



wwPDB EM Validation Summary Report ⓘ

Oct 31, 2022 – 02:04 pm GMT

PDB ID : 7ZN7
EMDB ID : EMD-14802
Title : Cryo-EM structure of RCMV-E E27 bound to human DDB1 (deltaBPB) and rat STAT2 CCD
Authors : Lauer, S.; Spahn, C.M.T.; Schwefel, D.
Deposited on : 2022-04-20
Resolution : 3.78 Å(reported)
Based on initial model : 6ZUE

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.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

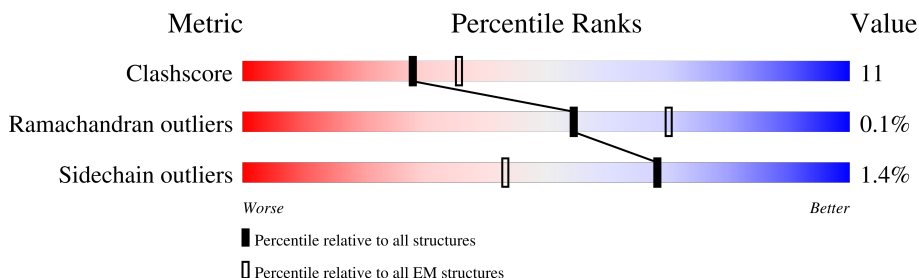
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.78 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	158937	4297
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 ≥ 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	840	
2	B	659	
3	D	845	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10497 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	783	6179	3927	1042	1176	34	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	PRO	-	expression tag	UNP Q16531
A	0	GLY	-	expression tag	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531

- Molecule 2 is a protein called B27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	400	3272	2074	586	590	22	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP K7Y9Z1
B	-1	PRO	-	expression tag	UNP K7Y9Z1
B	0	GLY	-	expression tag	UNP K7Y9Z1

- Molecule 3 is a protein called Signal transducer and activator of transcription.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	128	Total	C	N	O	S	0	0
			1045	665	188	188	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP Q5XI26
D	-1	PRO	-	expression tag	UNP Q5XI26
D	0	GLY	-	expression tag	UNP Q5XI26

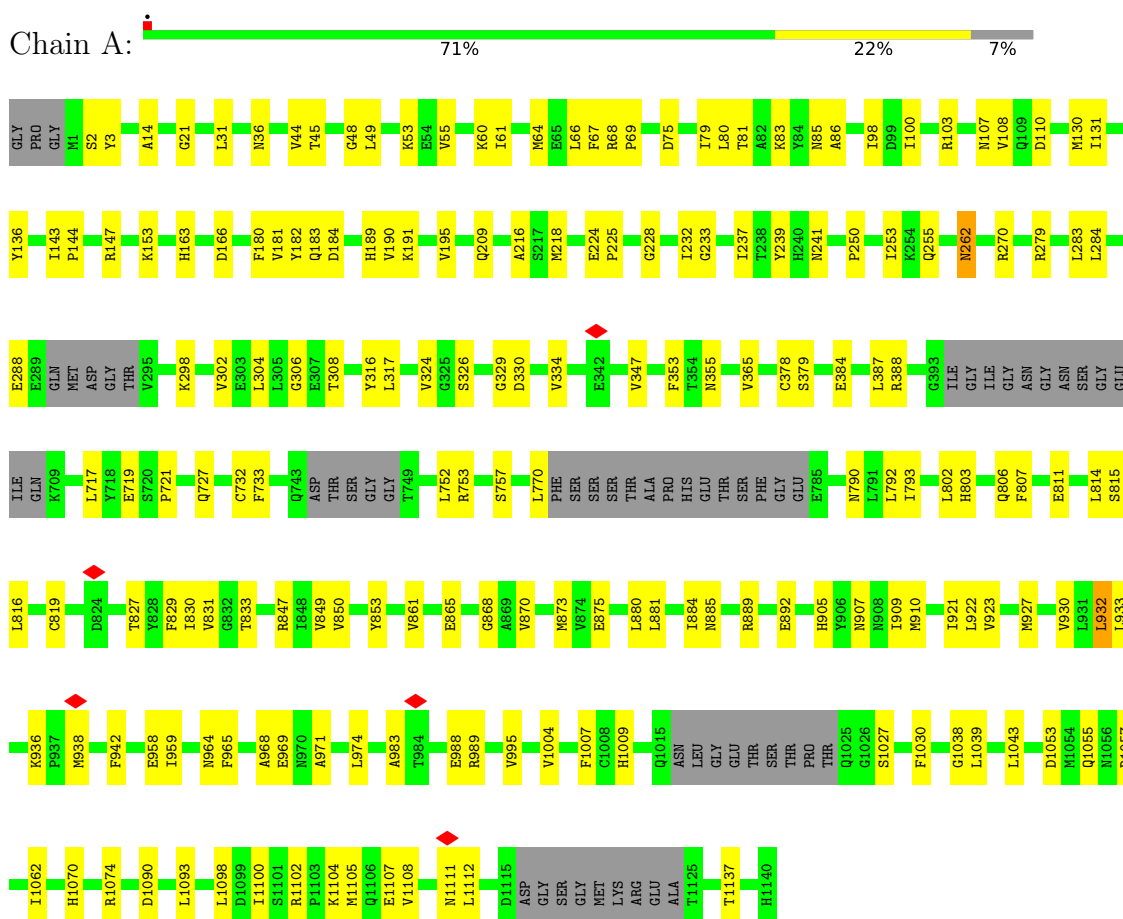
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	

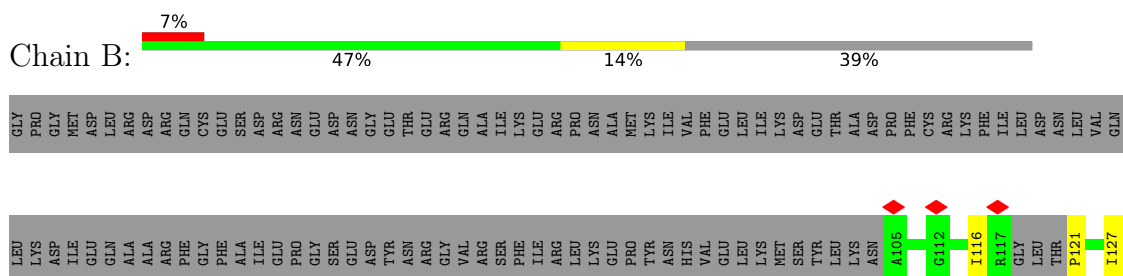
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA damage-binding protein 1



• Molecule 2: B27a



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	389784	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.694	Depositor
Minimum map value	-2.391	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	270.0, 270.0, 270.0	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.33	0/6286	0.57	0/8494
2	B	0.34	0/3334	0.55	0/4499
3	D	0.34	0/1050	0.65	0/1408
All	All	0.34	0/10670	0.57	0/14401

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	6179	0	6179	125	0
2	B	3272	0	3245	67	0
3	D	1045	0	1111	34	0
4	B	1	0	0	0	0
All	All	10497	0	10535	222	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 11.

The worst 5 of 222 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:B:487:ARG:O	2:B:491:ARG:HG3	1.86	0.76
1:A:103:ARG:NH1	1:A:147:ARG:HH12	1.84	0.75
1:A:830:ILE:HG12	1:A:850:VAL:HG23	1.69	0.73
1:A:182:TYR:HE1	1:A:191:LYS:HG3	1.54	0.72
1:A:1104:LYS:HA	1:A:1107:GLU:HG3	1.75	0.69

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	769/840 (92%)	714 (93%)	55 (7%)	0	100	100
2	B	386/659 (59%)	373 (97%)	12 (3%)	1 (0%)	41	74
3	D	120/845 (14%)	115 (96%)	5 (4%)	0	100	100
All	All	1275/2344 (54%)	1202 (94%)	72 (6%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	218	VAL

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	686/729 (94%)	682 (99%)	4 (1%)	86	92
2	B	351/579 (61%)	342 (97%)	9 (3%)	46	70
3	D	117/764 (15%)	114 (97%)	3 (3%)	46	70
All	All	1154/2072 (56%)	1138 (99%)	16 (1%)	68	82

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	220	LEU
3	D	159	LEU
2	B	215	LEU
2	B	336	LEU
2	B	208	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1034	ASN
2	B	209	GLN
2	B	508	HIS
2	B	319	HIS
1	A	262	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

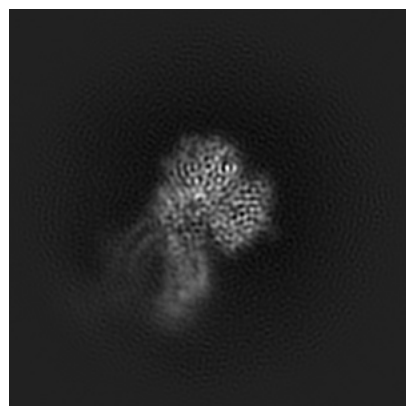
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14802. These allow visual inspection of the internal detail of the map and identification of artifacts.

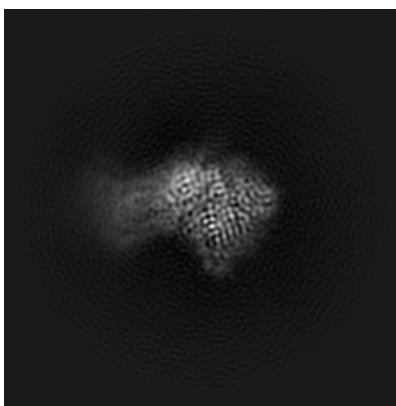
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

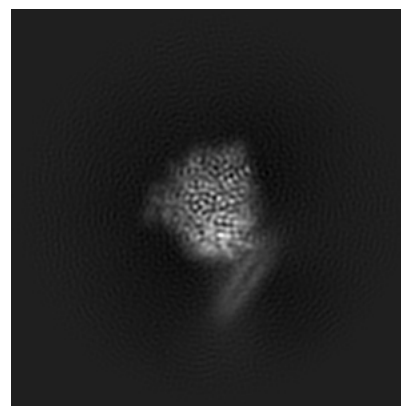
6.1.1 Primary map



X

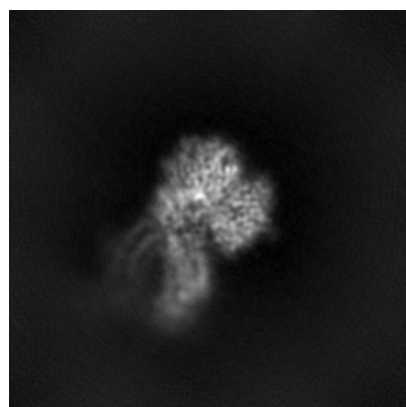


Y

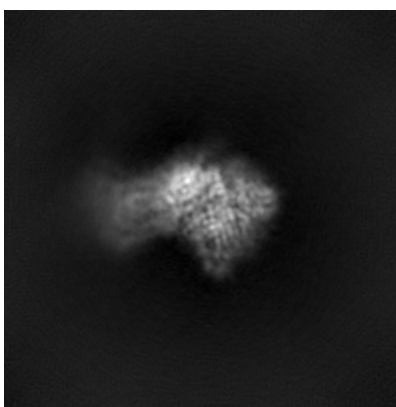


Z

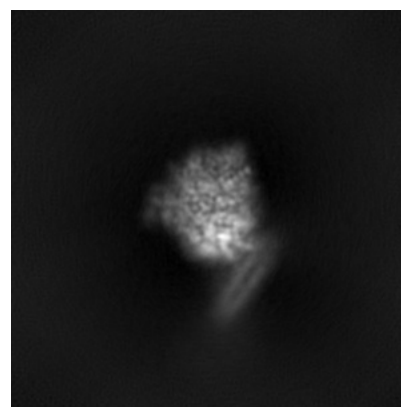
6.1.2 Raw map



X



Y

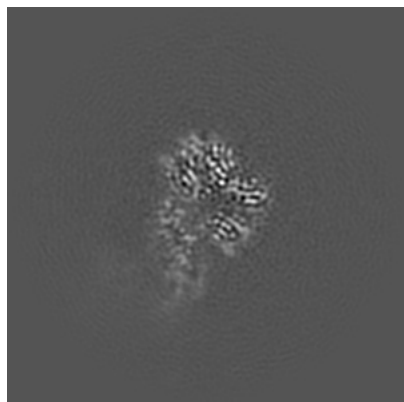


Z

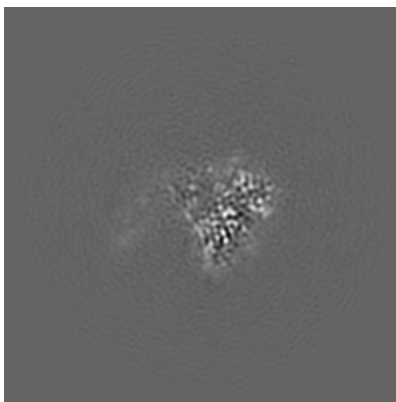
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

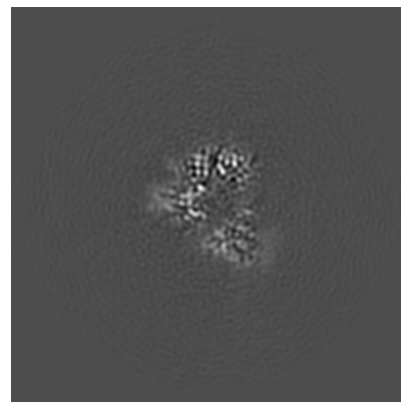
6.2.1 Primary map



X Index: 108

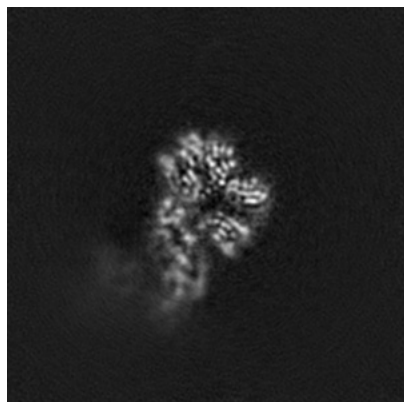


Y Index: 108

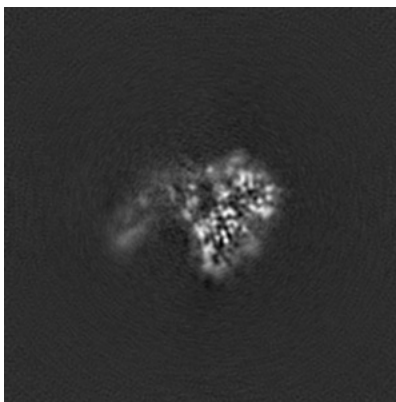


Z Index: 108

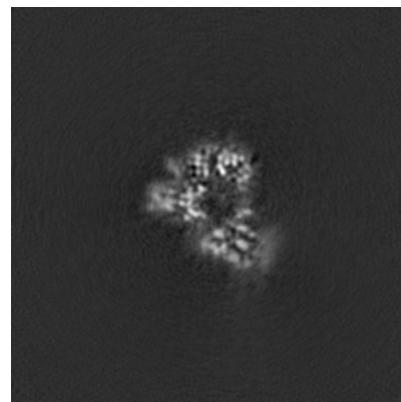
6.2.2 Raw map



X Index: 108



Y Index: 108

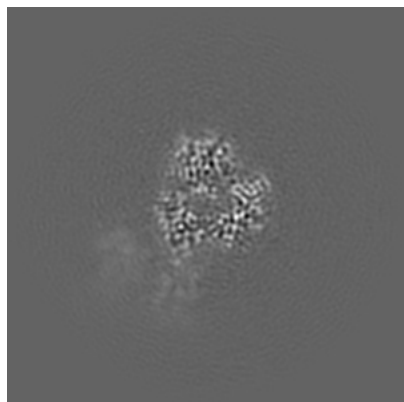


Z Index: 108

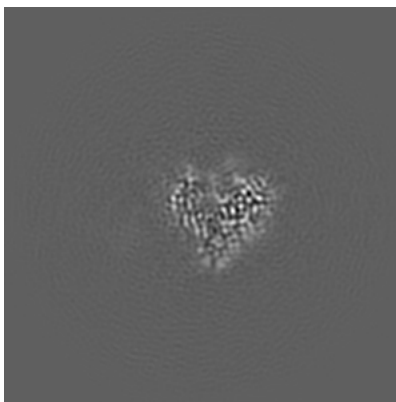
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

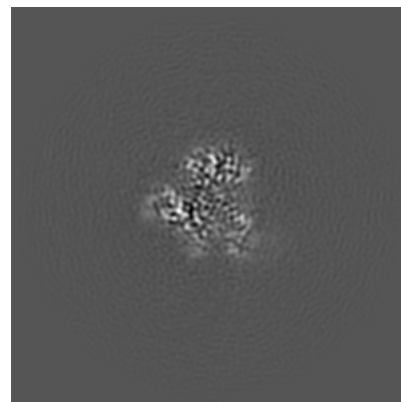
6.3.1 Primary map



X Index: 117

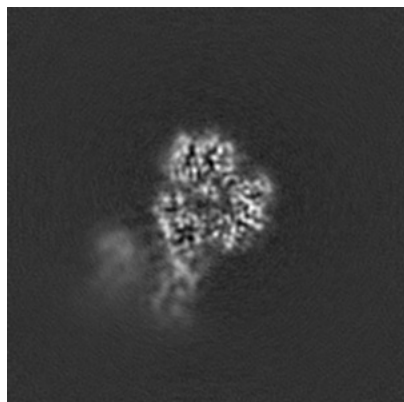


Y Index: 113

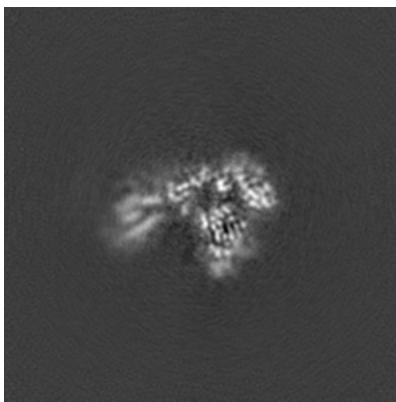


Z Index: 115

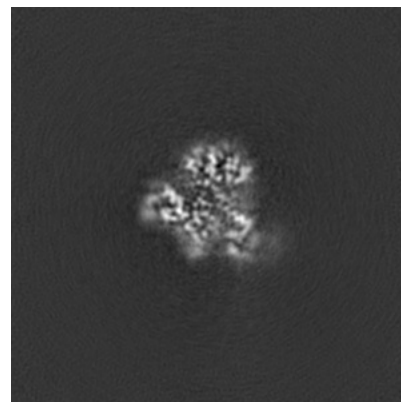
6.3.2 Raw map



X Index: 116



Y Index: 104

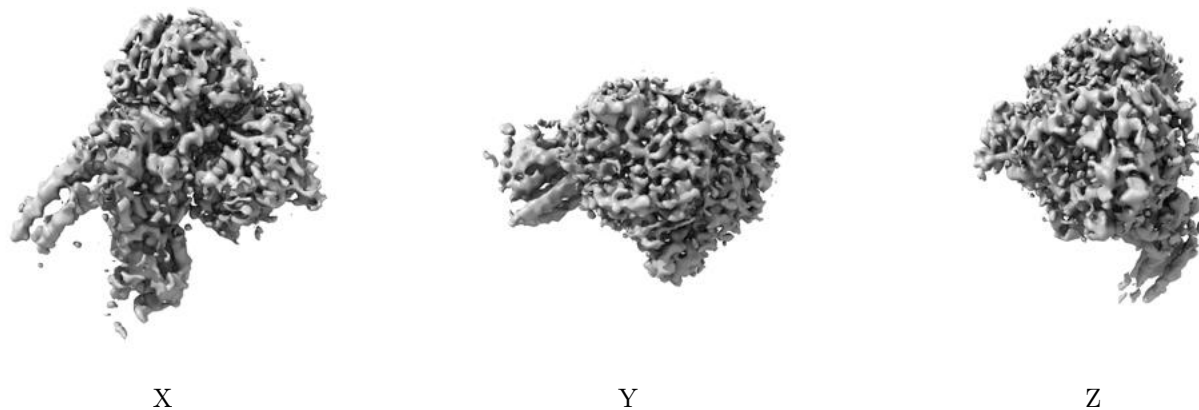


Z Index: 115

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

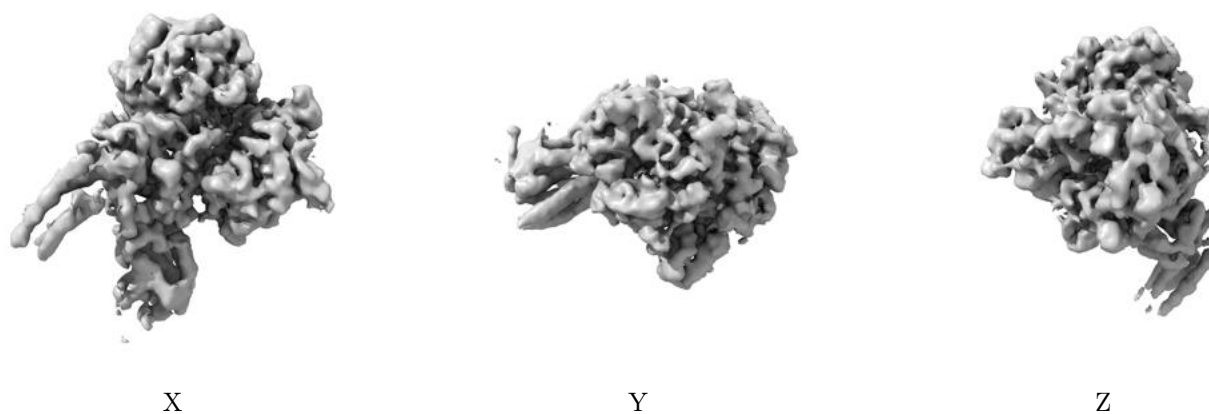
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

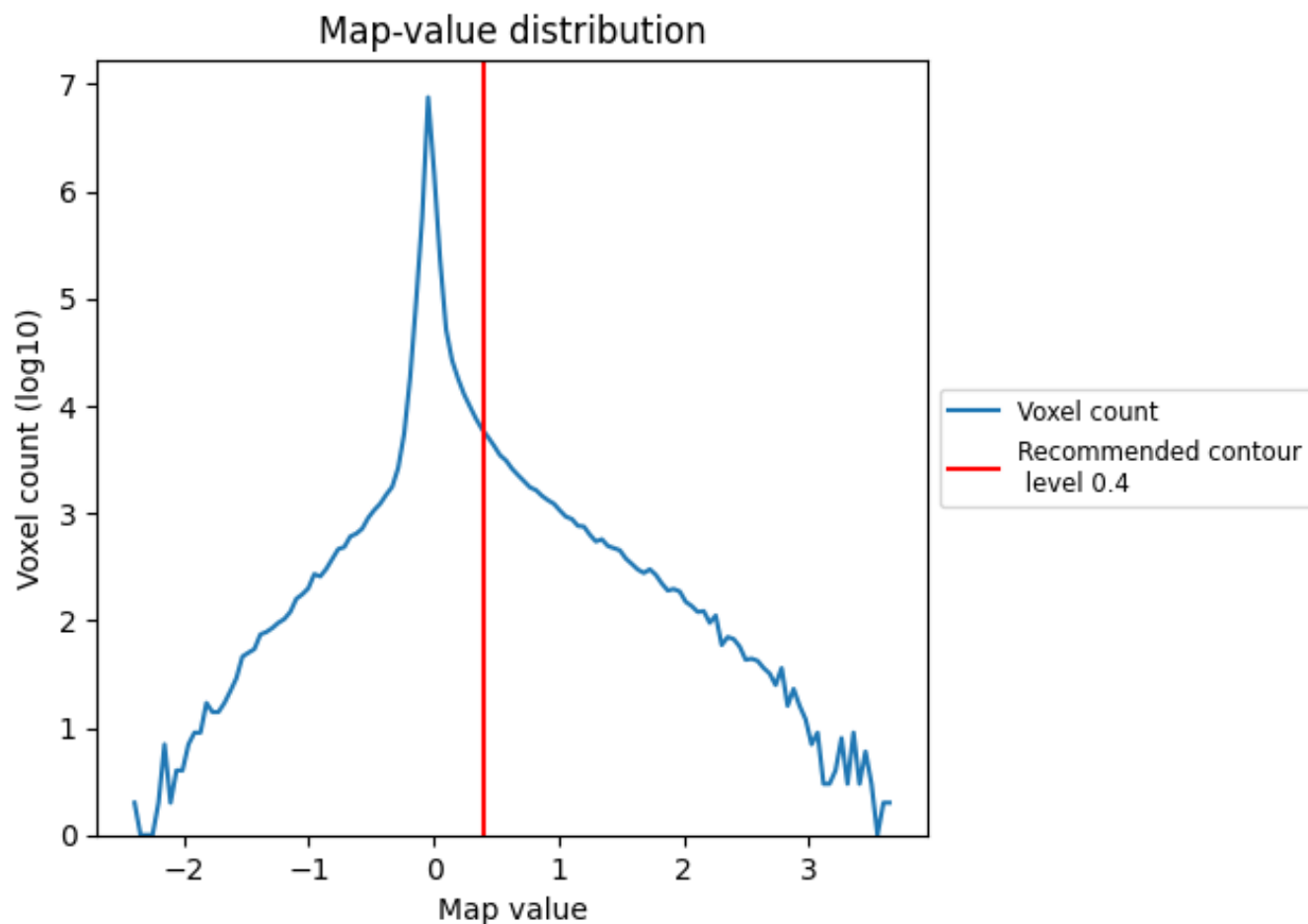
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

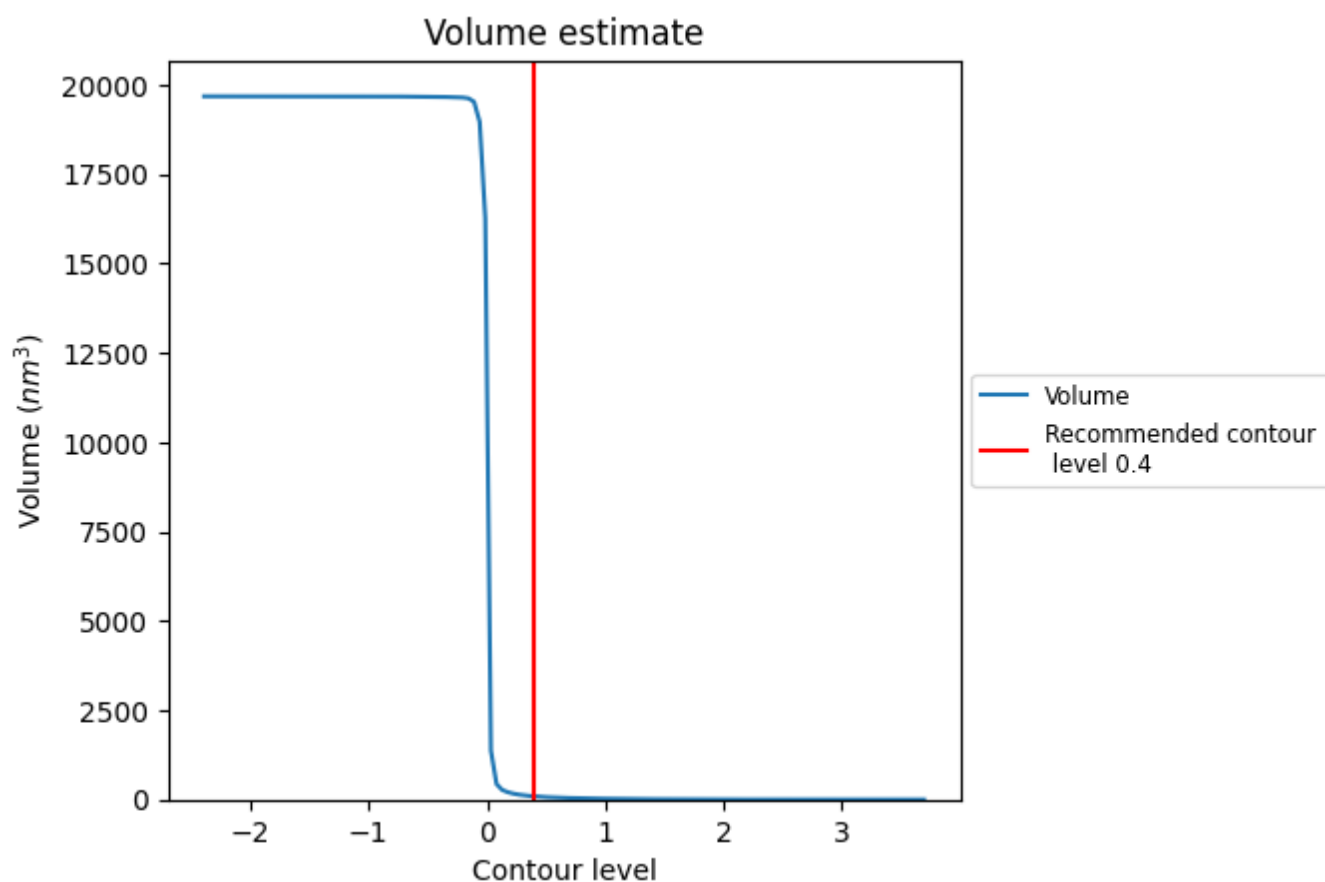
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

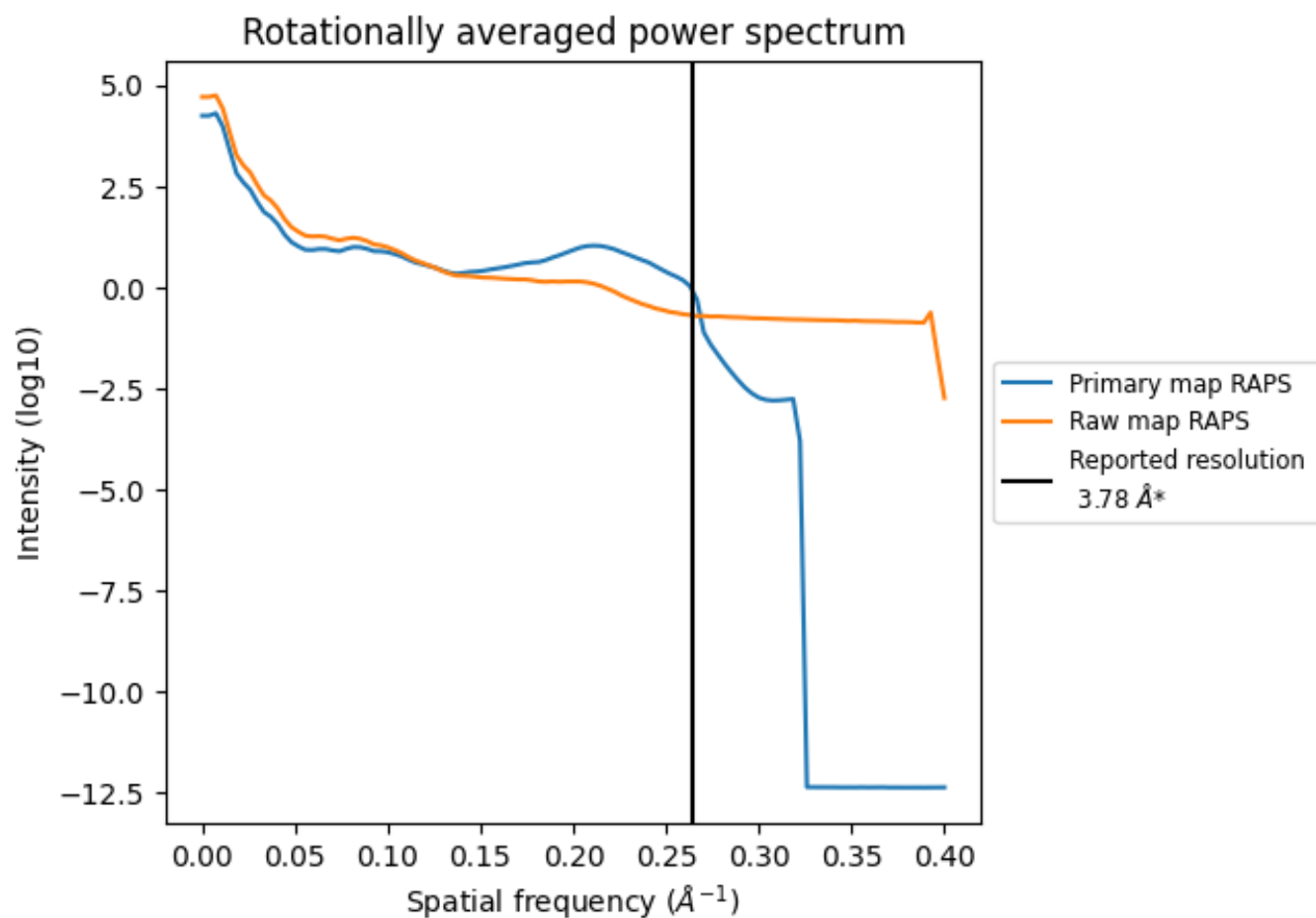
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm³; this corresponds to an approximate mass of 82 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 ⓘ

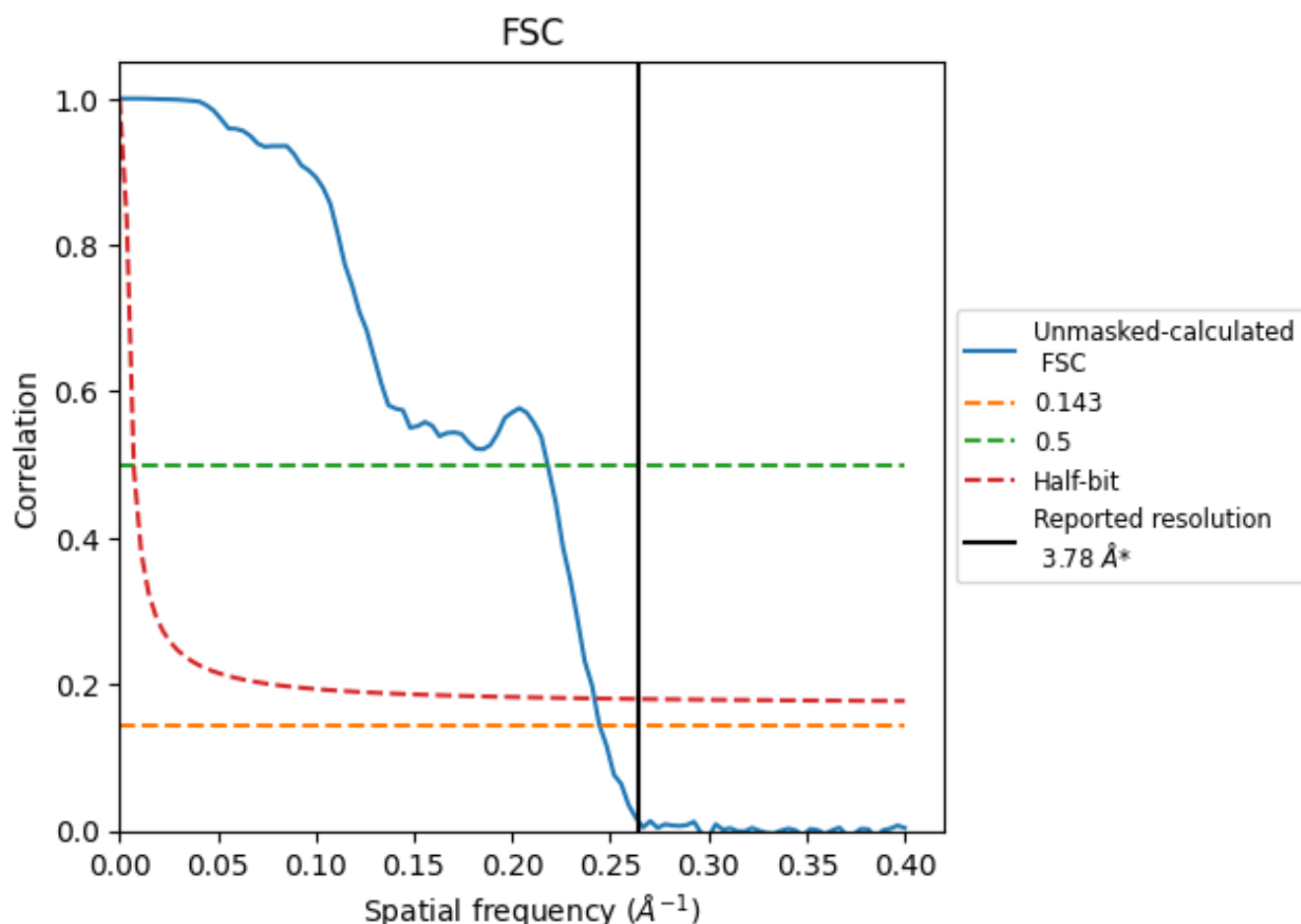


*Reported resolution corresponds to spatial frequency of 0.265 Å⁻¹

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 0.265 \AA^{-1}

8.2 Resolution estimates [i](#)

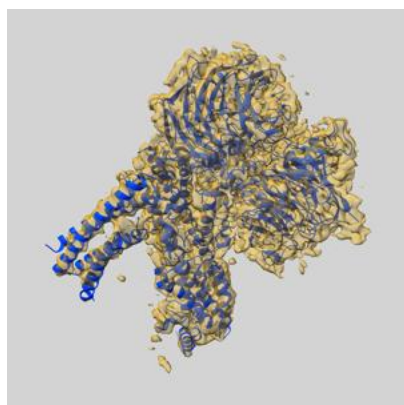
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	4.59	4.13

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

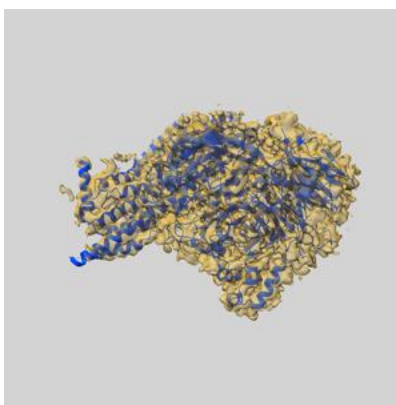
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14802 and PDB model 7ZN7. Per-residue inclusion information can be found in section [3](#) on page [5](#).

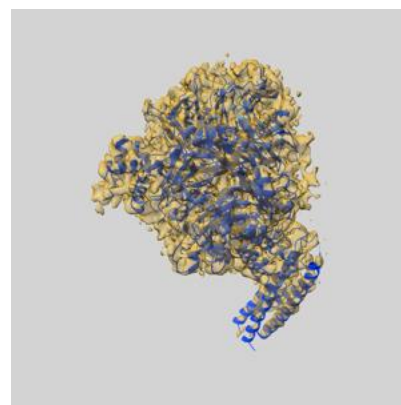
9.1 Map-model overlay [i](#)



X



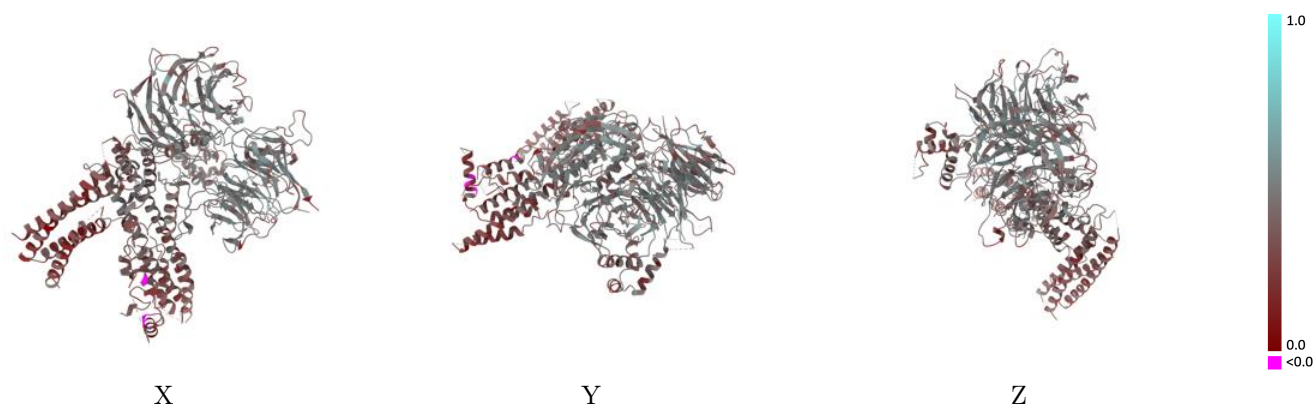
Y



Z

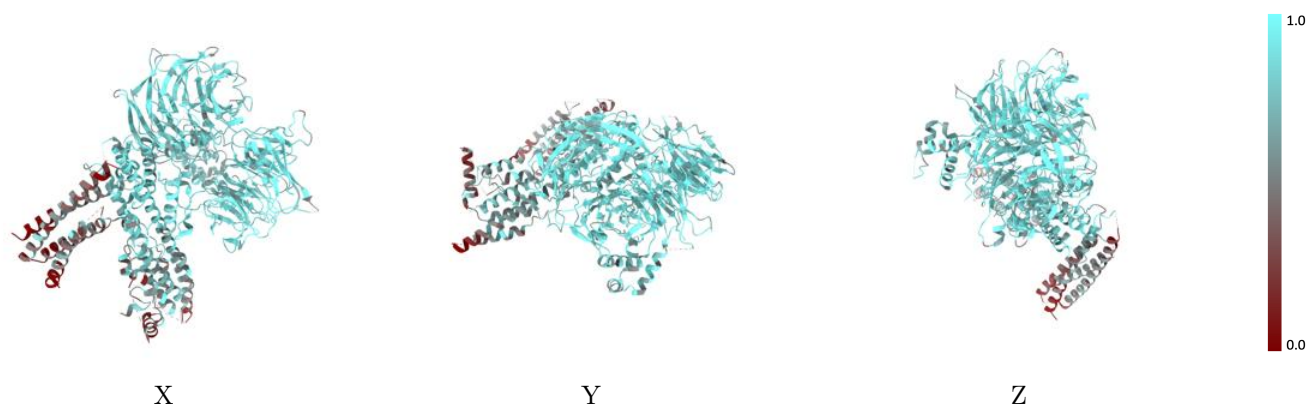
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



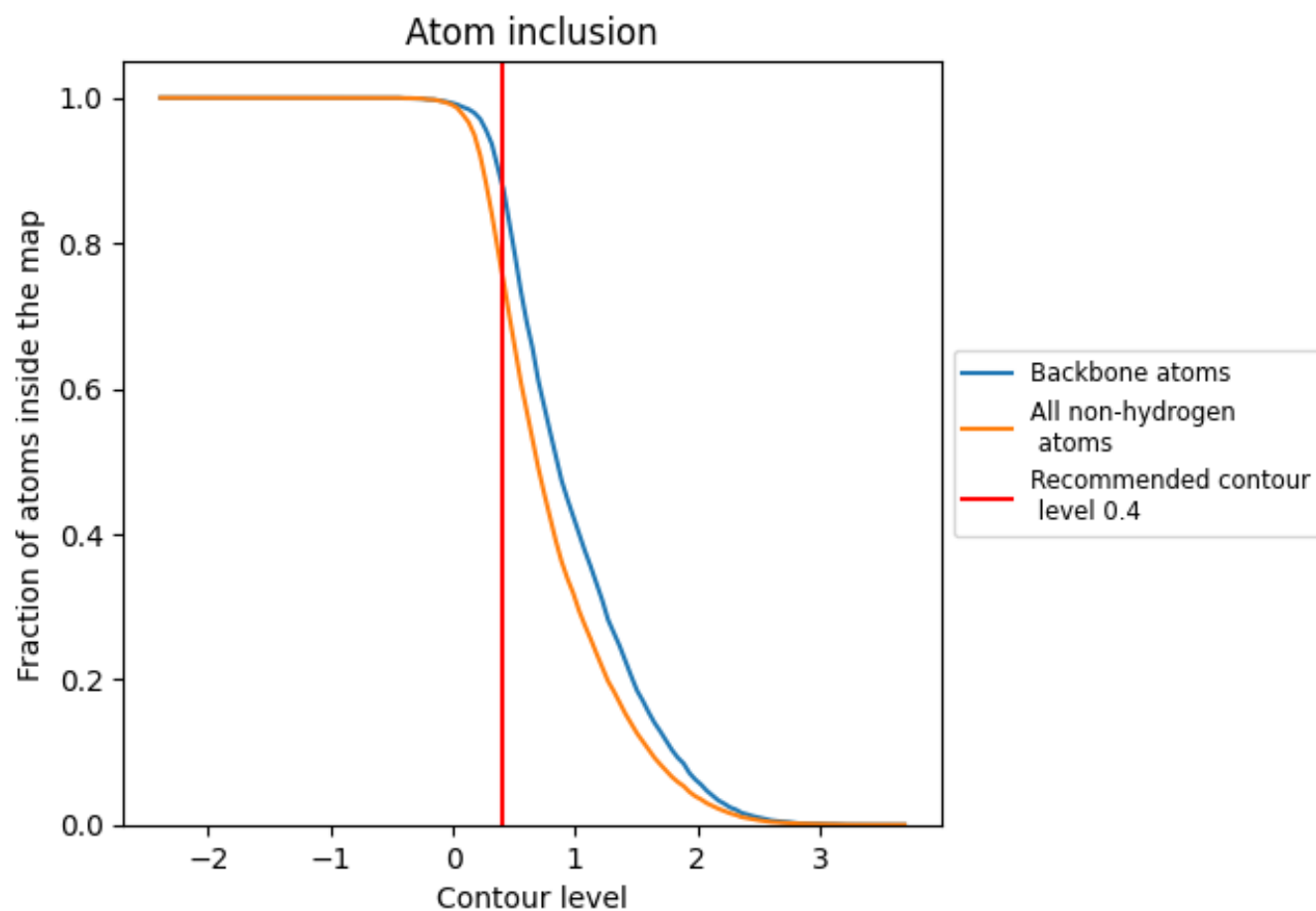
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7600	<div></div> 0.3950
A	<div></div> 0.8487	<div></div> 0.4400
B	<div></div> 0.7138	<div></div> 0.3530
D	<div></div> 0.3739	<div></div> 0.2650

