



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:22 AM UTC

PDB ID : 8CR9 / pdb_00008cr9
EMDB ID : EMD-16805
Title : Cryo-EM structure of PcrV/Fab(30-B8)
Authors : Yuan, B.; Simonis, A.; Marlovits, T.C.
Deposited on : 2023-03-08
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM Validation 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:

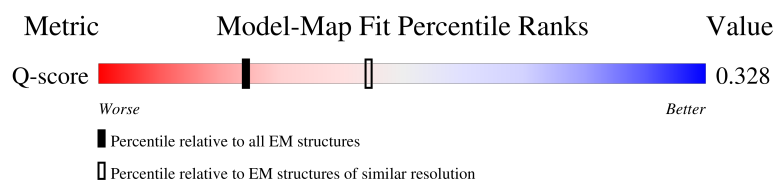
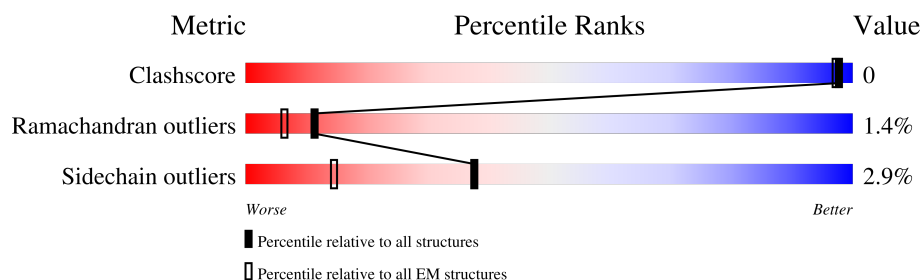
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	222	
2	B	217	
3	C	692	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8621 atoms, of which 4272 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 Heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	222	Total	C	H	N	O	S	0	0
			3300	1044	1634	290	326	6		

- Molecule 2 is a protein called light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	217	Total	C	H	N	O	S	0	0
			3290	1045	1621	278	341	5		

- Molecule 3 is a protein called Maltose/maltodextrin-binding periplasmic protein, Type III secretion protein PcrV.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	132	Total	C	H	N	O		0	0
			2031	641	1017	168	205			

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-397	MET	-	initiating methionine	UNP P0AEX9
C	-396	GLY	-	expression tag	UNP P0AEX9
C	-395	SER	-	expression tag	UNP P0AEX9
C	-394	TRP	-	expression tag	UNP P0AEX9
C	-393	SER	-	expression tag	UNP P0AEX9
C	-392	HIS	-	expression tag	UNP P0AEX9
C	-391	PRO	-	expression tag	UNP P0AEX9
C	-390	GLN	-	expression tag	UNP P0AEX9
C	-389	PHE	-	expression tag	UNP P0AEX9
C	-388	GLU	-	expression tag	UNP P0AEX9
C	-387	LYS	-	expression tag	UNP P0AEX9
C	-386	GLY	-	expression tag	UNP P0AEX9
C	-385	GLY	-	expression tag	UNP P0AEX9
C	-384	GLY	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-383	SER	-	expression tag	UNP P0AEX9
C	-382	GLY	-	expression tag	UNP P0AEX9
C	-381	GLY	-	expression tag	UNP P0AEX9
C	-380	GLY	-	expression tag	UNP P0AEX9
C	-379	SER	-	expression tag	UNP P0AEX9
C	-378	GLY	-	expression tag	UNP P0AEX9
C	-377	GLY	-	expression tag	UNP P0AEX9
C	-376	GLY	-	expression tag	UNP P0AEX9
C	-375	SER	-	expression tag	UNP P0AEX9
C	-374	TRP	-	expression tag	UNP P0AEX9
C	-373	SER	-	expression tag	UNP P0AEX9
C	-372	HIS	-	expression tag	UNP P0AEX9
C	-371	PRO	-	expression tag	UNP P0AEX9
C	-370	GLN	-	expression tag	UNP P0AEX9
C	-369	PHE	-	expression tag	UNP P0AEX9
C	-368	GLU	-	expression tag	UNP P0AEX9
C	-367	LYS	-	expression tag	UNP P0AEX9
C	-366	SER	-	expression tag	UNP P0AEX9
C	-365	GLY	-	expression tag	UNP P0AEX9
C	-364	LEU	-	expression tag	UNP P0AEX9
C	-363	VAL	-	expression tag	UNP P0AEX9
C	-362	PRO	-	expression tag	UNP P0AEX9
C	-361	ARG	-	expression tag	UNP P0AEX9
C	-360	GLY	-	expression tag	UNP P0AEX9
C	-359	SER	-	expression tag	UNP P0AEX9
C	-358	ALA	-	expression tag	UNP P0AEX9
C	-357	SER	-	expression tag	UNP P0AEX9
C	-356	LYS	-	expression tag	UNP P0AEX9
C	-355	THR	-	expression tag	UNP P0AEX9
C	-275	ALA	ASP	conflict	UNP P0AEX9
C	-274	ALA	LYS	conflict	UNP P0AEX9
C	-185	ALA	GLU	conflict	UNP P0AEX9
C	-184	ALA	ASN	conflict	UNP P0AEX9
C	-142	HIS	ALA	conflict	UNP P0AEX9
C	-138	HIS	LYS	conflict	UNP P0AEX9
C	-45	VAL	ALA	conflict	UNP P0AEX9
C	-40	VAL	ILE	conflict	UNP P0AEX9
C	21	PRO	SER	conflict	UNP G3XD49
C	225	LYS	SER	conflict	UNP G3XD49

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	292189	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 ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00548	Depositor
Map size (Å)	142.8, 142.8, 142.8	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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	0.80	0/1706	1.36	7/2320 (0.3%)
2	B	0.87	1/1706 (0.1%)	1.47	10/2319 (0.4%)
3	C	0.74	0/1031	1.24	0/1396
All	All	0.81	1/4443 (0.0%)	1.38	17/6035 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	4
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	47	LEU	CA-C	6.35	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	83	VAL	N-CA-C	7.79	119.58	112.17
1	A	47	TRP	CA-C-N	6.99	129.62	120.60
1	A	47	TRP	C-N-CA	6.99	129.62	120.60
2	B	101	PHE	CA-CB-CG	6.48	120.28	113.80
2	B	94	TYR	N-CA-C	5.53	116.67	108.60
1	A	48	VAL	N-CA-C	5.43	116.06	110.36
1	A	69	THR	CA-C-N	5.35	127.87	120.49
1	A	69	THR	C-N-CA	5.35	127.87	120.49
2	B	88	CYS	N-CA-C	5.30	116.90	108.79
1	A	44	ARG	NE-CZ-NH2	5.28	123.95	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	GLY	CA-C-N	5.28	126.44	119.84
2	B	102	GLY	C-N-CA	5.28	126.44	119.84
2	B	49	TYR	CA-C-N	5.26	131.59	121.54
2	B	49	TYR	C-N-CA	5.26	131.59	121.54
1	A	78	THR	N-CA-C	5.20	116.72	108.67
2	B	28	ASP	CA-C-N	5.10	131.15	121.97
2	B	28	ASP	C-N-CA	5.10	131.15	121.97

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	59	TYR	Sidechain
2	B	195	TYR	Sidechain
2	B	49	TYR	Sidechain
2	B	90	TYR	Sidechain
2	B	91	TYR	Sidechain

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	1666	1634	1634	3	0
2	B	1669	1621	1621	1	0
3	C	1014	1017	1016	0	0
All	All	4349	4272	4271	4	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 0.

All (4) 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:60:TYR:CD2	1:A:64:VAL:HG22	2.46	0.50
2:B:36:TYR:CD2	2:B:101:PHE:CZ	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:CYS:SG	1:A:23:THR:N	2.92	0.43
1:A:36:TRP:CH2	1:A:96:CYS:SG	3.14	0.40

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	220/222 (99%)	186 (84%)	31 (14%)	3 (1%)	9	39
2	B	215/217 (99%)	192 (89%)	18 (8%)	5 (2%)	5	29
3	C	130/692 (19%)	125 (96%)	5 (4%)	0	100	100
All	All	565/1131 (50%)	503 (89%)	54 (10%)	8 (1%)	11	39

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	93	SER
2	B	96	HIS
2	B	99	VAL
1	A	102	PRO
2	B	208	VAL
1	A	52	ILE
1	A	55	GLY
2	B	29	ILE

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	185/185 (100%)	179 (97%)	6 (3%)	34	56
2	B	191/191 (100%)	183 (96%)	8 (4%)	26	49
3	C	112/556 (20%)	112 (100%)	0	100	100
All	All	488/932 (52%)	474 (97%)	14 (3%)	38	58

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	48	VAL
1	A	51	ILE
1	A	64	VAL
1	A	70	ILE
1	A	202	THR
2	B	4	LEU
2	B	6	GLN
2	B	11	VAL
2	B	58	VAL
2	B	66	GLU
2	B	89	GLN
2	B	119	PHE
2	B	206	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	77	ASN
1	A	206	ASN
2	B	6	GLN
3	C	149	GLN
3	C	153	ASN

5.3.3 RNA ⓘ

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-16805. These allow visual inspection of the internal detail of the map and identification of artifacts.

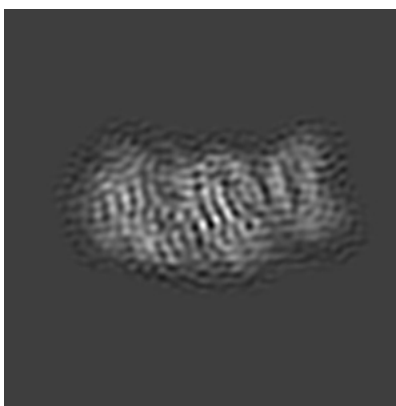
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

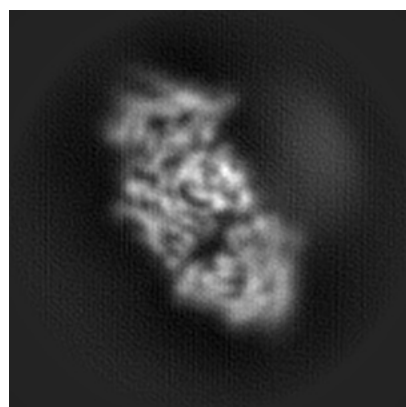


Y

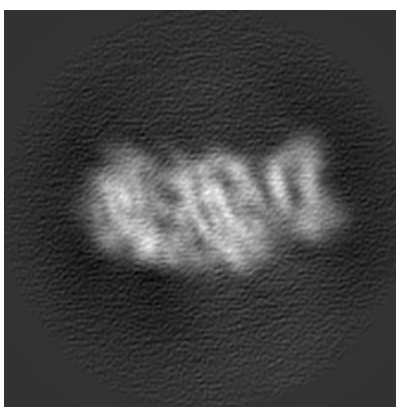


Z

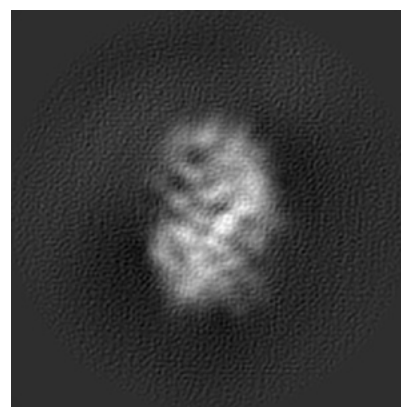
6.1.2 Raw map



X



Y

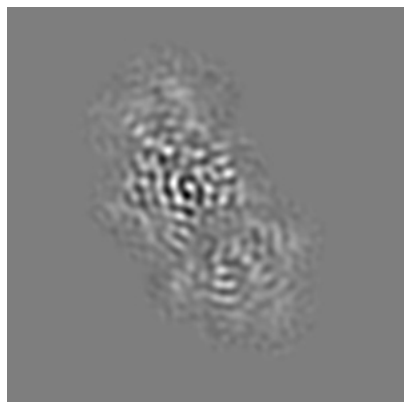


Z

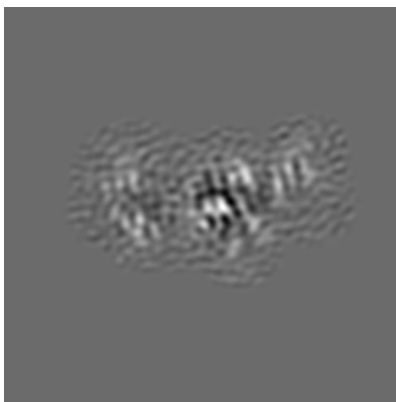
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 84

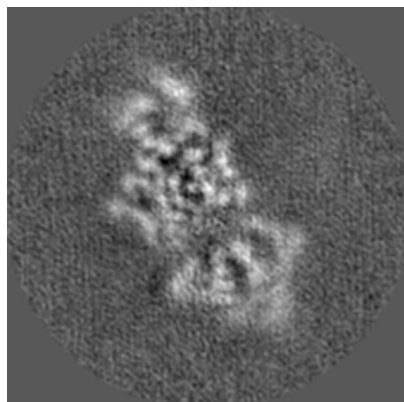


Y Index: 84

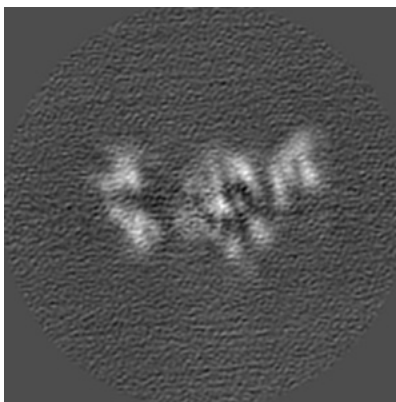


Z Index: 84

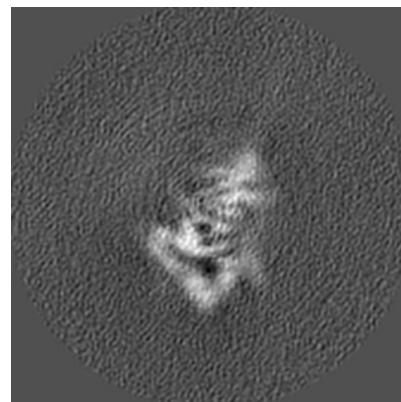
6.2.2 Raw map



X Index: 84



Y Index: 84

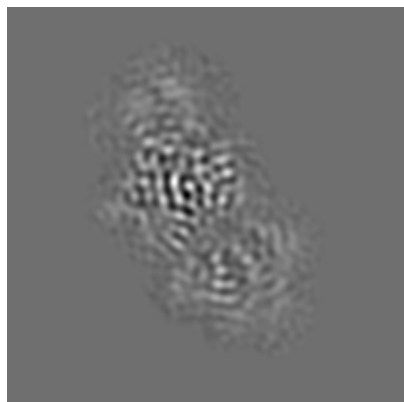


Z Index: 84

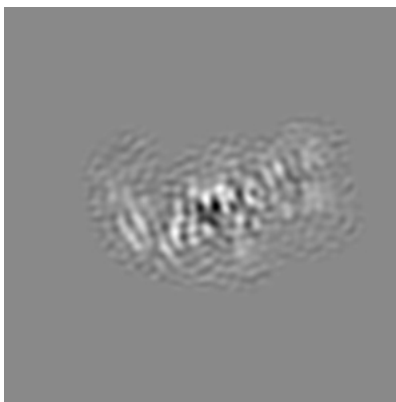
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 83

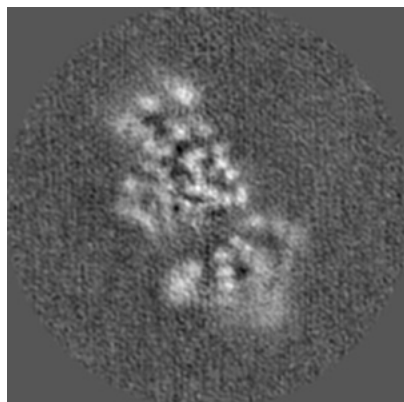


Y Index: 75

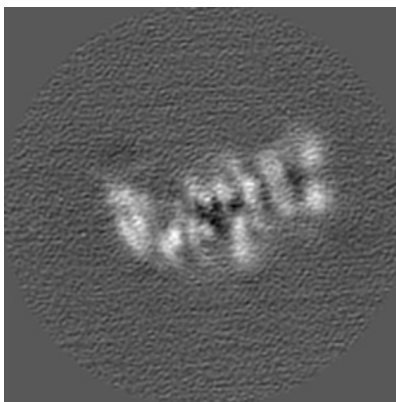


Z Index: 90

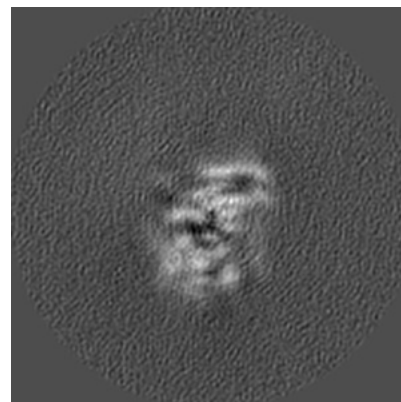
6.3.2 Raw map



X Index: 87



Y Index: 75

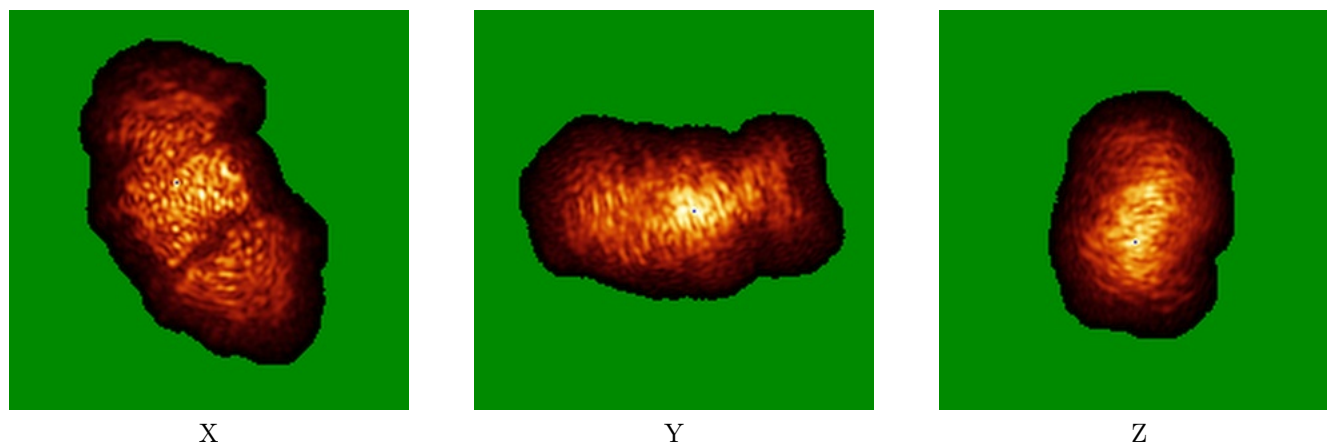


Z Index: 89

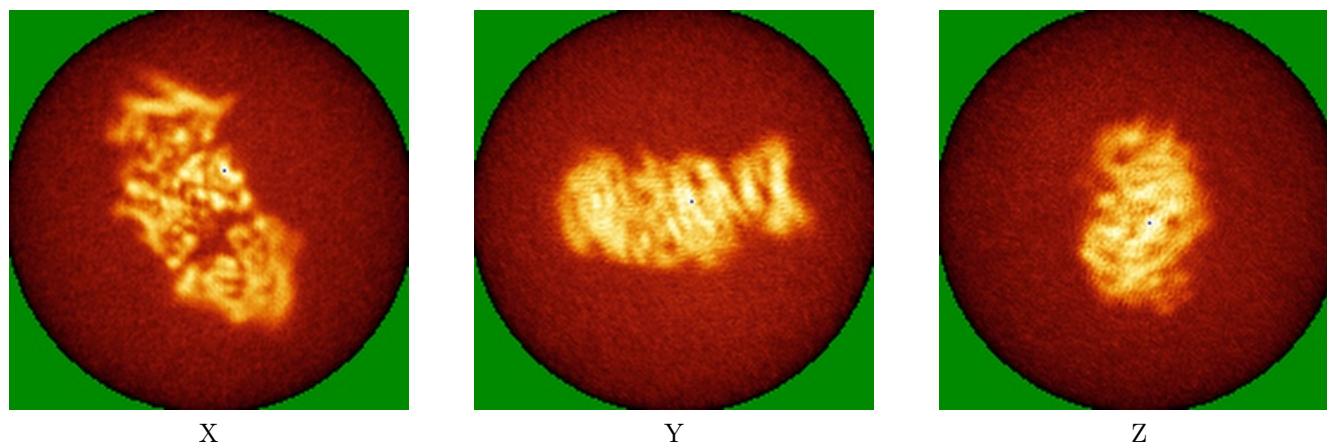
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

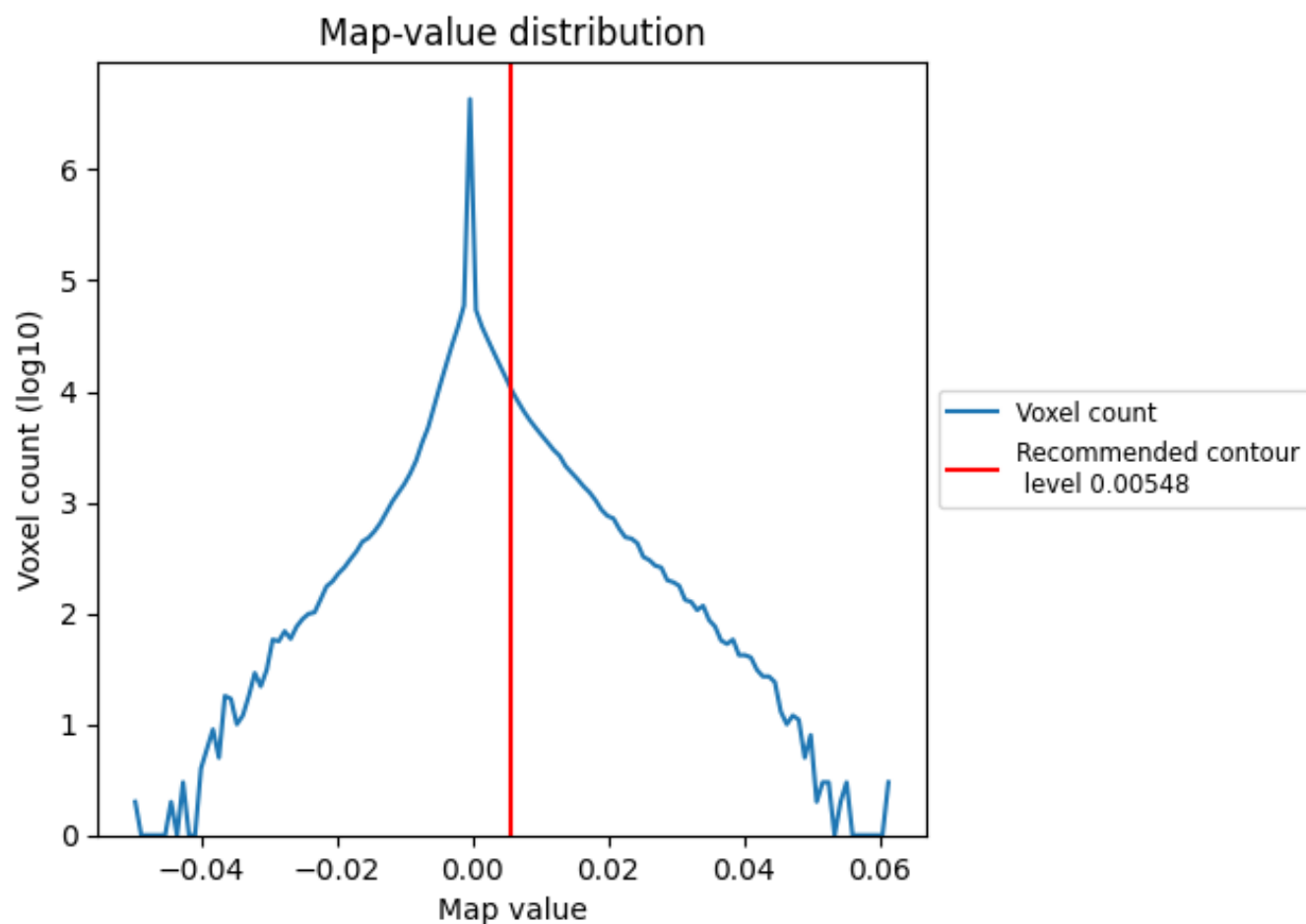
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

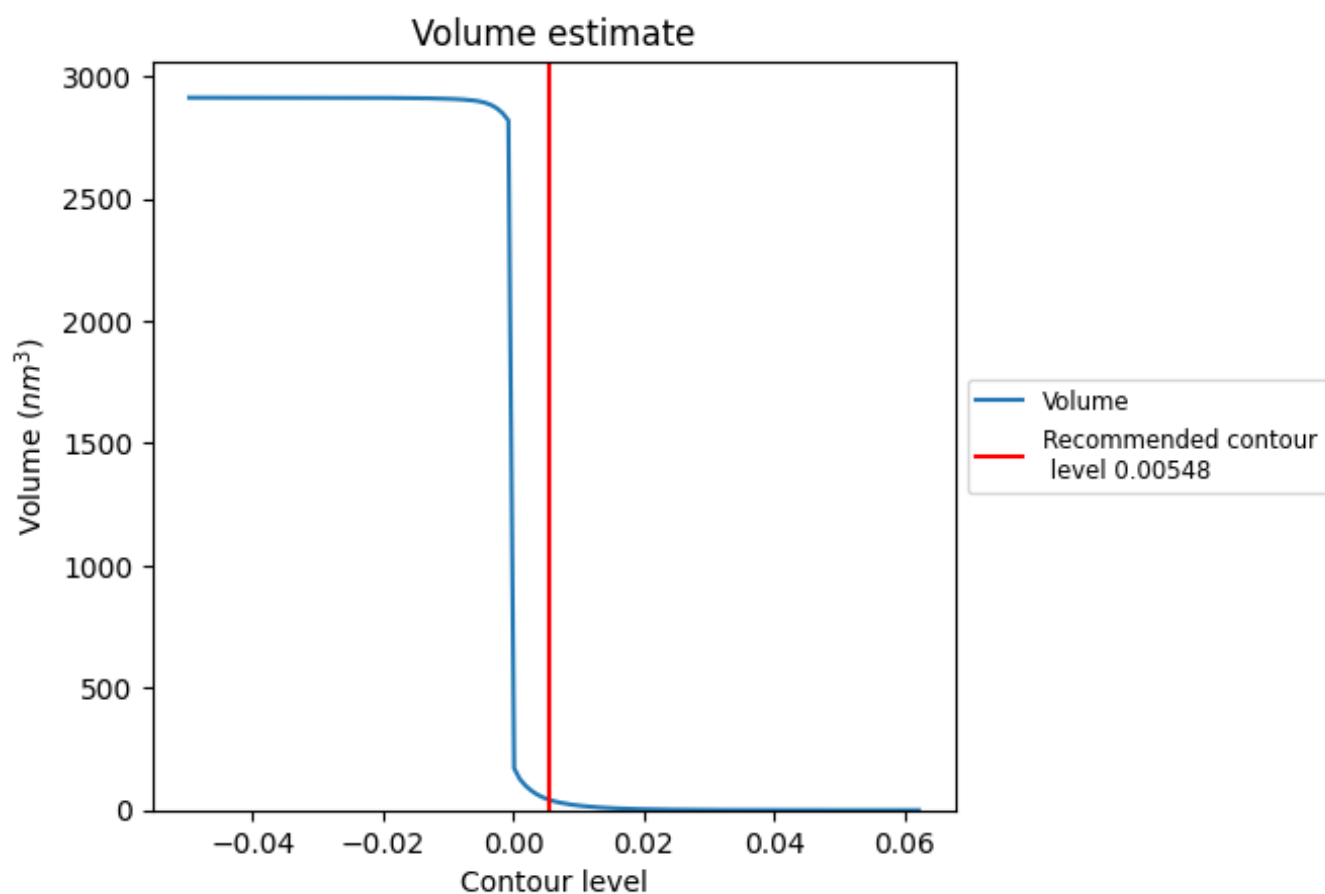
This section contains the results of statistical analysis of the map.

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.

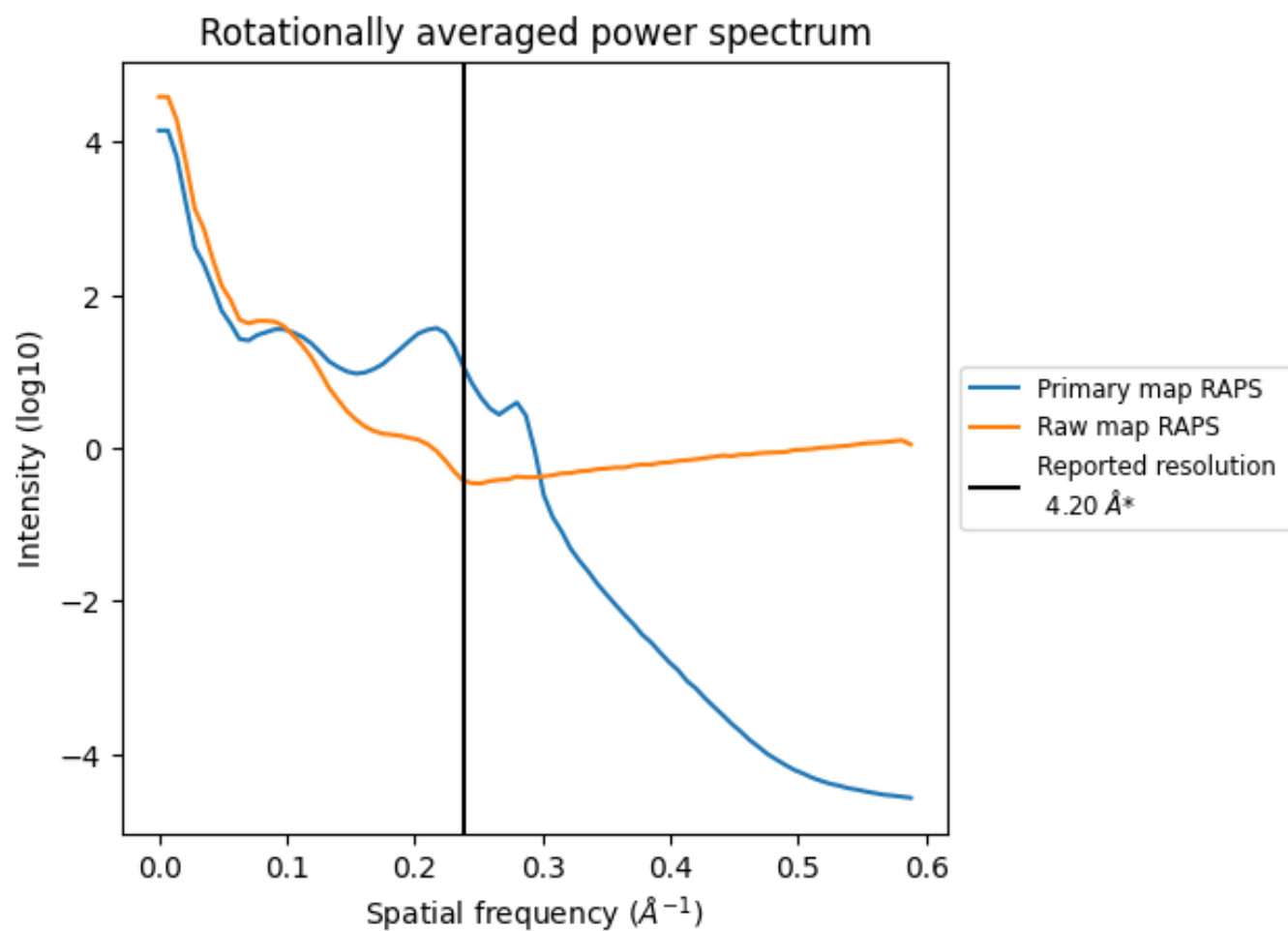
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 42 nm³; this corresponds to an approximate mass of 38 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 ⓘ

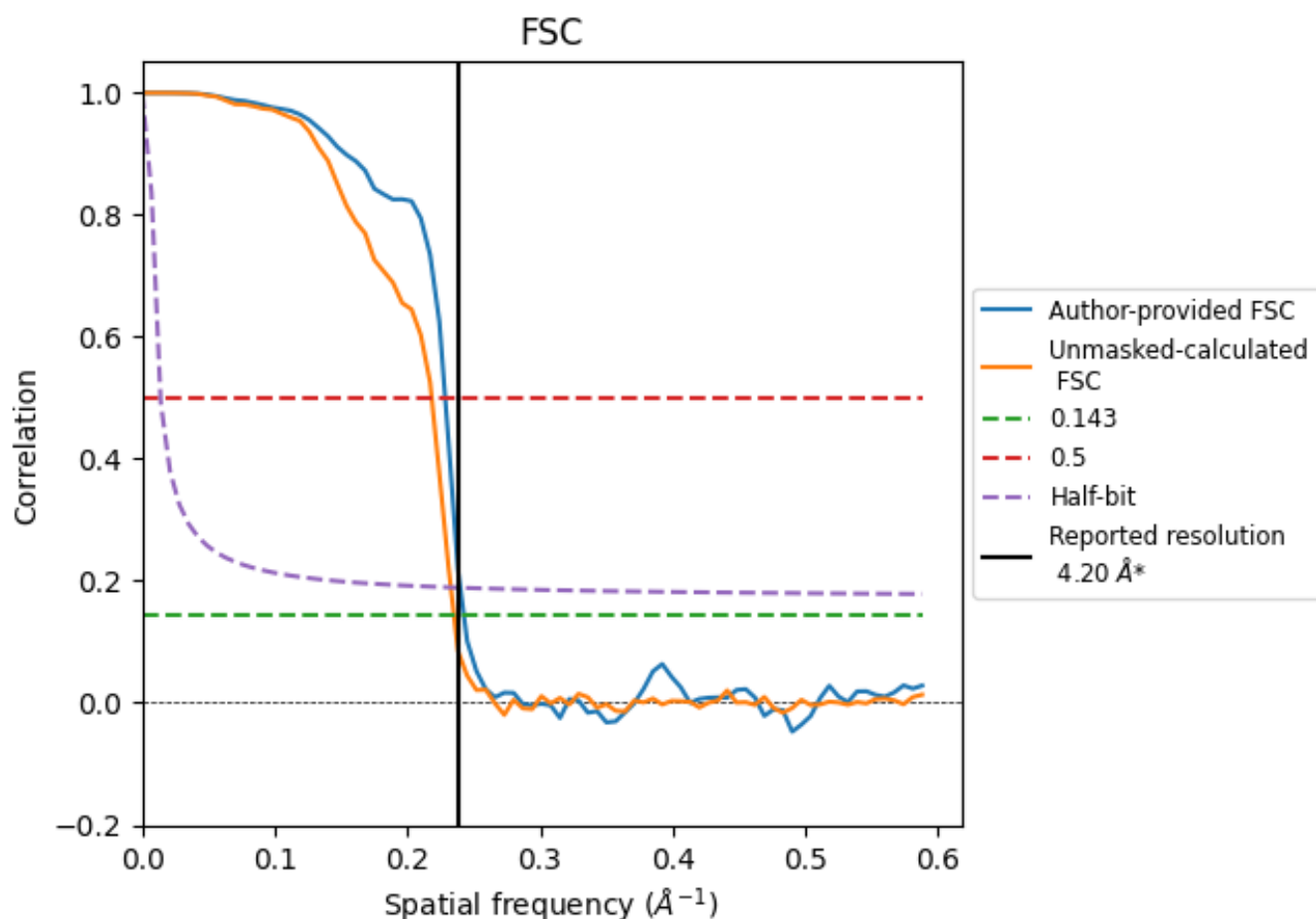


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

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 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.12	4.38	4.17
Unmasked-calculated*	4.25	4.58	4.30

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

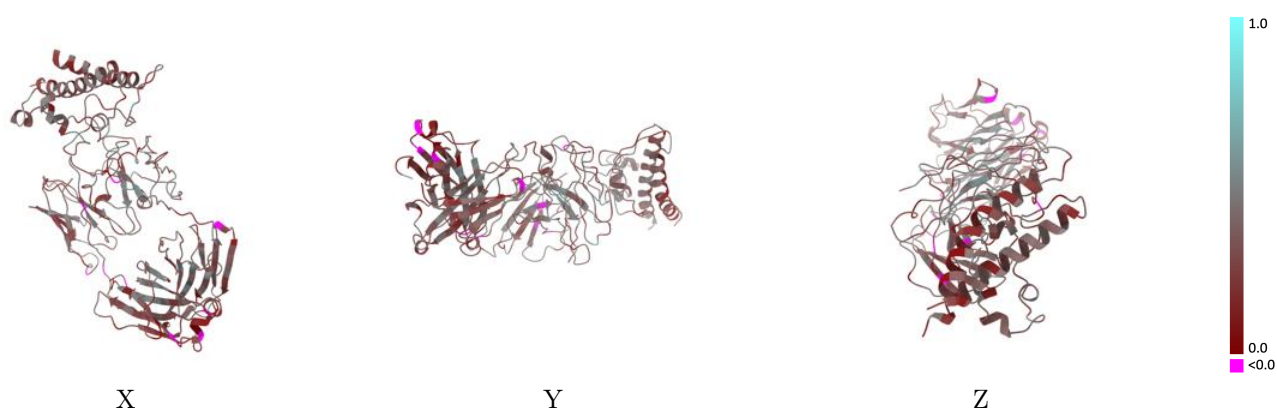
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16805 and PDB model 8CR9. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

This section was not generated.

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

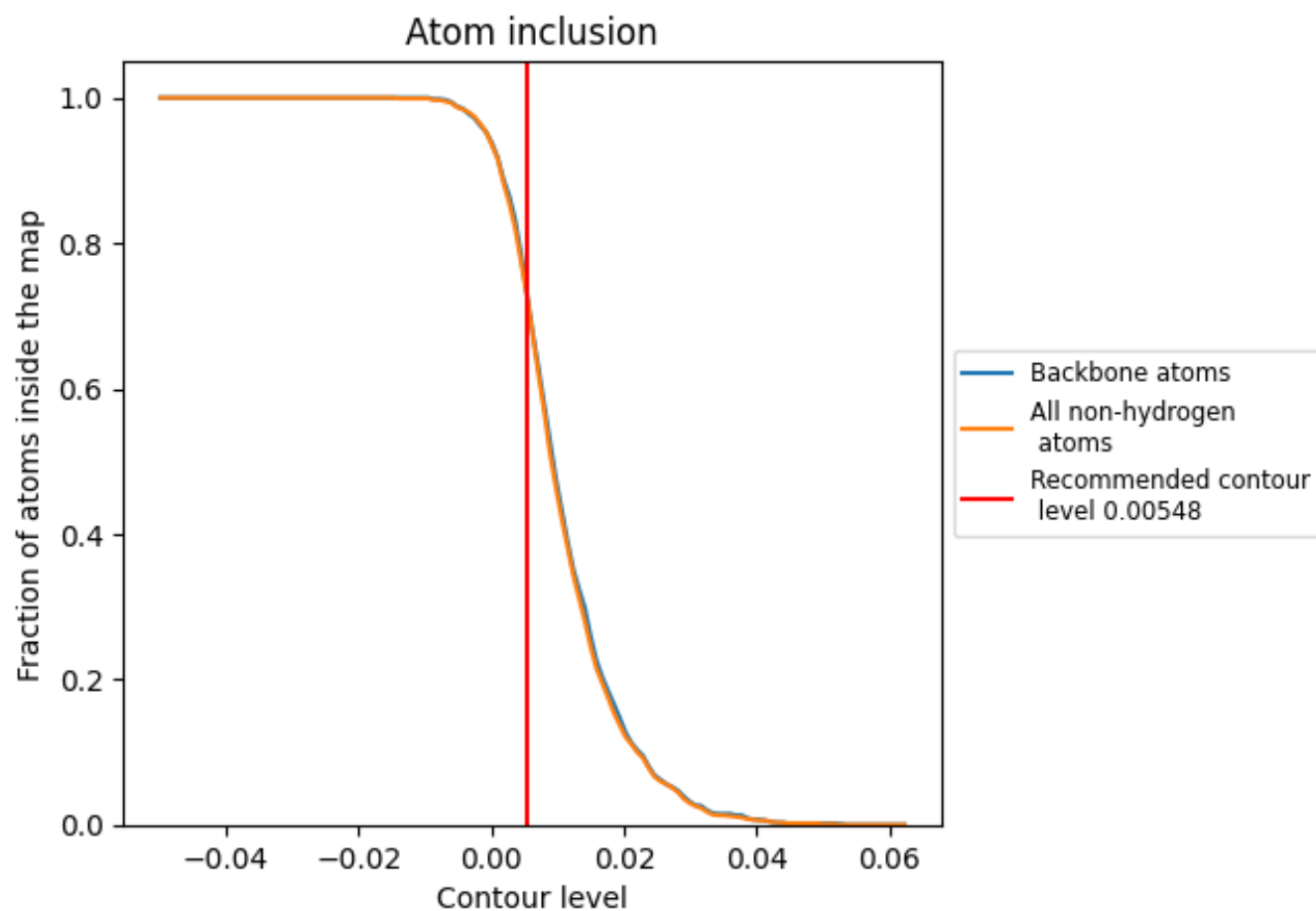


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.00548) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7230	0.3280
A	0.7390	0.3500
B	0.6750	0.3050
C	0.7400	0.3310

