



wwPDB EM Validation Summary Report ⓘ

Nov 24, 2021 – 02:13 pm GMT

PDB ID : 7PIJ
EMDB ID : EMD-13438
Title : Structure of Staphylococcus capitis divalent metal ion transporter (DMT) by NabFab-fiducial assisted cryo-EM
Authors : Bloch, J.S.; Mukherjee, S.; Kowal, J.; Kossiakoff, A.A.; Locher, K.P.
Deposited on : 2021-08-20
Resolution : 3.78 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

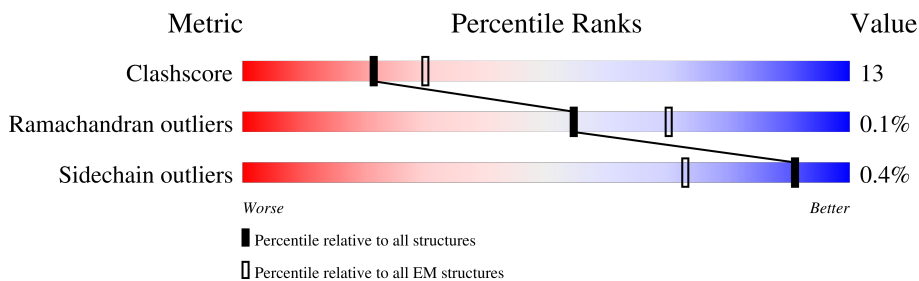
1 Overall quality at a glance

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	H	239	
2	L	215	
3	B	427	
4	N	131	
5	K	123	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8194 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 NabFab HC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	221	1678	1071	277	325	5	0	0

- Molecule 2 is a protein called NabFab LC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	208	1582	987	267	323	5	0	0

- Molecule 3 is a protein called Divalent metal cation transporter MntH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	398	3064	2032	489	530	13	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	MET	-	initiating methionine	UNP A0A4U9TNH6
B	42	SER	-	expression tag	UNP A0A4U9TNH6
B	449	ALA	-	expression tag	UNP A0A4U9TNH6
B	450	LEU	-	expression tag	UNP A0A4U9TNH6
B	451	GLU	-	expression tag	UNP A0A4U9TNH6
B	452	VAL	-	expression tag	UNP A0A4U9TNH6
B	453	LEU	-	expression tag	UNP A0A4U9TNH6
B	454	PHE	-	expression tag	UNP A0A4U9TNH6
B	455	GLN	-	expression tag	UNP A0A4U9TNH6
B	456	GLY	-	expression tag	UNP A0A4U9TNH6
B	457	PRO	-	expression tag	UNP A0A4U9TNH6
B	458	HIS	-	expression tag	UNP A0A4U9TNH6
B	459	HIS	-	expression tag	UNP A0A4U9TNH6
B	460	HIS	-	expression tag	UNP A0A4U9TNH6
B	461	HIS	-	expression tag	UNP A0A4U9TNH6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	462	HIS	-	expression tag	UNP A0A4U9TNH6
B	463	HIS	-	expression tag	UNP A0A4U9TNH6
B	464	HIS	-	expression tag	UNP A0A4U9TNH6
B	465	HIS	-	expression tag	UNP A0A4U9TNH6
B	466	HIS	-	expression tag	UNP A0A4U9TNH6
B	467	HIS	-	expression tag	UNP A0A4U9TNH6

- Molecule 4 is a protein called DMTNb16_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	121	Total	C	N	O	S	0	0
			924	566	173	182	3		

- Molecule 5 is a protein called Anti-Fab nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	120	Total	C	N	O	S	2	0
			930	578	162	184	6		

- Molecule 6 is water.

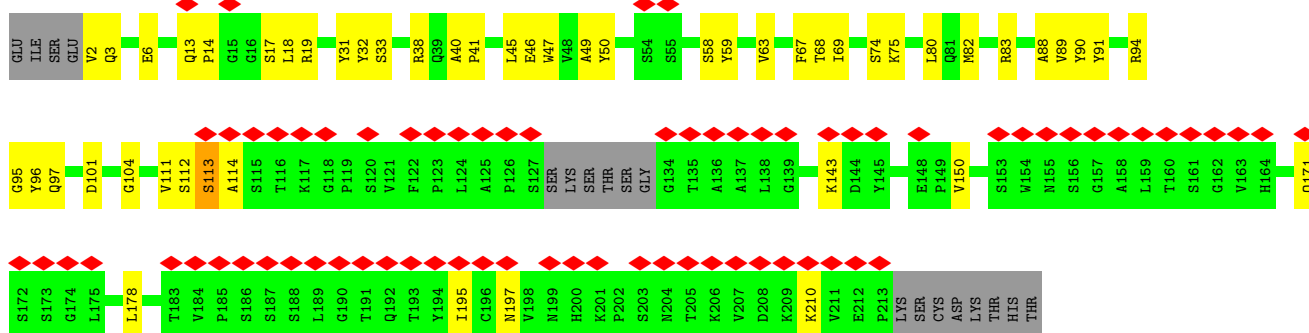
Mol	Chain	Residues	Atoms		AltConf
6	H	5	Total	O	0
			5	5	
6	L	4	Total	O	0
			4	4	
6	N	7	Total	O	0
			7	7	

3 Residue-property plots [i](#)


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.

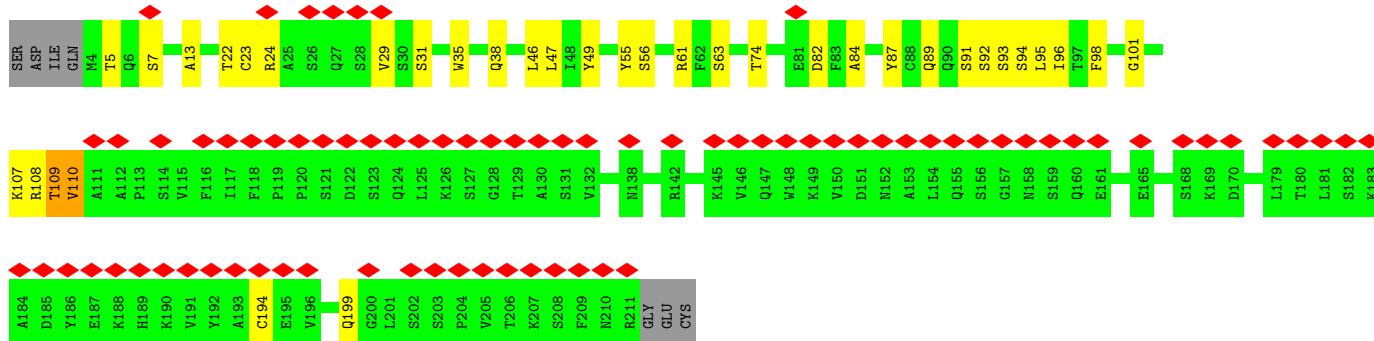
- Molecule 1: NabFab HC

Chain H: 



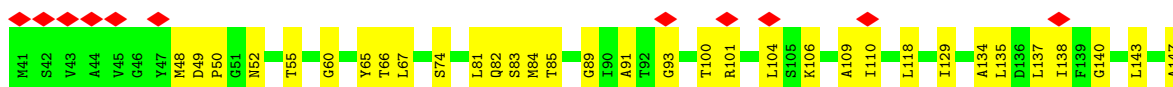
- Molecule 2: NabFab LC

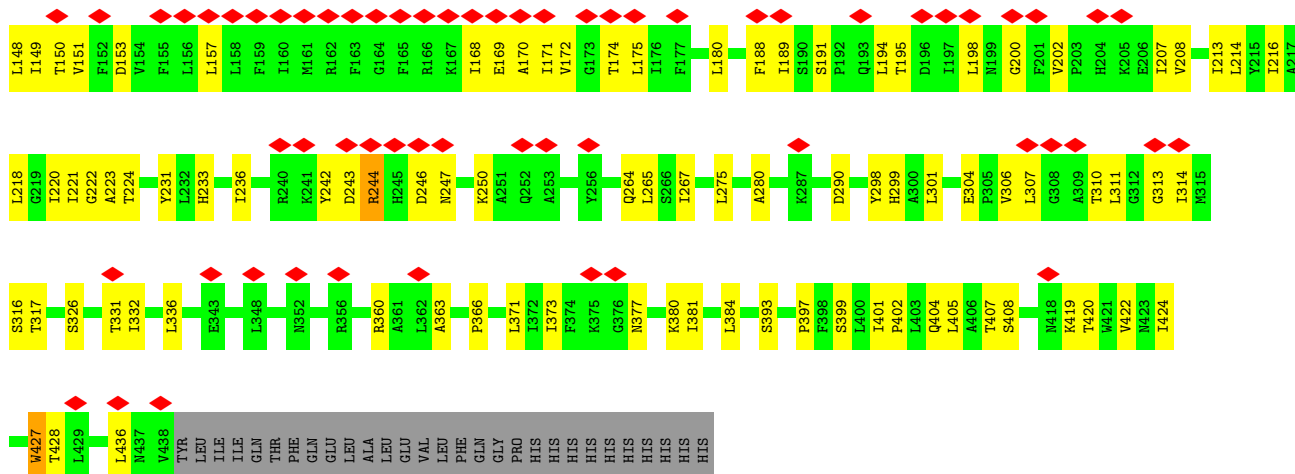
Chain L: 



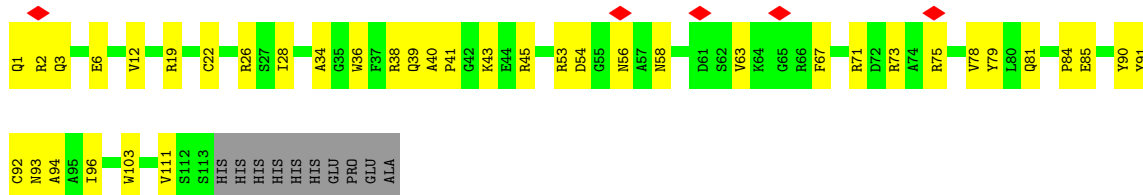
- Molecule 3: Divalent metal cation transporter MntH

Chain B: 

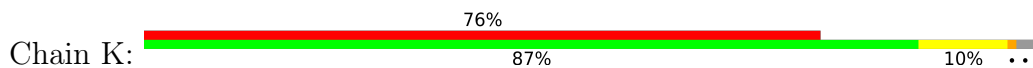




• Molecule 4: DMTNb16_4



• Molecule 5: Anti-Fab nanobody



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	433559	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 ($e^-/\text{\AA}^2$)	26	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	2.847	Depositor
Minimum map value	-1.921	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.365	Depositor
Map size (Å)	295.68002, 295.68002, 295.68002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.66, 0.66, 0.66	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	H	0.99	3/1727 (0.2%)	0.68	2/2360 (0.1%)
2	L	0.95	2/1614 (0.1%)	0.85	3/2190 (0.1%)
3	B	0.50	1/3125 (0.0%)	0.56	0/4252
4	N	0.59	0/939	0.56	0/1271
5	K	0.79	0/955	0.85	2/1290 (0.2%)
All	All	0.76	6/8360 (0.1%)	0.69	7/11363 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	113	SER	C-N	26.76	1.95	1.34
2	L	109	THR	C-N	23.34	1.87	1.34
2	L	194	CYS	CB-SG	-9.45	1.66	1.82
3	B	427	TRP	CB-CG	-6.80	1.38	1.50
1	H	150	VAL	CB-CG1	-5.48	1.41	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	109	THR	O-C-N	-20.59	89.76	122.70
1	H	113	SER	CA-C-N	-11.86	91.11	117.20
2	L	109	THR	CA-C-N	10.97	141.33	117.20
2	L	109	THR	C-N-CA	9.35	145.07	121.70
1	H	113	SER	C-N-CA	-7.83	102.14	121.70

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	H	1678	0	1598	39	0
2	L	1582	0	1549	43	0
3	B	3064	0	3245	97	0
4	N	924	0	903	31	0
5	K	930	0	880	22	0
6	H	5	0	0	1	0
6	L	4	0	0	1	0
6	N	7	0	0	1	0
All	All	8194	0	8175	207	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 13.

The worst 5 of 207 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:L:109:THR:C	2:L:110:VAL:N	1.87	1.28
2:L:199:GLN:CD	5:K:100:TYR:O	1.73	1.26
1:H:113:SER:C	1:H:114:ALA:N	1.95	1.19
2:L:199:GLN:NE2	5:K:100:TYR:O	1.79	1.13
1:H:112:SER:HG	1:H:114:ALA:N	1.44	1.12

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	H	217/239 (91%)	197 (91%)	20 (9%)	0	100 100
2	L	206/215 (96%)	185 (90%)	20 (10%)	1 (0%)	29 65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	396/427 (93%)	356 (90%)	40 (10%)	0	100	100
4	N	119/131 (91%)	89 (75%)	30 (25%)	0	100	100
5	K	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
All	All	1058/1135 (93%)	945 (89%)	112 (11%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	110	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	H	182/200 (91%)	180 (99%)	2 (1%)	73	85
2	L	184/190 (97%)	184 (100%)	0	100	100
3	B	334/361 (92%)	333 (100%)	1 (0%)	92	96
4	N	97/106 (92%)	96 (99%)	1 (1%)	76	86
5	K	98/98 (100%)	98 (100%)	0	100	100
All	All	895/955 (94%)	891 (100%)	4 (0%)	91	95

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

Mol	Chain	Res	Type
1	H	50	TYR
1	H	197	ASN
3	B	244	ARG
4	N	26	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
5	K	5	GLN
4	N	76	ASN
3	B	299	HIS
3	B	233	HIS
4	N	39	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 monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1
2	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	113:SER	C	114:ALA	N	1.95
1	L	109:THR	C	110:VAL	N	1.87

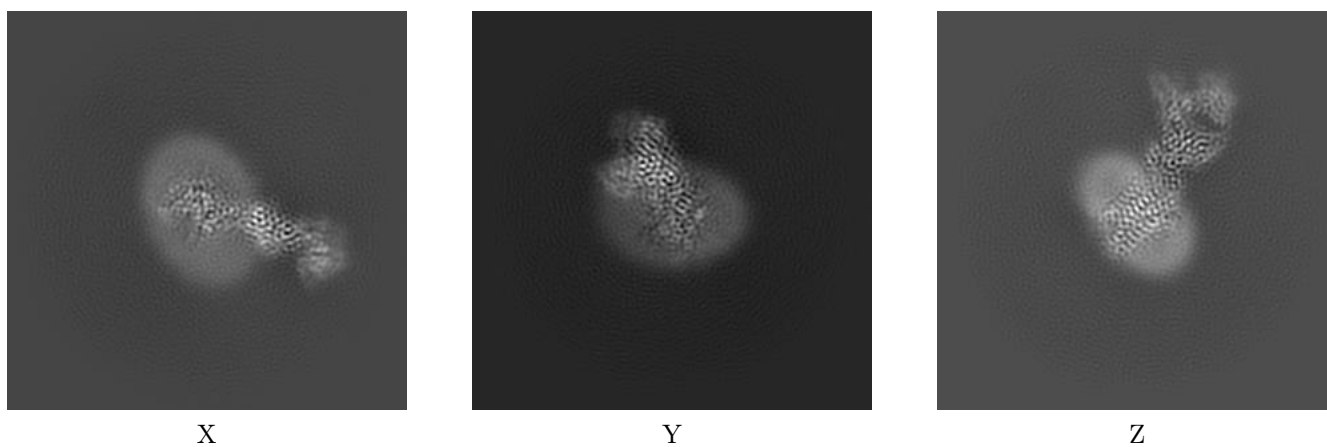
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13438. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

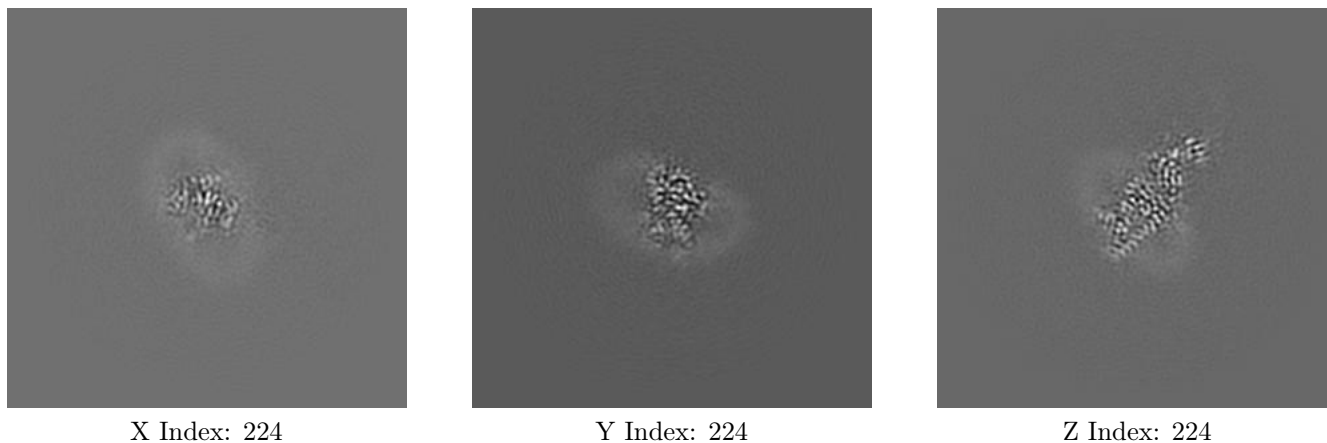
6.1.1 Primary map



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

6.2 Central slices [i](#)

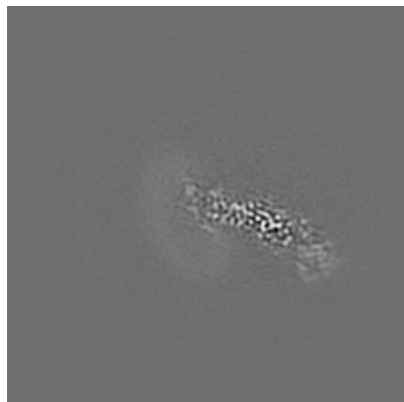
6.2.1 Primary map



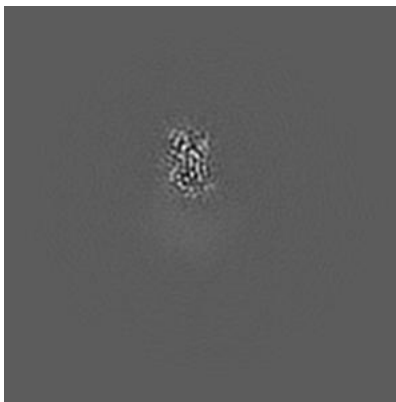
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

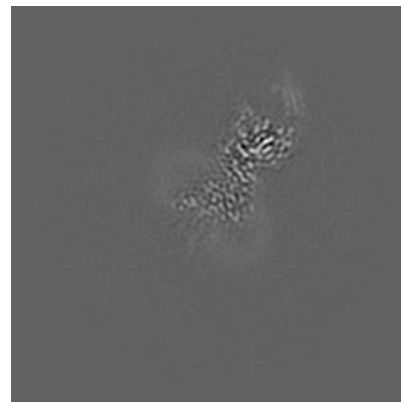
6.3.1 Primary map



X Index: 263



Y Index: 284

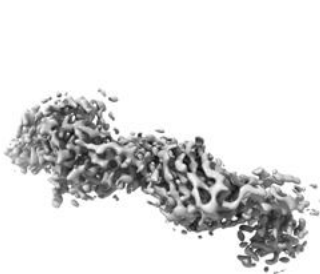


Z Index: 209

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.365. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

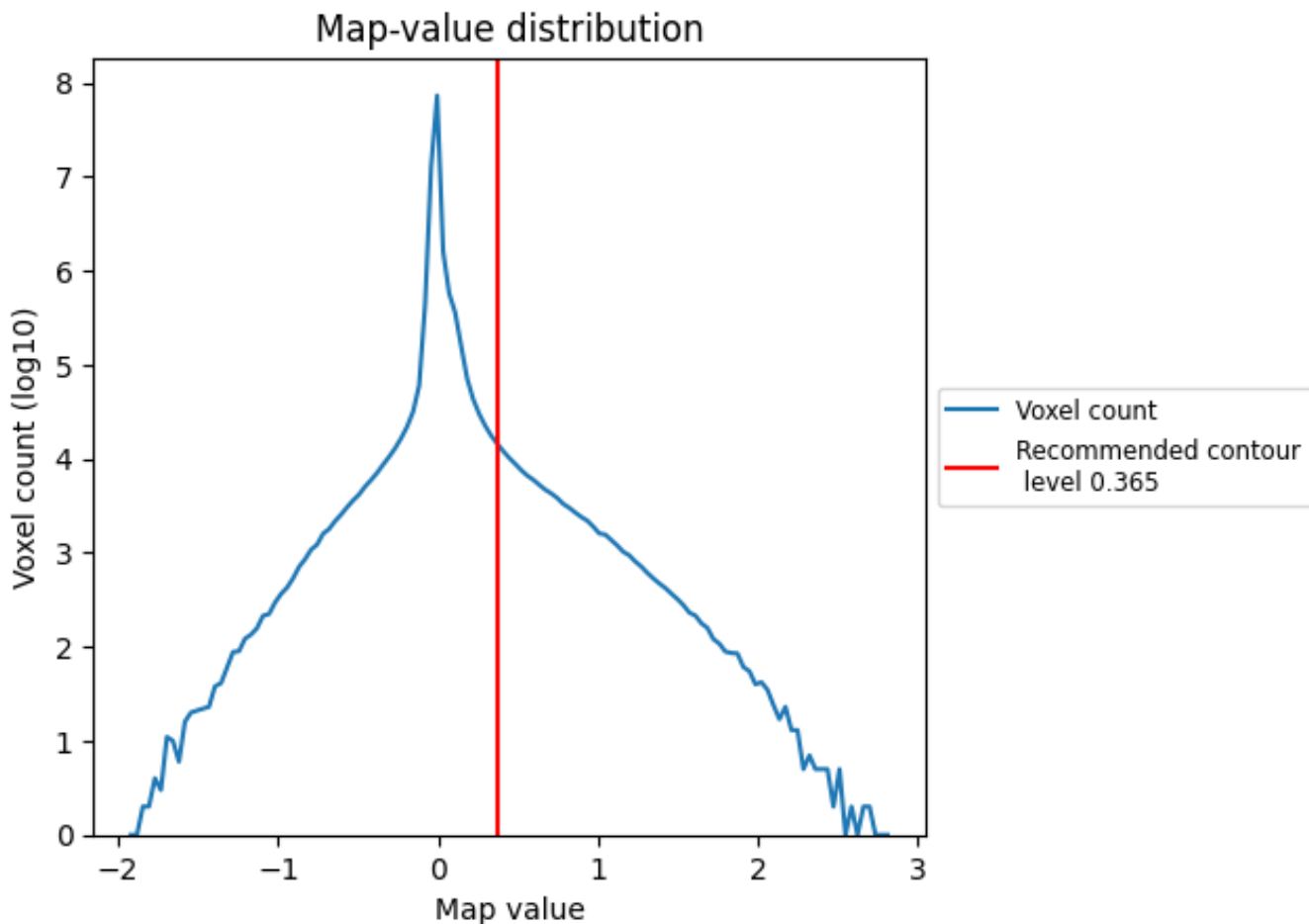
6.5 Mask visualisation

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

7 Map analysis [i](#)

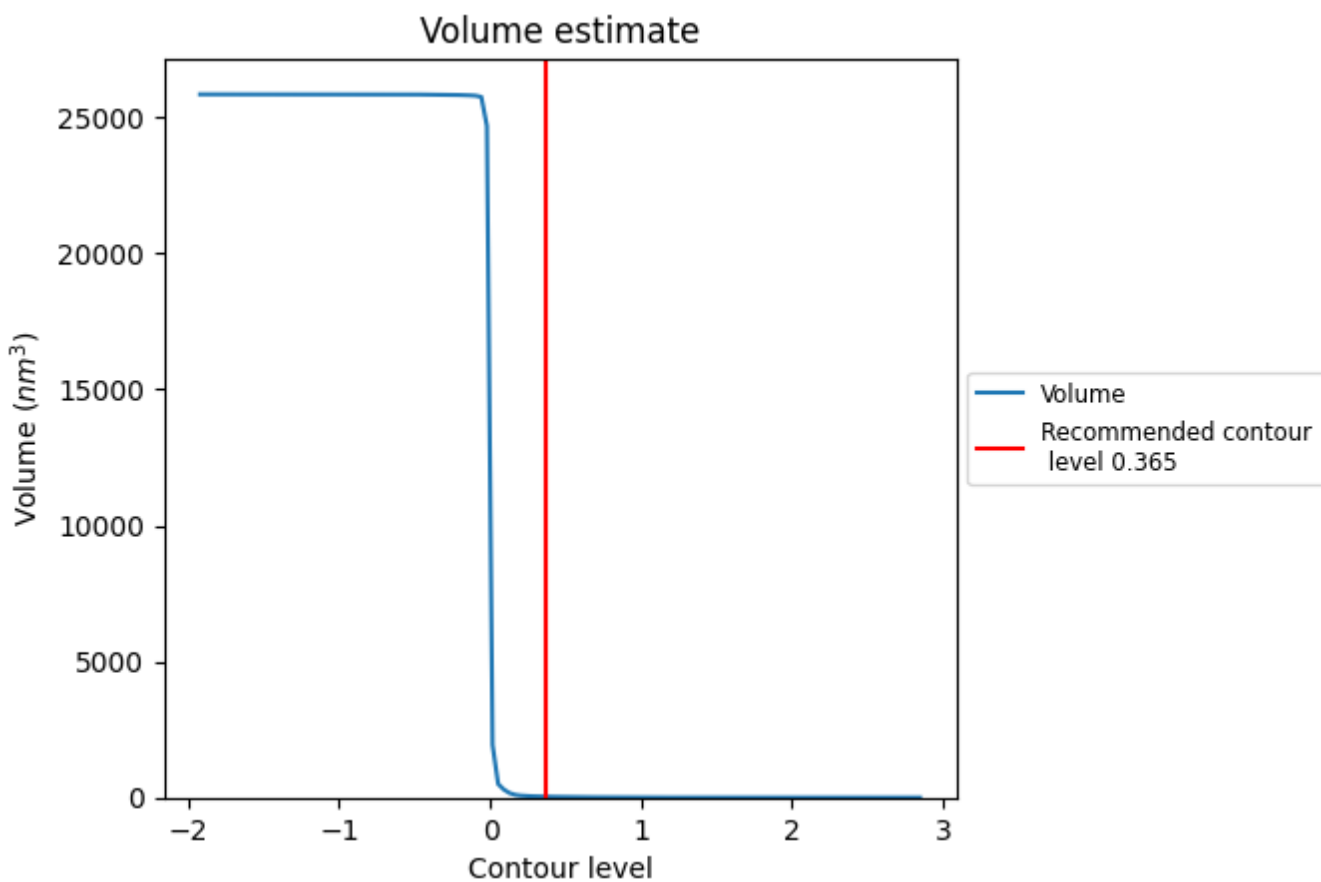
This section contains the results of statistical analysis of the map.

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.

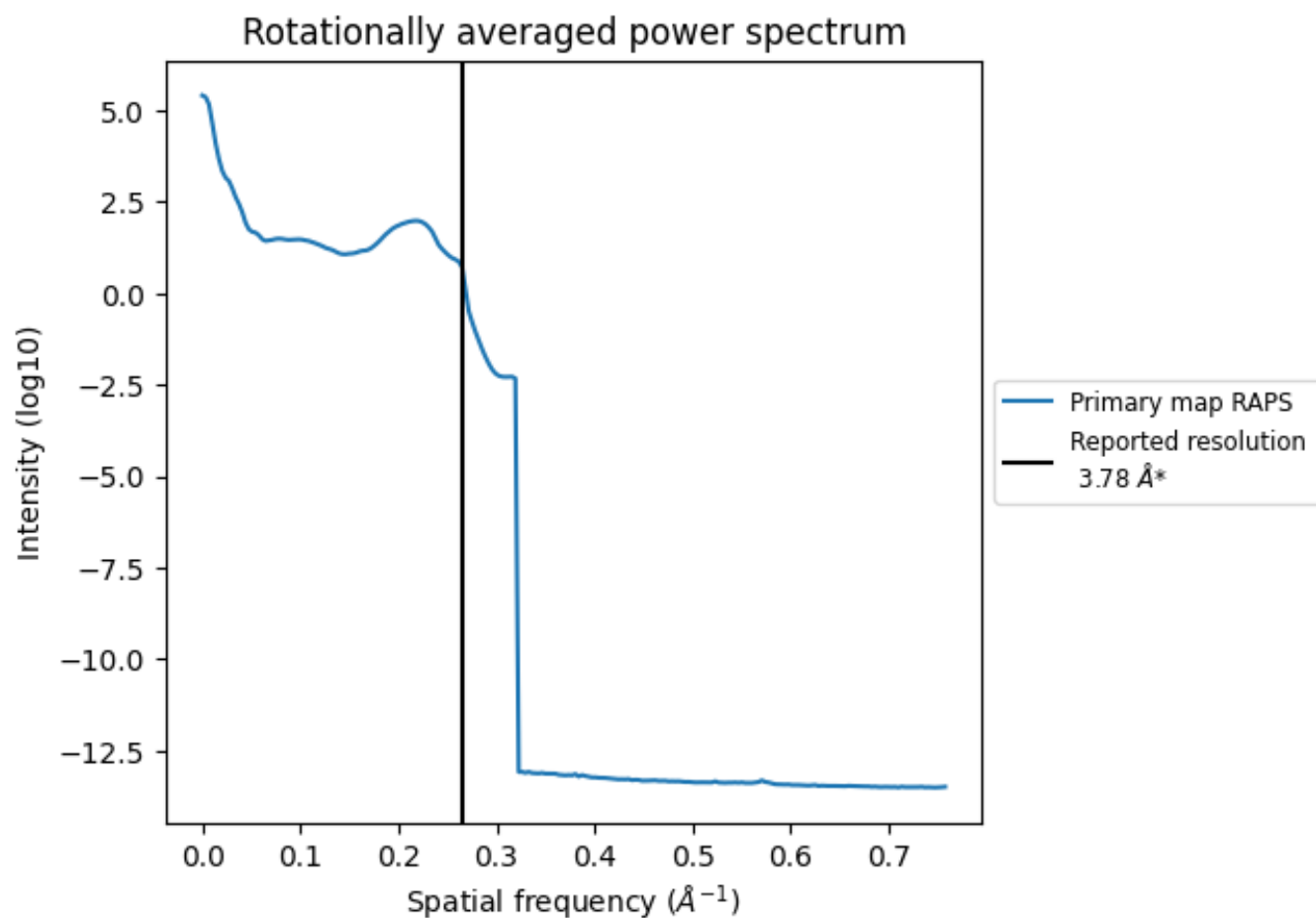
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33 nm³; this corresponds to an approximate mass of 30 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 [i](#)

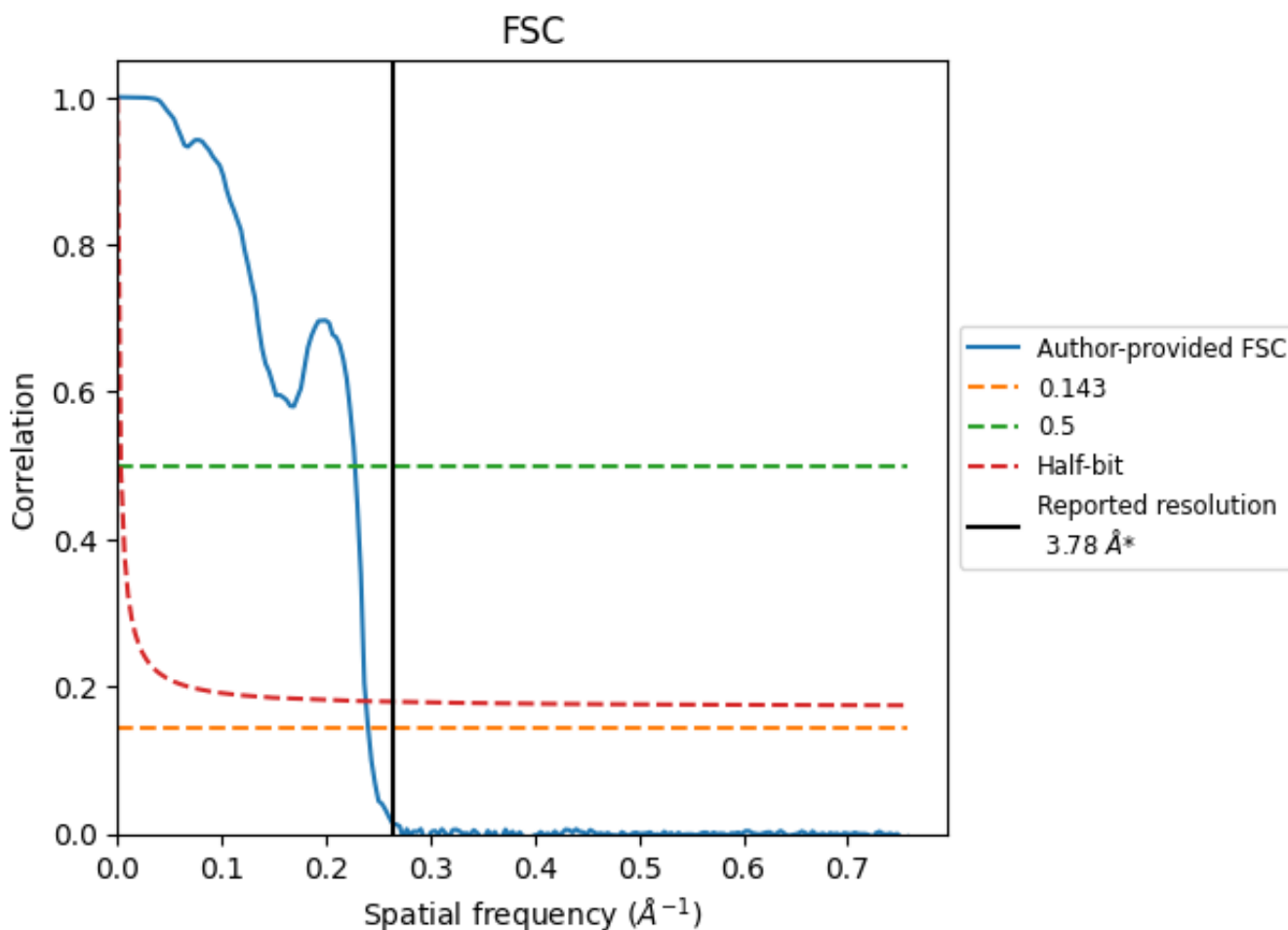


*Reported resolution corresponds to spatial frequency of 0.265 \AA^{-1}

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 Å⁻¹

8.2 Resolution estimates [i](#)

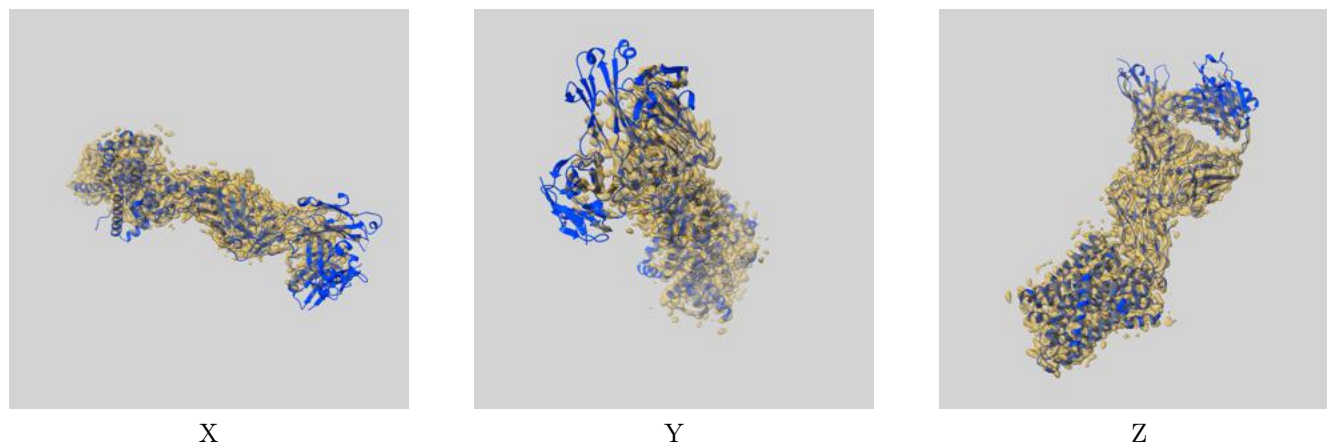
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.78	-	-
Author-provided FSC curve	4.16	4.39	4.20
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.78 by more than 10 %

9 Map-model fit [i](#)

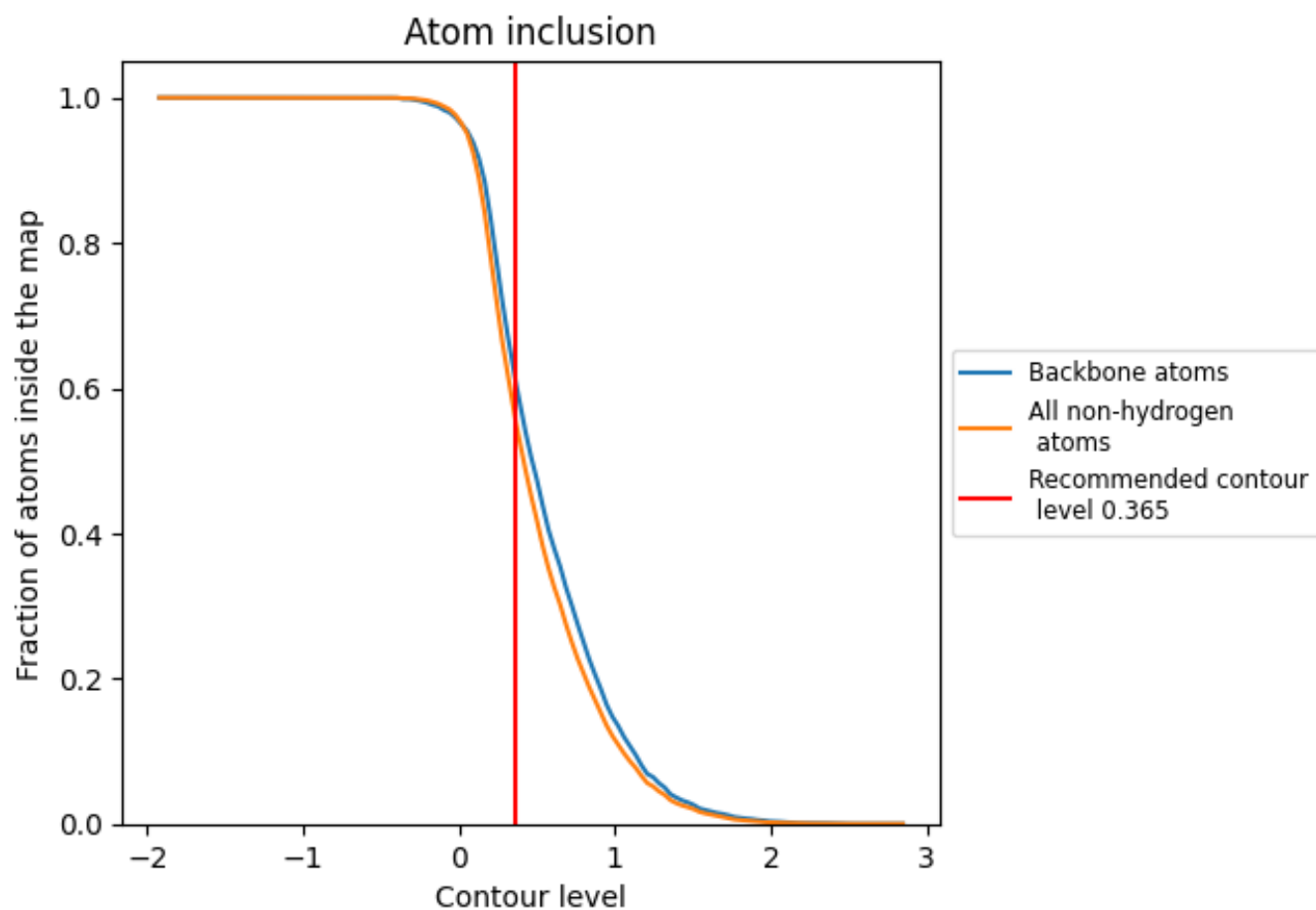
This section contains information regarding the fit between EMDB map EMD-13438 and PDB model 7PIJ. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.365 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 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.