



wwPDB EM Validation Summary Report ⓘ

Dec 29, 2024 – 09:18 AM EST

PDB ID : 7NS3
EMDB ID : EMD-12559
Title : Substrate receptor scaffolding module of yeast Chelator-GID SR4 E3 ubiquitin
ligase bound to Fbp1 substrate
Authors : Sherpa, D.; Chrustowicz, J.; Prabu, J.R.; Schulman, B.A.
Deposited on : 2021-03-05
Resolution : 3.50 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) : 2.40

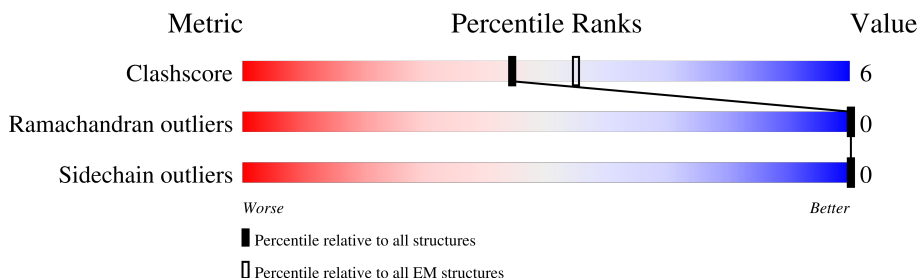
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	5	921	
2	8	493	
3	1	958	
4	9	516	
5	4	362	
6	Fb	348	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14445 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 Vacuolar import and degradation protein 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	762	Total	C	N	O	S	0	0
			5919	3857	978	1046	38		

- Molecule 2 is a protein called Glucose-induced degradation protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	8	325	Total	C	N	O	S	0	0
			2597	1673	446	466	12		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	456	SER	-	expression tag	UNP P40208
8	457	ASP	-	expression tag	UNP P40208
8	458	GLU	-	expression tag	UNP P40208
8	459	ASN	-	expression tag	UNP P40208
8	460	LEU	-	expression tag	UNP P40208
8	461	TYR	-	expression tag	UNP P40208
8	462	PHE	-	expression tag	UNP P40208
8	463	GLN	-	expression tag	UNP P40208
8	464	SER	-	expression tag	UNP P40208
8	465	GLY	-	expression tag	UNP P40208
8	466	TRP	-	expression tag	UNP P40208
8	467	SER	-	expression tag	UNP P40208
8	468	HIS	-	expression tag	UNP P40208
8	469	PRO	-	expression tag	UNP P40208
8	470	GLN	-	expression tag	UNP P40208
8	471	PHE	-	expression tag	UNP P40208
8	472	GLU	-	expression tag	UNP P40208
8	473	LYS	-	expression tag	UNP P40208
8	474	GLY	-	expression tag	UNP P40208
8	475	GLY	-	expression tag	UNP P40208
8	476	GLY	-	expression tag	UNP P40208

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Chain	Residue	Modelled	Actual	Comment	Reference
8	477	SER	-	expression tag	UNP P40208
8	478	GLY	-	expression tag	UNP P40208
8	479	GLY	-	expression tag	UNP P40208
8	480	GLY	-	expression tag	UNP P40208
8	481	SER	-	expression tag	UNP P40208
8	482	GLY	-	expression tag	UNP P40208
8	483	GLY	-	expression tag	UNP P40208
8	484	SER	-	expression tag	UNP P40208
8	485	ALA	-	expression tag	UNP P40208
8	486	TRP	-	expression tag	UNP P40208
8	487	SER	-	expression tag	UNP P40208
8	488	HIS	-	expression tag	UNP P40208
8	489	PRO	-	expression tag	UNP P40208
8	490	GLN	-	expression tag	UNP P40208
8	491	PHE	-	expression tag	UNP P40208
8	492	GLU	-	expression tag	UNP P40208
8	493	LYS	-	expression tag	UNP P40208

- Molecule 3 is a protein called BJ4_G0018240.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	424	Total	C	N	O	S	0	0
			3272	2120	541	600	11		

- Molecule 4 is a protein called Protein FYV10.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	9	136	Total	C	N	O	S	0	0
			1065	703	178	182	2		

- Molecule 5 is a protein called Vacuolar import and degradation protein 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	199	Total	C	N	O	S	0	0
			1570	1018	257	290	5		

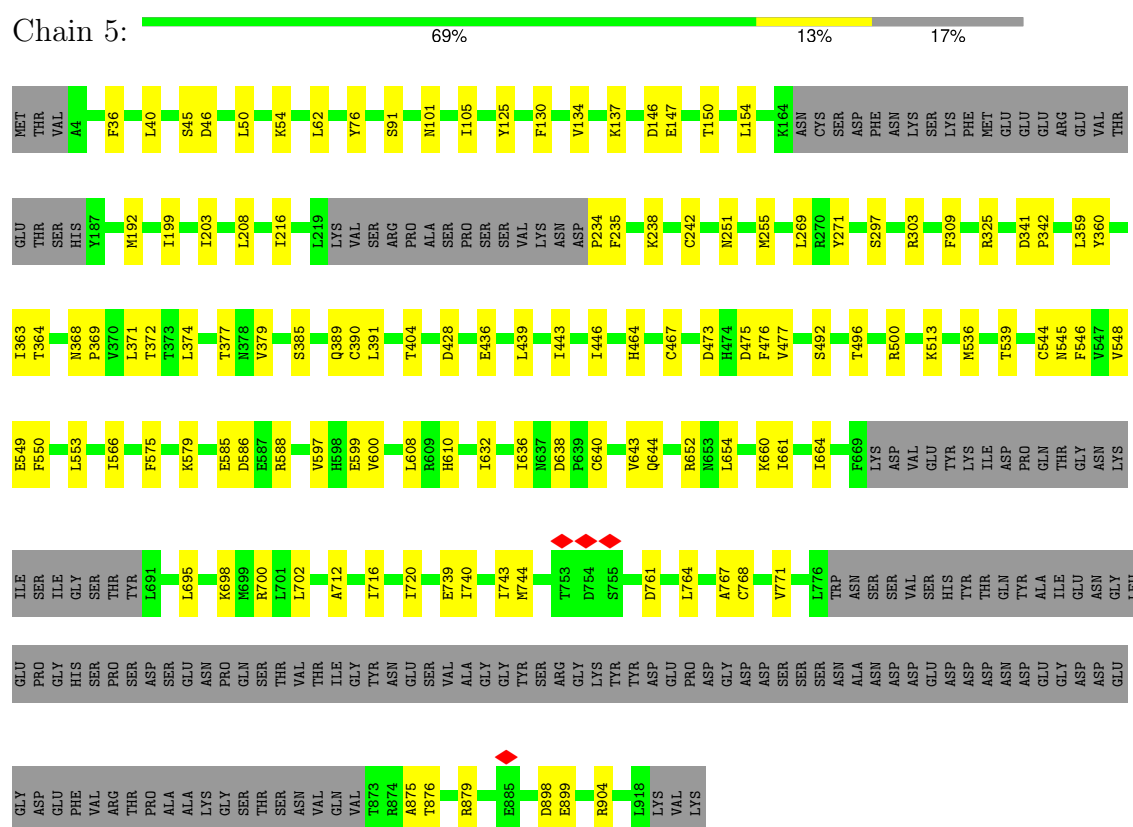
- Molecule 6 is a protein called Fructose-bisphosphatase.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	Fb	3	Total	C	N	O	0	0
			22	15	3	4		

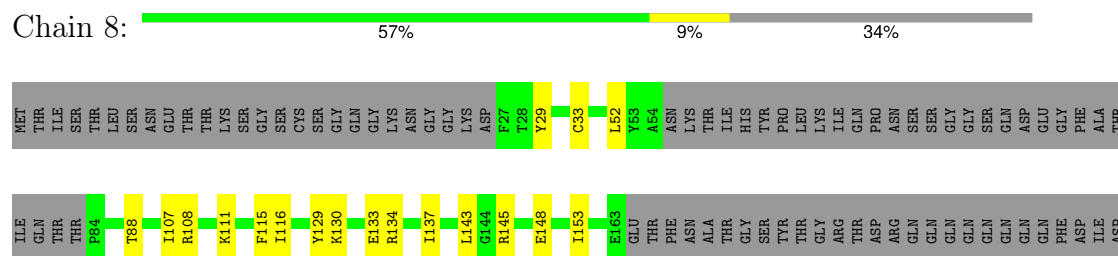
3 Residue-property plots

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: Vacuolar import and degradation protein 28



- Molecule 2: Glucose-induced degradation protein 8



MET	ARG	THR	LYS	GLU
P1	ALA	HIS	GLN	GLN
T2	GLU	LEU	PRO	ALA
L3	LEU	VAL	GLN	GLY
VAL	VAL	LEU	ALA	GLY
ASN	ASN	THR	LYS	LYS
GLY	LEU	LEU	ASN	ALA
PRO	VAL	GLY	ASN	VAL
ARG	GLY	ASP	ASN	ASN
LEU	LEU	PRO	LYS	ASP
ASP	ALA	VAL	ARG	ARG
ASP	GLY	ASP	PHE	GLY
THR	ALA	GLY	SER	GLU
ASP	SER	SER	ALA	ARG
ILE	ASN	THR	ARG	ILE
ILE	PHE	LEU	THR	ILE
THR	THR	ASP	TYR	THR
PRO	GLY	ASP	VAL	LEU
ARG	ASP	THR	GLY	LEU
PHE	VAL	ASN	SER	VAL
ILE	GLN	VAL	MET	PRO
ILE	GLN	SER	VAL	SER
GLU	LYS	GLY	ALA	HIS
HIS	LEU	PHE	ASP	ILE
GLN	PRO	ILE	VAL	ASP
LYS	ILE	ALA	HIS	LYS
LEU	PHE	THR	ARG	SER
THR	VAL	HIS	THR	THR
ASP	LEU	THR	ILE	GLY
ILE	LEU	PRO	PRO	SER
LYS	ASN	PRO	PHE	GLY
PHE	ALA	GLN	ALA	GLU
ASN	LYS	LYS	TYR	GLY
ASP	MET	SER	ASN	THR
ALA	ARG	GLY	GLU	LEU
THR	ALA	THR	ASN	LEU
GLY	SER	ILE	ILE	TYR
ASP	GLY	ASP	ILE	GLY
PHE	ILE	VAL	ASN	ASN
THR	ILE	LEU	GLY	GLY
VAL	LYS	ARG	ASN	LYS
LEU	VAL	CYS	THR	LEU
LEU	LEU	CYS	GLY	LEU
VAL	VAL	LYS	THR	TYR
ARG	VAL	GLY	ALA	ALA
ASP	GLY	LEU	ILE	PHE
ASP	THR	TYR	ARG	PRO
GLY	GLY	TRP	THR	MET
GLU	SER	ASN	PHE	GLU
ARG	ALA	GLU	ILE	ALA
ILE	ARG	THR	THR	PHE
ILE	THR	ILE	ILE	LEU
LEU	PRO	LYS	GLY	LEU
ASP	ASN	SER	LYS	GLN
THR	THR	THR	GLN	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74929	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 ($e^-/\text{\AA}^2$)	79.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.203	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.045	Depositor
Map size (\AA)	455.04, 455.04, 455.04	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.58, 1.58, 1.58	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	5	0.28	0/6032	0.43	0/8191
2	8	0.28	0/2648	0.43	0/3579
3	1	0.29	0/3342	0.43	0/4542
4	9	0.26	0/1087	0.39	0/1471
5	4	0.28	0/1614	0.46	0/2192
6	Fb	0.19	0/22	0.56	0/29
All	All	0.28	0/14745	0.43	0/20004

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	5	5919	0	5942	78	0
2	8	2597	0	2539	35	0
3	1	3272	0	3063	46	0
4	9	1065	0	1007	12	0
5	4	1570	0	1426	22	0
6	Fb	22	0	27	0	0
All	All	14445	0	14004	175	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 175 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)
1:5:652:ARG:NH2	5:4:358:SER:OG	2.08	0.86
5:4:163:LEU:HB3	5:4:185:ALA:HB3	1.70	0.74
1:5:134:VAL:HG21	1:5:199:ILE:HD11	1.75	0.69
5:4:117:THR:HG23	5:4:150:ASP:HB2	1.77	0.66
5:4:218:GLU:O	5:4:222:ASN:ND2	2.28	0.66

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	5	752/921 (82%)	711 (94%)	41 (6%)	0	100	100
2	8	309/493 (63%)	290 (94%)	19 (6%)	0	100	100
3	1	406/958 (42%)	375 (92%)	31 (8%)	0	100	100
4	9	128/516 (25%)	119 (93%)	9 (7%)	0	100	100
5	4	191/362 (53%)	177 (93%)	14 (7%)	0	100	100
6	Fb	1/348 (0%)	1 (100%)	0	0	100	100
All	All	1787/3598 (50%)	1673 (94%)	114 (6%)	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	5	636/849 (75%)	636 (100%)	0	100	100
2	8	279/439 (64%)	279 (100%)	0	100	100
3	1	333/864 (38%)	333 (100%)	0	100	100
4	9	105/487 (22%)	105 (100%)	0	100	100
5	4	161/329 (49%)	161 (100%)	0	100	100
6	Fb	3/295 (1%)	3 (100%)	0	100	100
All	All	1517/3263 (46%)	1517 (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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	4	222	ASN

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.

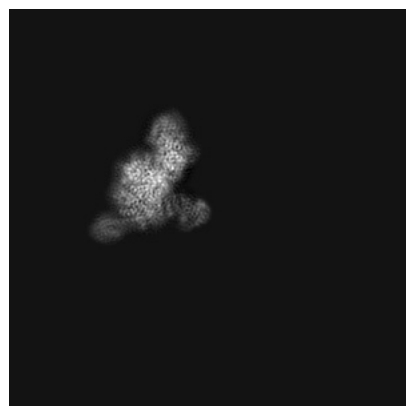
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12559. These allow visual inspection of the internal detail of the map and identification of artifacts.

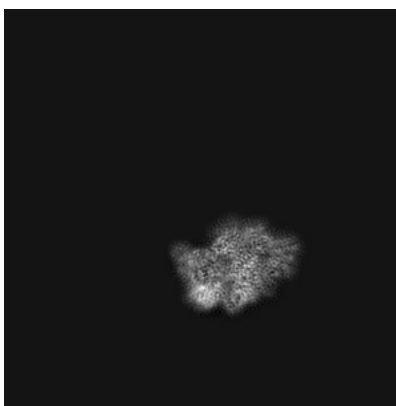
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

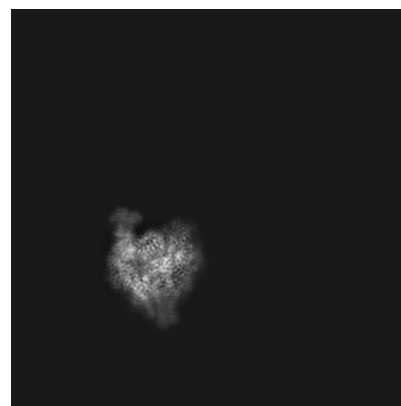
6.1.1 Primary map



X

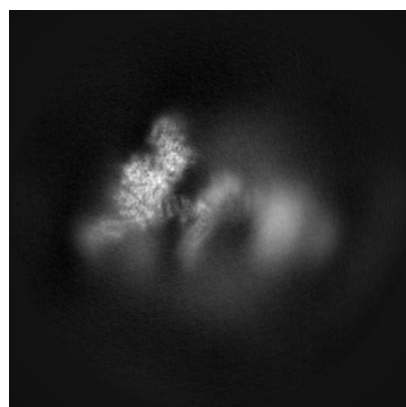


Y

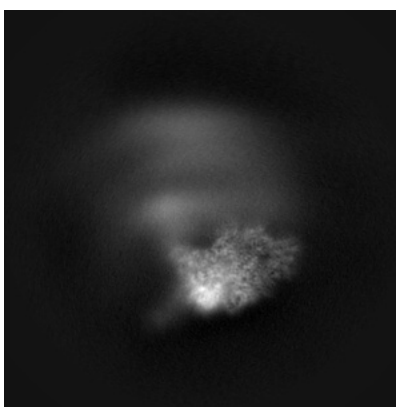


Z

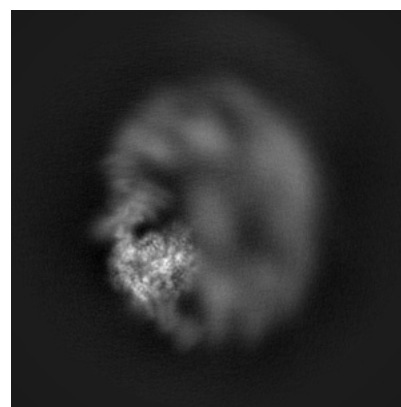
6.1.2 Raw map



X



Y

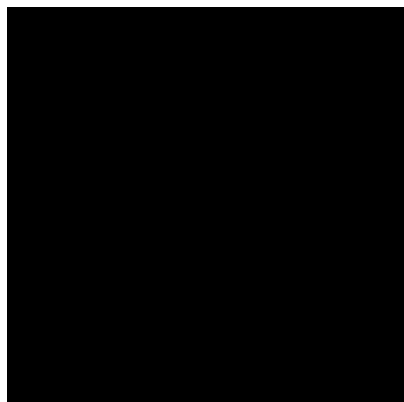


Z

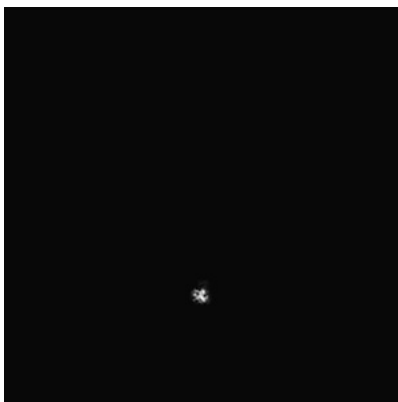
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

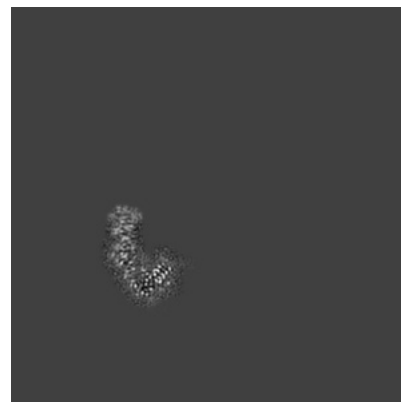
6.2.1 Primary map



X Index: 144

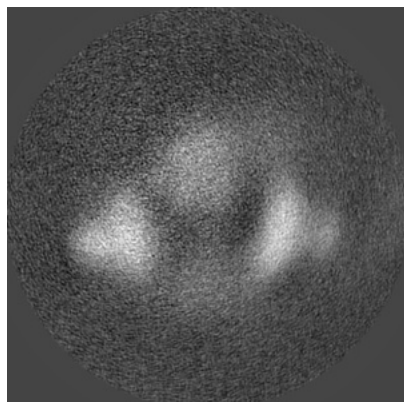


Y Index: 144

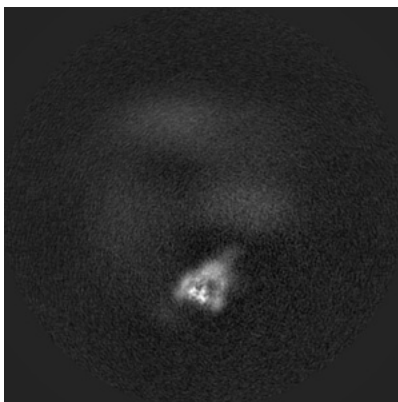


Z Index: 144

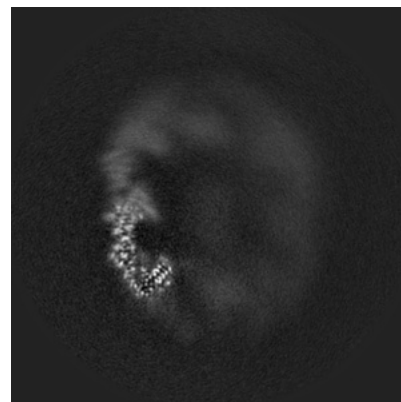
6.2.2 Raw map



X Index: 144



Y Index: 144

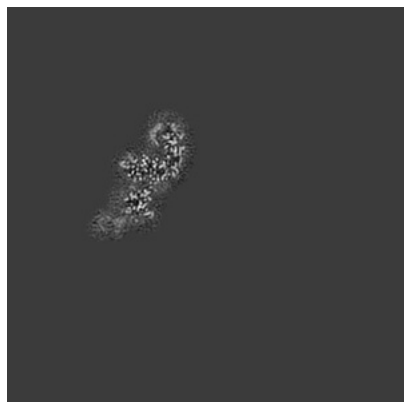


Z Index: 144

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

6.3 Largest variance slices [i](#)

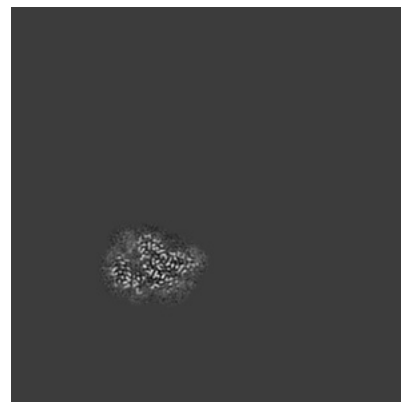
6.3.1 Primary map



X Index: 103

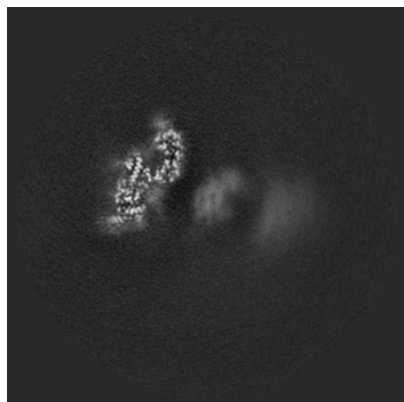


Y Index: 102

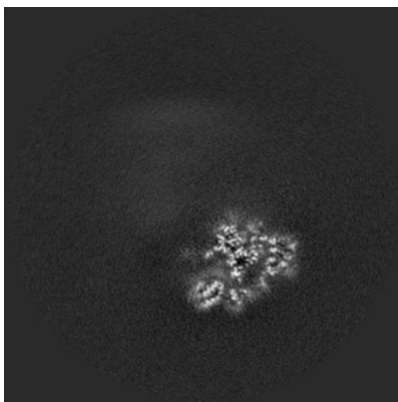


Z Index: 167

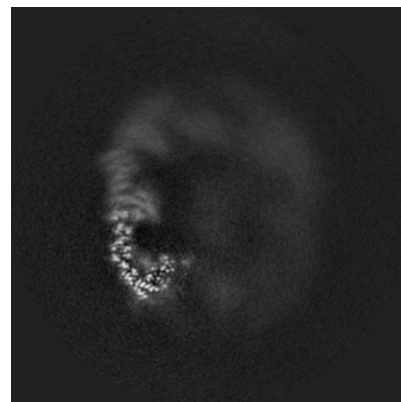
6.3.2 Raw map



X Index: 96



Y Index: 108

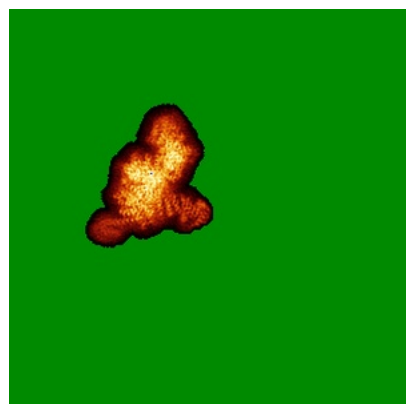


Z Index: 148

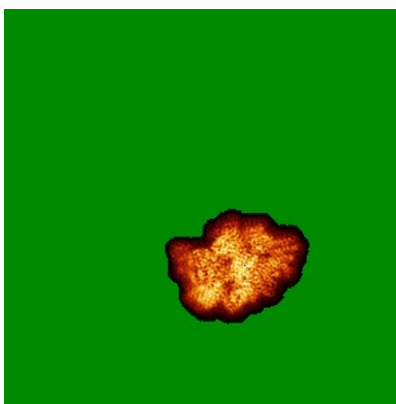
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

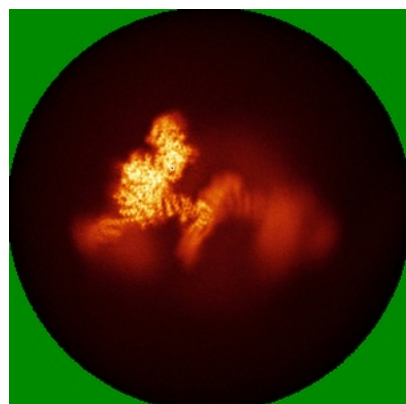


Y

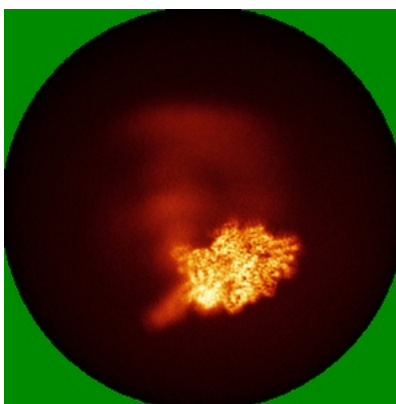


Z

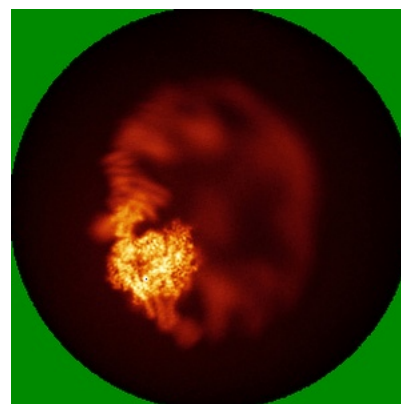
6.4.2 Raw map



X



Y

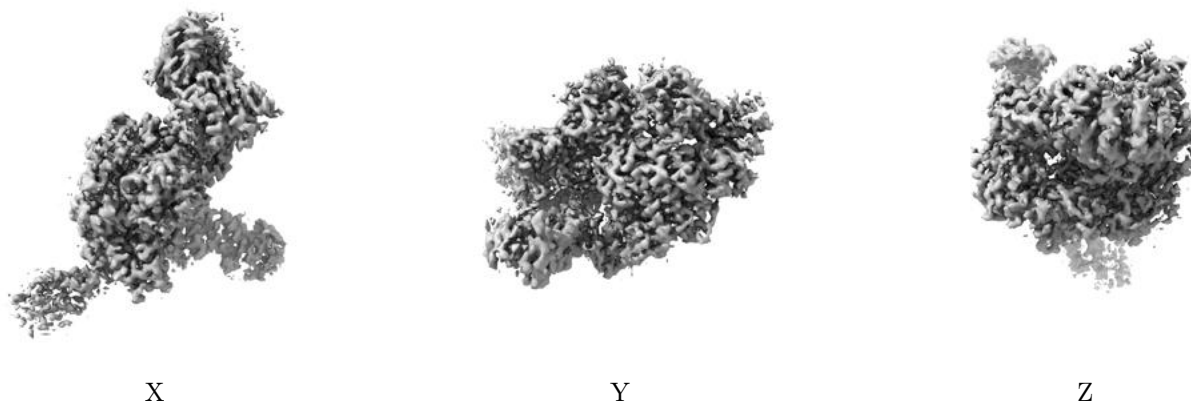


Z

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.

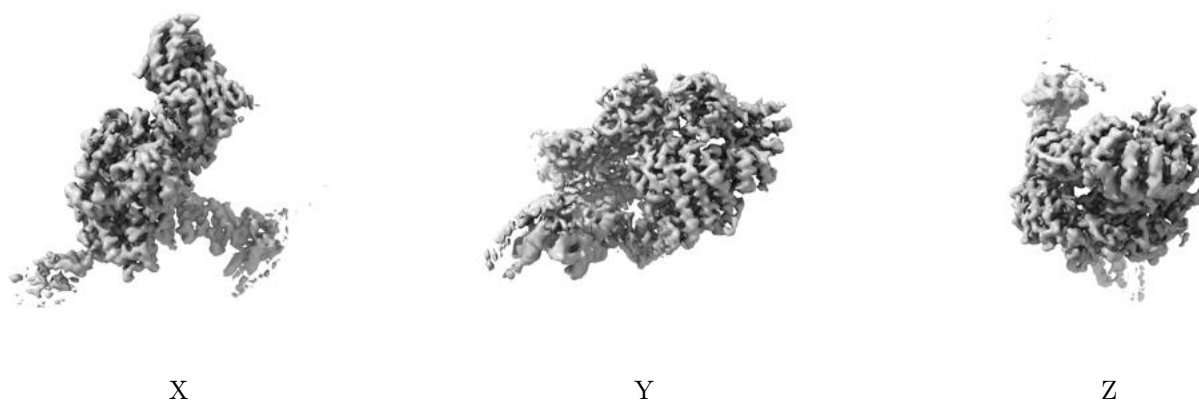
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. 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.

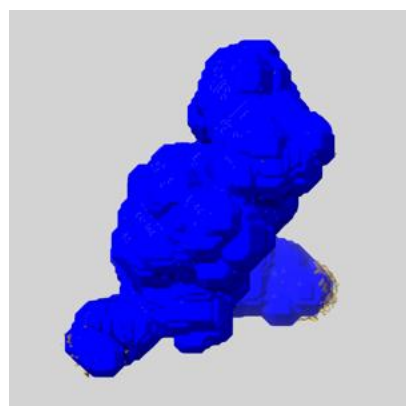
6.6 Mask visualisation [i](#)

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

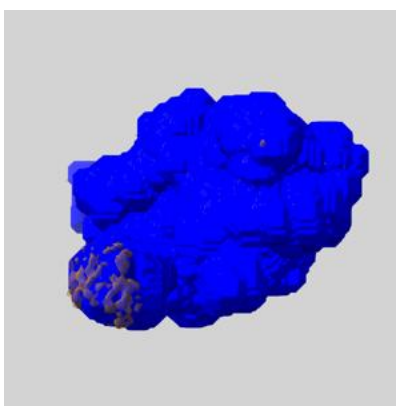
A mask typically either:

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

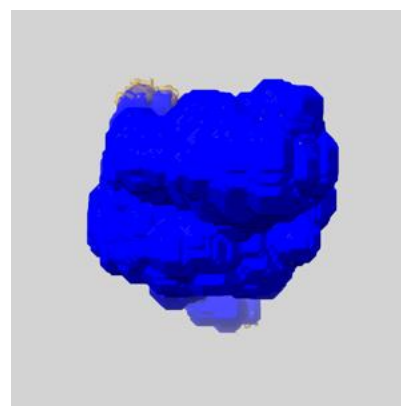
6.6.1 emd_12559_msk_1.map [i](#)



X



Y

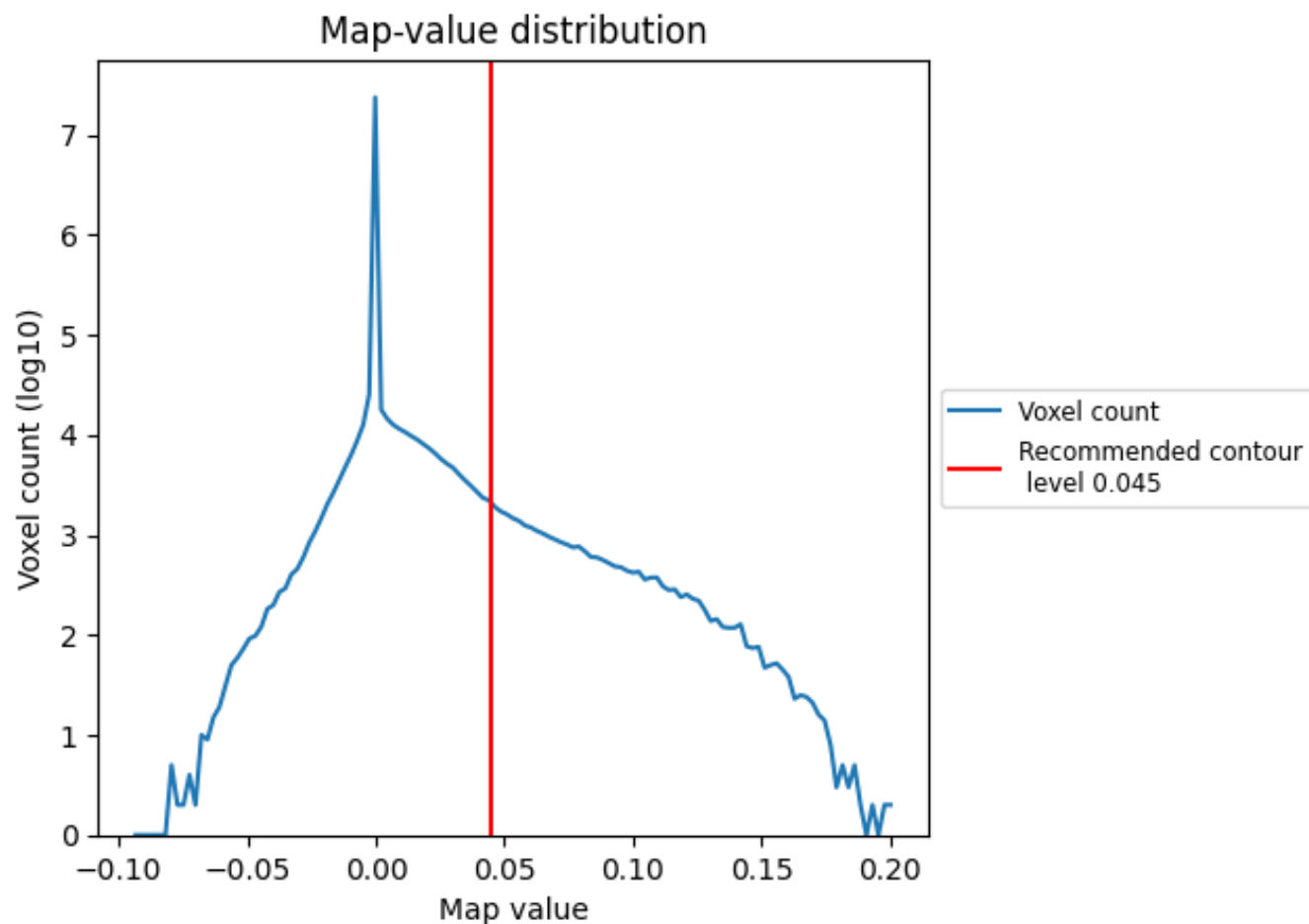


Z

7 Map analysis [i](#)

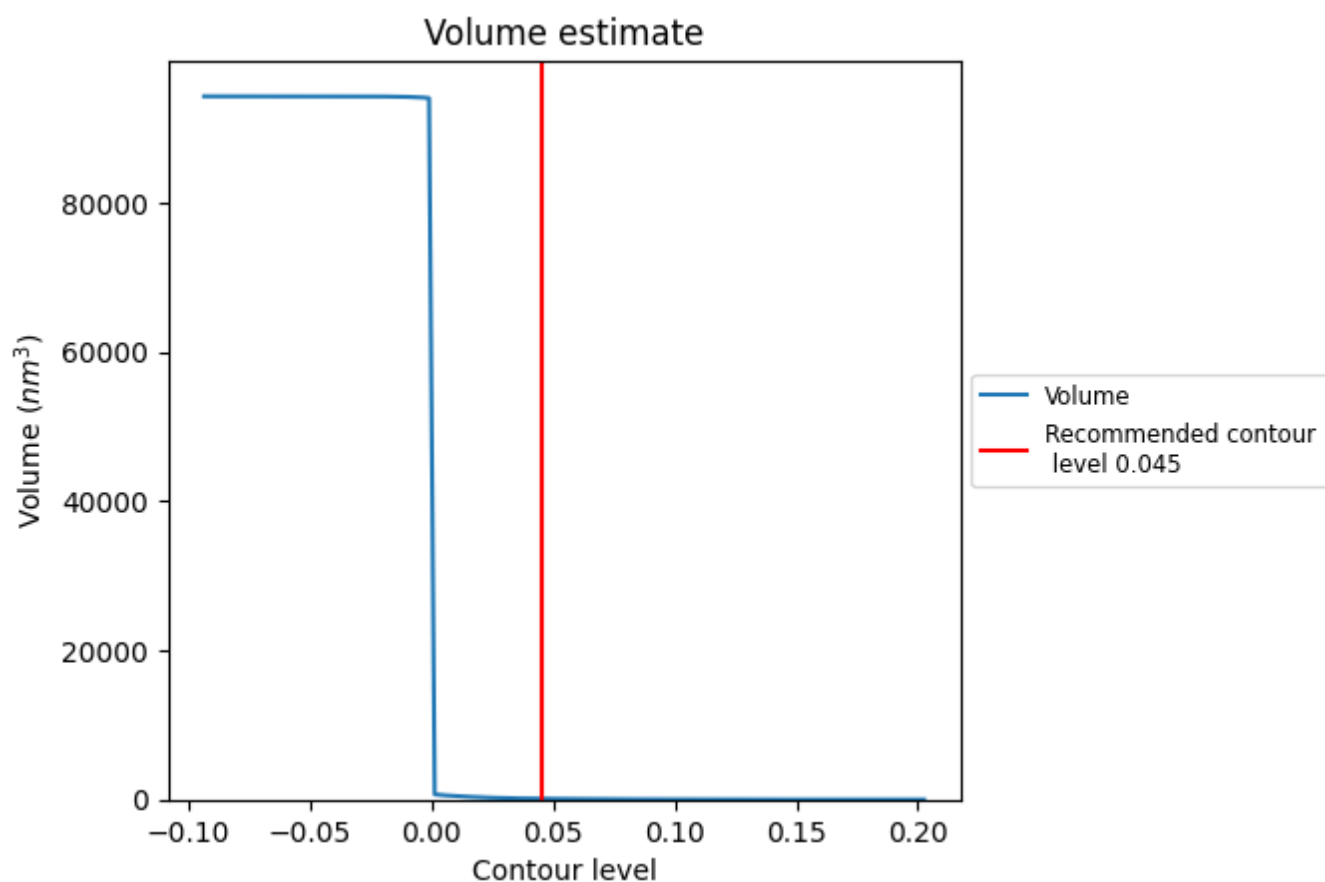
This section contains the results of statistical analysis of the map.

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.

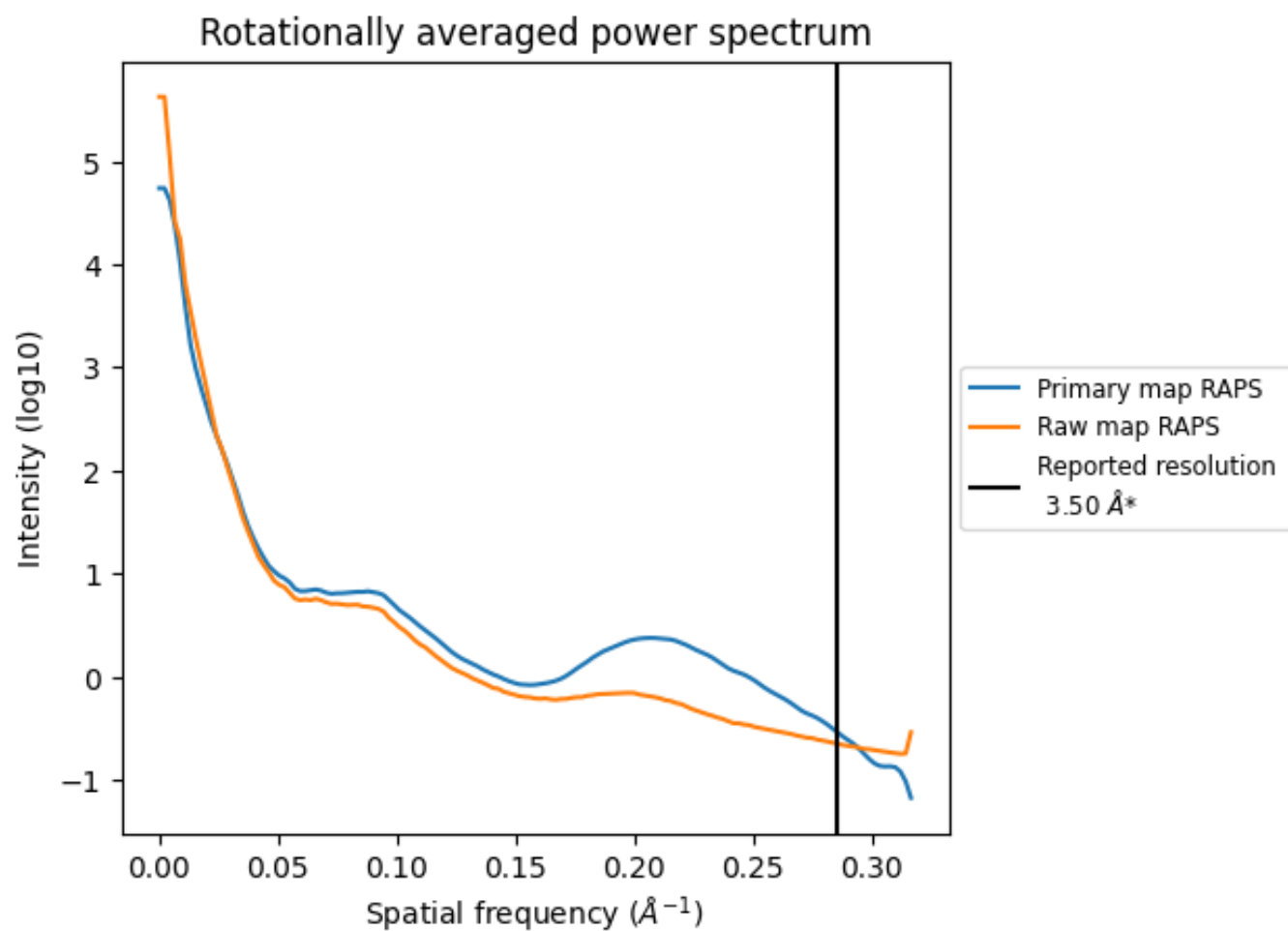
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 113 nm³; this corresponds to an approximate mass of 102 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 ⓘ

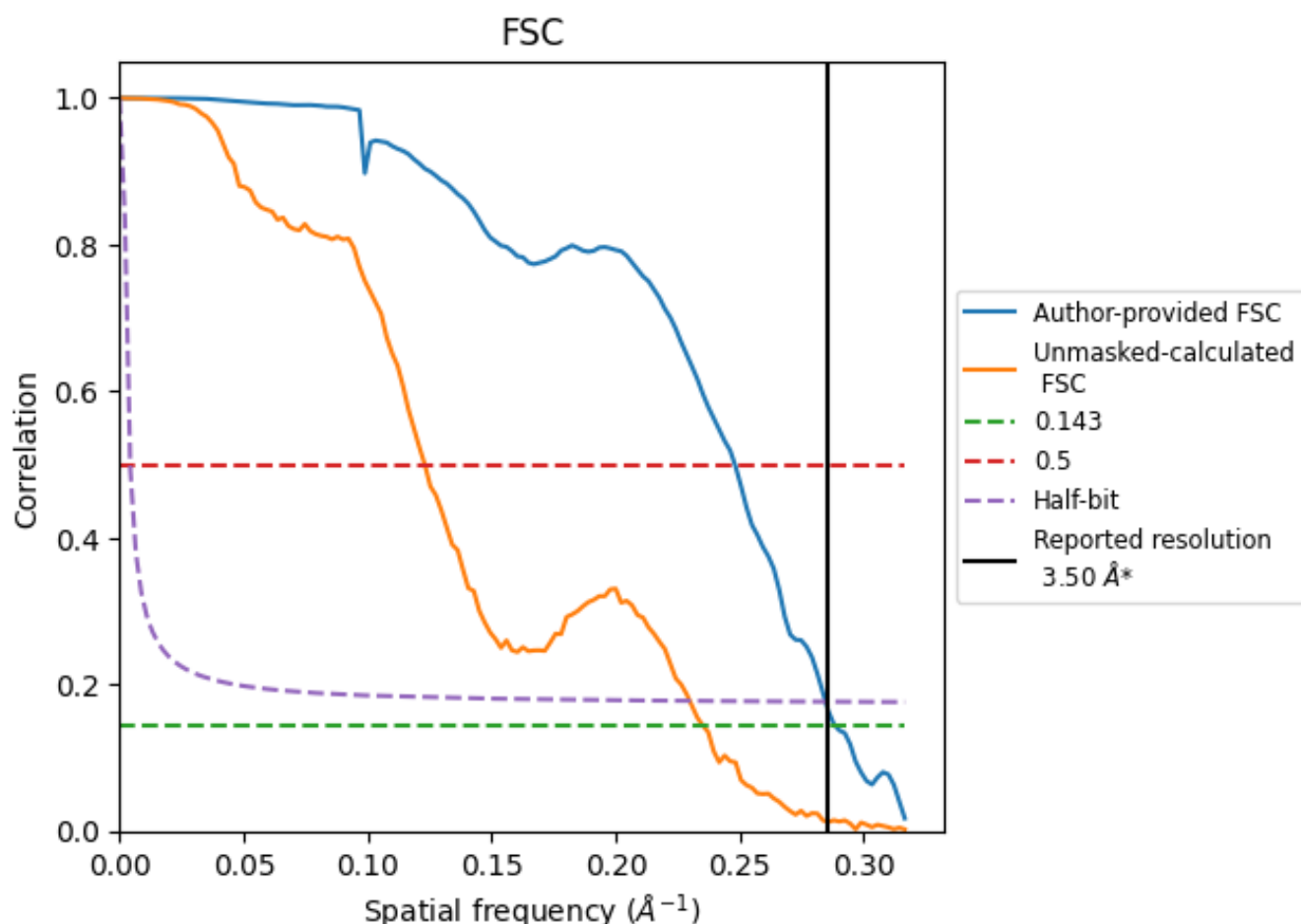


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

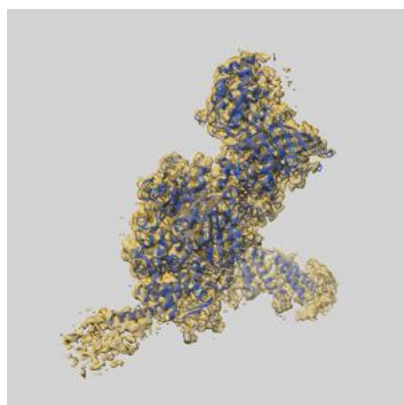
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.47	4.03	3.51
Unmasked-calculated*	4.25	8.13	4.35

*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 4.25 differs from the reported value 3.5 by more than 10 %

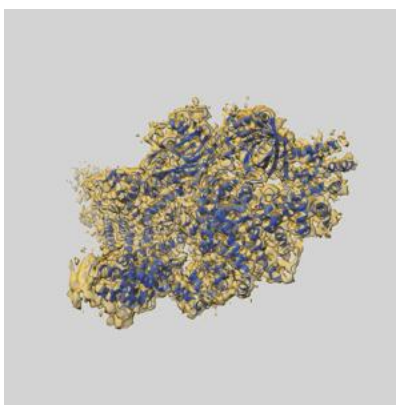
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12559 and PDB model 7NS3. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

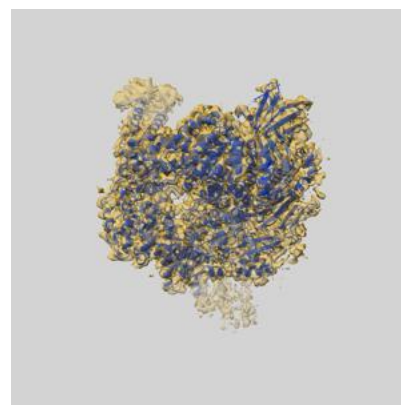
9.1 Map-model overlay [i](#)



X



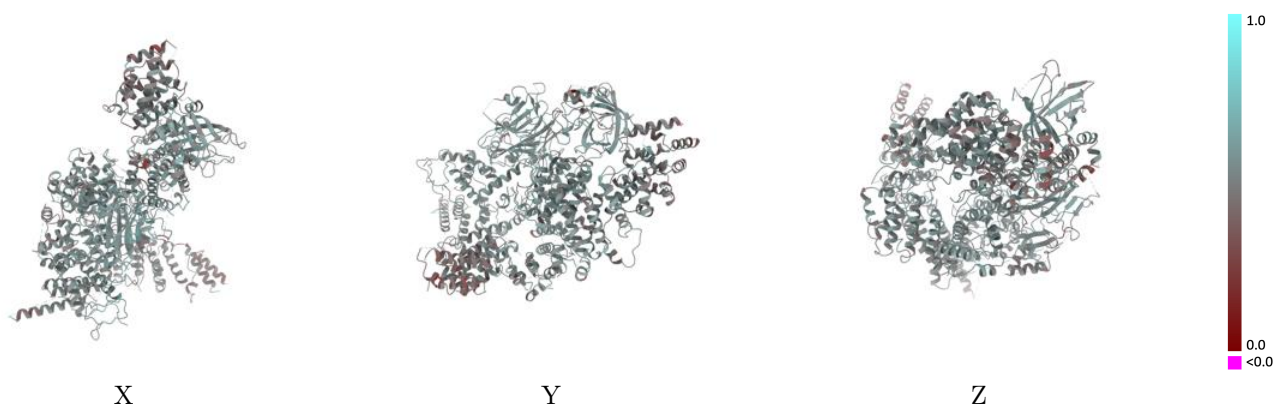
Y



Z

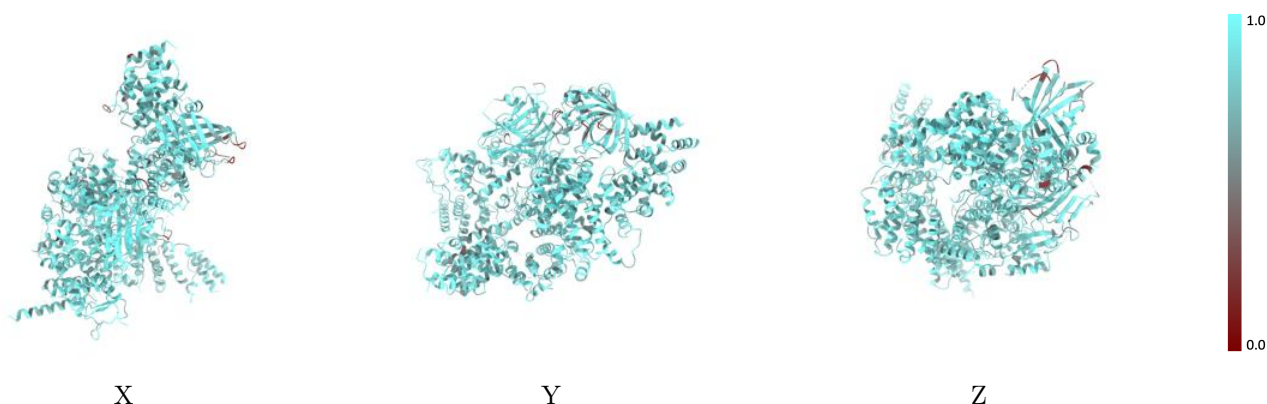
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



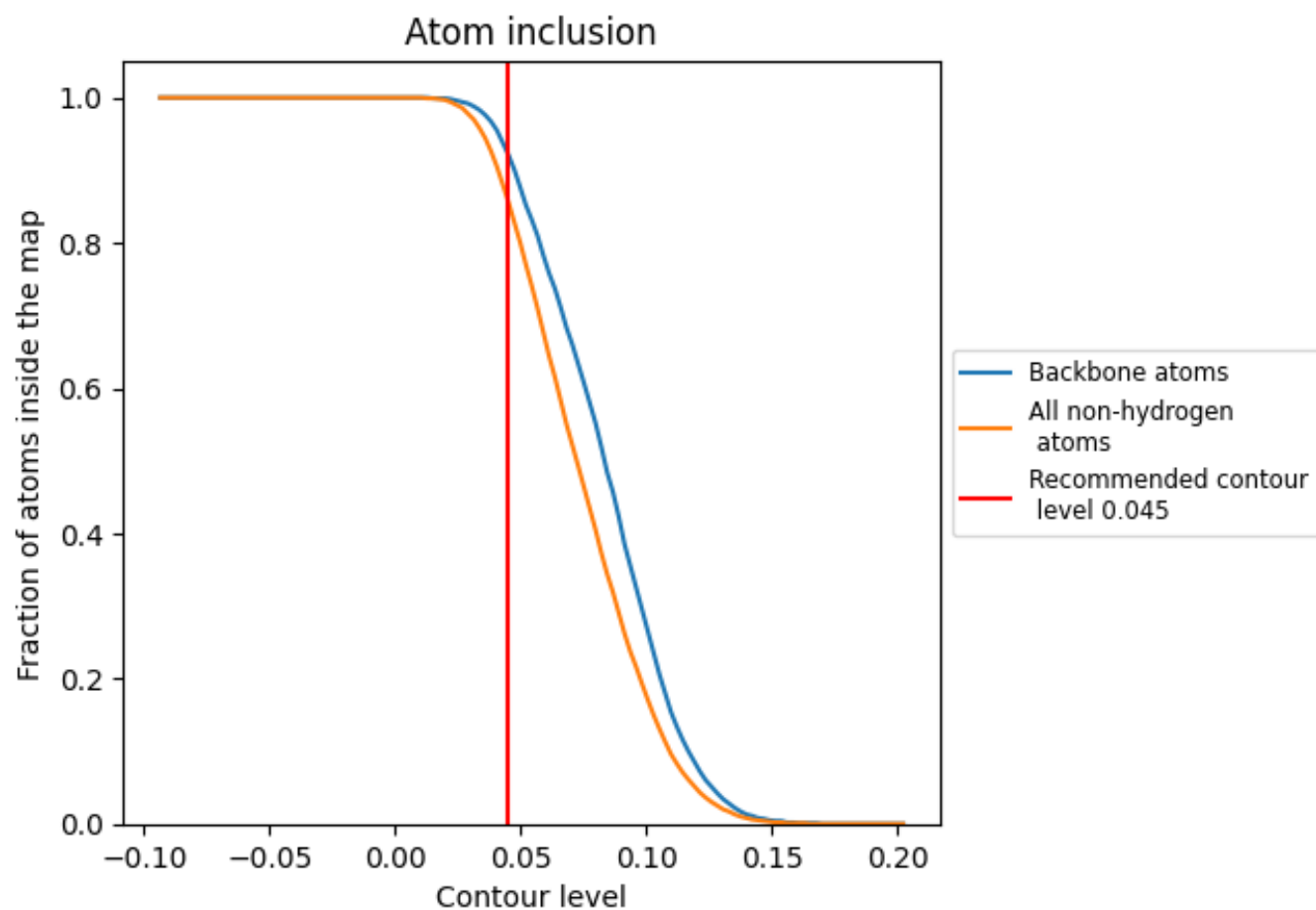
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8590	<div><div></div></div> 0.5200
1	<div><div></div></div> 0.8730	<div><div></div></div> 0.5310
4	<div><div></div></div> 0.8050	<div><div></div></div> 0.5310
5	<div><div></div></div> 0.8690	<div><div></div></div> 0.5200
8	<div><div></div></div> 0.8670	<div><div></div></div> 0.5280
9	<div><div></div></div> 0.8240	<div><div></div></div> 0.4540
Fb	<div><div></div></div> 0.5910	<div><div></div></div> 0.4920

1.0

0.0

<0.0