



## wwPDB EM Validation Summary Report ⓘ

Sep 1, 2025 – 01:26 pm BST

PDB ID : 9QCO / pdb\_00009qco  
EMDB ID : EMD-53017  
Title : NTNHA70 complex from Clostridium botulinum Serotype B1  
Authors : Krc, A.; Persson Kosenina, S.; Masuyer, G.; Stenmark, P.  
Deposited on : 2025-03-04  
Resolution : 2.76 Å (reported)  
Based on initial model : .

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev126  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.45.1

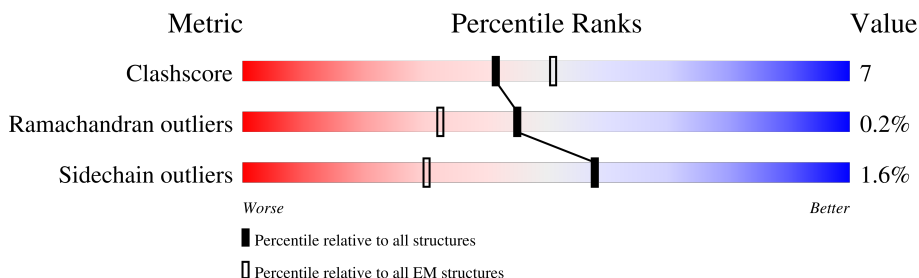
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.76 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  $\geq 3$ , 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	1197	
2	B	626	
2	C	626	
2	D	626	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19569 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.

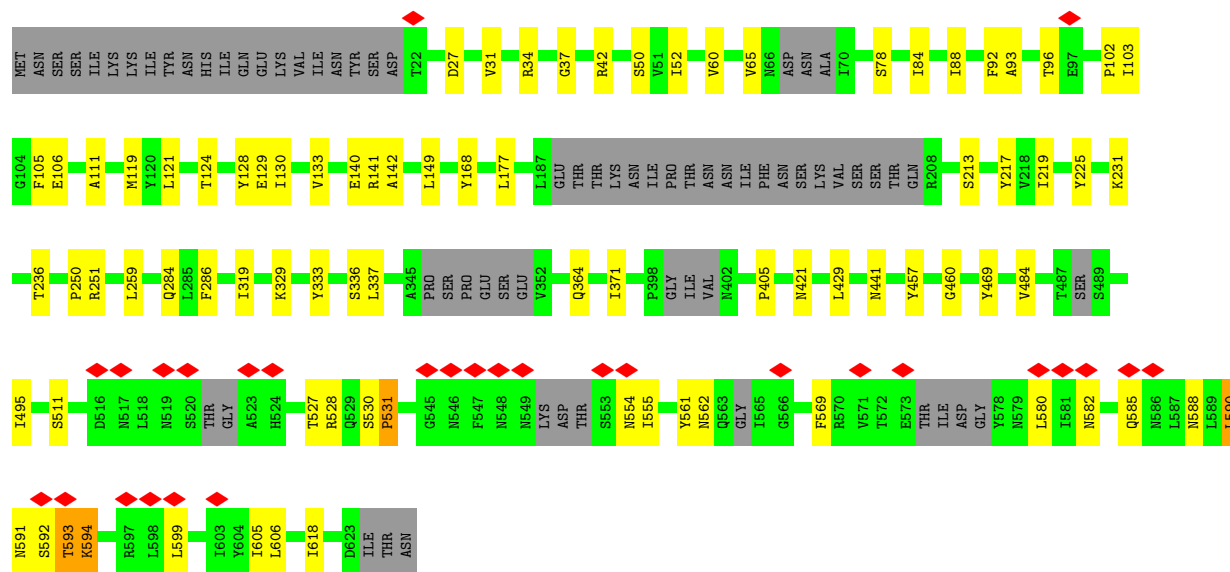
- Molecule 1 is a protein called Botulinum neurotoxin type B1, nontoxic-nonhemagglutinin component, NTNH.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1034	Total	C	N	O	S	0	0
			7457	4867	1216	1355	19		

- Molecule 2 is a protein called Hemagglutinin component HA70.

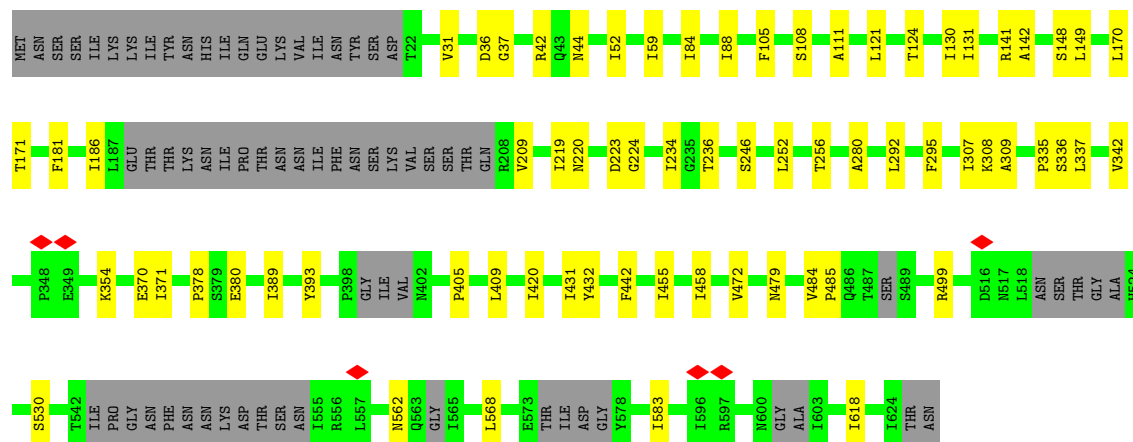
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	559	Total	C	N	O	S	0	0
			4081	2633	678	764	6		
2	C	555	Total	C	N	O	S	0	0
			3954	2568	655	725	6		
2	D	568	Total	C	N	O	S	0	0
			4077	2633	686	753	5		





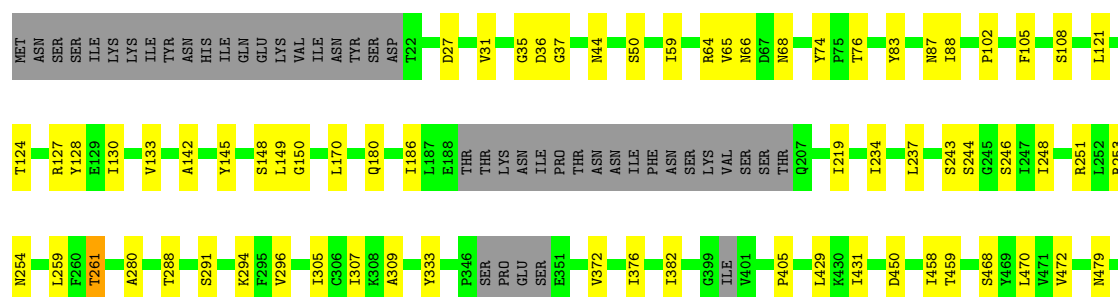
• Molecule 2: Hemagglutinin component HA70

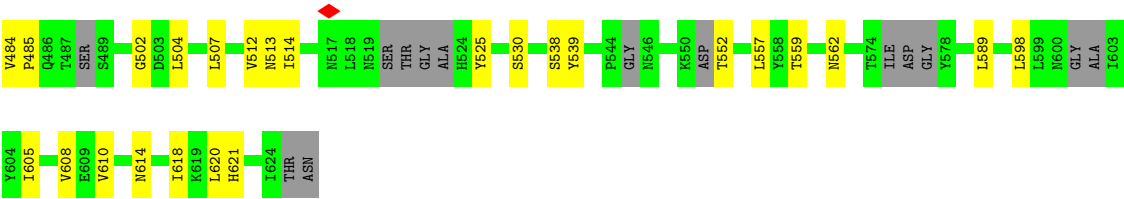
Chain C: 78% 11% 11%



• Molecule 2: Hemagglutinin component HA70

Chain D: 76% 15% 9%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	355719	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	52.124	Depositor
Minimum map value	-30.364	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	1.181	Depositor
Recommended contour level	7.44	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	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	0.26	3/7626 (0.0%)	0.50	11/10442 (0.1%)
2	B	0.22	1/4163 (0.0%)	0.39	3/5694 (0.1%)
2	C	0.15	0/4035	0.42	5/5529 (0.1%)
2	D	0.12	0/4158	0.35	1/5688 (0.0%)
All	All	0.21	4/19982 (0.0%)	0.43	20/27353 (0.1%)

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	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	531	PRO	N-CD	-8.32	1.36	1.47
1	A	551	PRO	N-CD	-7.38	1.37	1.47
1	A	569	TYR	CA-C	-5.84	1.44	1.52
1	A	558	TYR	CA-C	-5.06	1.46	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	568	ASN	N-CA-C	-8.31	103.73	114.04
2	D	514	ILE	N-CA-CB	-7.46	103.16	111.66
1	A	695	GLU	CB-CA-C	-6.91	99.46	110.86
2	C	380	GLU	N-CA-C	6.89	120.22	110.50
2	C	378	PRO	N-CA-C	-6.35	105.92	113.86



There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	368	TYR	Peptide
2	C	499	ARG	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	7457	0	6534	107	0
2	B	4081	0	3652	51	0
2	C	3954	0	3457	41	0
2	D	4077	0	3562	59	0
All	All	19569	0	17205	244	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 7.

The worst 5 of 244 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:SER:HB3	2:B:618:ILE:HB	1.50	0.93
2:B:588:ASN:O	2:B:592:SER:OG	1.91	0.87
1:A:509:THR:HG21	1:A:514:PHE:CE1	2.08	0.87
2:B:405:PRO:HA	2:B:484:VAL:O	1.75	0.86
1:A:349:ASP:OD1	1:A:350:ARG:HG3	1.76	0.84

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1016/1197 (85%)	964 (95%)	50 (5%)	2 (0%)	44	63
2	B	539/626 (86%)	516 (96%)	21 (4%)	2 (0%)	30	47
2	C	537/626 (86%)	505 (94%)	32 (6%)	0	100	100
2	D	548/626 (88%)	521 (95%)	27 (5%)	0	100	100
All	All	2640/3075 (86%)	2506 (95%)	130 (5%)	4 (0%)	45	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	925	ASP
2	B	590	LEU
2	B	594	LYS
1	A	369	PRO

### 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	666/1114 (60%)	653 (98%)	13 (2%)	50	70
2	B	380/570 (67%)	375 (99%)	5 (1%)	65	80
2	C	343/570 (60%)	340 (99%)	3 (1%)	75	86
2	D	356/570 (62%)	349 (98%)	7 (2%)	50	70
All	All	1745/2824 (62%)	1717 (98%)	28 (2%)	58	75

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	213	SER
2	D	620	LEU
2	B	606	LEU
2	D	557	LEU

*Continued on next page...*

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Mol	Chain	Res	Type
2	B	593	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	506	ASN
2	D	322	GLN
2	D	180	GLN
1	A	951	ASN
2	C	475	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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

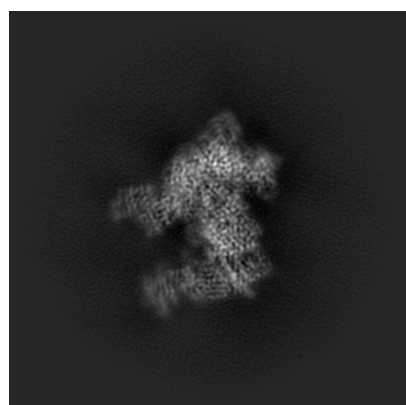
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53017. These allow visual inspection of the internal detail of the map and identification of artifacts.

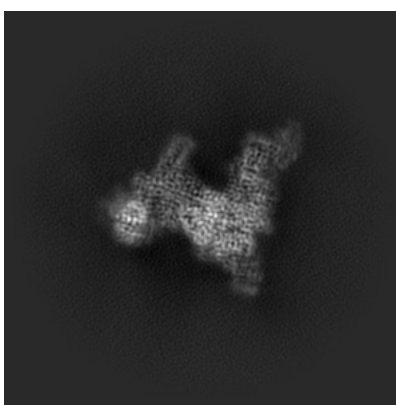
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

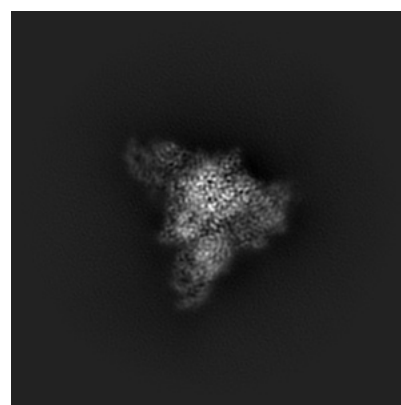
#### 6.1.1 Primary map



X



Y

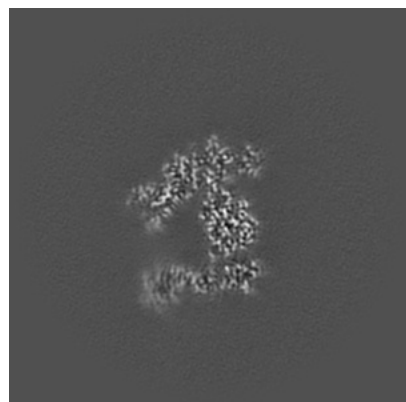


Z

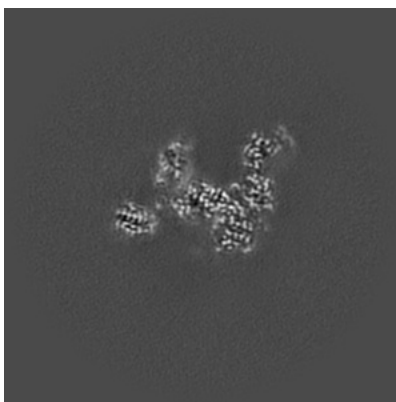
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

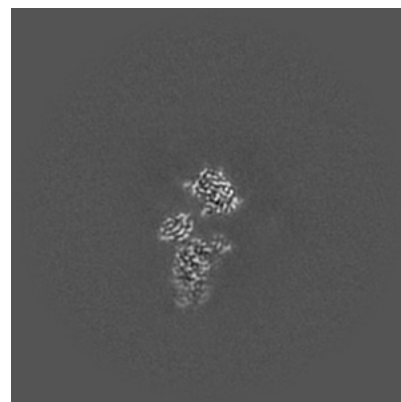
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

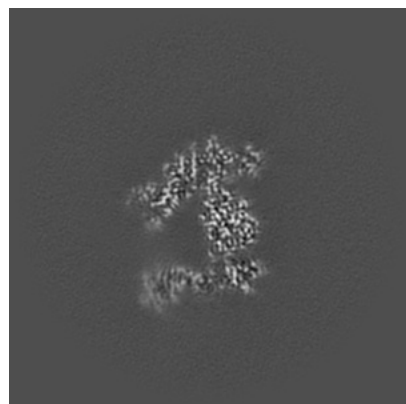


Z Index: 200

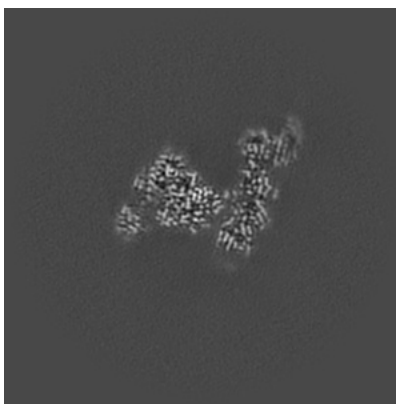
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

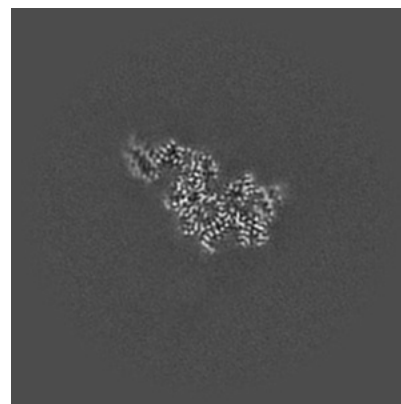
### 6.3.1 Primary map



X Index: 201



Y Index: 213

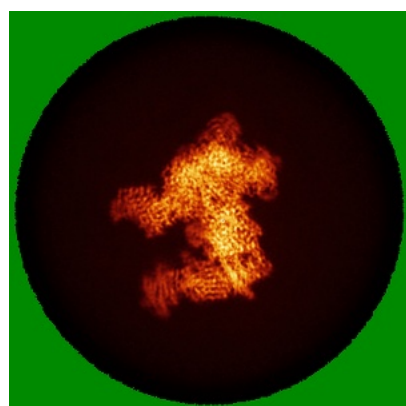


Z Index: 241

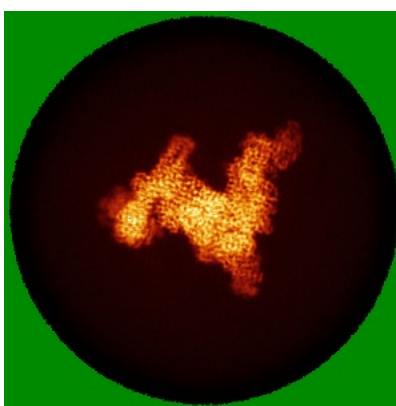
The images above show the largest variance slices of the map in three orthogonal directions.

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

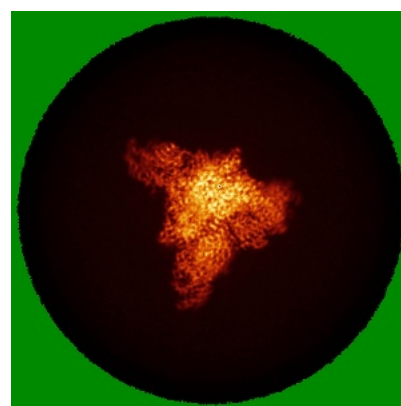
### 6.4.1 Primary map



X



Y

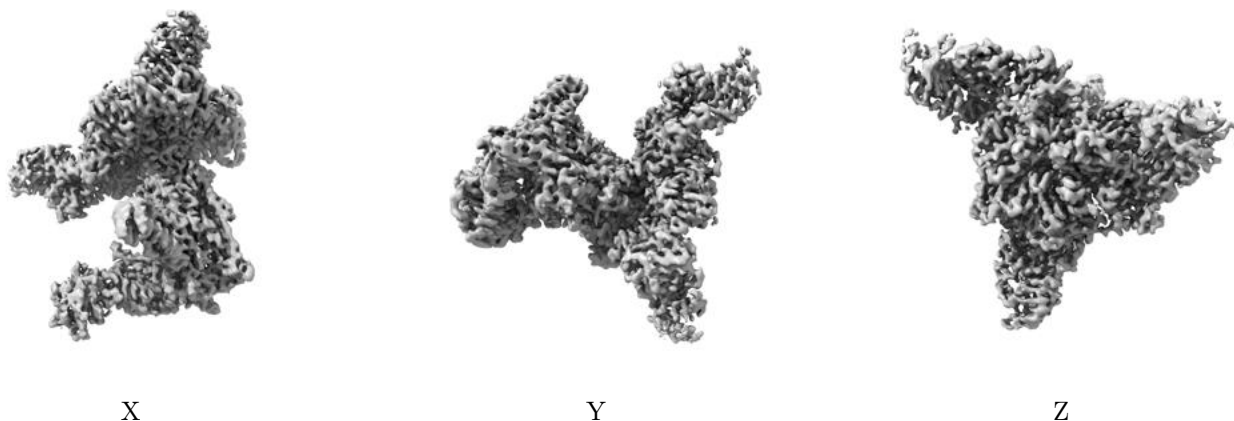


Z

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 7.44. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

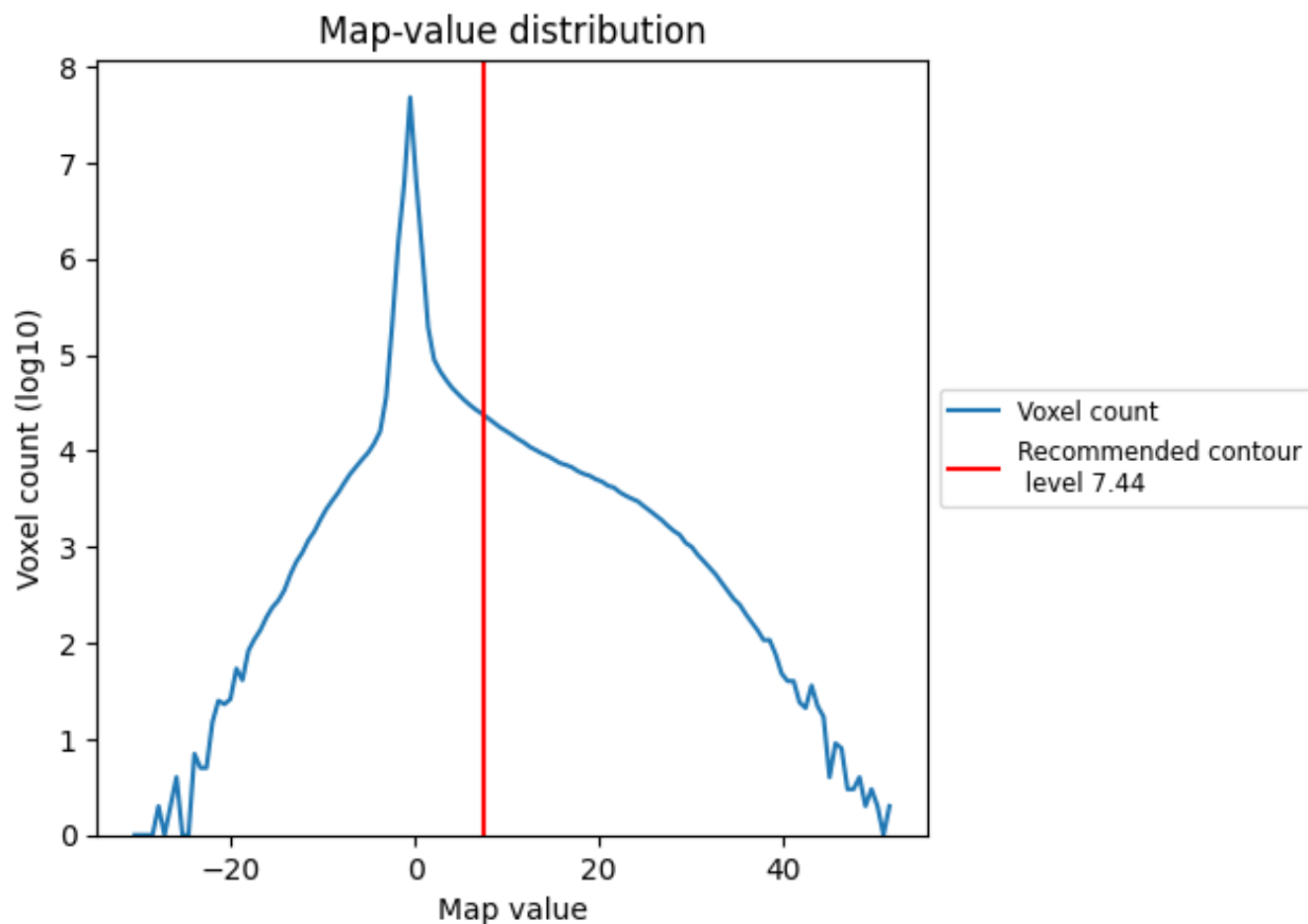
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

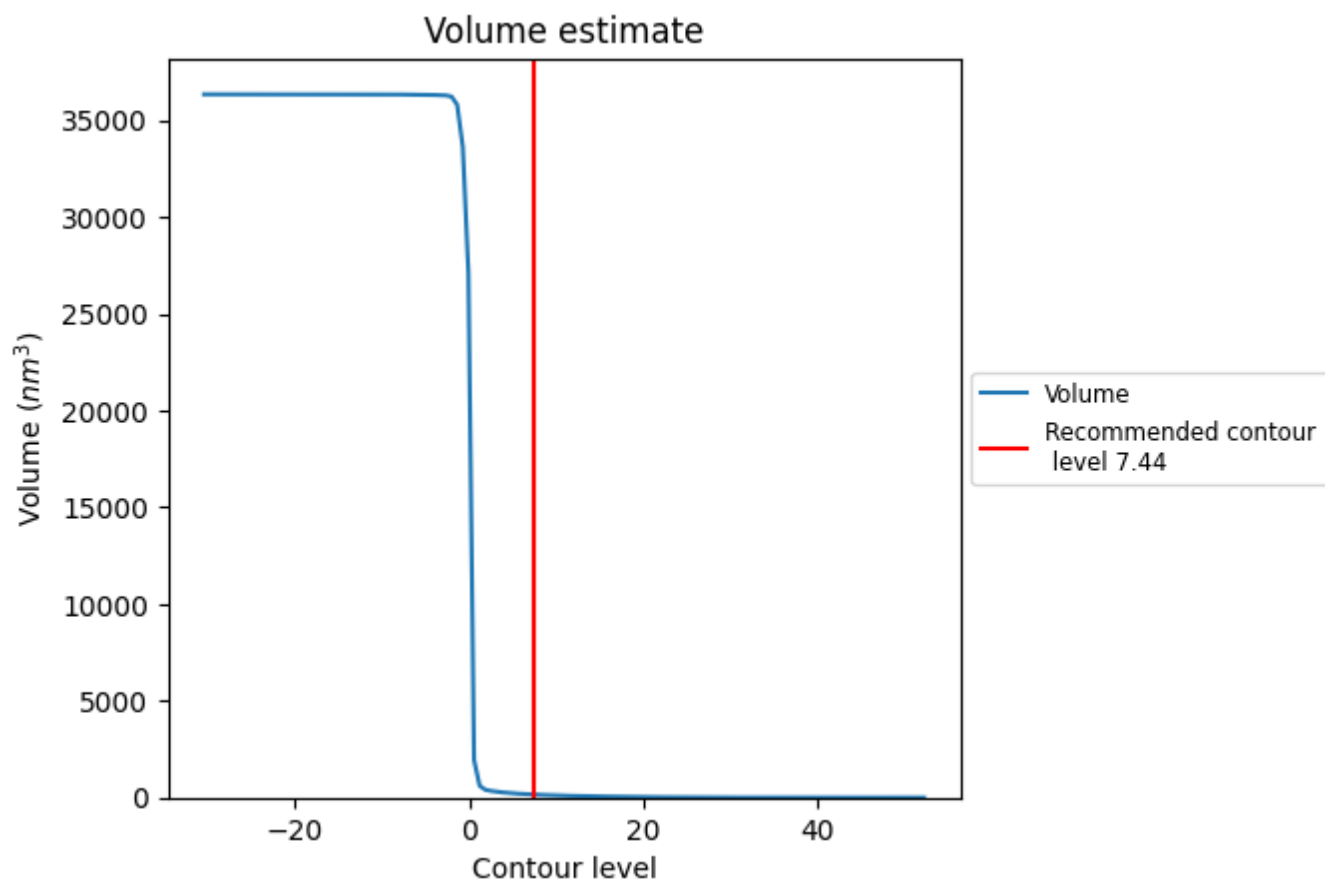
This section contains the results of statistical analysis of the map.

### 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](#)

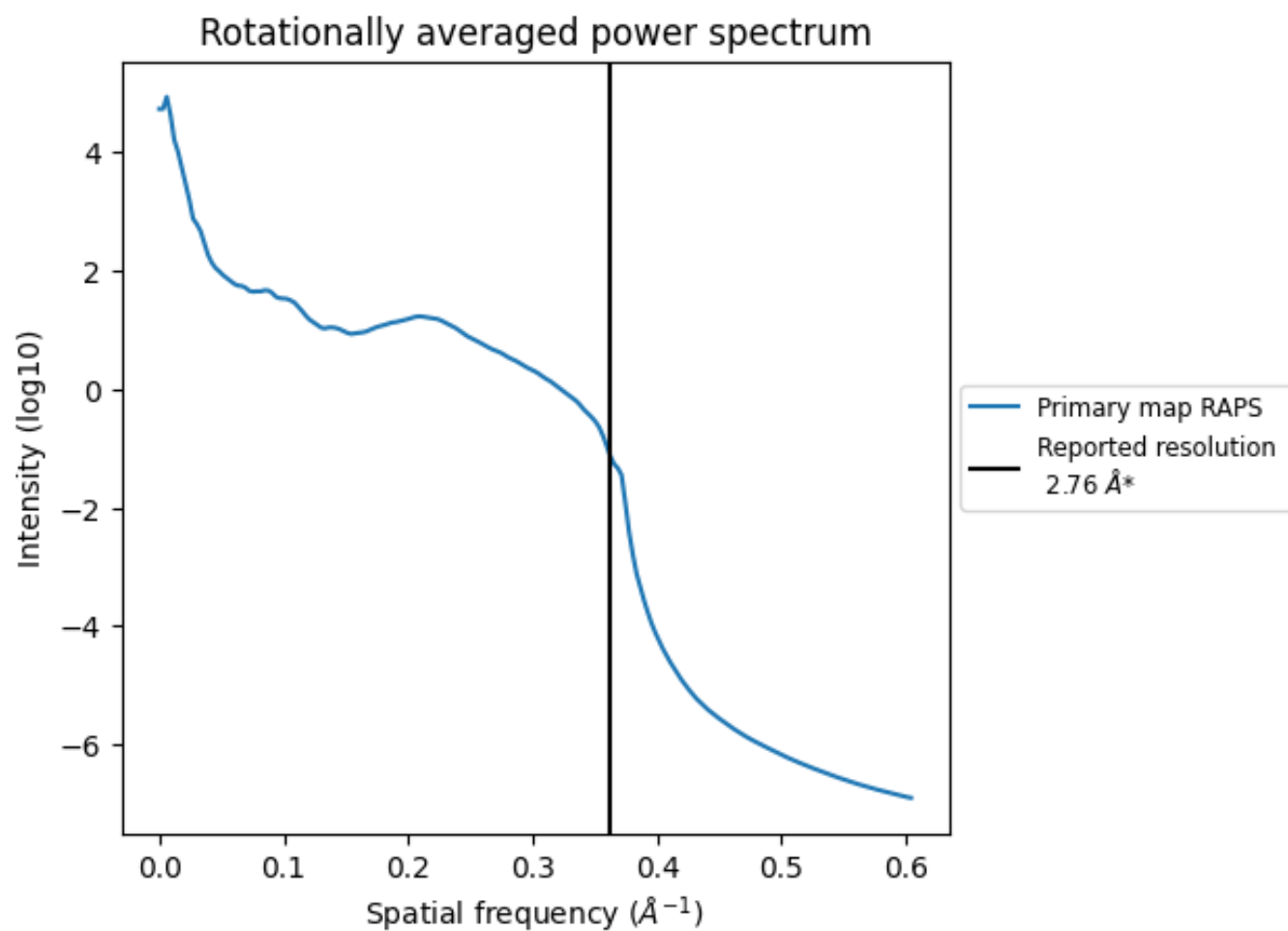


The volume at the recommended contour level is 155  $\text{nm}^3$ ; this corresponds to an approximate mass of 140 kDa.

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 0.362 Å<sup>-1</sup>

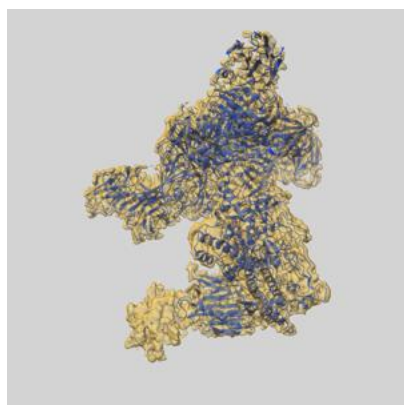
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

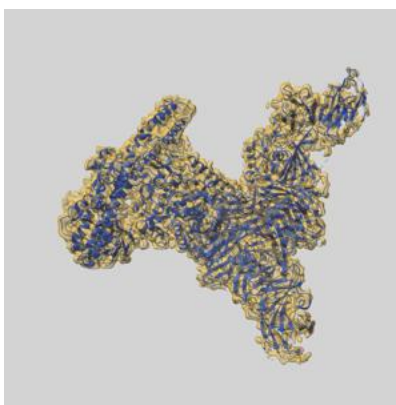
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53017 and PDB model 9QCO. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

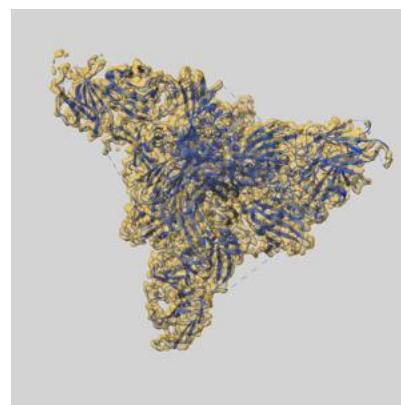
### 9.1 Map-model overlay [i](#)



X



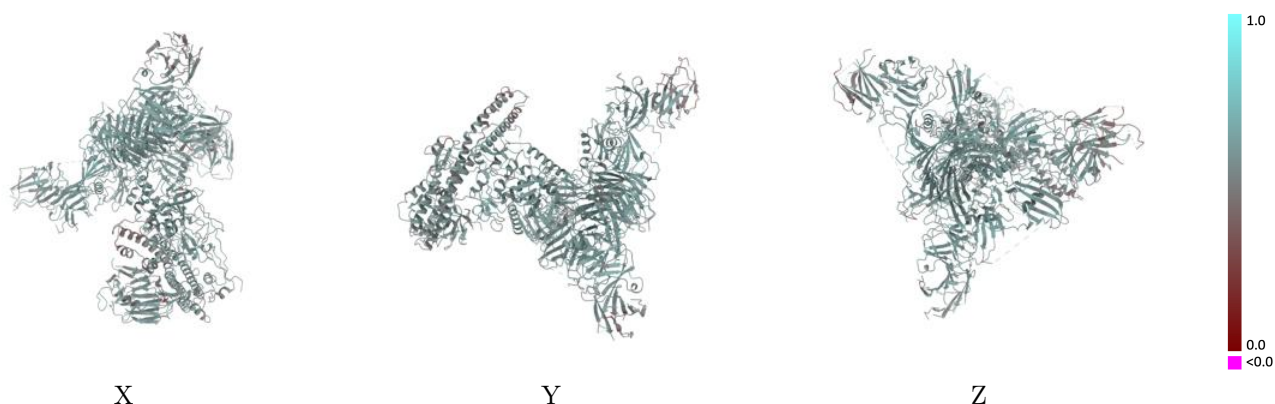
Y



Z

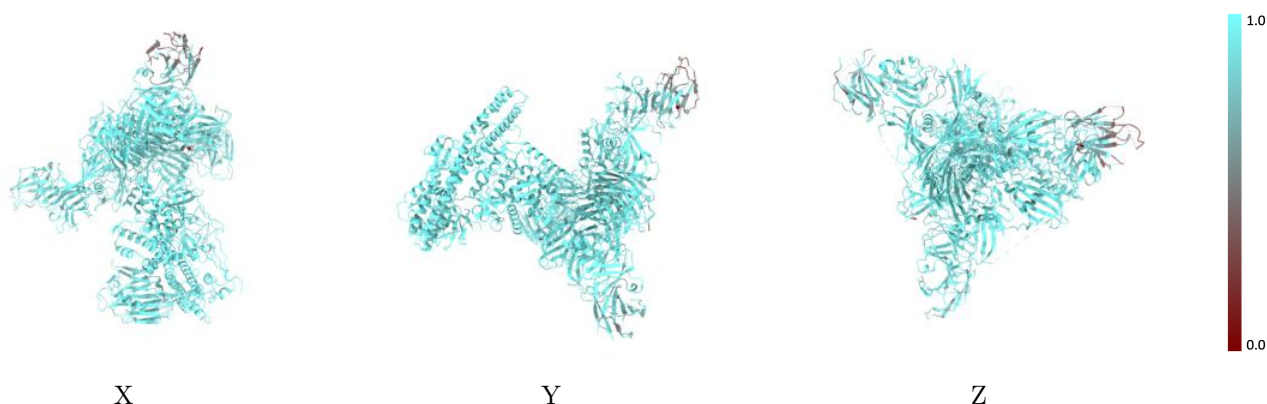
The images above show the 3D surface view of the map at the recommended contour level 7.44 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



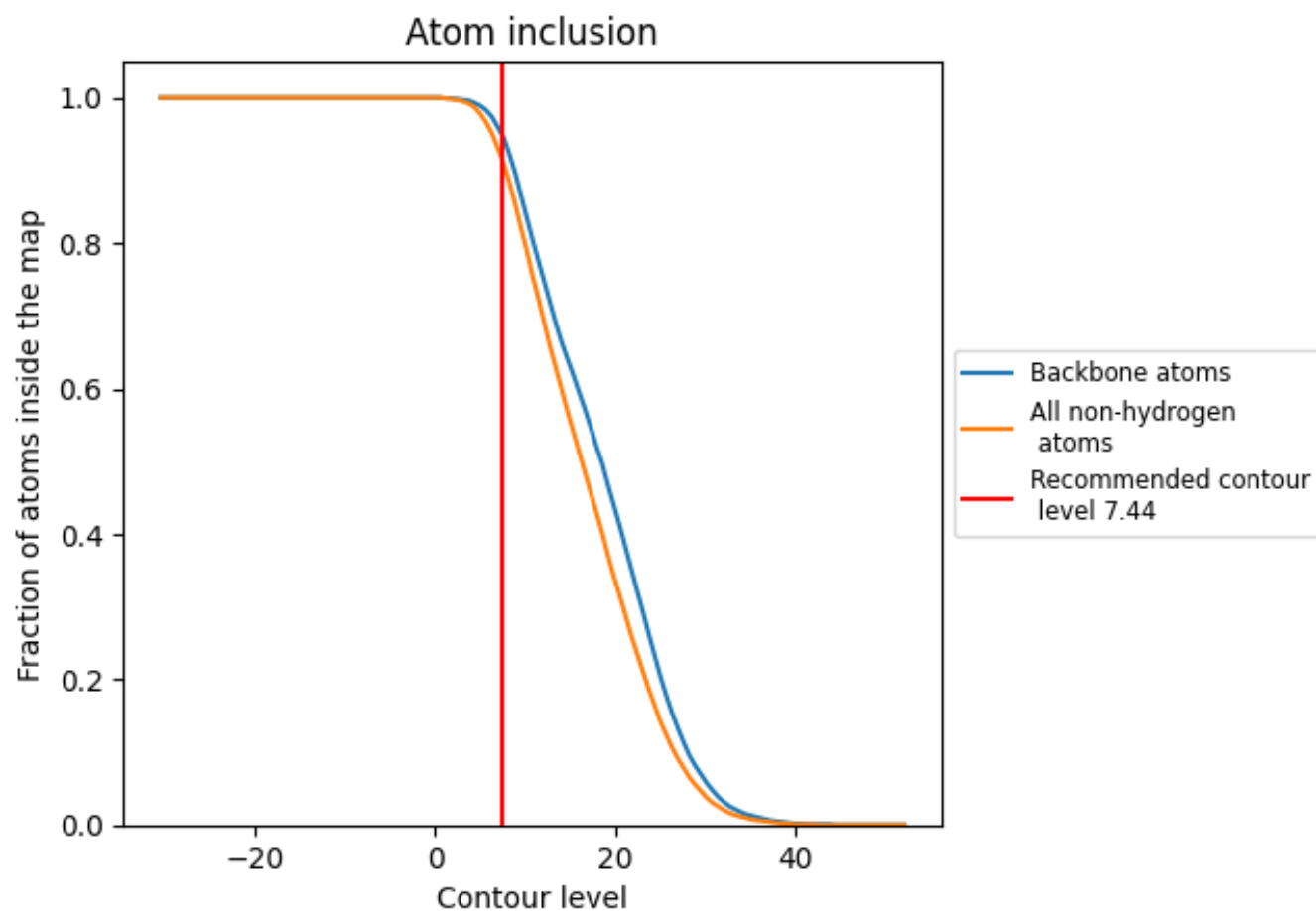
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7.44).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (7.44) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9180	<div></div> 0.5620
A	<div></div> 0.9520	<div></div> 0.5510
B	<div></div> 0.8520	<div></div> 0.5600
C	<div></div> 0.9110	<div></div> 0.5690
D	<div></div> 0.9270	<div></div> 0.5760

