



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 11:22 AM UTC

PDB ID : 9G93 / pdb_00009g93
EMDB ID : EMD-45459
Title : CryoET structure of the in vitro grown Bacillus anthracis Sap S-layer
Authors : Sogues, A.; Leigh, K.; Van der Verren, S.; Kudryashev, M.; Pak, A.; Hal-
ingstad, E.V.; Cecil, A.J.; Fioravanti, A.; Remaut, H.
Deposited on : 2024-07-24
Resolution : 7.20 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.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

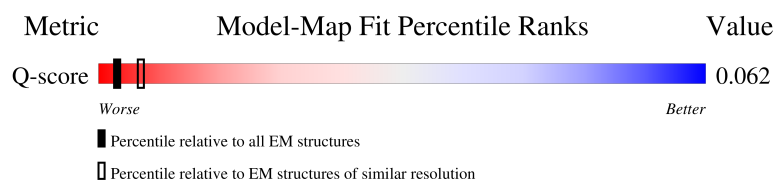
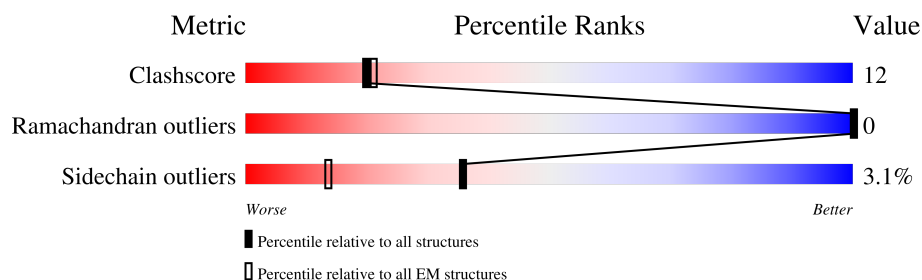
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.20 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	444 (6.70 - 7.70)

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	814	11% 61% 11% 27%
1	B	814	14% 63% 10% 27%
1	C	814	18% 62% 10% 27%
1	D	814	20% 63% 9% 27%

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Mol	Chain	Length	Quality of chain
1	E	814	20%62%11%27%
1	F	814	32%62%11%27%
1	G	814	12%29%5%66%
1	I	814	25%39%7%54%
1	J	814	11%27%6%66%
1	K	814	33%39%7%54%
1	L	814	6%10%89%

2 Entry composition

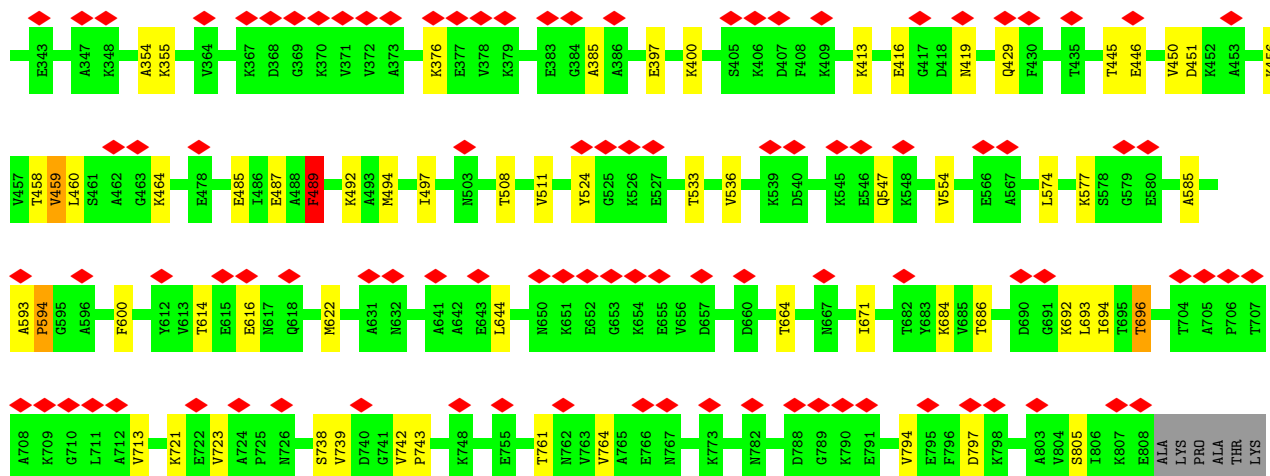
There is only 1 type of molecule in this entry. The entry contains 37178 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

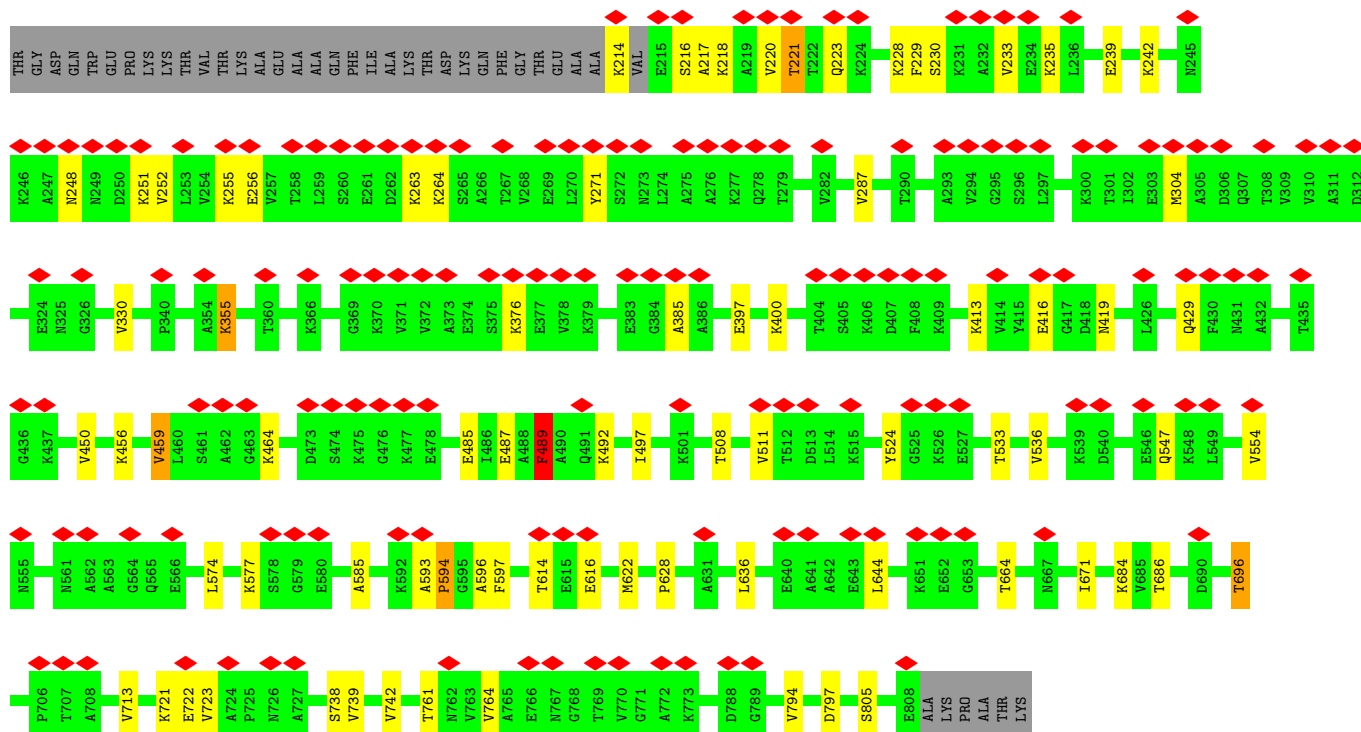
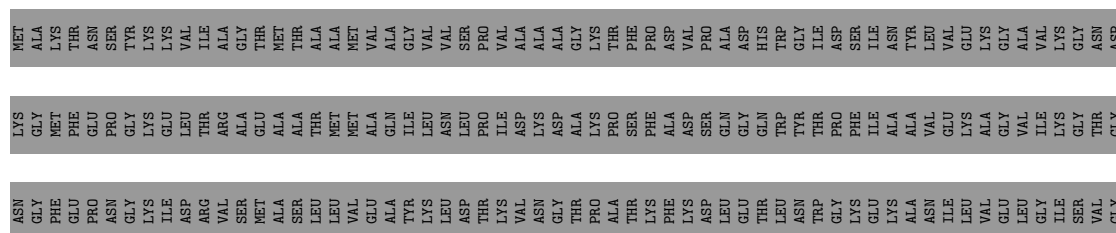
- Molecule 1 is a protein called S-layer protein sap.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	595	Total	C	N	O	S	0	0
			4456	2803	732	918	3		
1	B	595	Total	C	N	O	S	0	0
			4456	2803	732	918	3		
1	C	595	Total	C	N	O	S	0	0
			4456	2803	732	918	3		
1	D	595	Total	C	N	O	S	0	0
			4456	2803	732	918	3		
1	E	595	Total	C	N	O	S	0	0
			4456	2803	732	918	3		
1	F	595	Total	C	N	O	S	0	0
			4456	2803	732	918	3		
1	G	278	Total	C	N	O	S	0	0
			2097	1315	343	438	1		
1	I	376	Total	C	N	O	S	0	0
			2804	1761	458	584	1		
1	J	277	Total	C	N	O	S	0	0
			2088	1310	341	436	1		
1	L	88	Total	C	N	O	S	0	0
			649	406	103	139	1		
1	K	376	Total	C	N	O	S	0	0
			2804	1761	458	584	1		

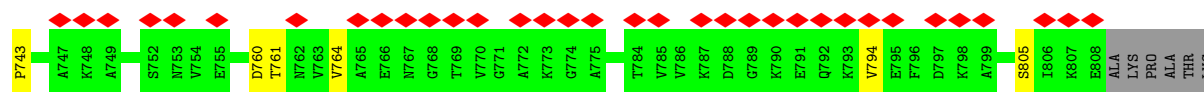




• Molecule 1: S-layer protein sap

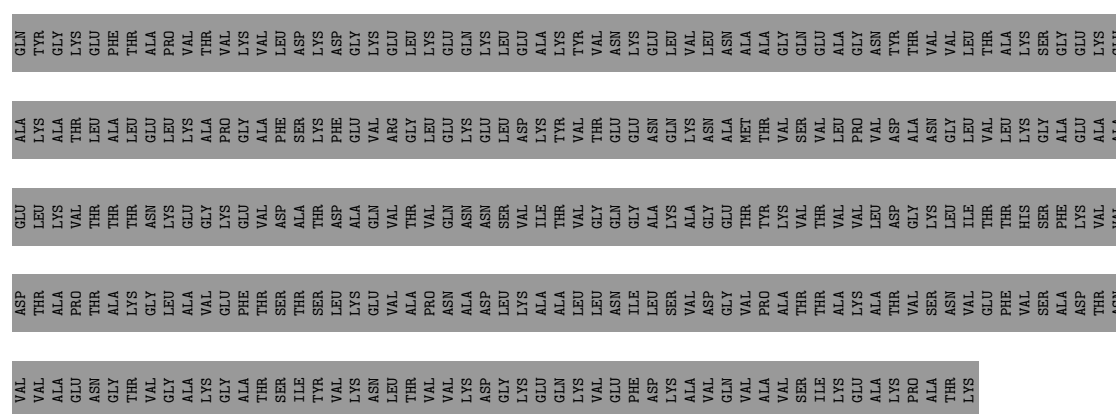
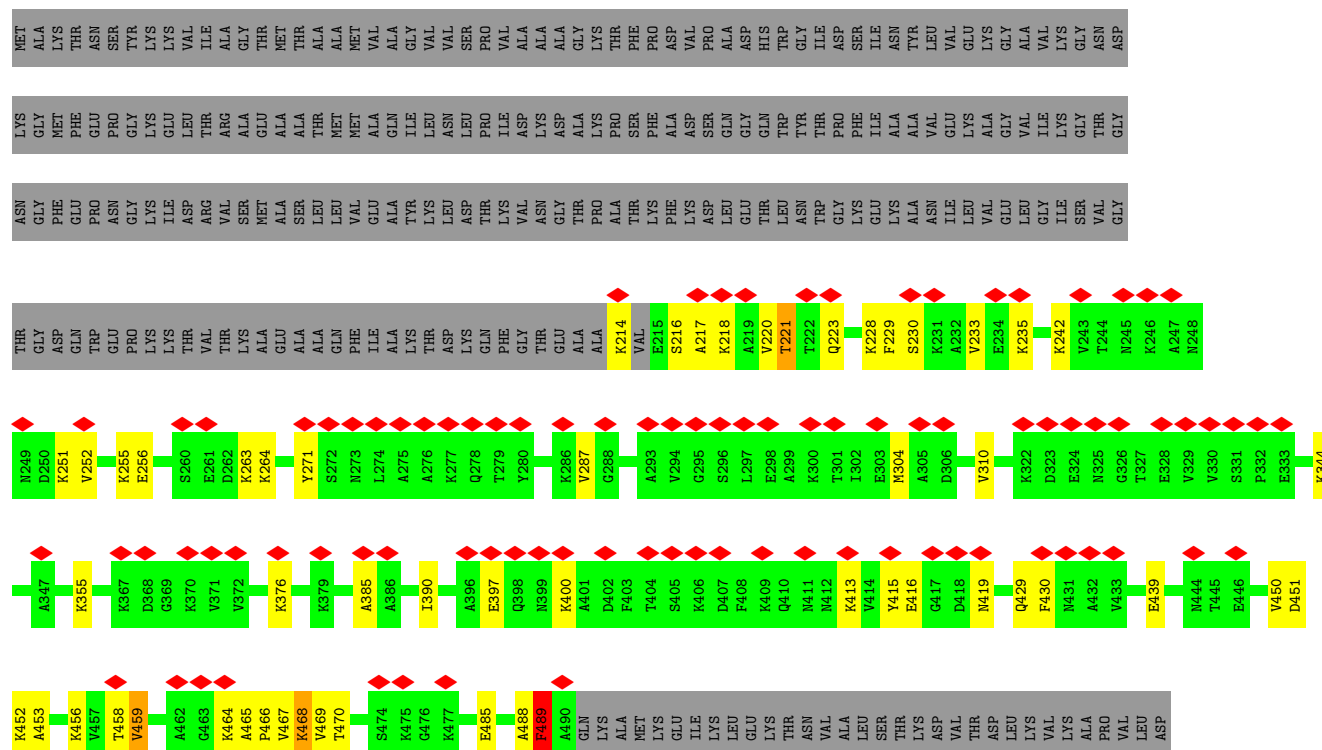


• Molecule 1: S-layer protein sap



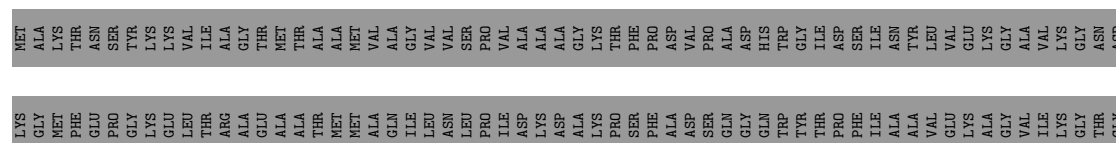
• Molecule 1: S-layer protein sap

Chain J: 11% 27% 6% 66%



• Molecule 1: S-layer protein sap

Chain L: 6% 10% 89%



D760	T761	N762	V763	V764	A765	E766	N767	G768	T769	V770	G771	A772	K773	G774	A775	K781	T784	V785	V786	K787	D788	G789	K790	E791	Q792	K793	V794	E795	F796	D797	K798	S805	I806	K807	E808	ALA	LYS	PRO	ALA	THR	LYS															
VAL	LEU	ASP	GLY	LYS	LEU	ILE	THR	THR	HIS	SER	PHE	LYS	VAL	VAL	ASP	THR	ALA	ALA	PRO	THR	ALA	LYS	G710	L711	A712	V713	E714	F715	T716	S717	T718	K721	E722	V723	A724	P725	N726	A727	D728	L729	K730	A731	A732	S738	V739	D740	G741	P743	T750	V751	S752	N753	V757	A759		
THR	LYS	ASP	THR	VAL	ASP	LEU	LYS	VAL	ALA	LYS	GLY	GLU	LYS	GLU	ASP	GLN	TYR	GLY	LYS	GLY	PHE	THR	PRO	ALA	THR	VAL	VAL	PRO	LYS	ALA	THR	LEU	LYS	GLU	GLN	LYS	LEU	ASP	GLU	ALA	LYS	TYR	VAL	GLU	GLN	ASN	LYS	GLU	LEU	VAL	LYS	ASN	ALA	THR	VAL	SER
GLY	ASN	TYR	THR	VAL	VAL	LEU	THR	VAL	LEU	ALA	LYS	SER	GLY	ALA	GLY	LYS	GLU	ALA	LYS	THR	LEU	ALA	GLU	THR	LYS	VAL	PRO	LYS	ALA	GLY	VAL	ARG	GLY	LEU	LYS	GLU	GLN	GLY	VAL	THR	TYR	VAL	GLU	GLN	ASN	ALA	GLN	LYS	ALA	THR	VAL	SER				
PRO	VAL	ASP	ALA	ASN	GLY	LEU	VAL	VAL	LEU	LYS	GLY	ALA	GLY	GLU	ALA	LYS	THR	THR	ASN	LYS	GLY	GLY	THR	ALA	THR	ASP	GLN	VAL	THR	VAL	GLN	ASN	SER	ILE	THR	VAL	GLY	GLN	GLY	ALA	LYS	ALA	THR	LYS	VAL	THR	VAL	THR	VAL							
VAL	LEU	ASP	GLY	LYS	LEU	ILE	THR	THR	HIS	SER	PHE	LYS	VAL	VAL	ASP	THR	ALA	ALA	PRO	THR	ALA	LYS	G710	L711	A712	V713	E714	F715	T716	S717	T718	K721	E722	V723	A724	P725	N726	A727	D728	L729	K730	A731	A732	S738	V739	D740	G741	P743	T750	V751	S752	N753	V757	A759		

4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	10126	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	156	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.084	Depositor
Minimum map value	-5.636	Depositor
Average map value	-0.058	Depositor
Map value standard deviation	0.834	Depositor
Recommended contour level	2.56	Depositor
Map size ($\text{\AA}$)	345.59998, 345.59998, 345.59998	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.7999998, 1.7999998, 1.7999998	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	A	0.45	2/4495 (0.0%)	0.63	2/6079 (0.0%)
1	B	0.45	2/4495 (0.0%)	0.63	2/6079 (0.0%)
1	C	0.45	2/4495 (0.0%)	0.62	2/6079 (0.0%)
1	D	0.45	2/4495 (0.0%)	0.61	2/6079 (0.0%)
1	E	0.46	2/4495 (0.0%)	0.62	2/6079 (0.0%)
1	F	0.45	2/4495 (0.0%)	0.62	2/6079 (0.0%)
1	G	0.68	3/2115 (0.1%)	0.68	5/2857 (0.2%)
1	I	0.61	3/2827 (0.1%)	0.64	3/3825 (0.1%)
1	J	0.68	3/2106 (0.1%)	0.70	6/2845 (0.2%)
1	K	0.49	2/2827 (0.1%)	0.62	1/3825 (0.0%)
1	L	0.51	2/654 (0.3%)	0.55	0/884
All	All	0.50	25/37499 (0.1%)	0.63	27/50710 (0.1%)

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	488	ALA	C-N	20.32	1.52	1.33
1	J	488	ALA	C-N	20.30	1.52	1.33
1	G	488	ALA	C-N	20.27	1.52	1.33
1	K	487	GLU	C-N	-11.44	1.17	1.33
1	E	487	GLU	C-N	-9.78	1.19	1.33

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	594	PRO	O-C-N	-11.75	109.75	123.03
1	A	594	PRO	O-C-N	-11.71	109.79	123.03
1	B	594	PRO	O-C-N	-11.61	109.91	123.03
1	F	594	PRO	O-C-N	-10.46	111.21	123.03
1	D	594	PRO	O-C-N	-10.12	111.60	123.03

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	4456	0	4624	179	0
1	B	4456	0	4624	109	0
1	C	4456	0	4624	136	0
1	D	4456	0	4624	88	0
1	E	4456	0	4624	207	0
1	F	4456	0	4624	157	0
1	G	2097	0	2158	36	0
1	I	2804	0	2892	85	0
1	J	2088	0	2150	54	0
1	K	2804	0	2892	81	0
1	L	649	0	663	4	0
All	All	37178	0	38499	941	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 12.

The worst 5 of 941 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:F:239:GLU:CB	1:F:742:VAL:CG1	1.77	1.62
1:B:239:GLU:CB	1:B:742:VAL:CG1	1.77	1.61
1:K:239:GLU:CB	1:K:742:VAL:CG1	1.77	1.60
1:I:239:GLU:CB	1:I:742:VAL:CG1	1.77	1.59
1:C:239:GLU:CB	1:C:742:VAL:CG1	1.77	1.58

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	593/814 (73%)	572 (96%)	21 (4%)	0	100	100
1	B	593/814 (73%)	572 (96%)	21 (4%)	0	100	100
1	C	593/814 (73%)	572 (96%)	21 (4%)	0	100	100
1	D	593/814 (73%)	572 (96%)	21 (4%)	0	100	100
1	E	593/814 (73%)	572 (96%)	21 (4%)	0	100	100
1	F	579/814 (71%)	560 (97%)	19 (3%)	0	100	100
1	G	276/814 (34%)	269 (98%)	7 (2%)	0	100	100
1	I	372/814 (46%)	364 (98%)	8 (2%)	0	100	100
1	J	275/814 (34%)	268 (98%)	7 (2%)	0	100	100
1	K	372/814 (46%)	364 (98%)	8 (2%)	0	100	100
1	L	86/814 (11%)	81 (94%)	5 (6%)	0	100	100
All	All	4925/8954 (55%)	4766 (97%)	159 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	491/659 (74%)	476 (97%)	15 (3%)	35	56
1	B	491/659 (74%)	476 (97%)	15 (3%)	35	56
1	C	491/659 (74%)	476 (97%)	15 (3%)	35	56
1	D	491/659 (74%)	476 (97%)	15 (3%)	35	56
1	E	491/659 (74%)	476 (97%)	15 (3%)	35	56
1	F	491/659 (74%)	476 (97%)	15 (3%)	35	56
1	G	233/659 (35%)	223 (96%)	10 (4%)	26	47
1	I	311/659 (47%)	302 (97%)	9 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	232/659 (35%)	223 (96%)	9 (4%)	28	49
1	K	311/659 (47%)	302 (97%)	9 (3%)	37	58
1	L	71/659 (11%)	70 (99%)	1 (1%)	59	72
All	All	4104/7249 (57%)	3976 (97%)	128 (3%)	36	56

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	376	LYS
1	K	216	SER
1	D	235	LYS
1	D	221	THR
1	K	221	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	223	GLN
1	L	318	GLN
1	K	223	GLN
1	J	223	GLN
1	D	620	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1
1	I	1
1	J	1
1	E	1
1	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	489:PHE	C	490:ALA	N	1.20
1	I	489:PHE	C	490:ALA	N	1.20
1	J	489:PHE	C	490:ALA	N	1.20
1	E	487:GLU	C	488:ALA	N	1.19
1	K	487:GLU	C	488:ALA	N	1.17

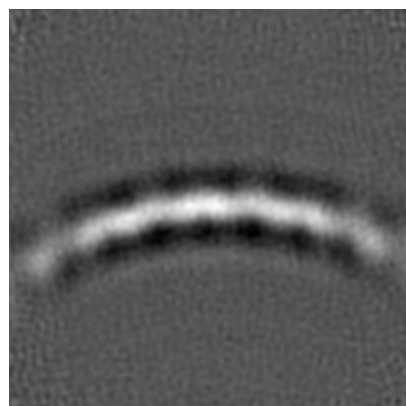
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45459. These allow visual inspection of the internal detail of the map and identification of artifacts.

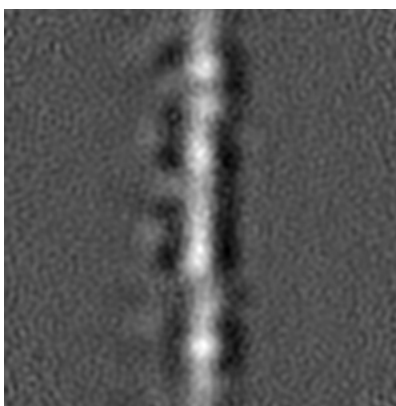
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

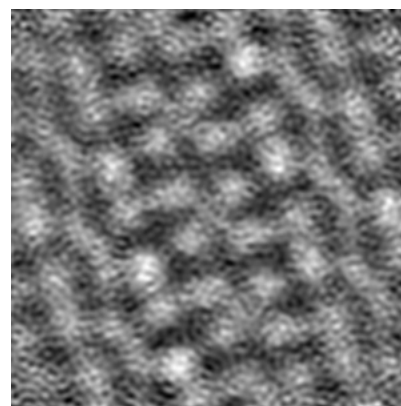
6.1.1 Primary map



X

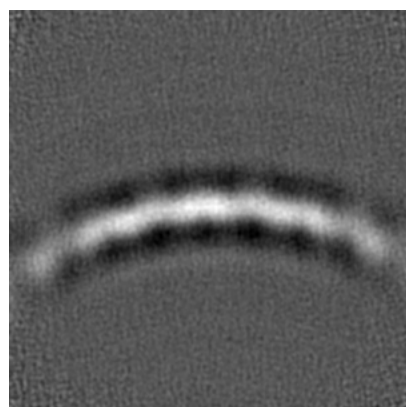


Y

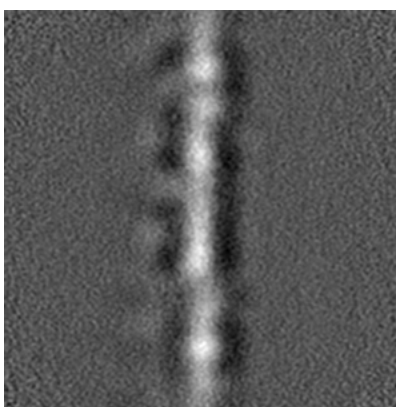


Z

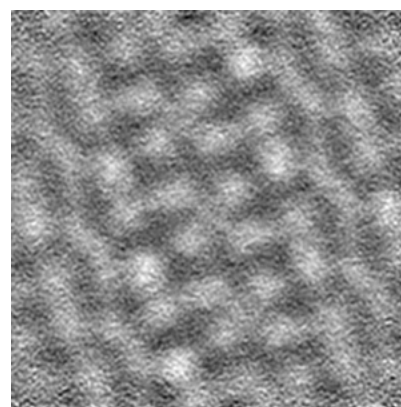
6.1.2 Raw map



X



Y



Z

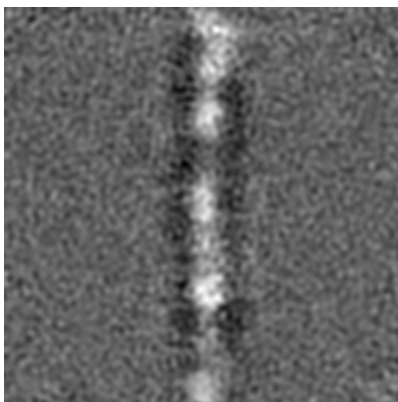
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

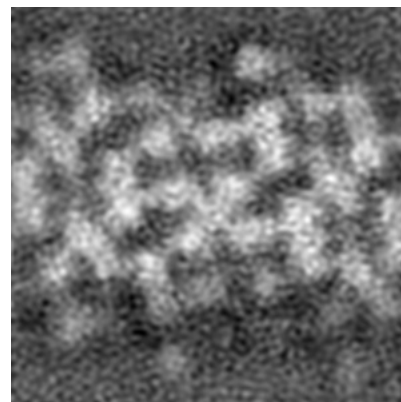
6.2.1 Primary map



X Index: 96

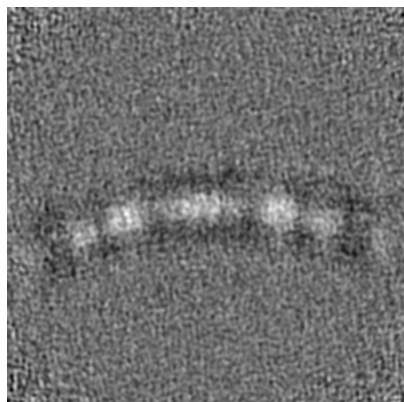


Y Index: 96

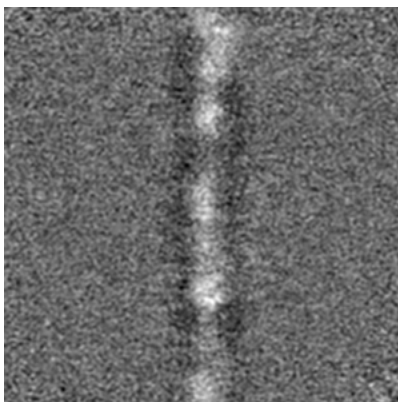


Z Index: 96

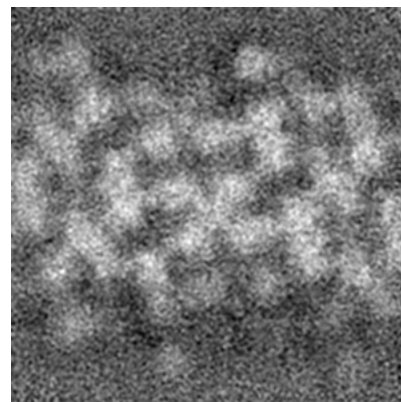
6.2.2 Raw map



X Index: 96



Y Index: 96



Z Index: 96

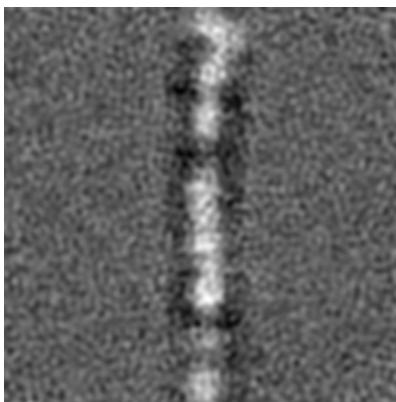
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

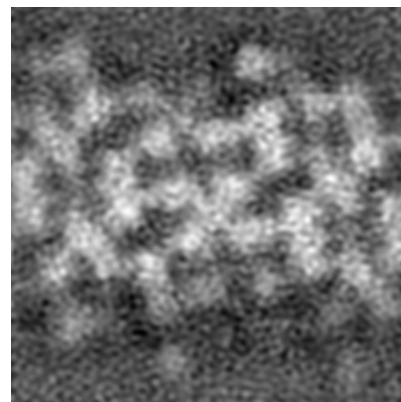
6.3.1 Primary map



X Index: 121

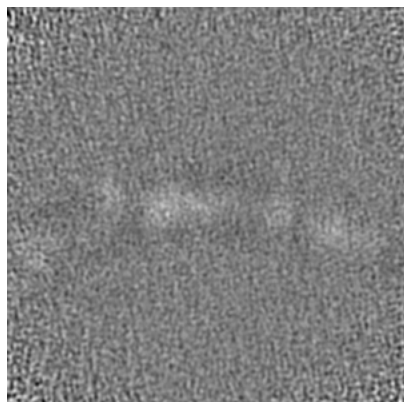


Y Index: 98

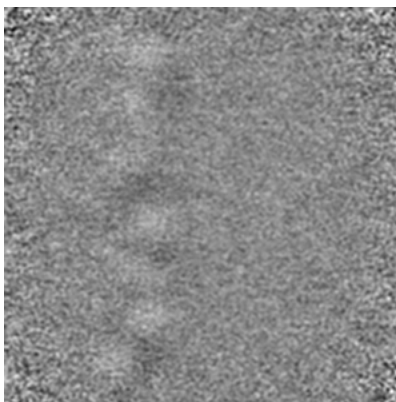


Z Index: 96

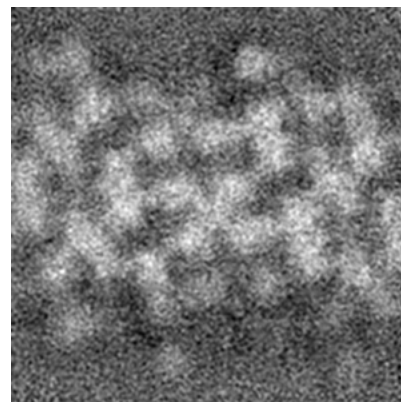
6.3.2 Raw map



X Index: 190



Y Index: 0

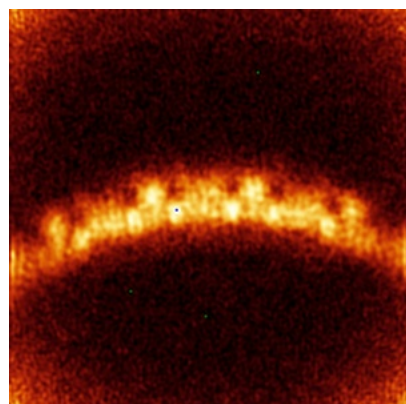


Z Index: 96

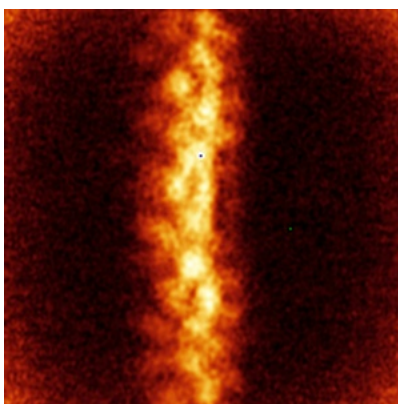
The images above show the largest variance slices of the map in three orthogonal directions.

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

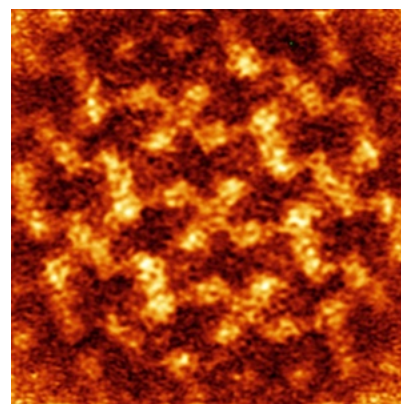
6.4.1 Primary map



X

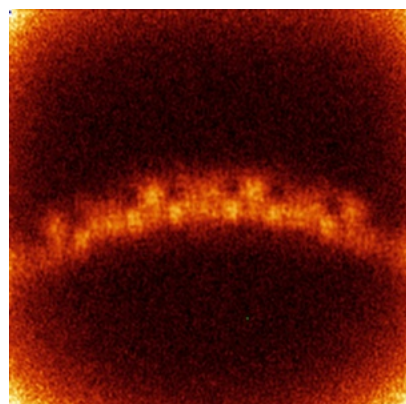


Y

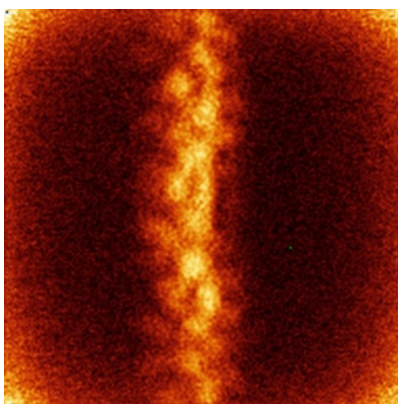


Z

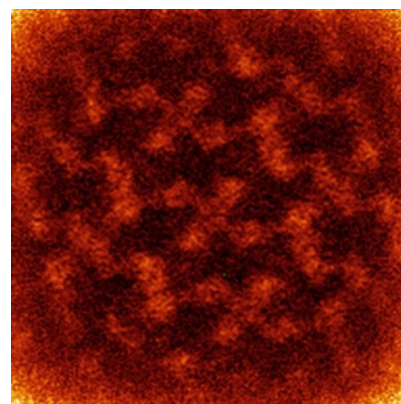
6.4.2 Raw map



X



Y

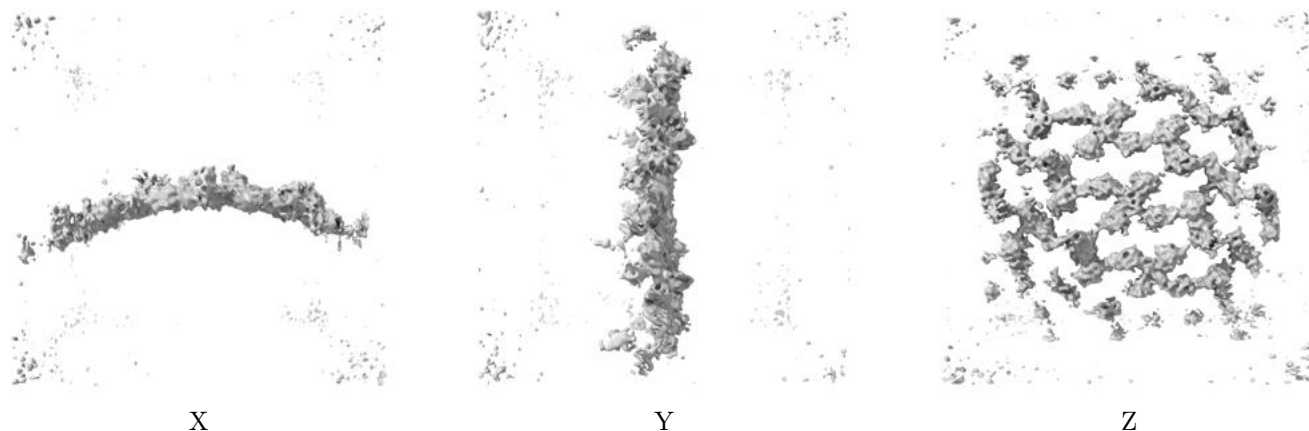


Z

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.

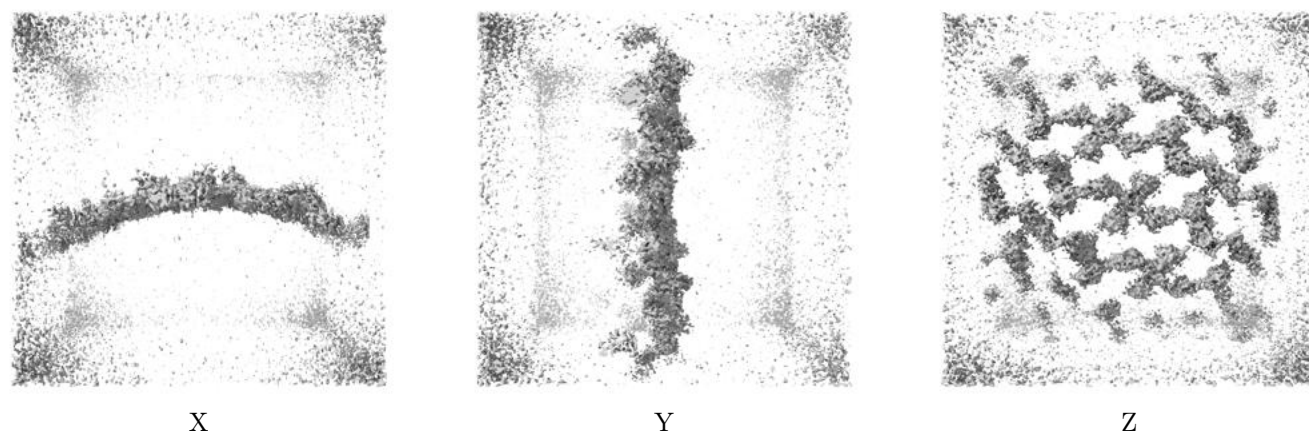
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.56. 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.

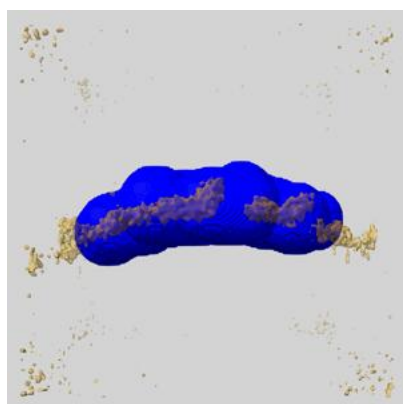
6.6 Mask visualisation [i](#)

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

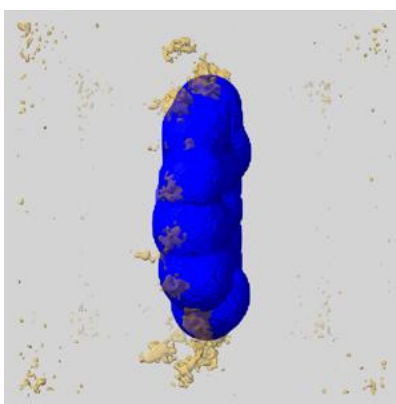
A mask typically either:

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

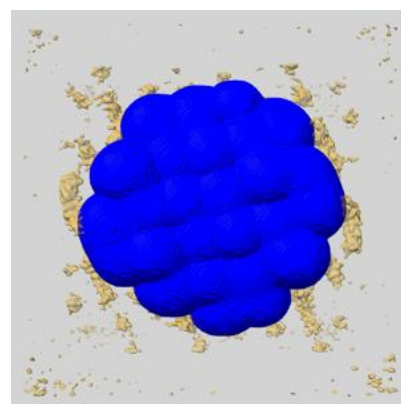
6.6.1 emd_45459_msk_1.map [i](#)



X



Y

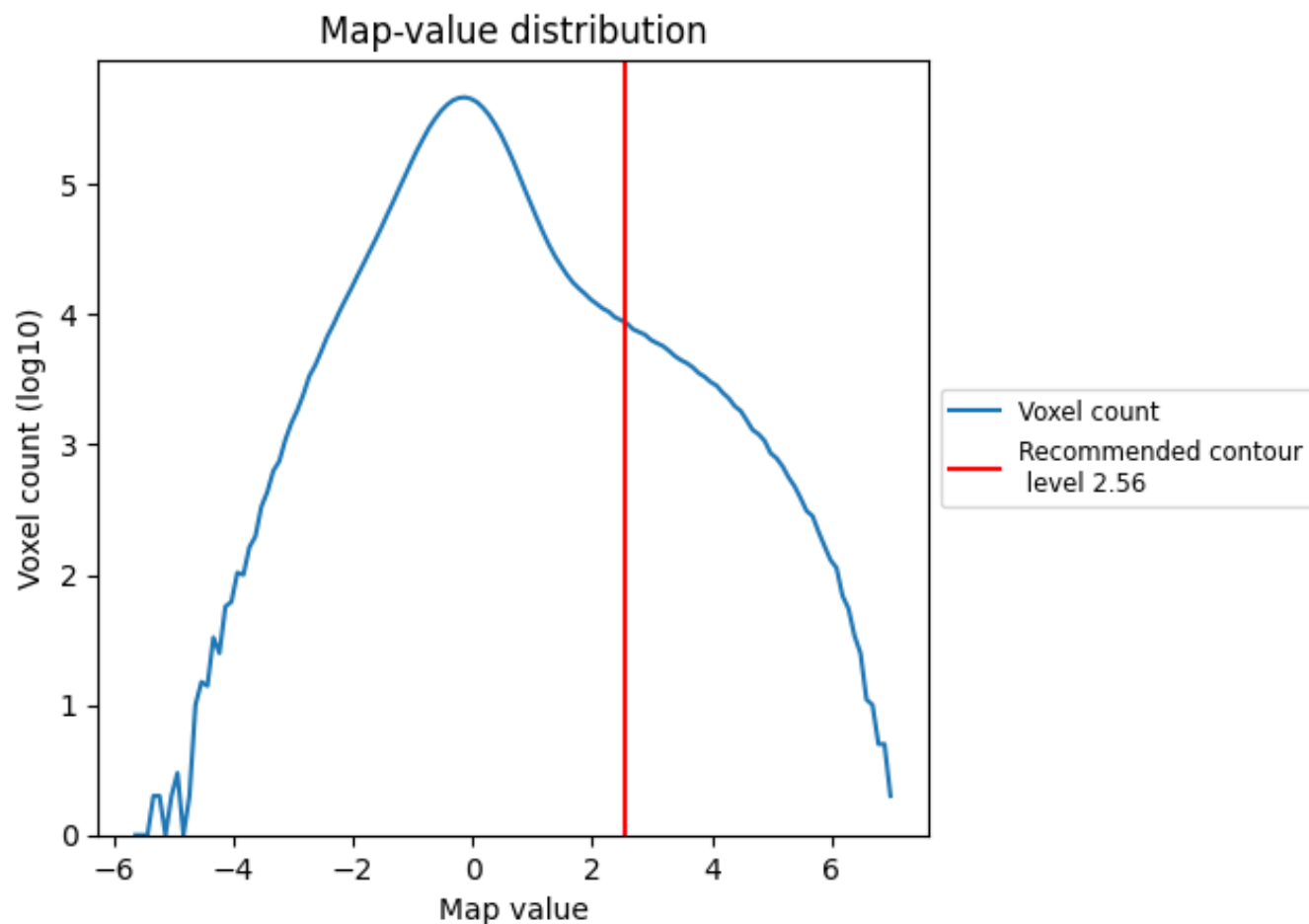


Z

7 Map analysis [i](#)

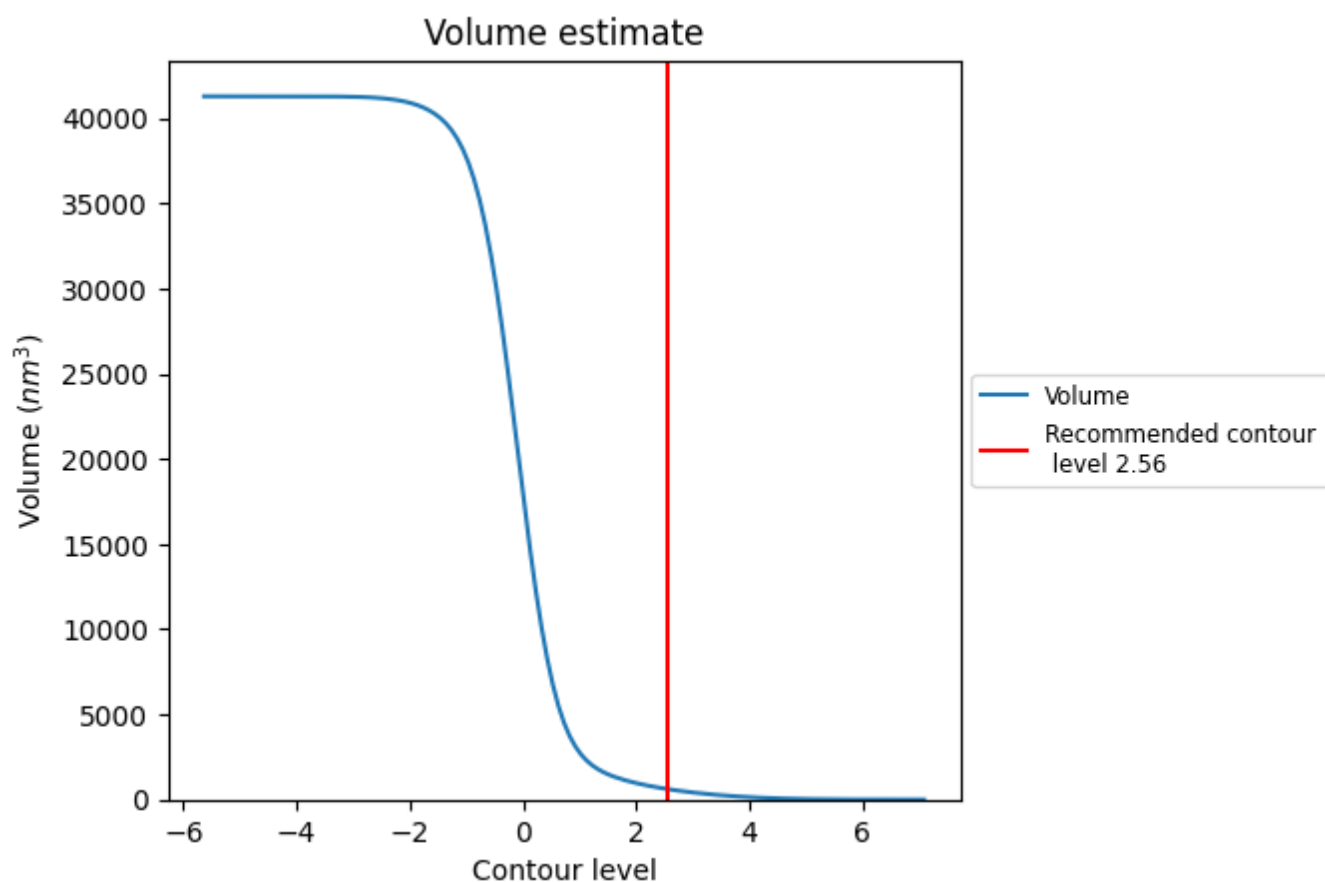
This section contains the results of statistical analysis of the map.

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.

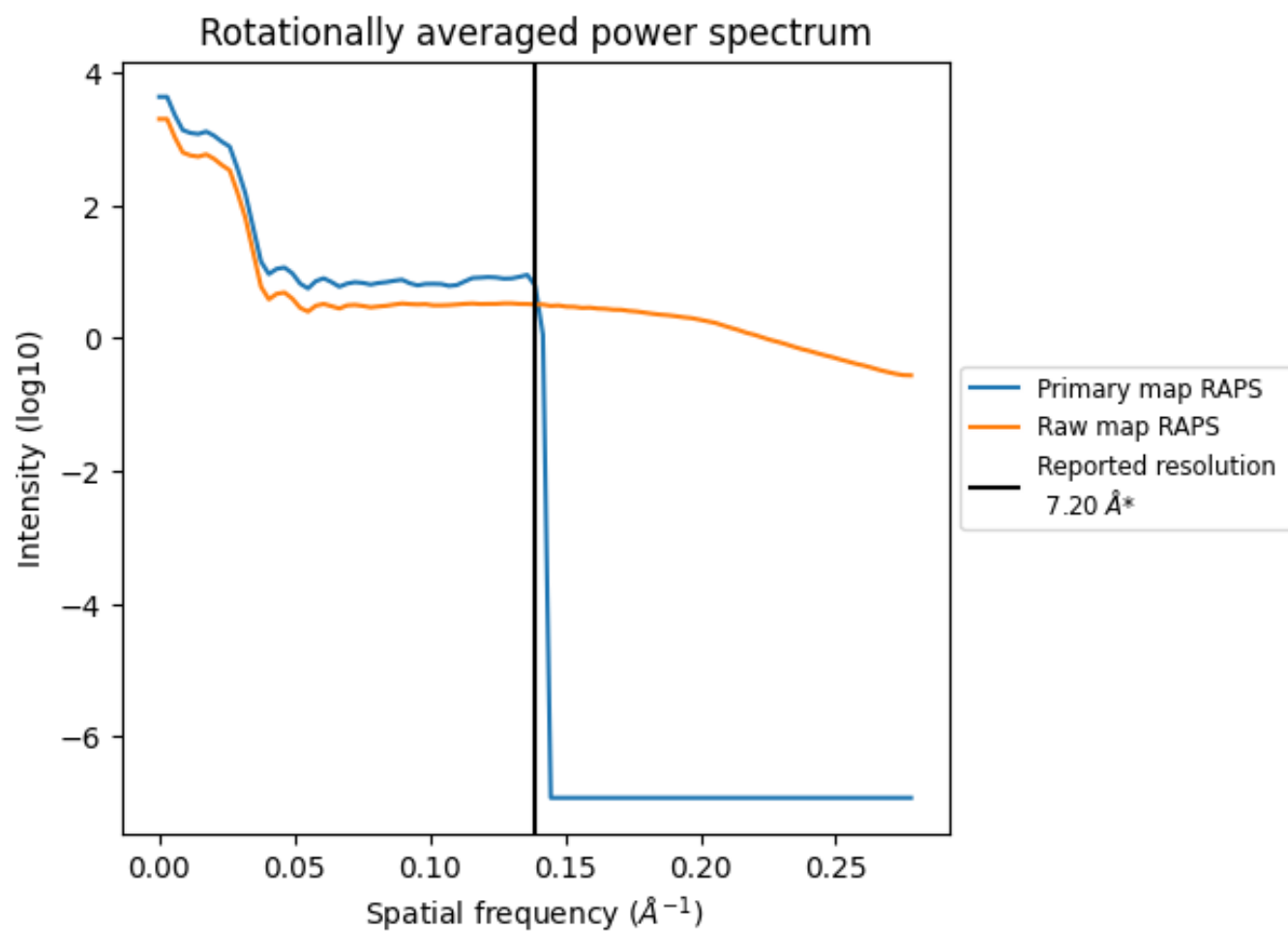
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 611 nm³; this corresponds to an approximate mass of 552 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 ⓘ

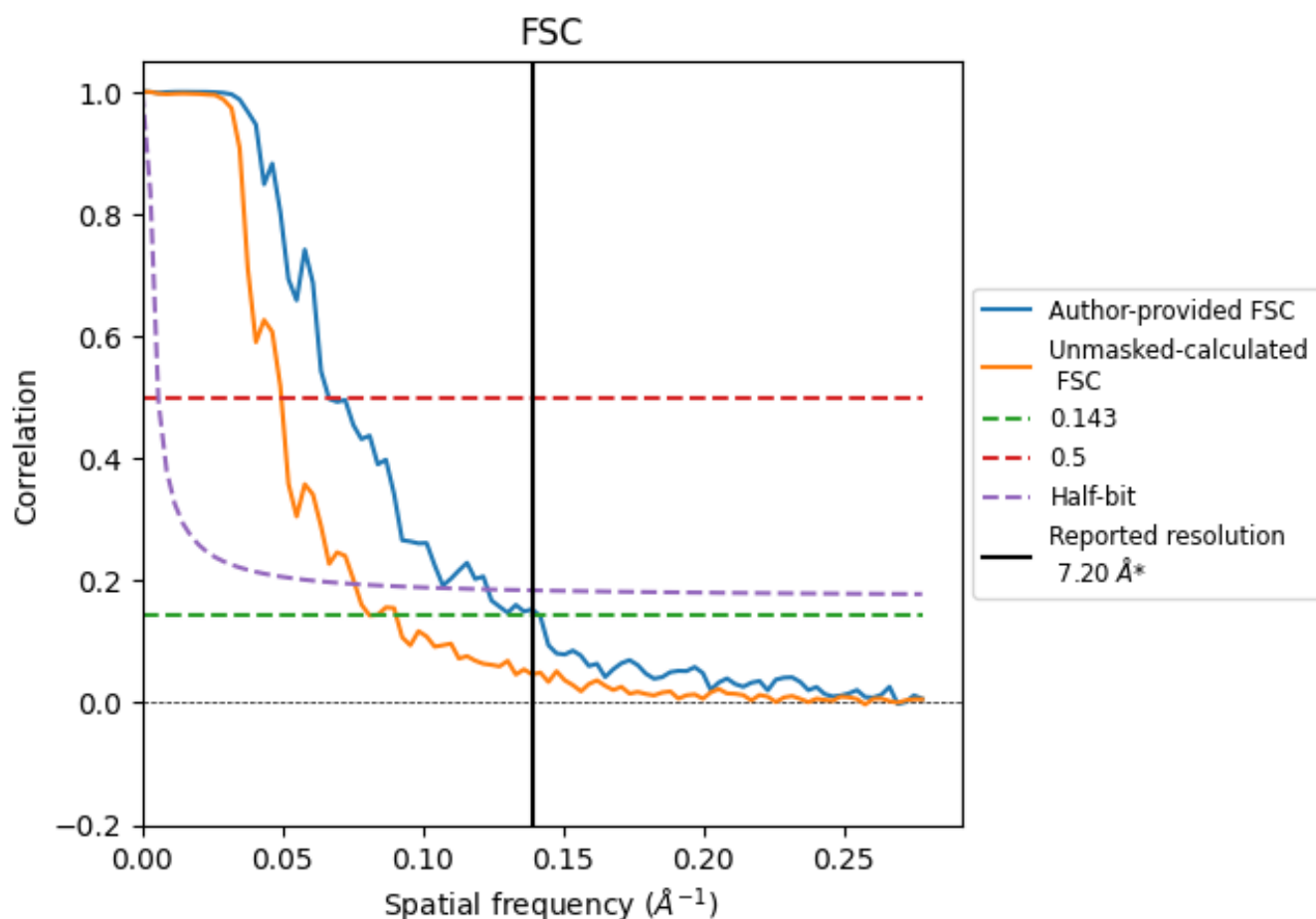


*Reported resolution corresponds to spatial frequency of 0.139 $\text{\AA}^{-1}$

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 0.139 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

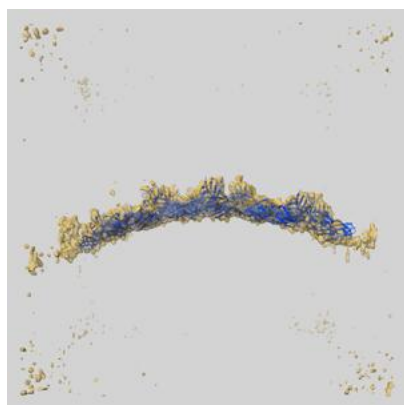
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.20	-	-
Author-provided FSC curve	7.07	15.06	8.12
Unmasked-calculated*	12.35	20.20	13.19

*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 12.35 differs from the reported value 7.2 by more than 10 %

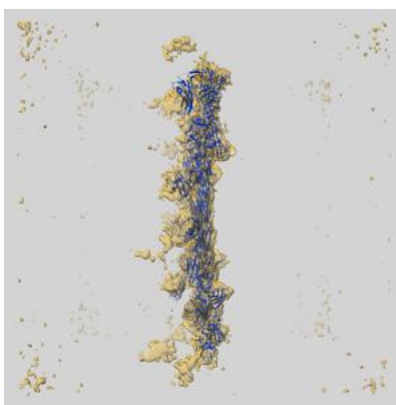
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45459 and PDB model 9G93. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

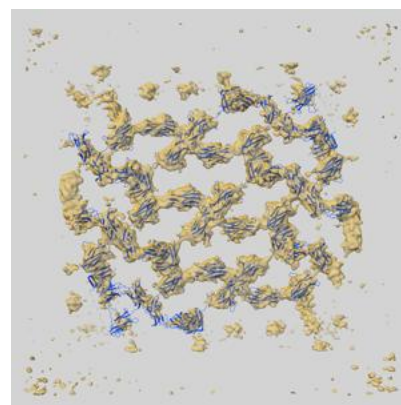
9.1 Map-model overlay [i](#)



X



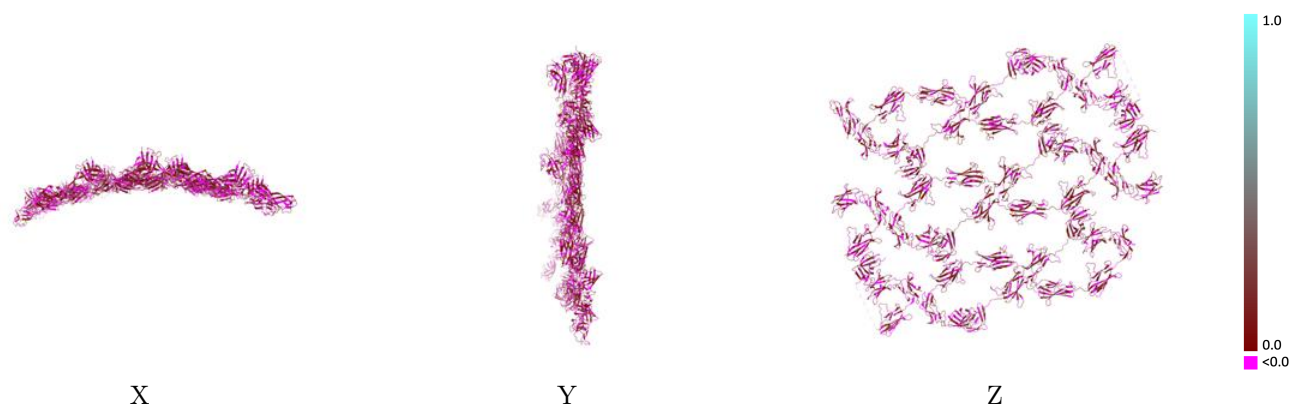
Y



Z

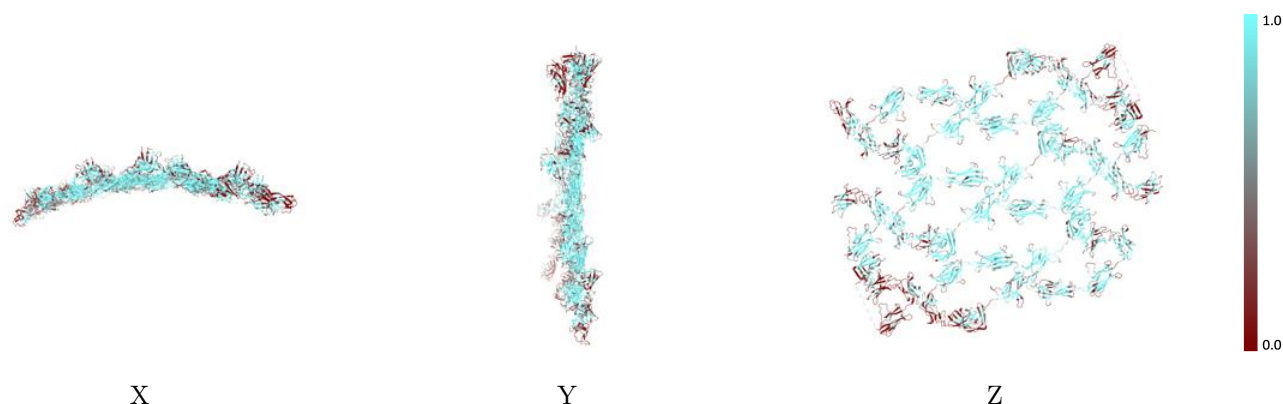
The images above show the 3D surface view of the map at the recommended contour level 2.56 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



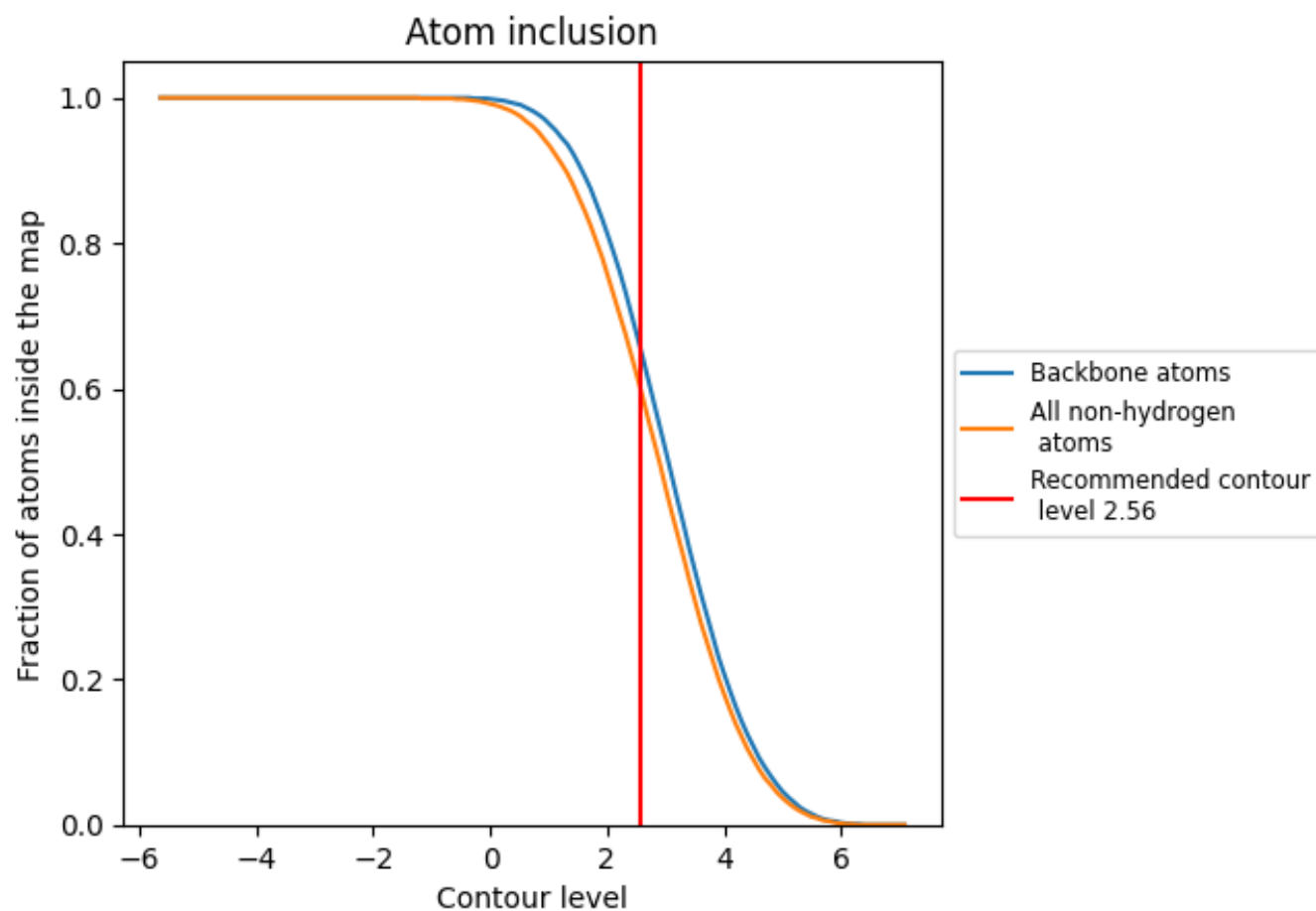
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.56).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 60% 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 (2.56) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6020	0.0620
A	0.7630	0.0850
B	0.7460	0.0760
C	0.6630	0.0650
D	0.6610	0.0650
E	0.6590	0.0630
F	0.5190	0.0550
G	0.5730	0.0480
I	0.4020	0.0440
J	0.5880	0.0540
K	0.2630	0.0420
L	0.3410	0.0550

1.0

0.0

<0.0