GLY	ALA	GLY
LEU	LEU	Y686	G550	V392	M325	LEU	GLY	GLY	ARG	SER
THR	THR	A687	I586	D404	M326	GLY	GLY	GLY	PRO	PRO
PRO	THR	A687	I586	D404	M326	LEU	GLY	SER	LEU	ALA
ARG	LEU	L688	V557	A327	A327	GLU	SER	GLY	GLY	PRO
ARG	ASN	I689	T558	M407	T328	PRO	GLY	GLY	GLY	GLY
GLN	ALA	N690	D008	D408	T328	PHE	HIS	ALA	THR	LEU
ALA	LEU	F691	E559	V330	V330	GLU	HIS	ALA	PRO	ALA
MET	GLN	S692	I560	I419	V331	ASP	GLN	GLY	SER	ALA
LYS	HIS	V693	T561	I423	T332	GLY	HIS	ARG	GLN	VAL
GLU	SER		N562	I423	T333	PHE	TYR	PHE	SER	GLY
MET	ILE	S701			T334	ALA	TYR	ARG	ARG	GLY
SER	ARG	P702	Y584	A426	L336	ASN	TYR	VAL	PHE	THR
ILE	LEU	G703	G585		L336	GLY	ASP	ASN	GLN	PRO
ASP	SER	W704	L586	E429	T338	GLU	THR	PHE	VAL	SER
GLN	GLY		L586		T338	GLU	HIS	VAL	ASP	ALA
ALA	VAL	A707	M593	L438	S339	SER	THR	ASP	LEU	ALA
LYS	GLU				A340	THR	ASN	PRO	VAL	ALA
GLN	ASN	N712	S587		I341	PRO	THR	ALA	SER	LEU
GLN	HIS	W713			A342	THR	TYR	ALA	GLU	ALA
ARG	VAL	W714	I607	D448	T343	ARG	TYR	ALA	ASN	ALA
TRP	LYS	I715		F449	T343	ASP	LEU	SER	ASN	ALA
LEU	ASN		T611	T453	G345	ALA	ARG	SER	GLY	ALA
ILE	PHE	L718	L612	P456	F346	VAL	THR	ALA	ARG	VAL
LYS	ARG	G719	S613		V347	VAL	PHE	GLU	ALA	VAL
ASN	PRO				R348	THR	HIS	ASP	ALA	LEU
GLN	GLN	L722	A622	F465	G349	THR	ASN	LEU	ALA	GLY
CYS	CYS	C723	P623	E471	G350	ALA	THR	SER	ALA	ALA
LEU	LEU	C724	F626		R351	GLU	MET	ASP	ALA	ALA
LYS	VAL	I725		M476	A352	LYS	ALA	ALA	ALA	ALA
PHE	MET	W726	V726		R352	GLY	VAL	GLY	SER	PRO
TYR	THR	M727	P636	P479	V353	VAL	PRO	VAL	ALA	VAL
ALA	GLY	F728	A637		Y354	VAL	ARG	VAL	ALA	VAL
PRO	ALA	V729		T466	L355	VAL	PRO	GLY	ALA	PRO
VAL	PRO		M640		L355	VAL	ILE	VAL	ALA	PRO
HIS	ASN	A735	F641	S489	L356	LYS	ASP	ASP	ALA	ASP
ALA	SER		A642	V490	S357	PHE	HIS	GLY	ALA	ALA
ASP	ARG	Y739	K643		R358	TRP	TYR	PRO	ALA	ALA
LEU	PRO		K643	F495	S359	ARG	ASN	ASN	GLY	PRO
ASP	ALA	V742		P496	L360	THR	HIS	VAL	ALA	ALA
ARG	LEU		K647		G361	THR	ALA	SER	GLY	SER
GLU	LEU	L743	I648	T489	G361	ALA	THR	ALA	GLY	ALA
GLY	HIS	G744		G500	P362	ALA	ALA	PHE	GLY	ARG
ALA	LEU	L745	N649	I501	E363	ASN	GLN	GLN	ALA	ASP
GLN	VAL	I746	Y746	L502	A367	LEU	LEU	GLY	LYS	GLY
TYR	HIS	Y748	L652	A503	A367	GLY	GLY	GLY	GLY	GLY
LEU	ASP		R653		I371	GLU	ASP	THR	THR	VAL
LEU	THR	Y751	G654	P519	I371	LYS	GLY	THR	PRO	ARG
MET	PHE	K752		T658	F372	LEU	THR	VAL	ALA	ASP
GLN	LYS	K753		I526	A373	LEU	VAL	VAL	ALA	ASP
ALA	ASN		L663		V378	GLU	LEU	LEU	ASP	GLY
GLY	VAL	PRO	L667	T530	A381	ARG	SER	SER	GLY	GLY
		ASP	L667		M382					

[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90803	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 ( $e^-/\text{\AA}^2$ )	10	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	2.476	Depositor
Minimum map value	-1.989	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	0.40	0/3097	0.47	0/4247
1	B	0.40	0/3097	0.47	0/4247
All	All	0.40	0/6194	0.47	0/8494

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

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	3031	0	2605	92	0
1	B	3031	0	2605	91	0
All	All	6062	0	5210	183	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 16.

The worst 5 of 183 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)
1:A:338:THR:HA	1:A:341:ILE:HD12	1.54	0.89
1:B:338:THR:HA	1:B:341:ILE:HD12	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:HD12	1:A:533:TYR:HE1	1.49	0.78
1:B:304:LEU:HD12	1:B:533:TYR:HE1	1.49	0.77
1:B:351:ARG:O	1:B:355:LEU:N	2.18	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	464/1212 (38%)	407 (88%)	57 (12%)	0	100	100
1	B	464/1212 (38%)	407 (88%)	57 (12%)	0	100	100
All	All	928/2424 (38%)	814 (88%)	114 (12%)	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	233/984 (24%)	233 (100%)	0	100	100
1	B	233/984 (24%)	233 (100%)	0	100	100
All	All	466/1968 (24%)	466 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	398	HIS
1	A	398	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 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.

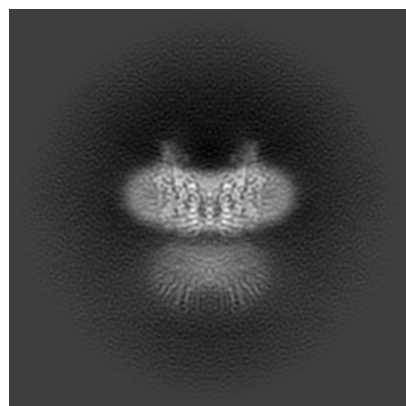
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20537. These allow visual inspection of the internal detail of the map and identification of artifacts.

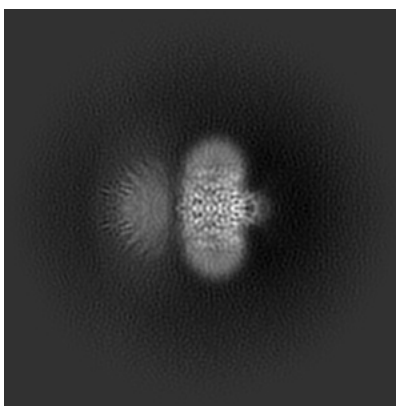
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

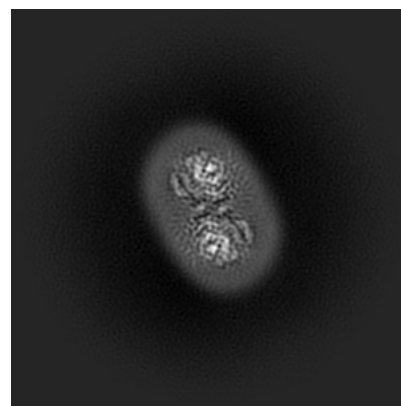
#### 6.1.1 Primary map



X

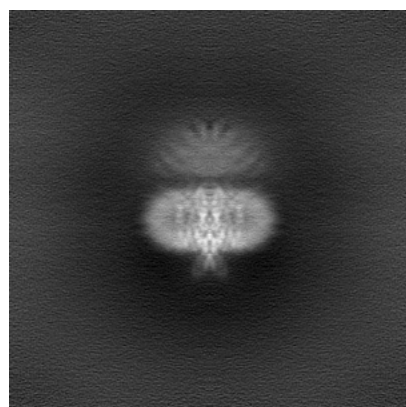


Y

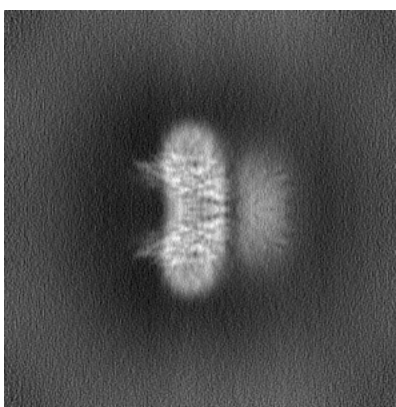


Z

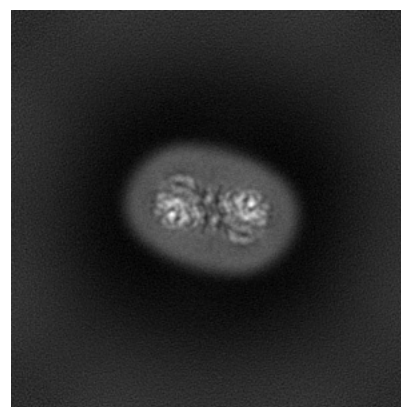
#### 6.1.2 Raw map



X



Y

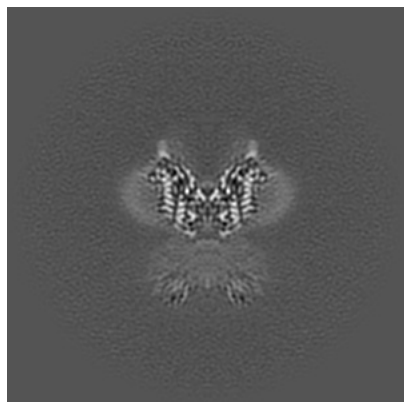


Z

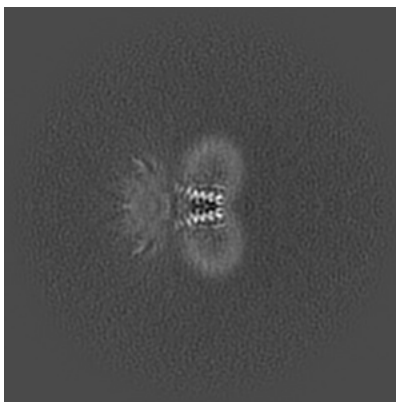
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

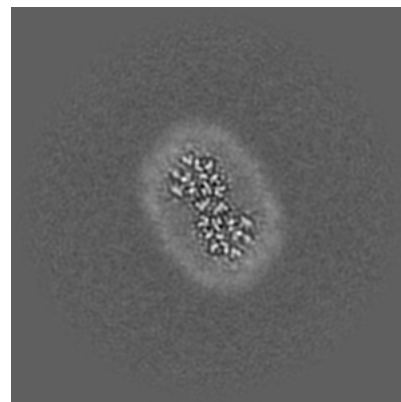
### 6.2.1 Primary map



X Index: 150

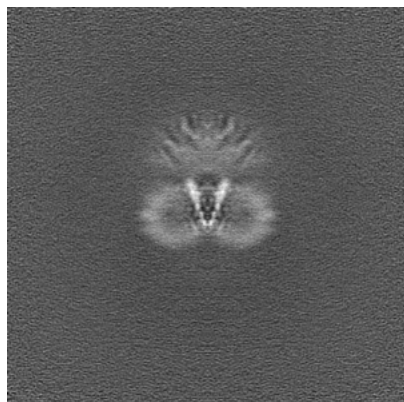


Y Index: 150

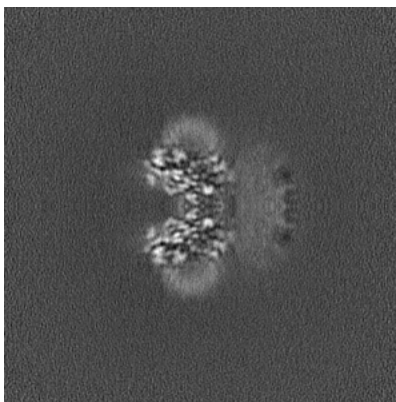


Z Index: 150

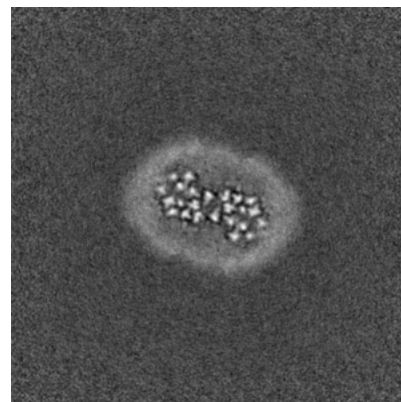
### 6.2.2 Raw map



X Index: 150



Y Index: 150

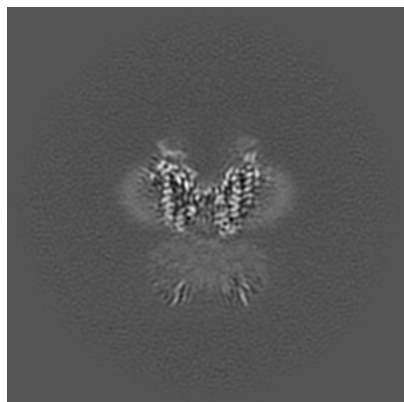


Z Index: 150

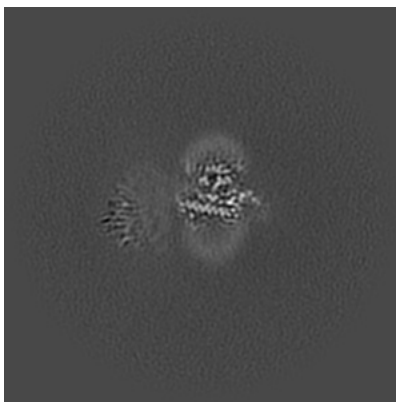
The images above show central slices of the map in three orthogonal directions.

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

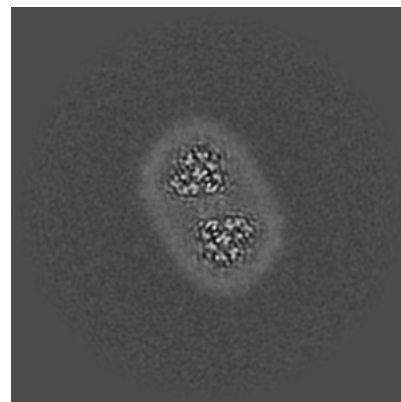
### 6.3.1 Primary map



X Index: 152

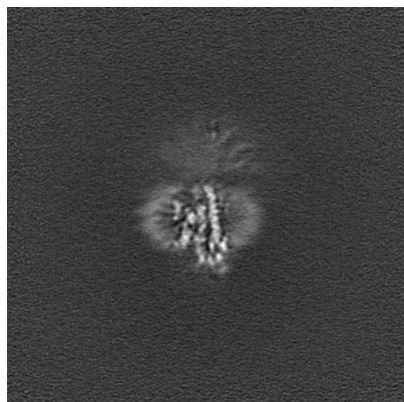


Y Index: 129

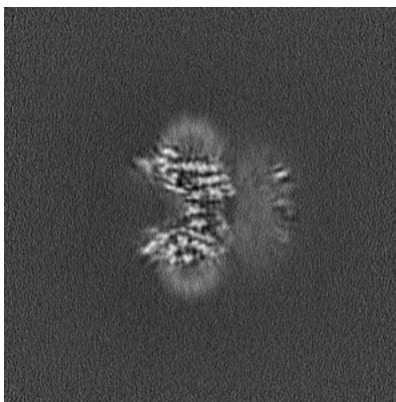


Z Index: 167

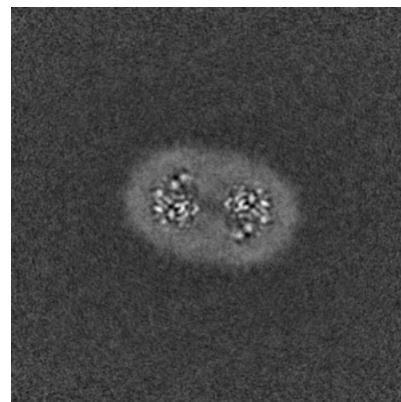
### 6.3.2 Raw map



X Index: 179



Y Index: 154



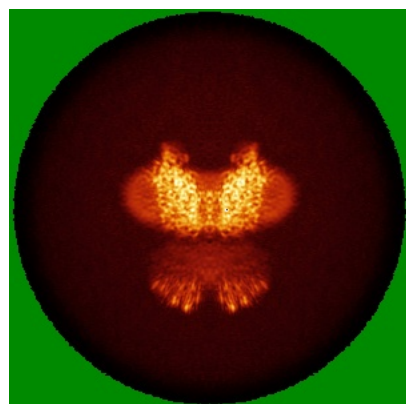
Z Index: 128

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

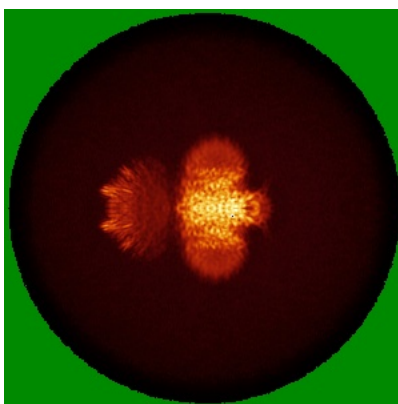


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

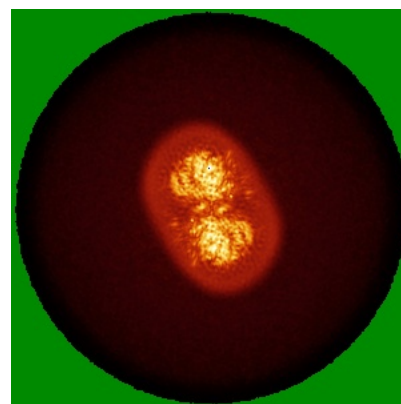
### 6.4.1 Primary map



X

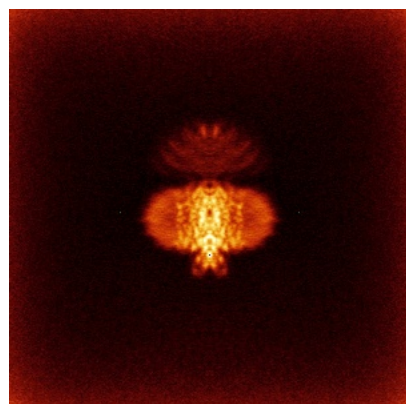


Y

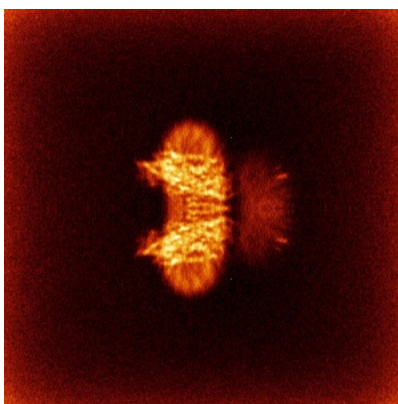


Z

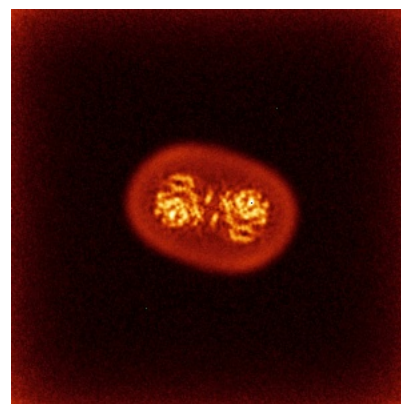
### 6.4.2 Raw map



X



Y

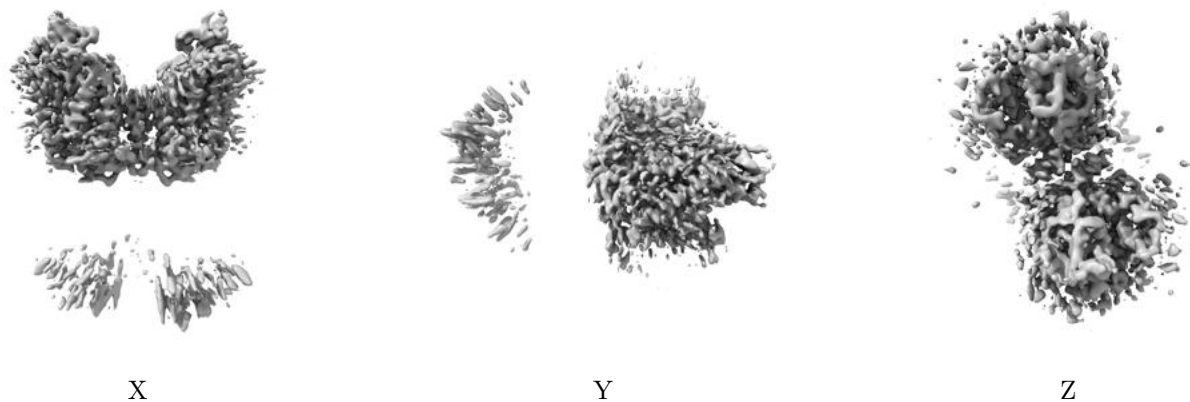


Z

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.

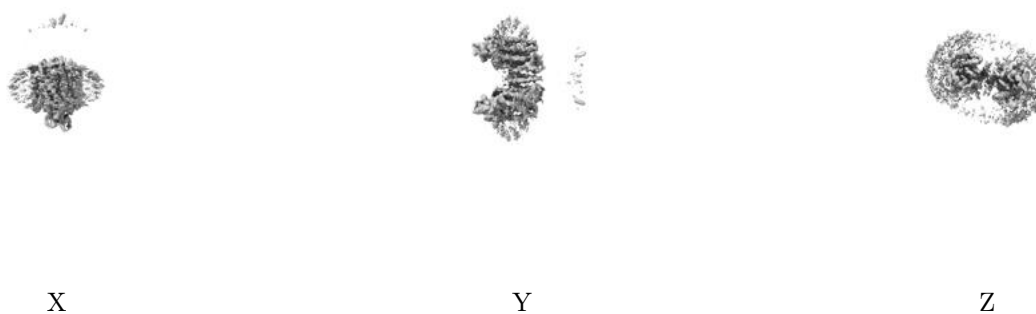
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

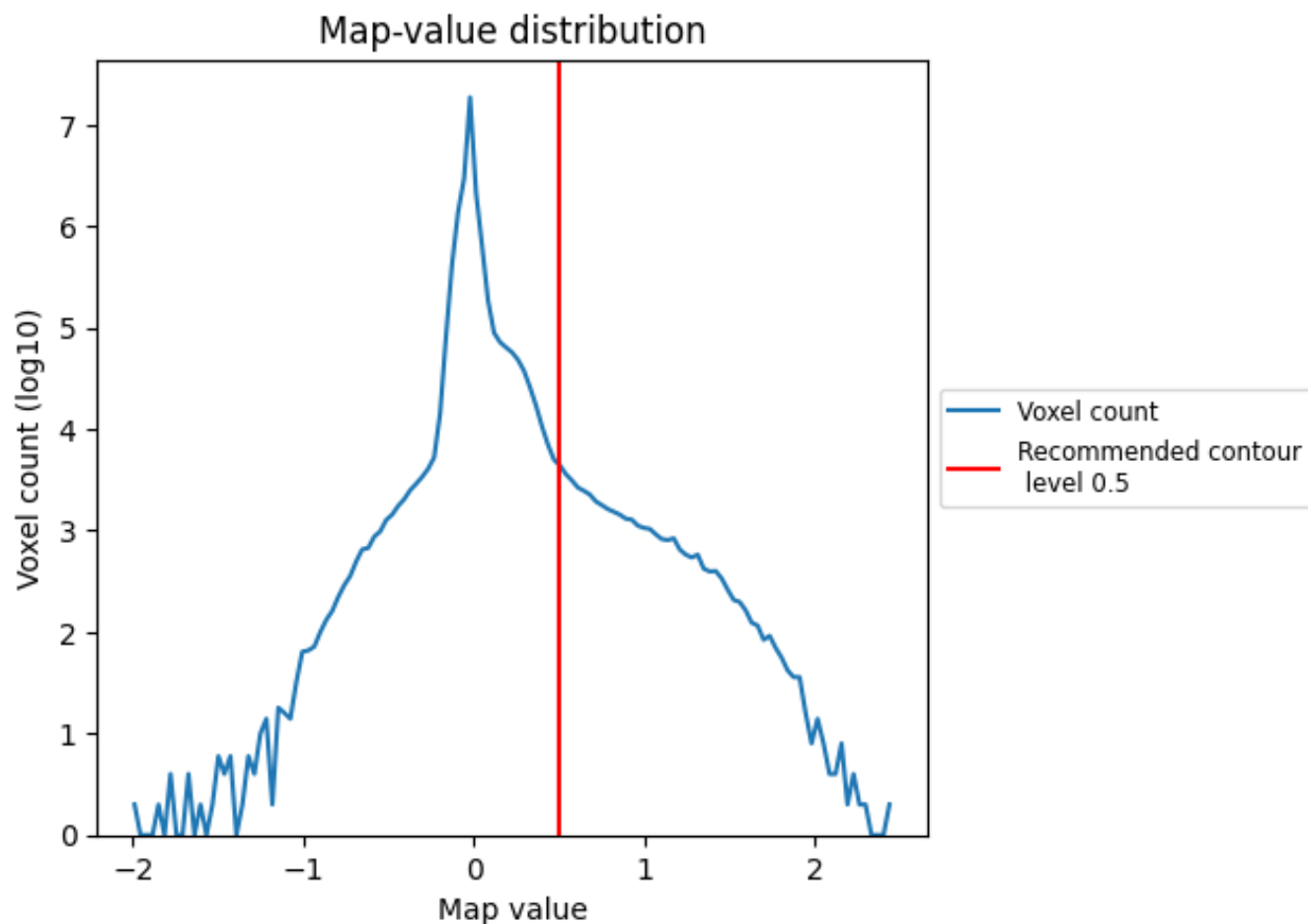
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

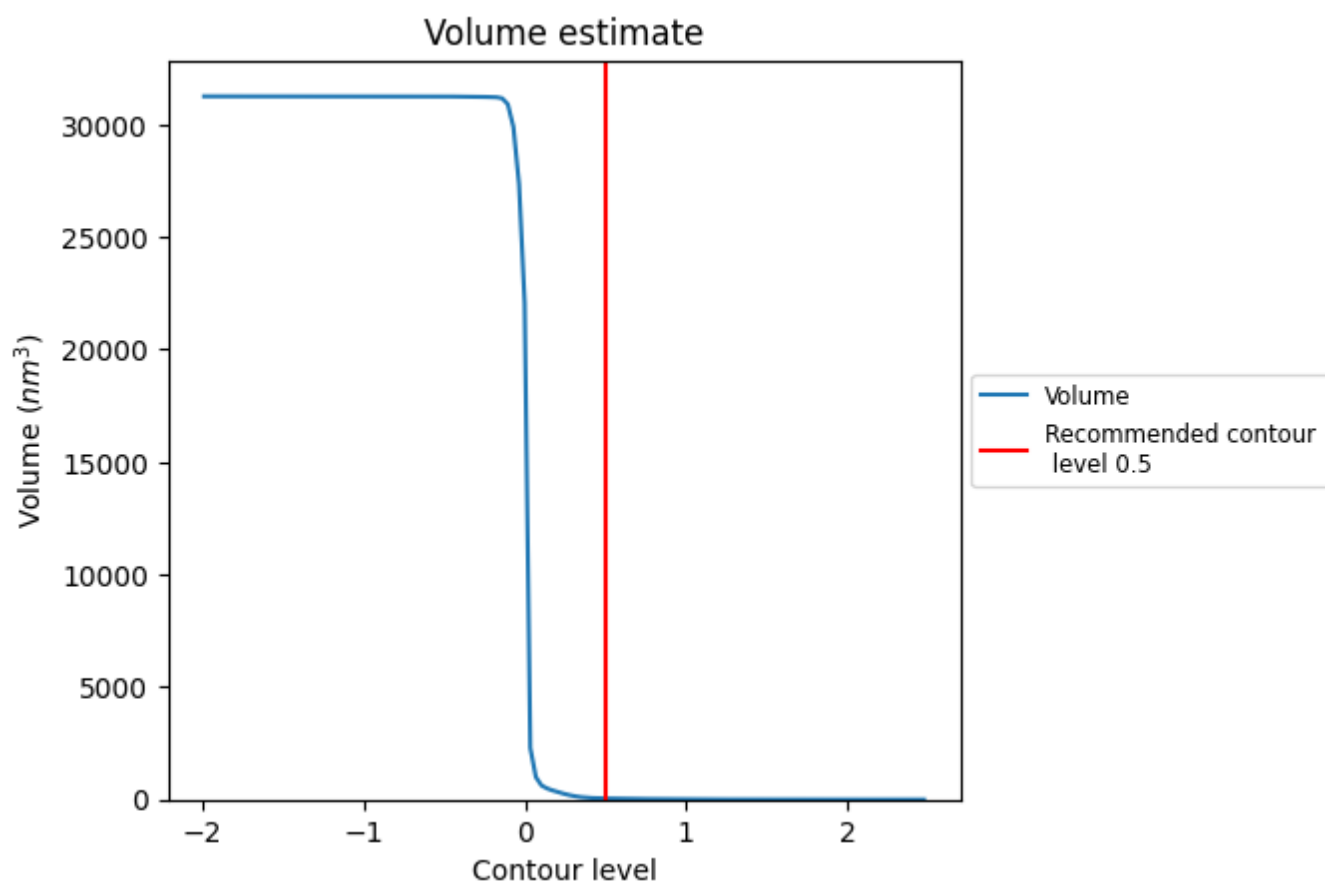
### 7.1 Map-value distribution [i](#)



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.



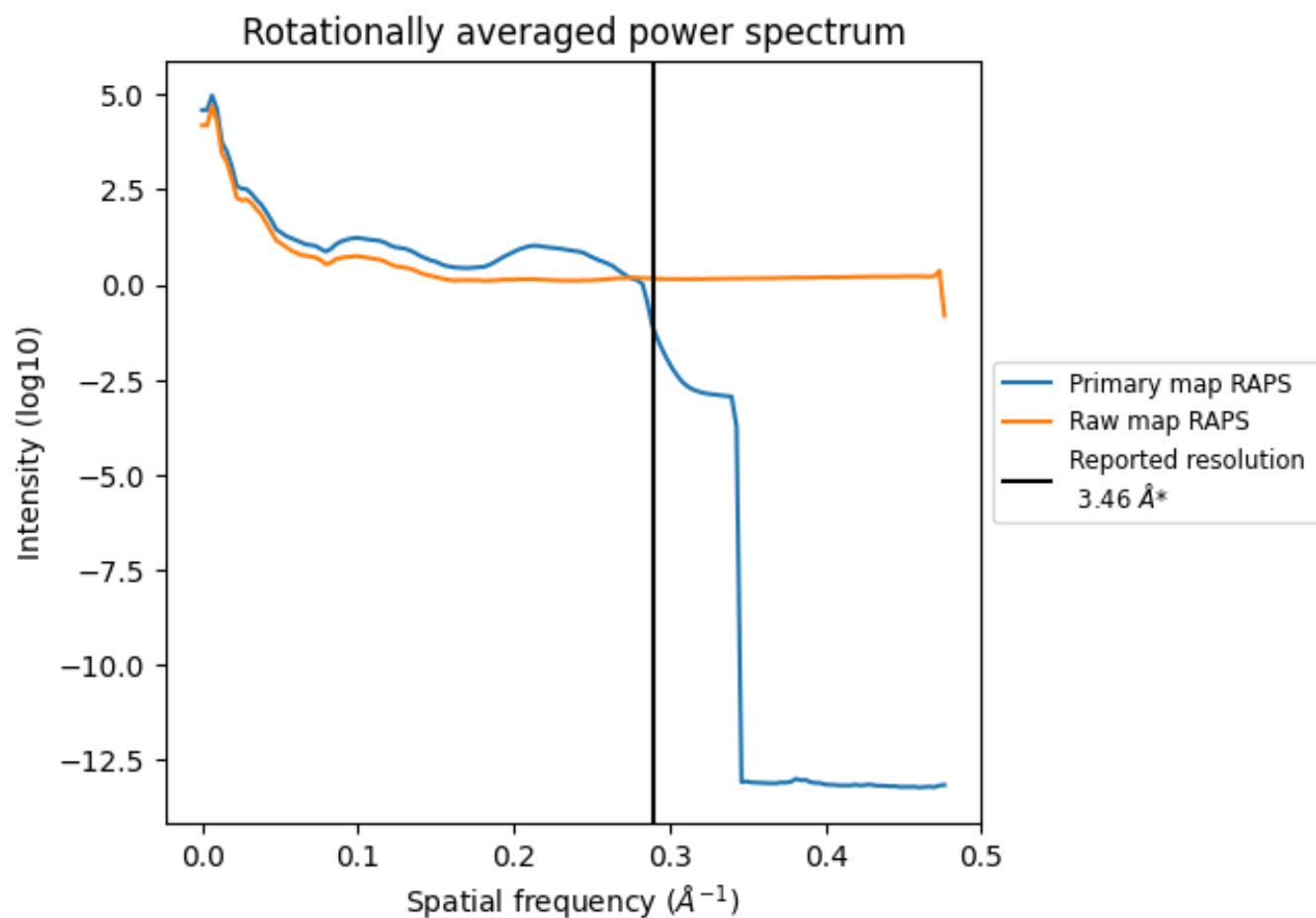
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49 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 ⓘ

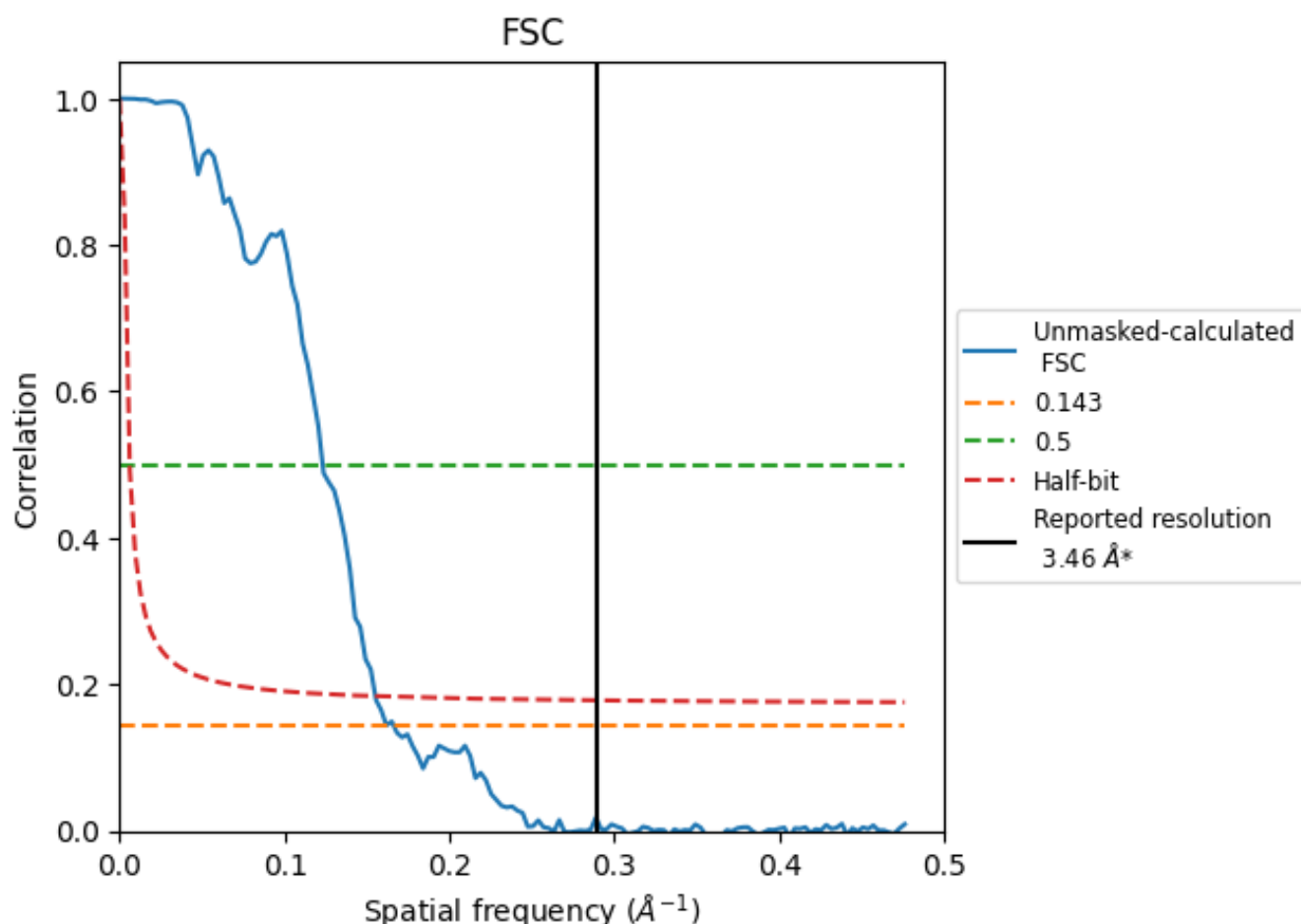


\*Reported resolution corresponds to spatial frequency of 0.289 Å<sup>-1</sup>

## 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 0.289 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

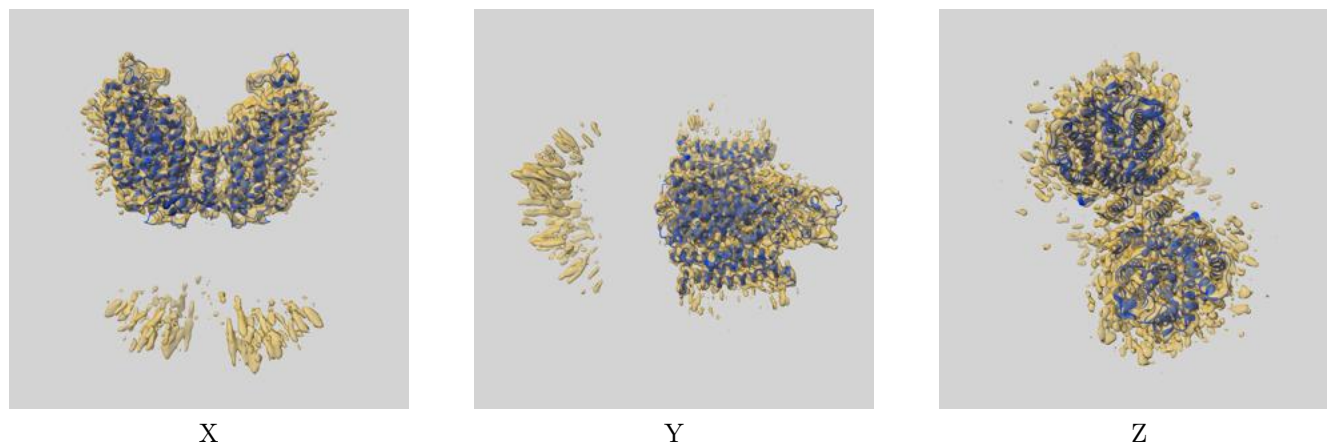
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.01	8.12	6.44

\*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 6.01 differs from the reported value 3.46 by more than 10 %

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

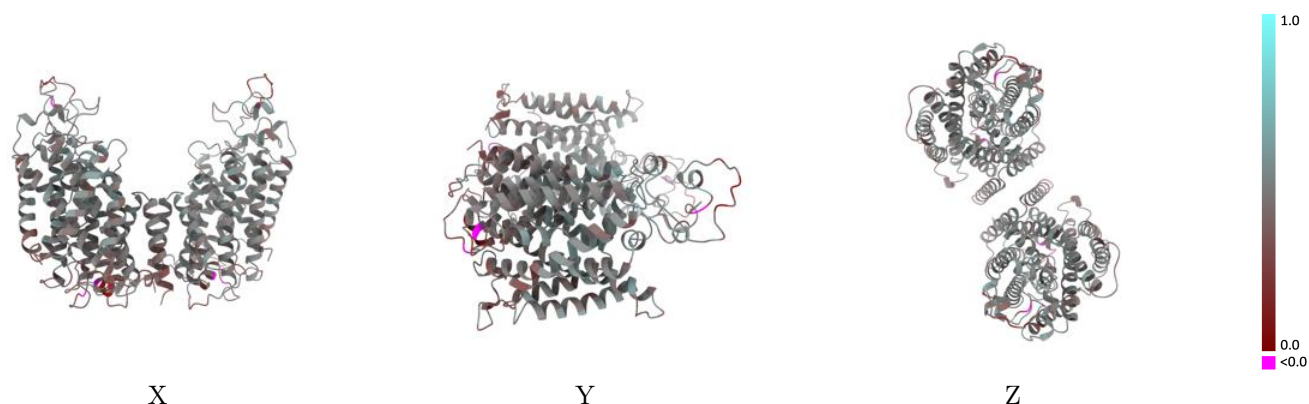
This section contains information regarding the fit between EMDB map EMD-20537 and PDB model 6PZT. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

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



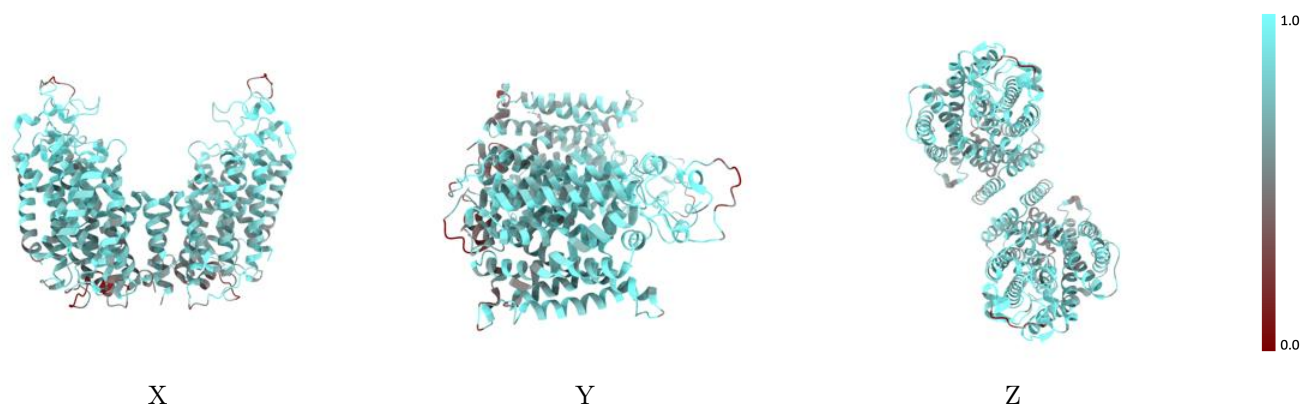
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



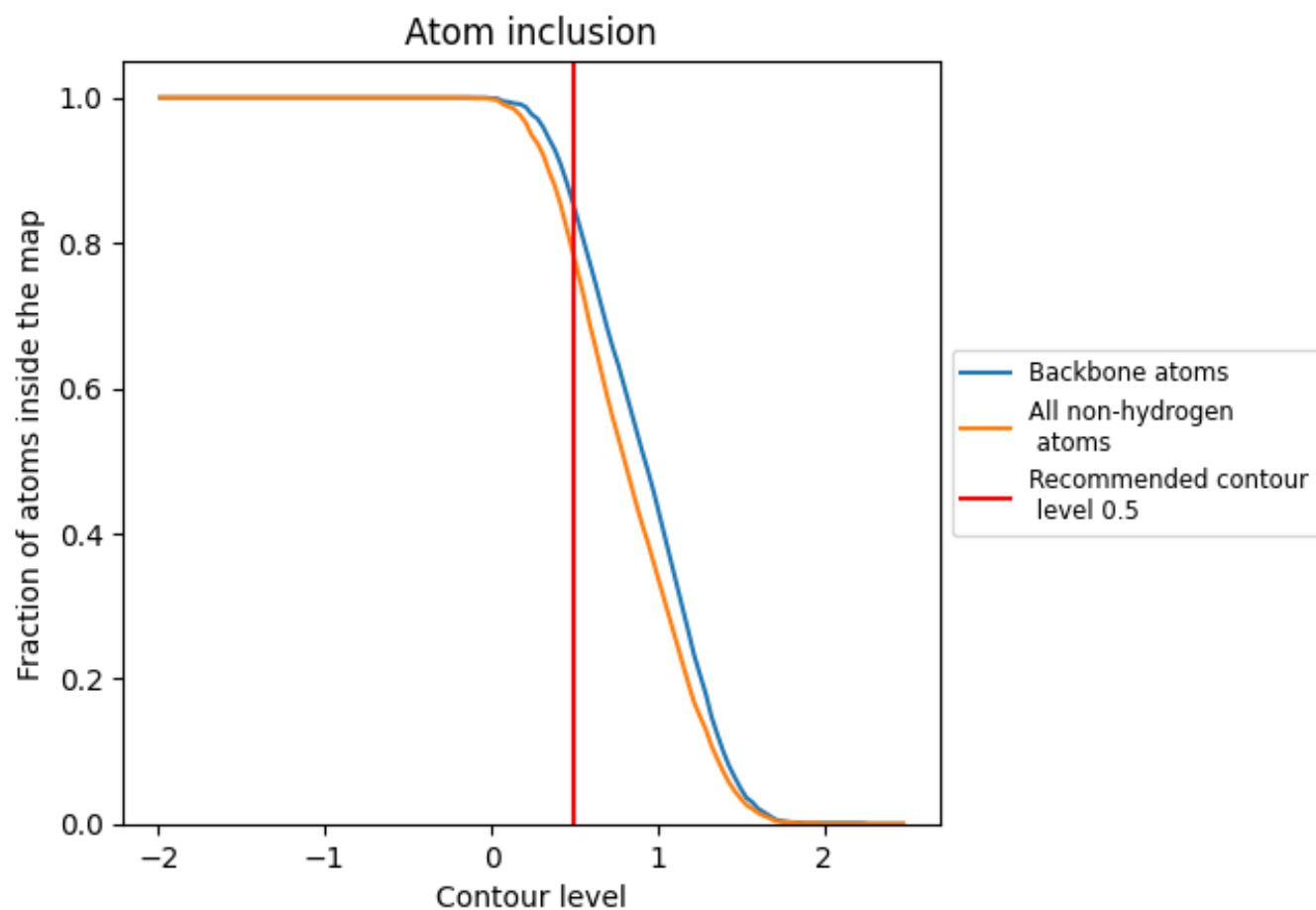
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7780	<div></div> 0.4540
A	<div></div> 0.7780	<div></div> 0.4550
B	<div></div> 0.7780	<div></div> 0.4540

