



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 10:08 AM UTC

PDB ID : 7OMM / pdb_00007omm
EMDB ID : EMD-12990
Title : Cryo-EM structure of *N. gonorrhoeae* LptDE in complex with ProMacrobodies (MBPs have not been built de novo)
Authors : Botte, M.; Ni, D.; Schenck, S.; Zimmermann, I.; Chami, M.; Bocquet, N.; Egloff, P.; Bucher, D.; Trabuco, M.; Cheng, R.K.Y.; Brunner, J.D.; Seeger, M.A.; Stahlberg, H.; Hennig, M.
Deposited on : 2021-05-24
Resolution : 3.40 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:

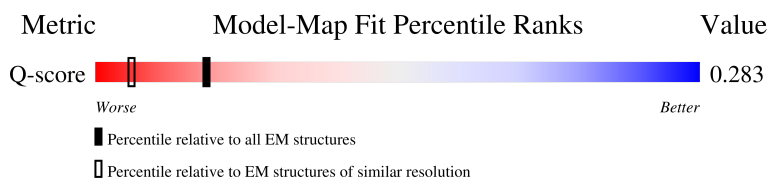
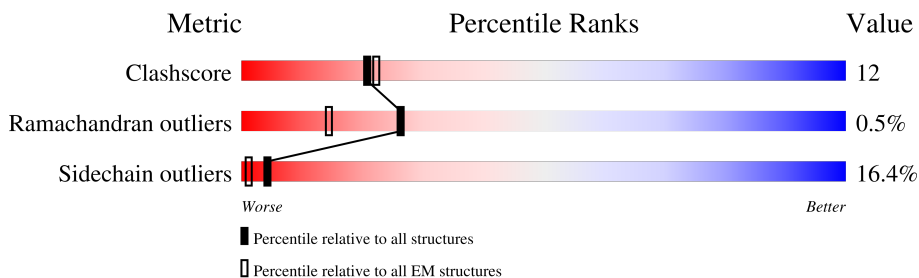
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.40 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	14717 (2.90 - 3.90)

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	801	<p>8% (red), 59% (green), 26% (yellow), 13% (grey)</p>
2	B	165	<p>5% (red), 61% (green), 16% (yellow), 22% (grey)</p>
3	C	520	<p>69% (green), 79% (green), 12% (yellow), 8% (grey)</p>
4	D	526	<p>69% (green), 43% (green), 34% (yellow), 15% (orange), 7% (grey)</p>

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 13981 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 LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	698	5462	3430	985	1038	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	SER	ALA	conflict	UNP Q5F651

- Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	128	1020	640	179	198	3	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	160	HIS	-	expression tag	UNP A0A5K1Q6A7
B	161	HIS	-	expression tag	UNP A0A5K1Q6A7
B	162	HIS	-	expression tag	UNP A0A5K1Q6A7
B	163	HIS	-	expression tag	UNP A0A5K1Q6A7
B	164	HIS	-	expression tag	UNP A0A5K1Q6A7
B	165	HIS	-	expression tag	UNP A0A5K1Q6A7

- Molecule 3 is a protein called ProMacrobody 21,Maltodextrin-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	479	3731	2397	614	710	10	0	0

There are 37 discrepancies between the modelled and reference sequences:

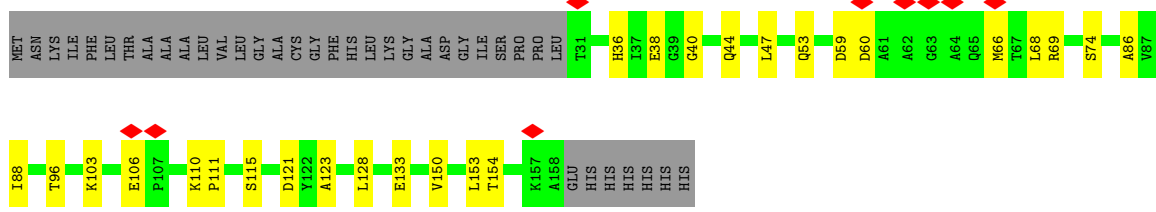
Chain	Residue	Modelled	Actual	Comment	Reference
C	484	PRO	-	expression tag	UNP A0A0F8L1I7
C	485	GLY	-	expression tag	UNP A0A0F8L1I7
C	486	SER	-	expression tag	UNP A0A0F8L1I7
C	487	GLY	-	expression tag	UNP A0A0F8L1I7
C	488	GLY	-	expression tag	UNP A0A0F8L1I7
C	489	GLY	-	expression tag	UNP A0A0F8L1I7
C	490	SER	-	expression tag	UNP A0A0F8L1I7
C	491	ALA	-	expression tag	UNP A0A0F8L1I7
C	492	TRP	-	expression tag	UNP A0A0F8L1I7
C	493	SER	-	expression tag	UNP A0A0F8L1I7
C	494	HIS	-	expression tag	UNP A0A0F8L1I7
C	495	PRO	-	expression tag	UNP A0A0F8L1I7
C	496	GLN	-	expression tag	UNP A0A0F8L1I7
C	497	PHE	-	expression tag	UNP A0A0F8L1I7
C	498	GLU	-	expression tag	UNP A0A0F8L1I7
C	499	LYS	-	expression tag	UNP A0A0F8L1I7
C	500	GLY	-	expression tag	UNP A0A0F8L1I7
C	501	GLY	-	expression tag	UNP A0A0F8L1I7
C	502	GLY	-	expression tag	UNP A0A0F8L1I7
C	503	SER	-	expression tag	UNP A0A0F8L1I7
C	504	GLY	-	expression tag	UNP A0A0F8L1I7
C	505	GLY	-	expression tag	UNP A0A0F8L1I7
C	506	GLY	-	expression tag	UNP A0A0F8L1I7
C	507	SER	-	expression tag	UNP A0A0F8L1I7
C	508	GLY	-	expression tag	UNP A0A0F8L1I7
C	509	GLY	-	expression tag	UNP A0A0F8L1I7
C	510	SER	-	expression tag	UNP A0A0F8L1I7
C	511	ALA	-	expression tag	UNP A0A0F8L1I7
C	512	TRP	-	expression tag	UNP A0A0F8L1I7
C	513	SER	-	expression tag	UNP A0A0F8L1I7
C	514	HIS	-	expression tag	UNP A0A0F8L1I7
C	515	PRO	-	expression tag	UNP A0A0F8L1I7
C	516	GLN	-	expression tag	UNP A0A0F8L1I7
C	517	PHE	-	expression tag	UNP A0A0F8L1I7
C	518	GLU	-	expression tag	UNP A0A0F8L1I7
C	519	LYS	-	expression tag	UNP A0A0F8L1I7
C	520	ALA	-	expression tag	UNP A0A0F8L1I7

- Molecule 4 is a protein called ProMacrobody 51, Maltodextrin-binding protein.

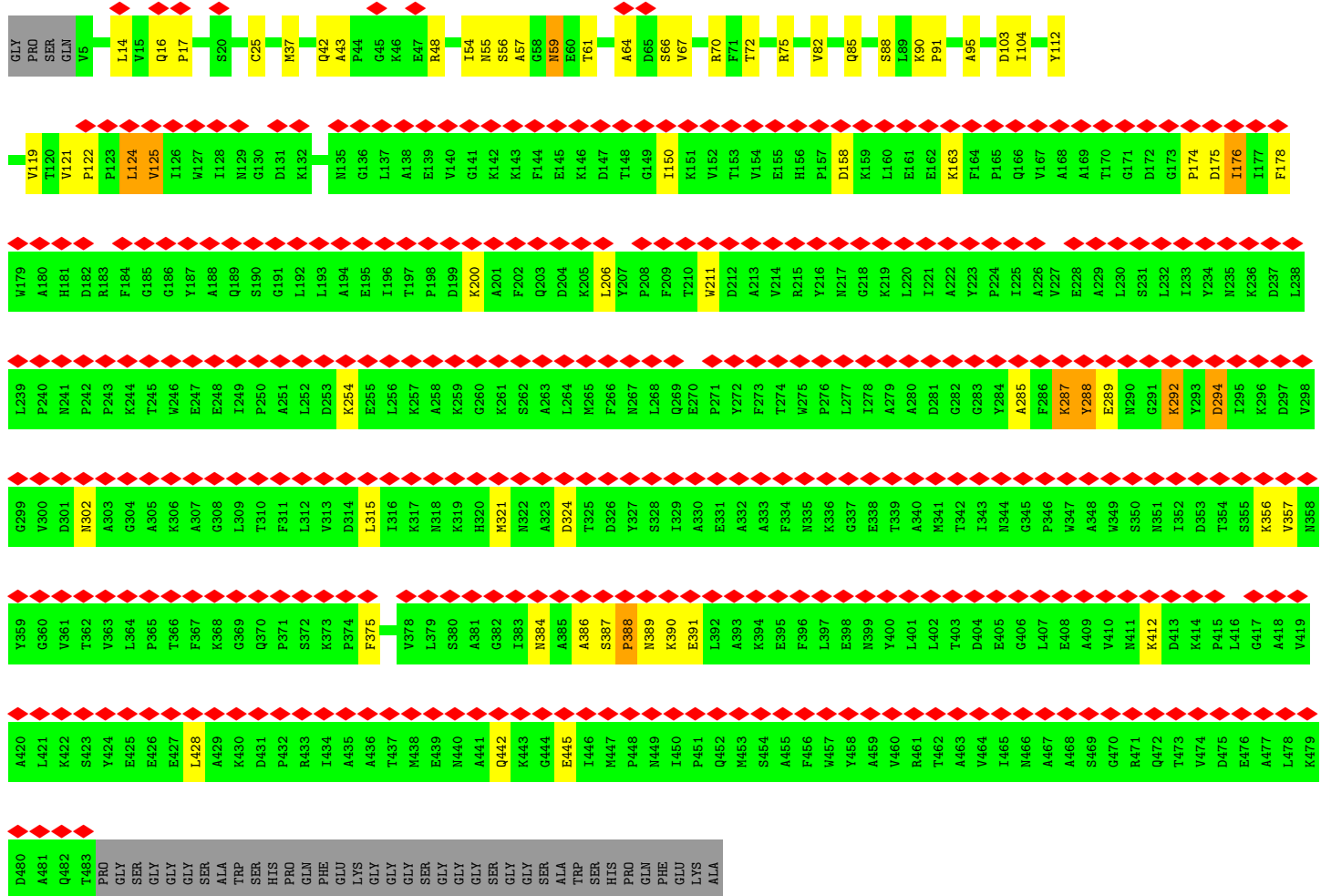
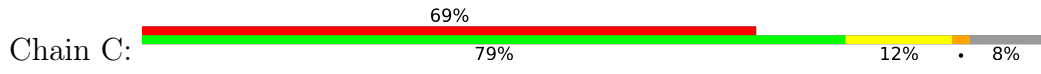
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	489	3768	2422	614	723	9	0	0

There are 37 discrepancies between the modelled and reference sequences:

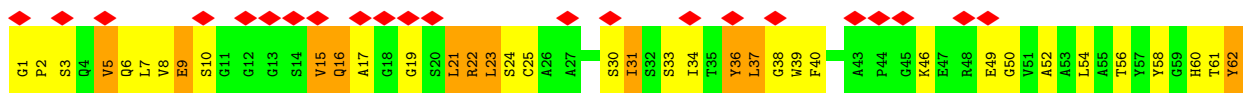
Chain	Residue	Modelled	Actual	Comment	Reference
D	490	PRO	-	expression tag	UNP A0A0F8L1I7
D	491	GLY	-	expression tag	UNP A0A0F8L1I7
D	492	SER	-	expression tag	UNP A0A0F8L1I7
D	493	GLY	-	expression tag	UNP A0A0F8L1I7
D	494	GLY	-	expression tag	UNP A0A0F8L1I7
D	495	GLY	-	expression tag	UNP A0A0F8L1I7
D	496	SER	-	expression tag	UNP A0A0F8L1I7
D	497	ALA	-	expression tag	UNP A0A0F8L1I7
D	498	TRP	-	expression tag	UNP A0A0F8L1I7
D	499	SER	-	expression tag	UNP A0A0F8L1I7
D	500	HIS	-	expression tag	UNP A0A0F8L1I7
D	501	PRO	-	expression tag	UNP A0A0F8L1I7
D	502	GLN	-	expression tag	UNP A0A0F8L1I7
D	503	PHE	-	expression tag	UNP A0A0F8L1I7
D	504	GLU	-	expression tag	UNP A0A0F8L1I7
D	505	LYS	-	expression tag	UNP A0A0F8L1I7
D	506	GLY	-	expression tag	UNP A0A0F8L1I7
D	507	GLY	-	expression tag	UNP A0A0F8L1I7
D	508	GLY	-	expression tag	UNP A0A0F8L1I7
D	509	SER	-	expression tag	UNP A0A0F8L1I7
D	510	GLY	-	expression tag	UNP A0A0F8L1I7
D	511	GLY	-	expression tag	UNP A0A0F8L1I7
D	512	GLY	-	expression tag	UNP A0A0F8L1I7
D	513	SER	-	expression tag	UNP A0A0F8L1I7
D	514	GLY	-	expression tag	UNP A0A0F8L1I7
D	515	GLY	-	expression tag	UNP A0A0F8L1I7
D	516	SER	-	expression tag	UNP A0A0F8L1I7
D	517	ALA	-	expression tag	UNP A0A0F8L1I7
D	518	TRP	-	expression tag	UNP A0A0F8L1I7
D	519	SER	-	expression tag	UNP A0A0F8L1I7
D	520	HIS	-	expression tag	UNP A0A0F8L1I7
D	521	PRO	-	expression tag	UNP A0A0F8L1I7
D	522	GLN	-	expression tag	UNP A0A0F8L1I7
D	523	PHE	-	expression tag	UNP A0A0F8L1I7
D	524	GLU	-	expression tag	UNP A0A0F8L1I7
D	525	LYS	-	expression tag	UNP A0A0F8L1I7
D	526	ALA	-	expression tag	UNP A0A0F8L1I7



● Molecule 3: ProMacrobody 21, Maltodextrin-binding protein



● Molecule 4: ProMacrobody 51, Maltodextrin-binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184206	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.965	Depositor
Minimum map value	-1.718	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.45	Depositor
Map size (\AA)	344.4, 344.4, 344.4	wwPDB
Map dimensions	390, 390, 390	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8830769, 0.8830769, 0.8830769	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	0.44	0/5594	0.73	8/7569 (0.1%)
2	B	0.15	0/1034	0.36	0/1400
3	C	0.79	0/3829	1.40	6/5208 (0.1%)
4	D	0.98	0/3865	1.30	8/5260 (0.2%)
All	All	0.71	0/14322	1.10	22/19437 (0.1%)

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	181	ASP	N-CA-C	9.31	121.03	111.07
4	D	137	ASP	N-CA-C	-8.71	101.78	111.28
1	A	662	ARG	CB-CA-C	-7.34	103.83	110.44
4	D	402	PHE	CA-CB-CG	7.00	120.80	113.80
4	D	78	ALA	N-CA-C	-6.93	104.64	113.23

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	5462	0	5221	131	0
2	B	1020	0	1024	20	0
3	C	3731	0	3645	33	0
4	D	3768	0	3692	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13981	0	13582	331	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 331 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)
4:D:131:VAL:HB	4:D:180:PRO:HB3	1.36	1.07
4:D:333:TYR:O	4:D:333:TYR:HD1	1.40	1.04
4:D:401:GLU:OE1	4:D:401:GLU:O	1.82	0.97
4:D:333:TYR:CD1	4:D:333:TYR:C	2.43	0.91
4:D:333:TYR:O	4:D:333:TYR:CD1	2.28	0.87

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	671/801 (84%)	551 (82%)	116 (17%)	4 (1%)	21	50
2	B	126/165 (76%)	118 (94%)	8 (6%)	0	100	100
3	C	477/520 (92%)	457 (96%)	17 (4%)	3 (1%)	21	50
4	D	487/526 (93%)	464 (95%)	21 (4%)	2 (0%)	30	59
All	All	1761/2012 (88%)	1590 (90%)	162 (9%)	9 (0%)	26	54

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	PRO
3	C	390	LYS

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Mol	Chain	Res	Type
4	D	163	PRO
1	A	207	ASP
1	A	265	ALA

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	556/632 (88%)	509 (92%)	47 (8%)	10	33
2	B	108/136 (79%)	108 (100%)	0	100	100
3	C	384/409 (94%)	359 (94%)	25 (6%)	15	42
4	D	387/409 (95%)	223 (58%)	164 (42%)	0	0
All	All	1435/1586 (90%)	1199 (84%)	236 (16%)	4	10

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	117	GLU
4	D	445	GLU
4	D	195	GLN
4	D	437	ASP
4	D	386	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	466	ASN
4	D	60	HIS
4	D	4	GLN
4	D	87	ASN
1	A	434	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 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.

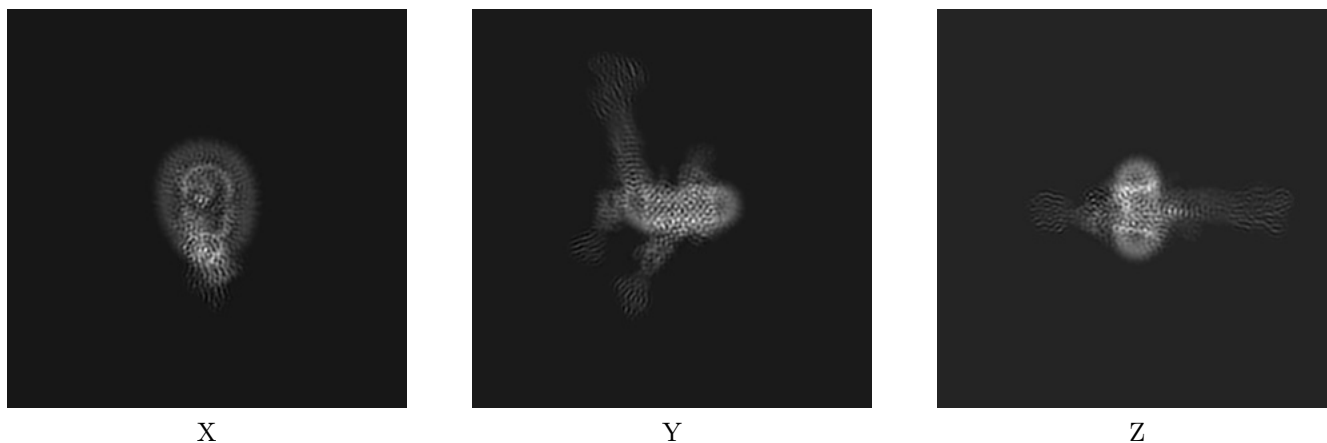
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12990. 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](#)

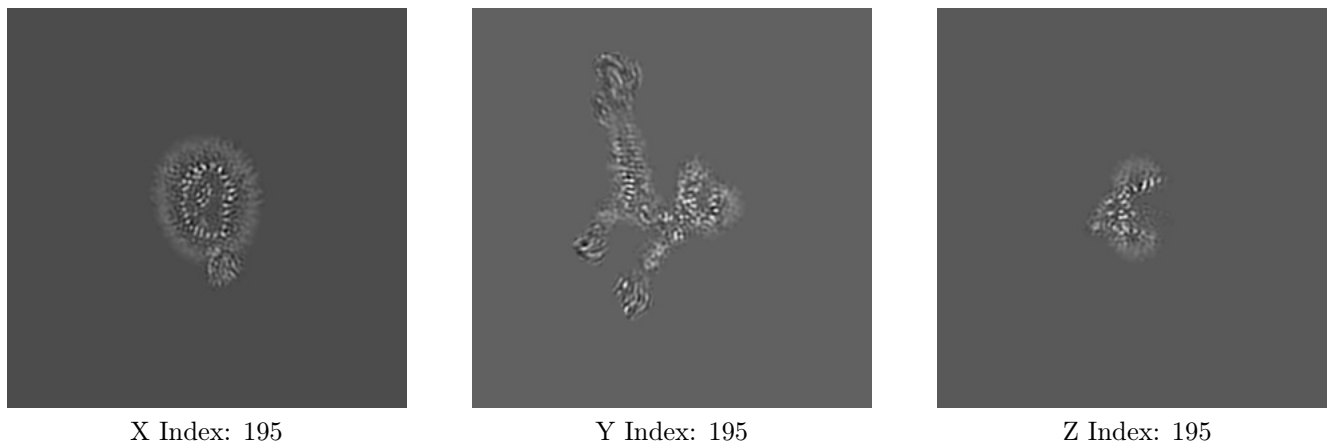
6.1.1 Primary map



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

6.2 Central slices [i](#)

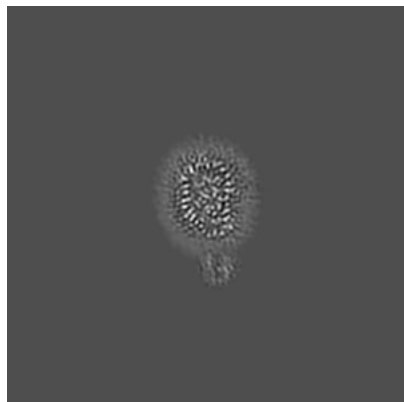
6.2.1 Primary map



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

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

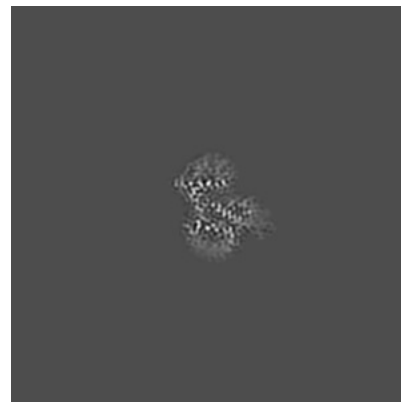
6.3.1 Primary map



X Index: 185



Y Index: 189



Z Index: 216

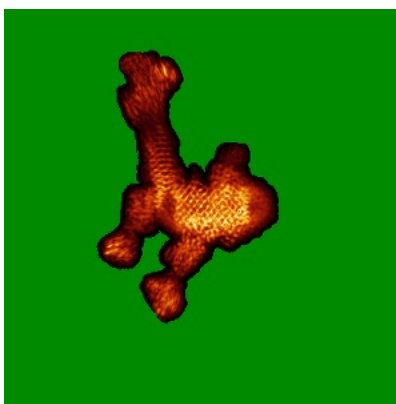
The images above show the largest variance slices of the map in three orthogonal directions.

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

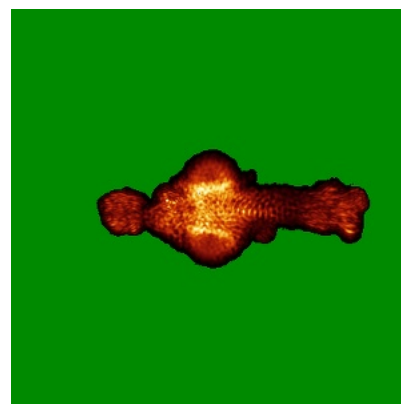
6.4.1 Primary map



X



Y

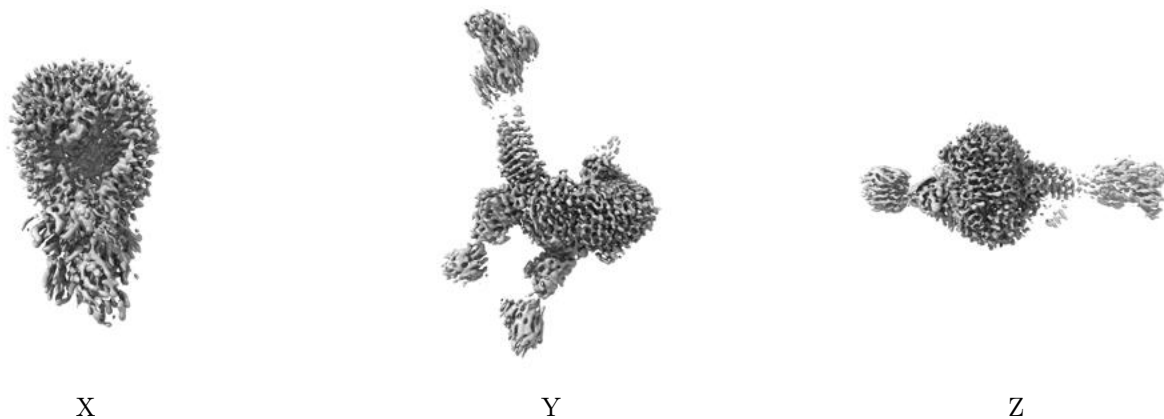


Z

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

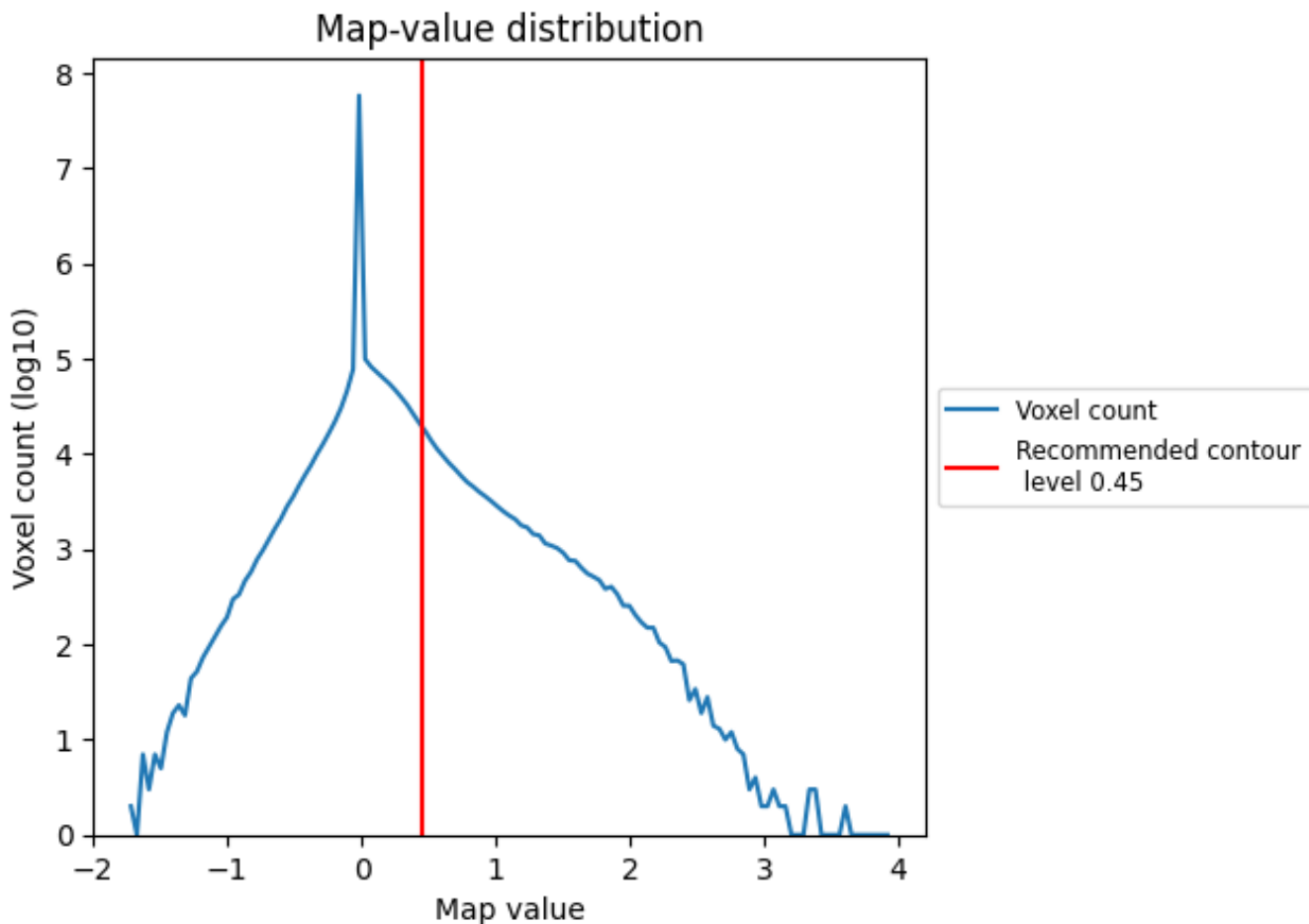
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

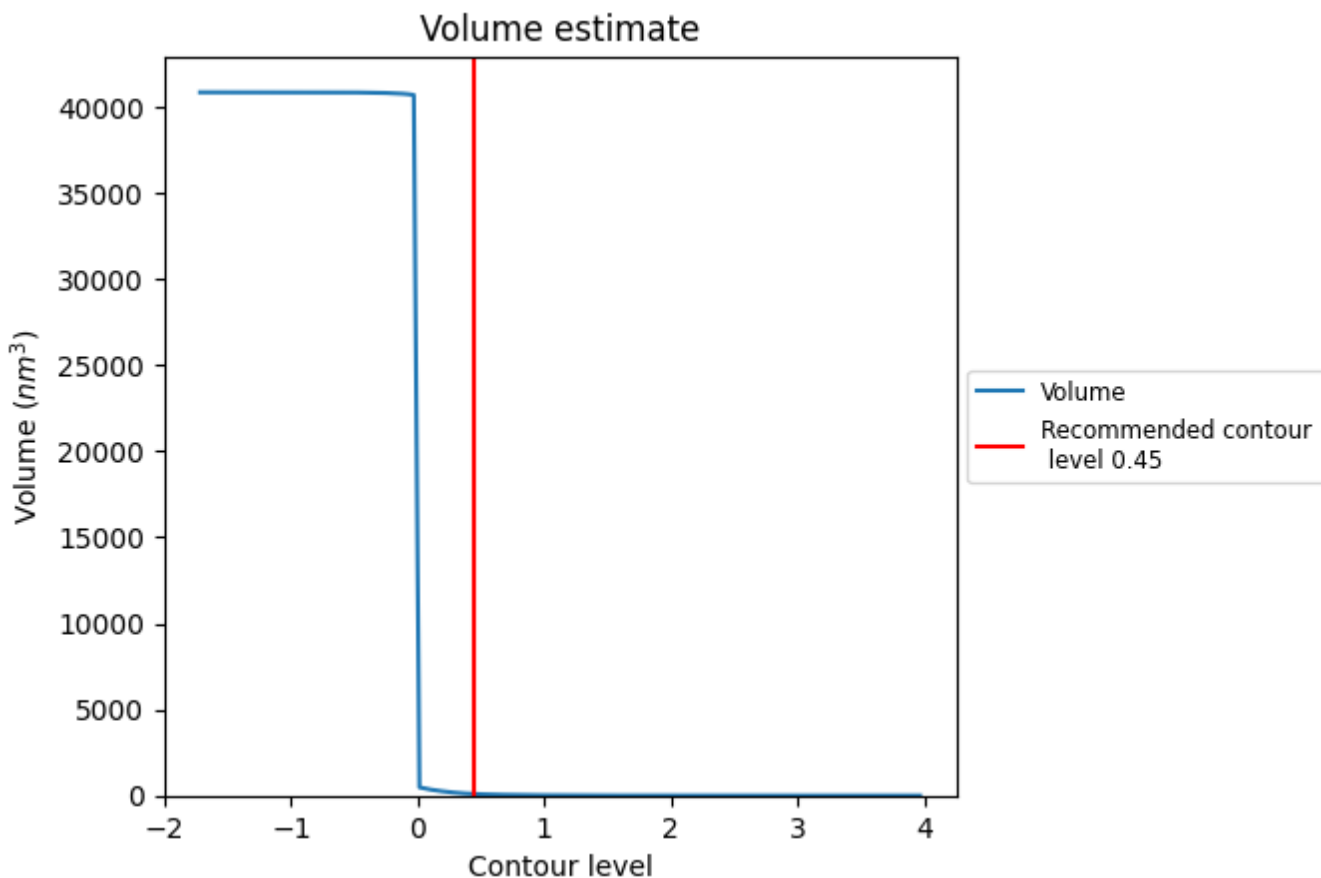
This section contains the results of statistical analysis of the map.

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.

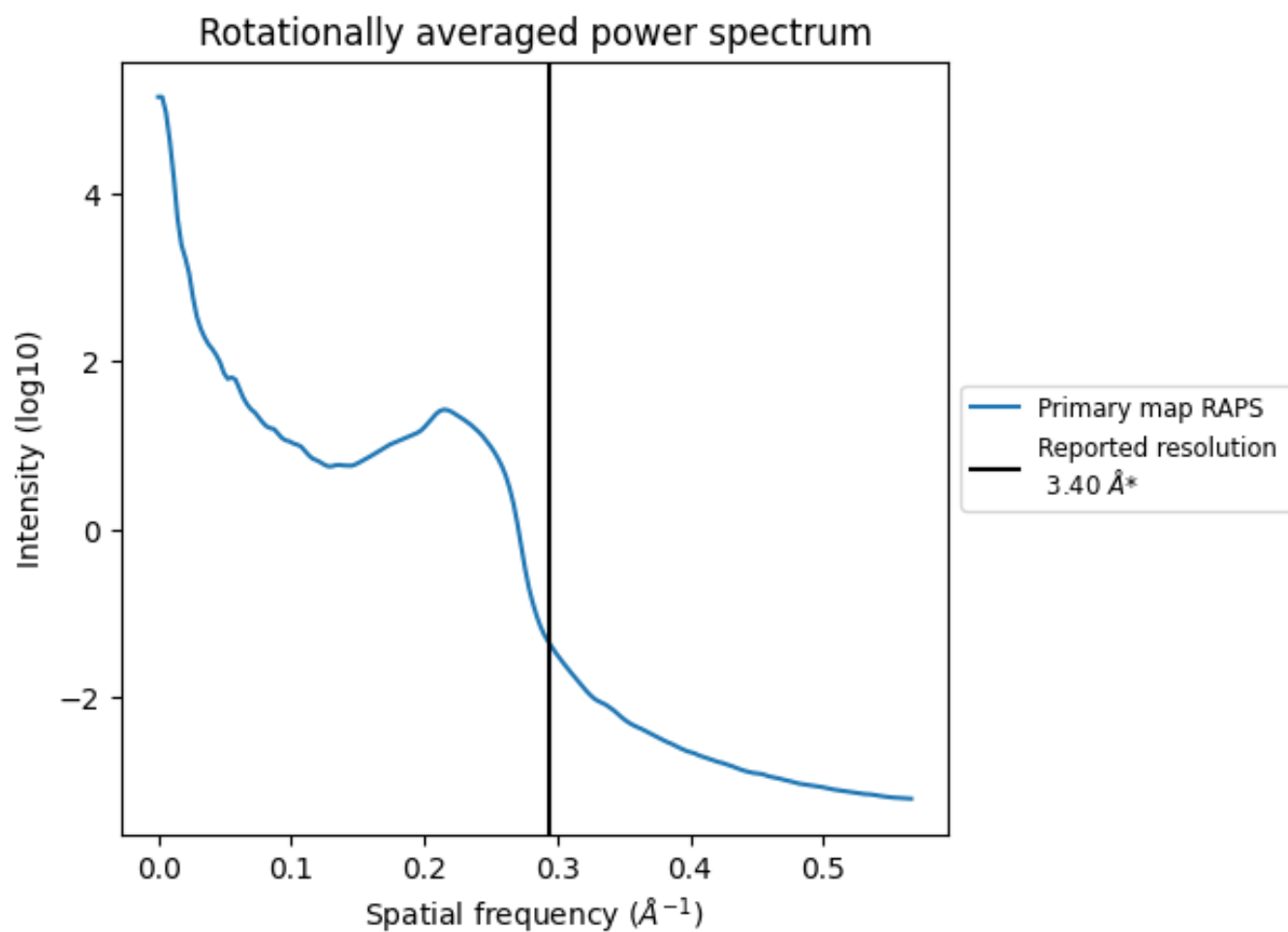
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 91 nm³; this corresponds to an approximate mass of 82 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 0.294\AA^{-1}

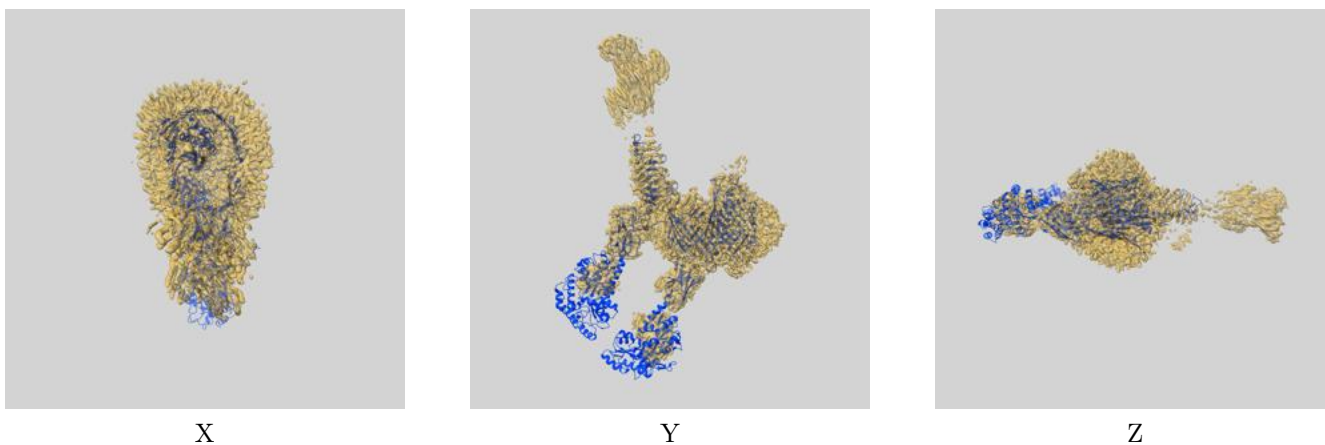
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

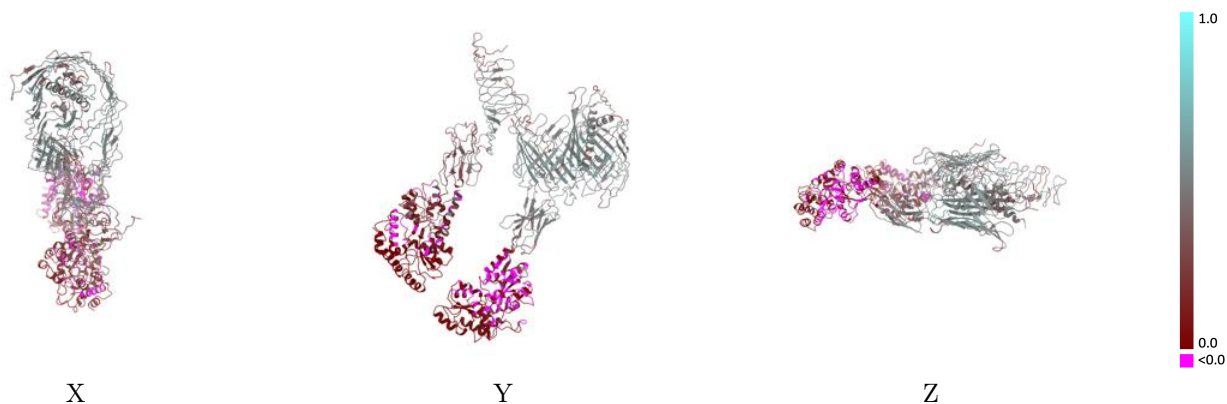
This section contains information regarding the fit between EMDB map EMD-12990 and PDB model 7OMM. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.45 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 [\(i\)](#)

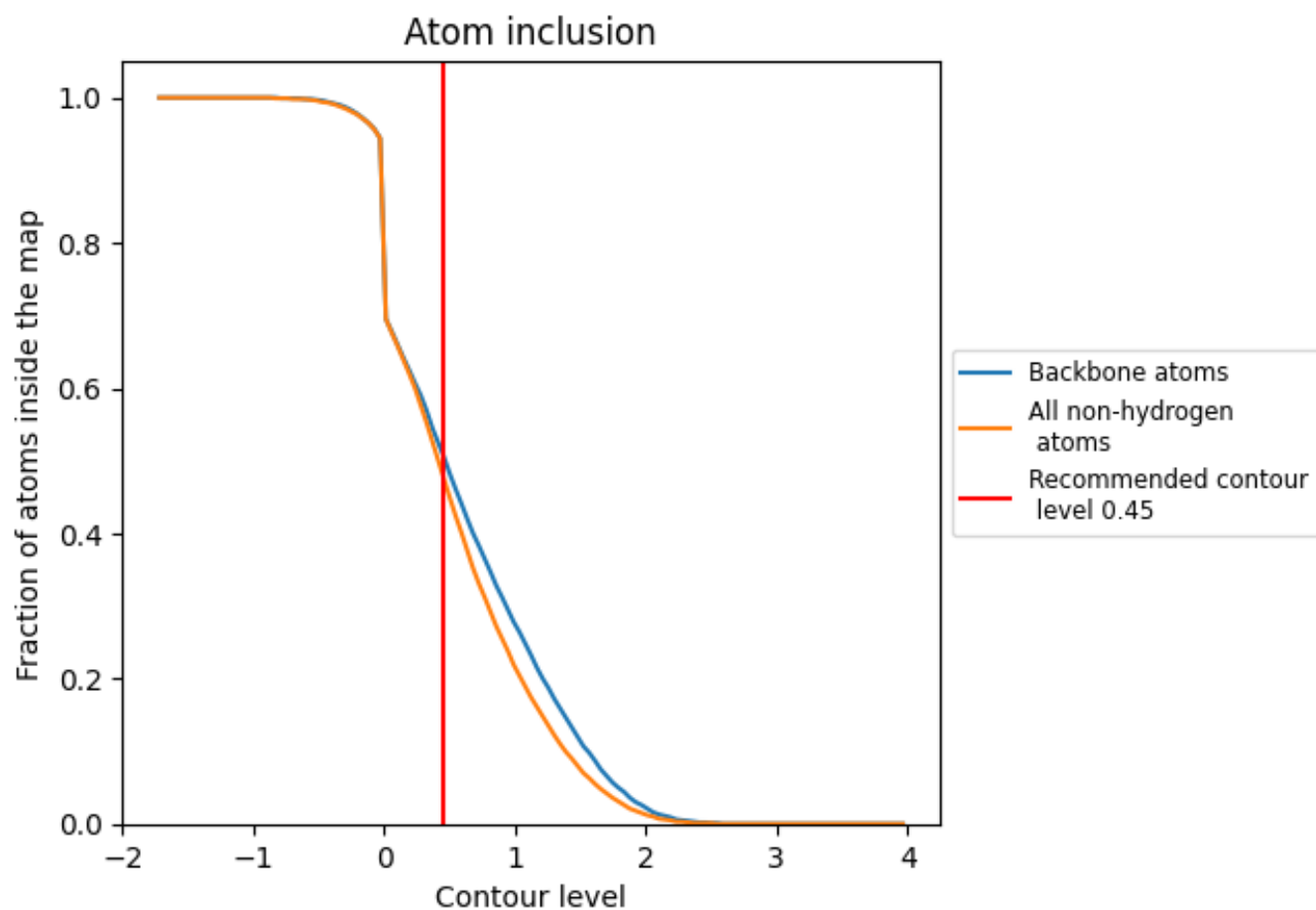


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4780	0.2830
A	0.7840	0.4720
B	0.7480	0.4570
C	0.2330	0.1050
D	0.2110	0.1380

