



wwPDB EM Validation Summary Report ⓘ

Jul 17, 2024 – 03:09 pm BST

PDB ID : 8QX8
EMDB ID : EMD-18701
Title : Endosomal membrane tethering complex CORVET
Authors : Shvarev, D.; Ungermann, C.; Moeller, A.
Deposited on : 2023-10-23
Resolution : 4.60 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

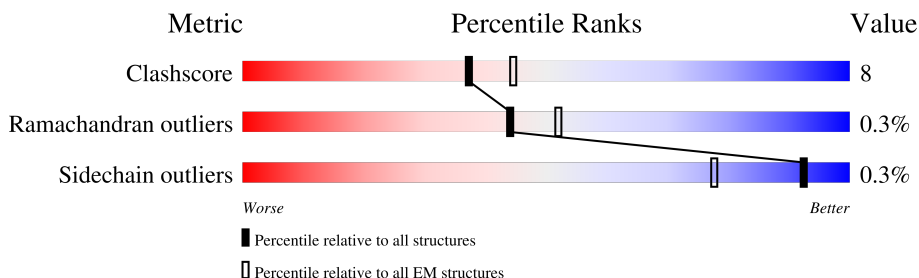
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	F	1298	
2	D	691	
3	B	798	
4	A	1029	
5	E	1011	
6	C	918	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30086 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 Vacuolar protein sorting-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	1117	7530	4743	1310	1455	22	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1275	ASP	-	expression tag	UNP P39702
F	1276	TYR	-	expression tag	UNP P39702
F	1277	LYS	-	expression tag	UNP P39702
F	1278	ASP	-	expression tag	UNP P39702
F	1279	ASP	-	expression tag	UNP P39702
F	1280	ASP	-	expression tag	UNP P39702
F	1281	ASP	-	expression tag	UNP P39702
F	1282	LYS	-	expression tag	UNP P39702
F	1283	ASP	-	expression tag	UNP P39702
F	1284	TYR	-	expression tag	UNP P39702
F	1285	LYS	-	expression tag	UNP P39702
F	1286	ASP	-	expression tag	UNP P39702
F	1287	ASP	-	expression tag	UNP P39702
F	1288	ASP	-	expression tag	UNP P39702
F	1289	ASP	-	expression tag	UNP P39702
F	1290	LYS	-	expression tag	UNP P39702
F	1291	ASP	-	expression tag	UNP P39702
F	1292	TYR	-	expression tag	UNP P39702
F	1293	LYS	-	expression tag	UNP P39702
F	1294	ASP	-	expression tag	UNP P39702
F	1295	ASP	-	expression tag	UNP P39702
F	1296	ASP	-	expression tag	UNP P39702
F	1297	ASP	-	expression tag	UNP P39702
F	1298	LYS	-	expression tag	UNP P39702

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	613	Total	C	N	O	S	0	0
			4939	3157	818	944	20		

- Molecule 3 is a protein called Vacuolar protein sorting-associated protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	728	Total	C	N	O	S	0	0
			5966	3852	974	1112	28		

- Molecule 4 is a protein called E3 ubiquitin-protein ligase PEP5.

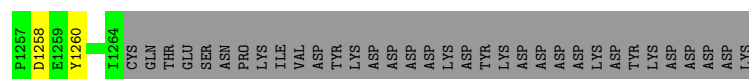
Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	969	Total	C	N	O	S	0	0
			6264	3911	1137	1206	10		

- Molecule 5 is a protein called Vacuolar protein sorting-associated protein 3.

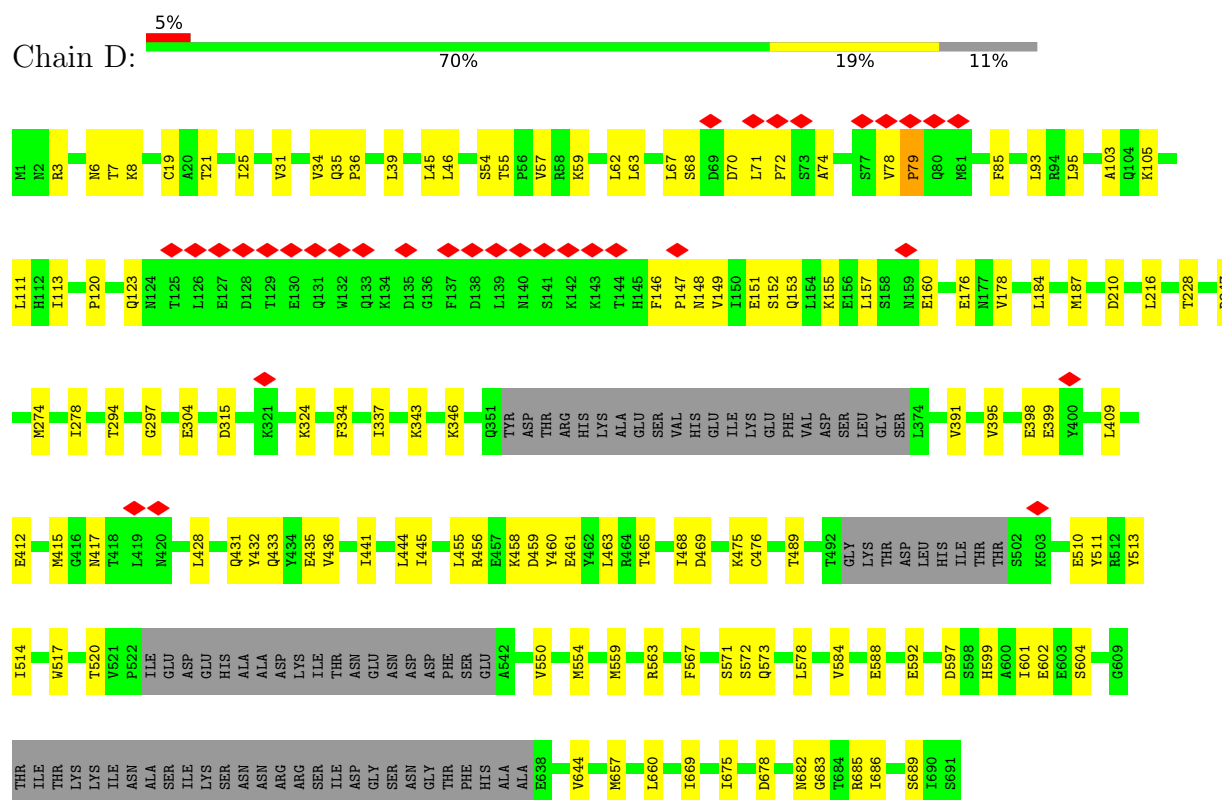
Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	216	Total	C	N	O	0	0
			1077	645	216	216		

- Molecule 6 is a protein called Vacuolar membrane protein PEP3.

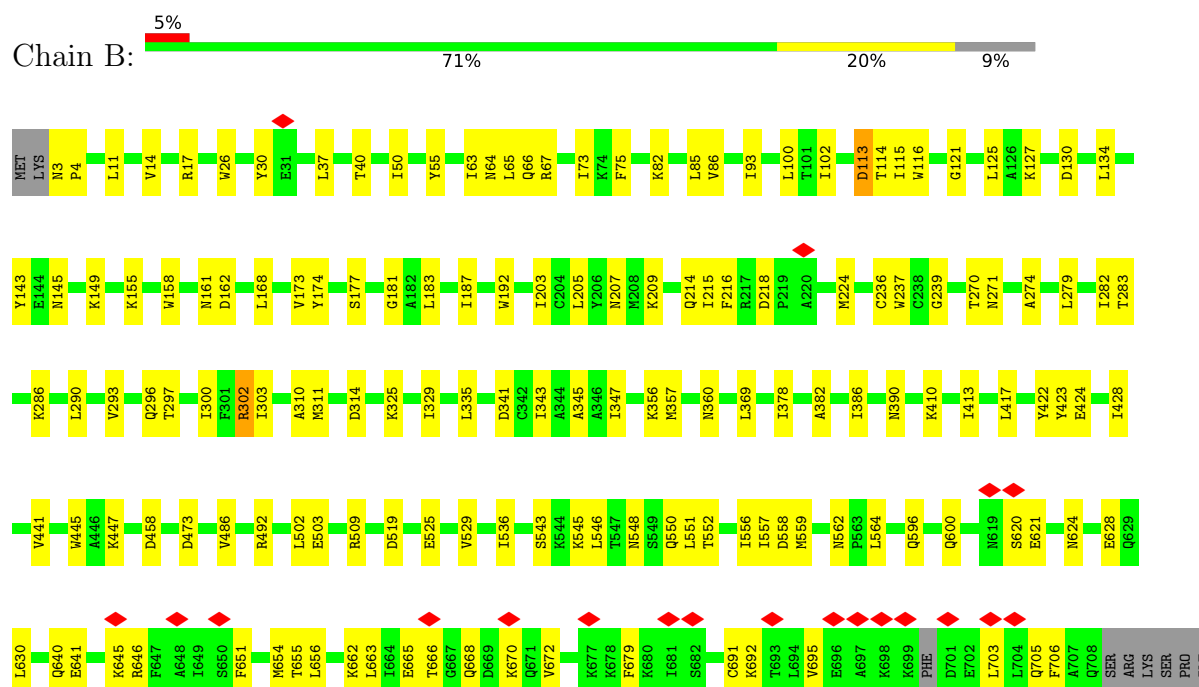
Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	800	Total	C	N	O	S	0	0
			4310	2611	841	851	7		

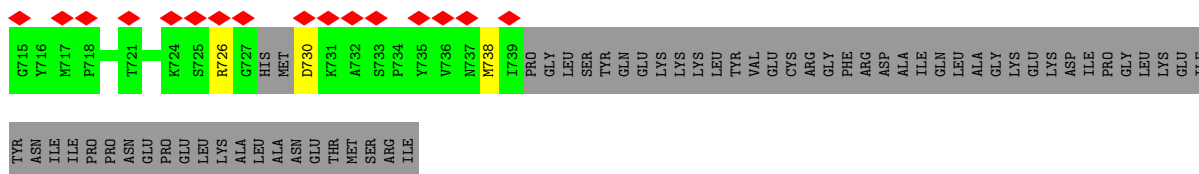


• Molecule 2: Vacuolar protein sorting-associated protein 33



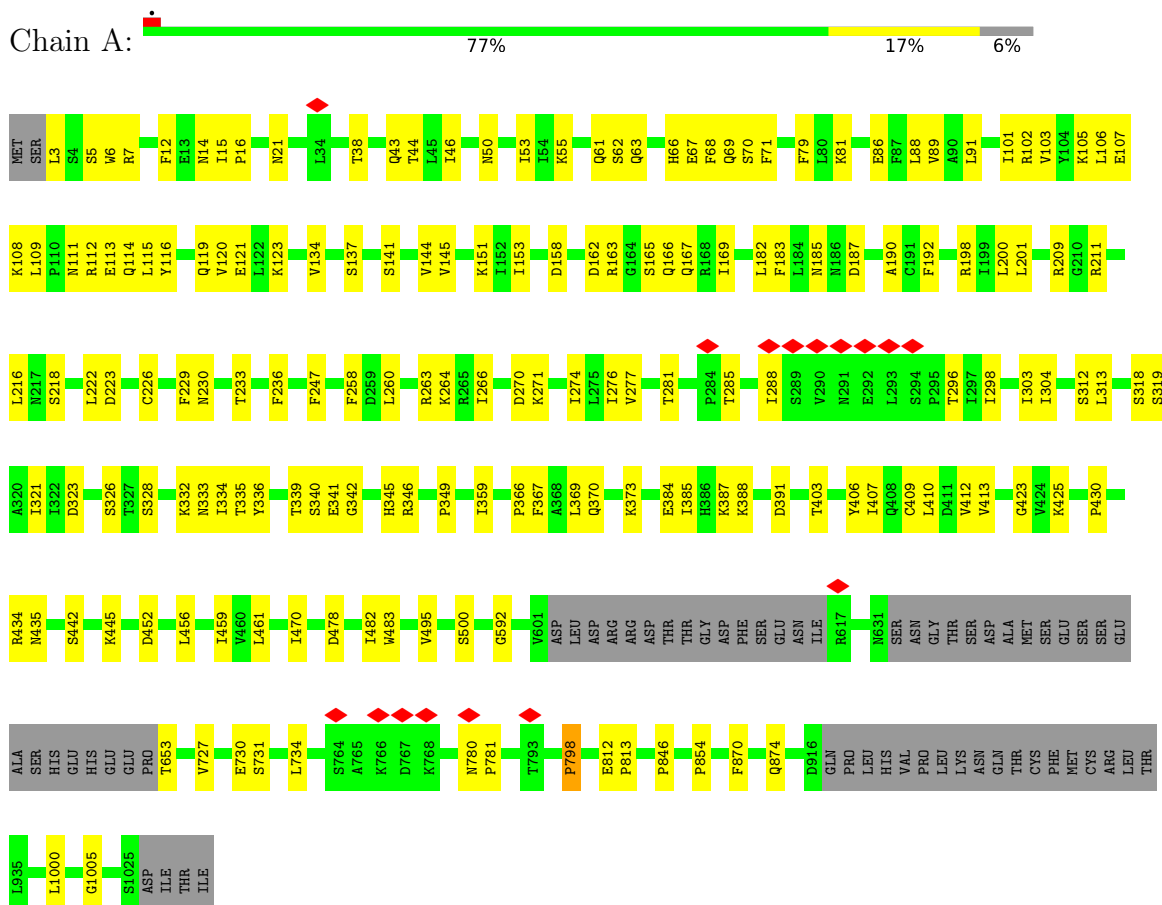
• Molecule 3: Vacuolar protein sorting-associated protein 16

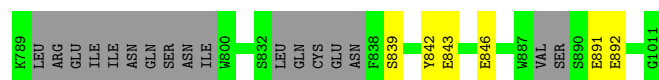




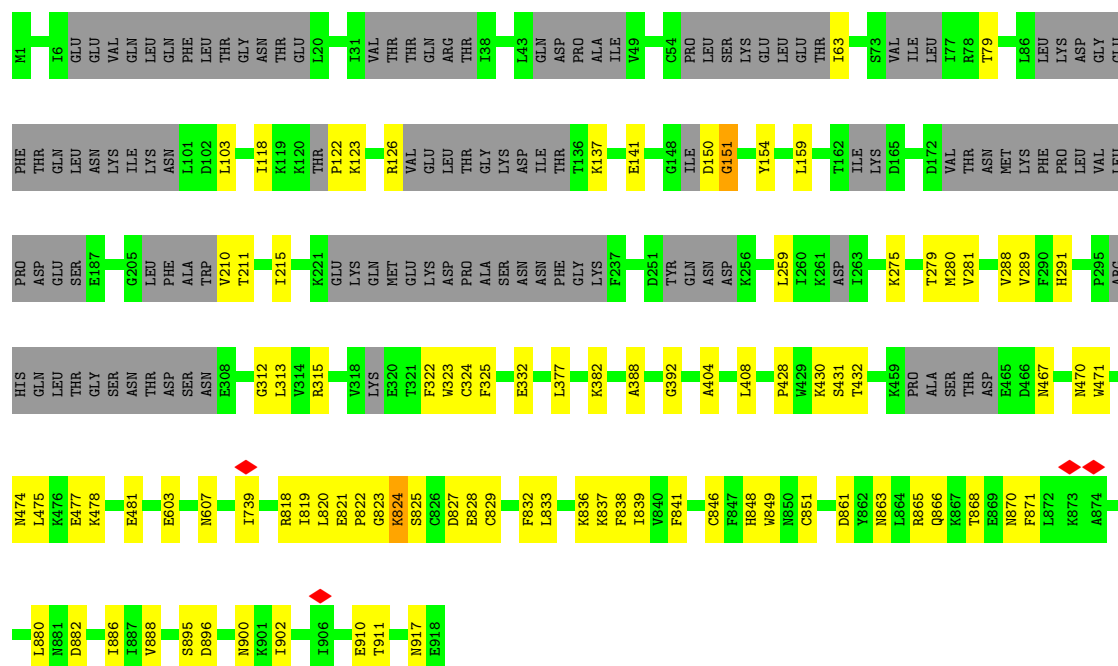
• Molecule 4: E3 ubiquitin-protein ligase PEP5

Chain A:





Chain C: 77% 10% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.989	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.32	Depositor
Map size (Å)	814.8, 814.8, 814.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.037, 2.037, 2.037	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	F	0.24	0/7620	0.43	0/10404
2	D	0.24	0/5026	0.49	2/6802 (0.0%)
3	B	0.24	0/6084	0.49	0/8214
4	A	0.24	0/6334	0.48	5/8677 (0.1%)
5	E	0.24	0/1073	0.34	0/1494
6	C	0.25	0/4308	0.41	0/5946
All	All	0.24	0/30445	0.46	7/41537 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	79	PRO	N-CA-CB	6.55	111.16	103.30
4	A	854	PRO	N-CA-CB	6.06	110.57	103.30
4	A	781	PRO	N-CA-CB	5.89	110.37	103.30
4	A	846	PRO	N-CA-CB	5.84	110.31	103.30
4	A	798	PRO	N-CA-CB	5.80	110.27	103.30

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	F	7530	0	6130	118	0
2	D	4939	0	4932	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5966	0	6024	103	0
4	A	6264	0	4946	105	0
5	E	1077	0	437	2	0
6	C	4310	0	2266	73	0
All	All	30086	0	24735	450	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 8.

The worst 5 of 450 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)
6:C:828:GLU:HG3	6:C:851:CYS:SG	1.63	1.38
6:C:828:GLU:CG	6:C:851:CYS:SG	2.27	1.22
3:B:270:THR:HG22	3:B:271:ASN:H	1.15	1.08
6:C:828:GLU:CG	6:C:851:CYS:HG	1.71	1.00
6:C:828:GLU:HG3	6:C:851:CYS:HG	0.77	0.93

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	F	1077/1298 (83%)	998 (93%)	79 (7%)	0	100	100
2	D	603/691 (87%)	562 (93%)	39 (6%)	2 (0%)	41	76
3	B	720/798 (90%)	621 (86%)	98 (14%)	1 (0%)	51	85
4	A	961/1029 (93%)	838 (87%)	119 (12%)	4 (0%)	34	72
5	E	208/1011 (21%)	197 (95%)	9 (4%)	2 (1%)	15	54
6	C	762/918 (83%)	699 (92%)	58 (8%)	5 (1%)	22	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4331/5745 (75%)	3915 (90%)	402 (9%)	14 (0%)	44	76

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	78	VAL
2	D	79	PRO
5	E	892	GLU
6	C	428	PRO
6	C	151	GLY

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	F	586/1203 (49%)	585 (100%)	1 (0%)	93	96
2	D	559/640 (87%)	558 (100%)	1 (0%)	93	96
3	B	668/730 (92%)	667 (100%)	1 (0%)	93	96
4	A	443/952 (46%)	441 (100%)	2 (0%)	88	93
6	C	96/873 (11%)	95 (99%)	1 (1%)	76	86
All	All	2352/4398 (54%)	2346 (100%)	6 (0%)	92	95

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	7	ARG
4	A	410	LEU
6	C	824	LYS
2	D	324	LYS
1	F	561	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	642	GLN
2	D	186	ASN
2	D	417	ASN
3	B	390	ASN
4	A	230	ASN

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](#)

There are no chain breaks in this entry.

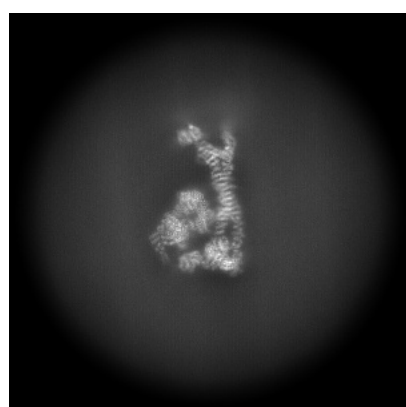
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18701. These allow visual inspection of the internal detail of the map and identification of artifacts.

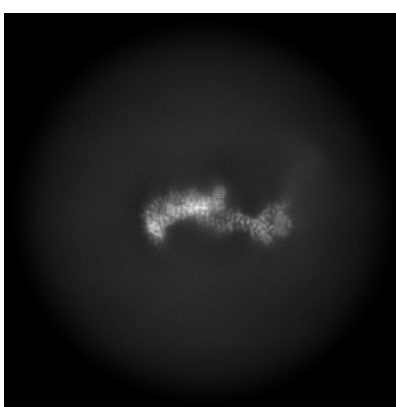
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

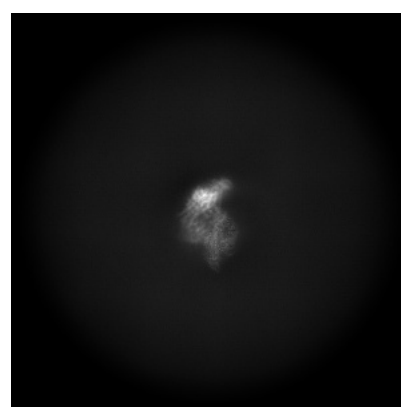
6.1.1 Primary map



X



Y

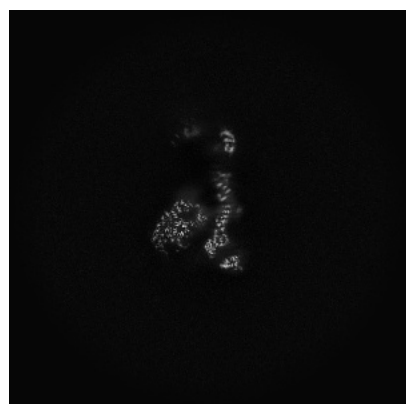


Z

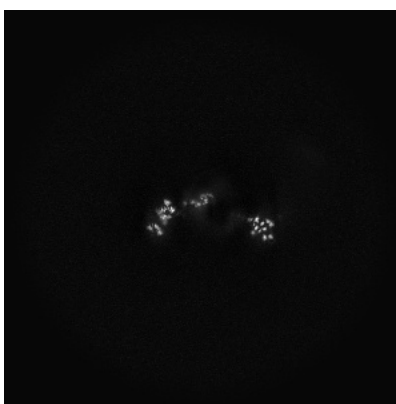
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200



Y Index: 200

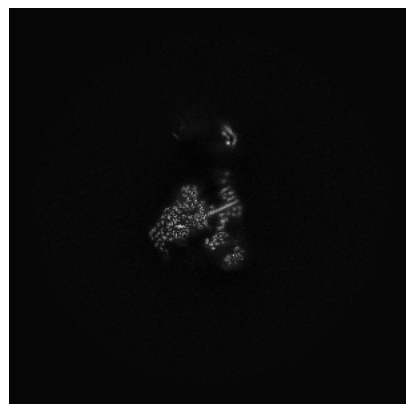


Z Index: 200

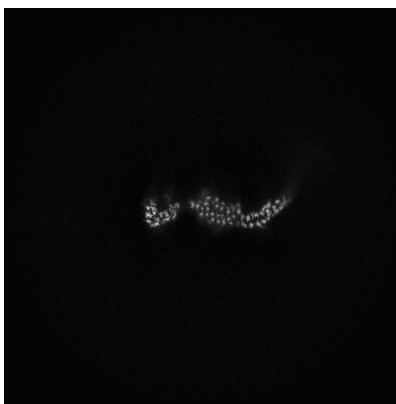
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 204



Y Index: 217

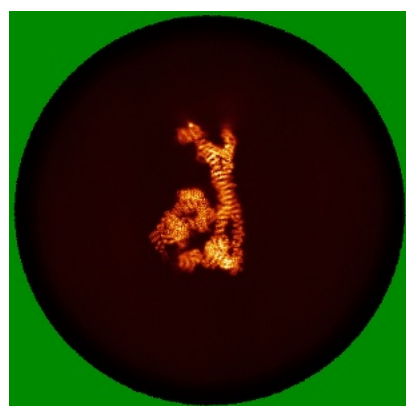


Z Index: 149

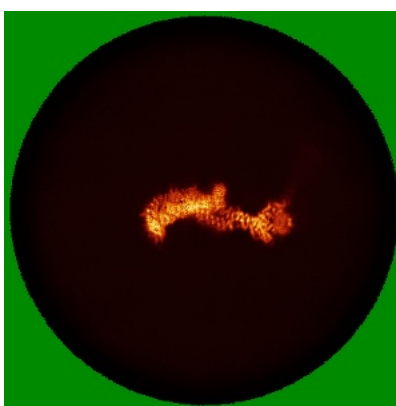
The images above show the largest variance slices of the map in three orthogonal directions.

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

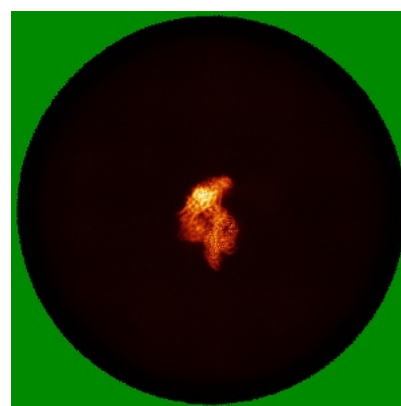
6.4.1 Primary map



X



Y

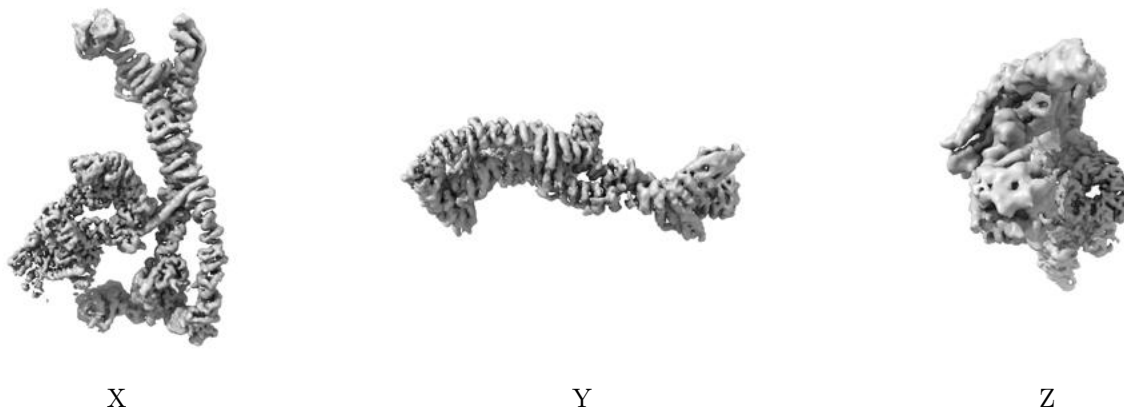


Z

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

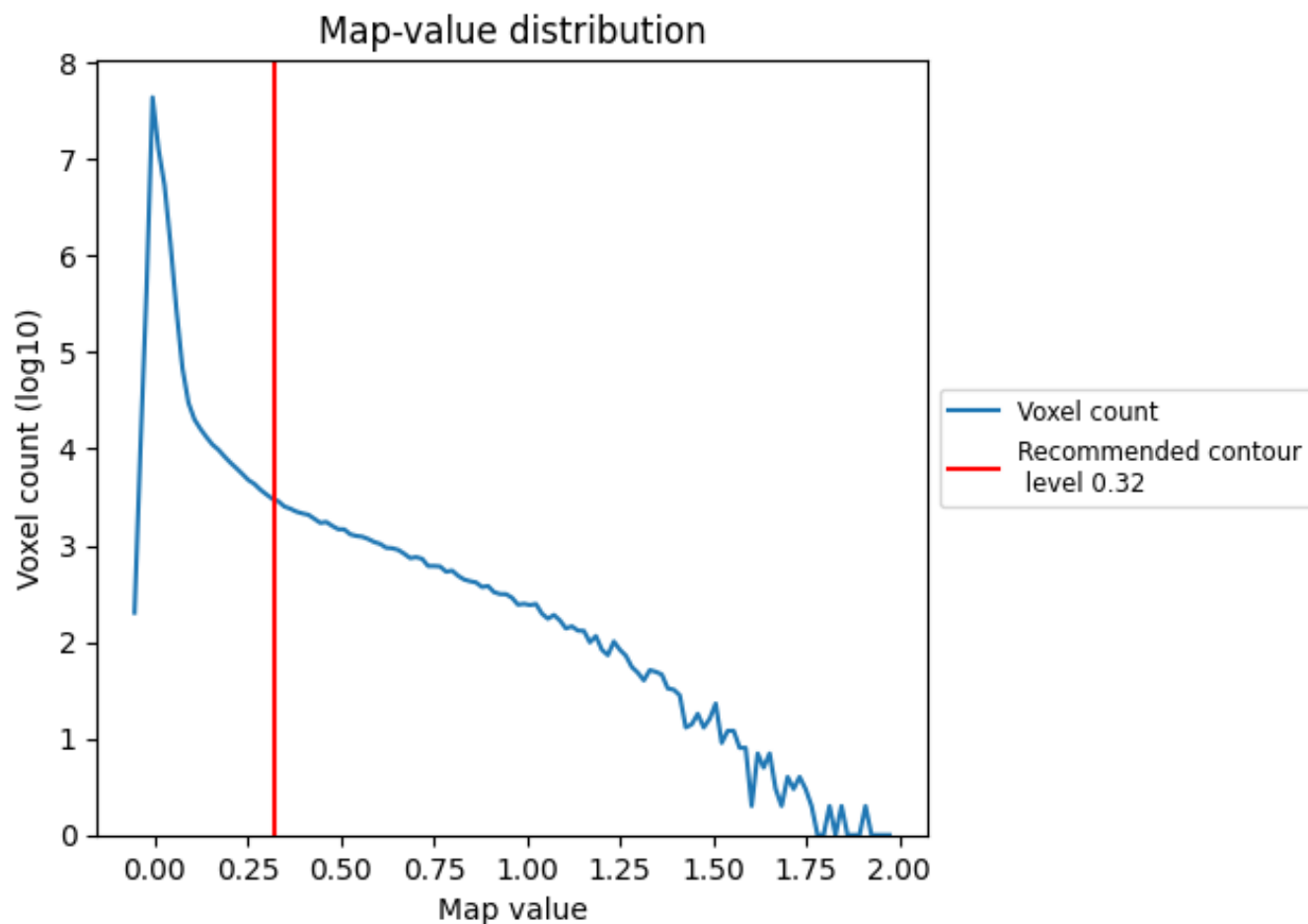
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

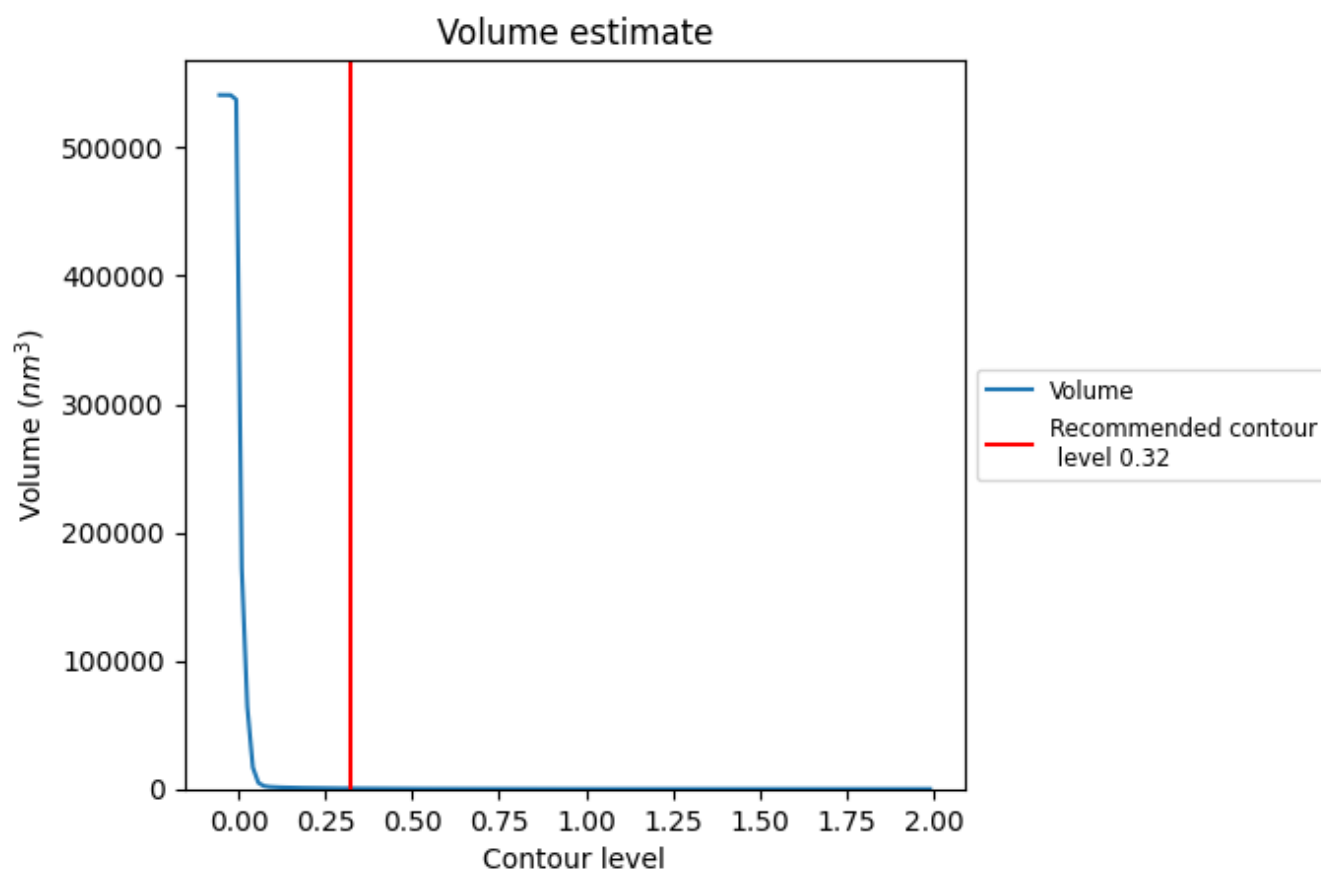
This section contains the results of statistical analysis of the map.

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.

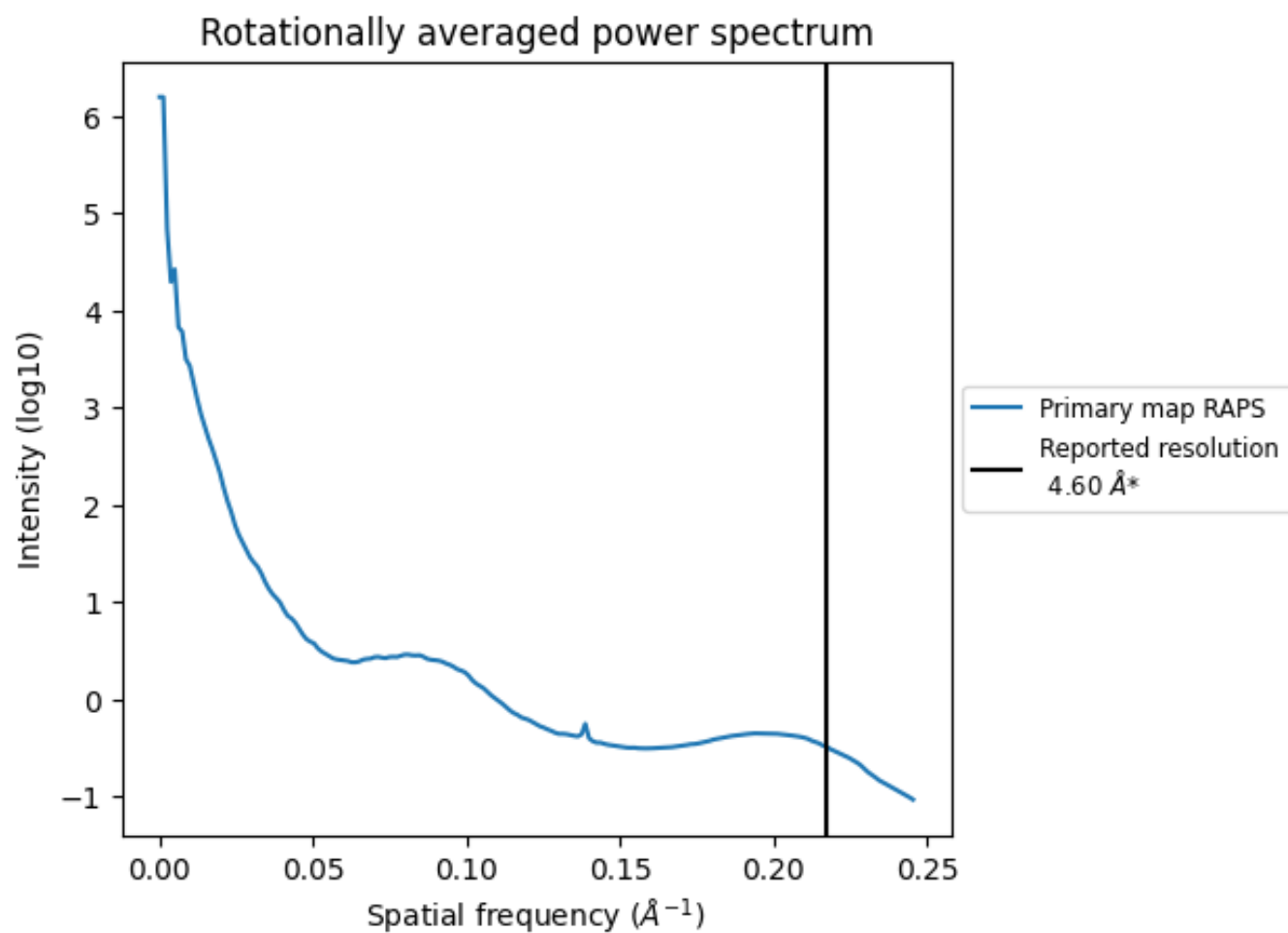
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 418 nm^3 ; this corresponds to an approximate mass of 378 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 0.217 Å⁻¹

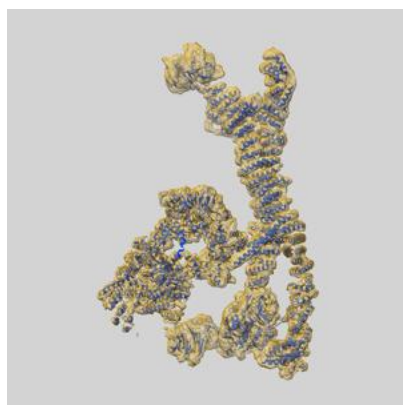
8 Fourier-Shell correlation

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

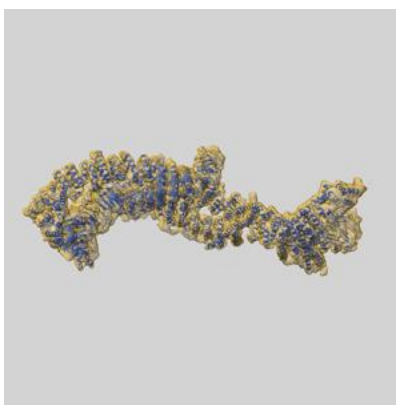
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18701 and PDB model 8QX8. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

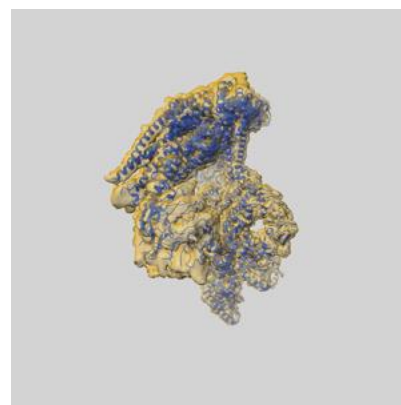
9.1 Map-model overlay [i](#)



X



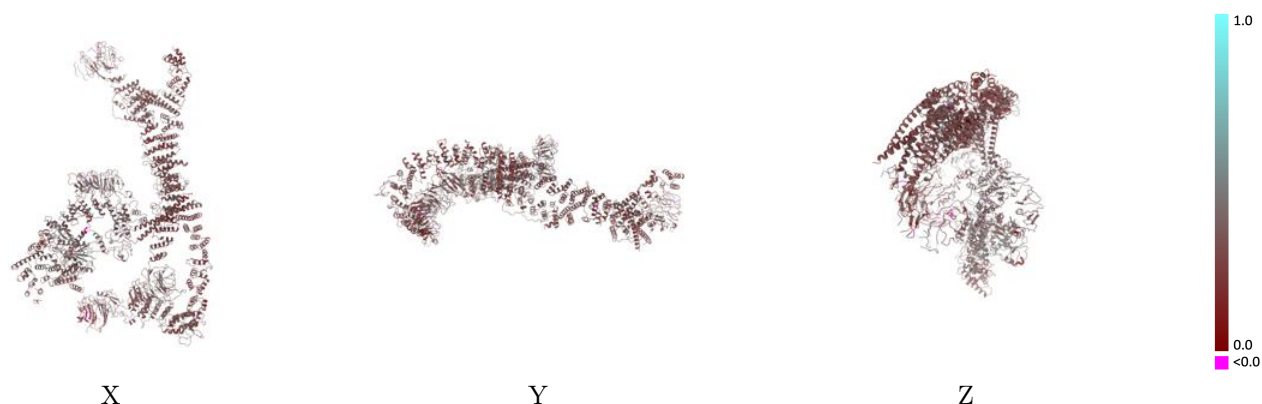
Y



Z

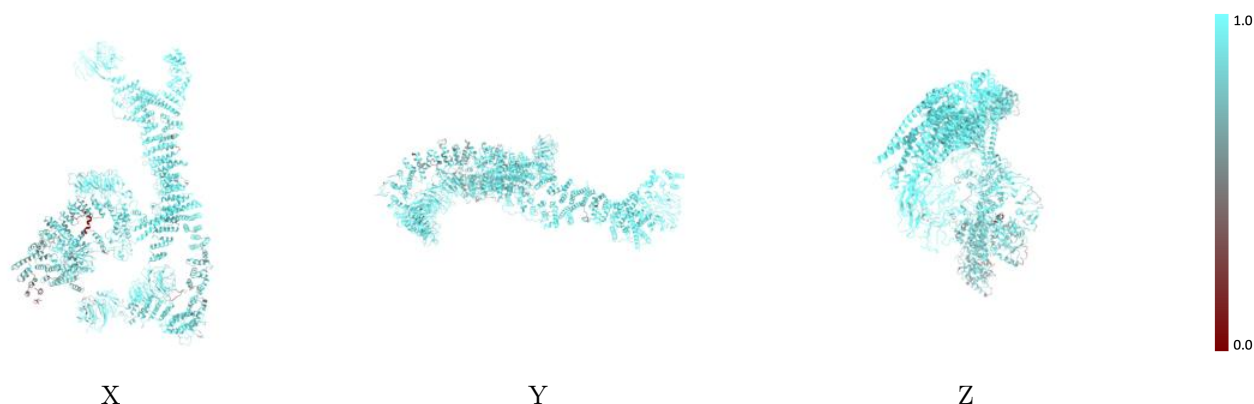
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



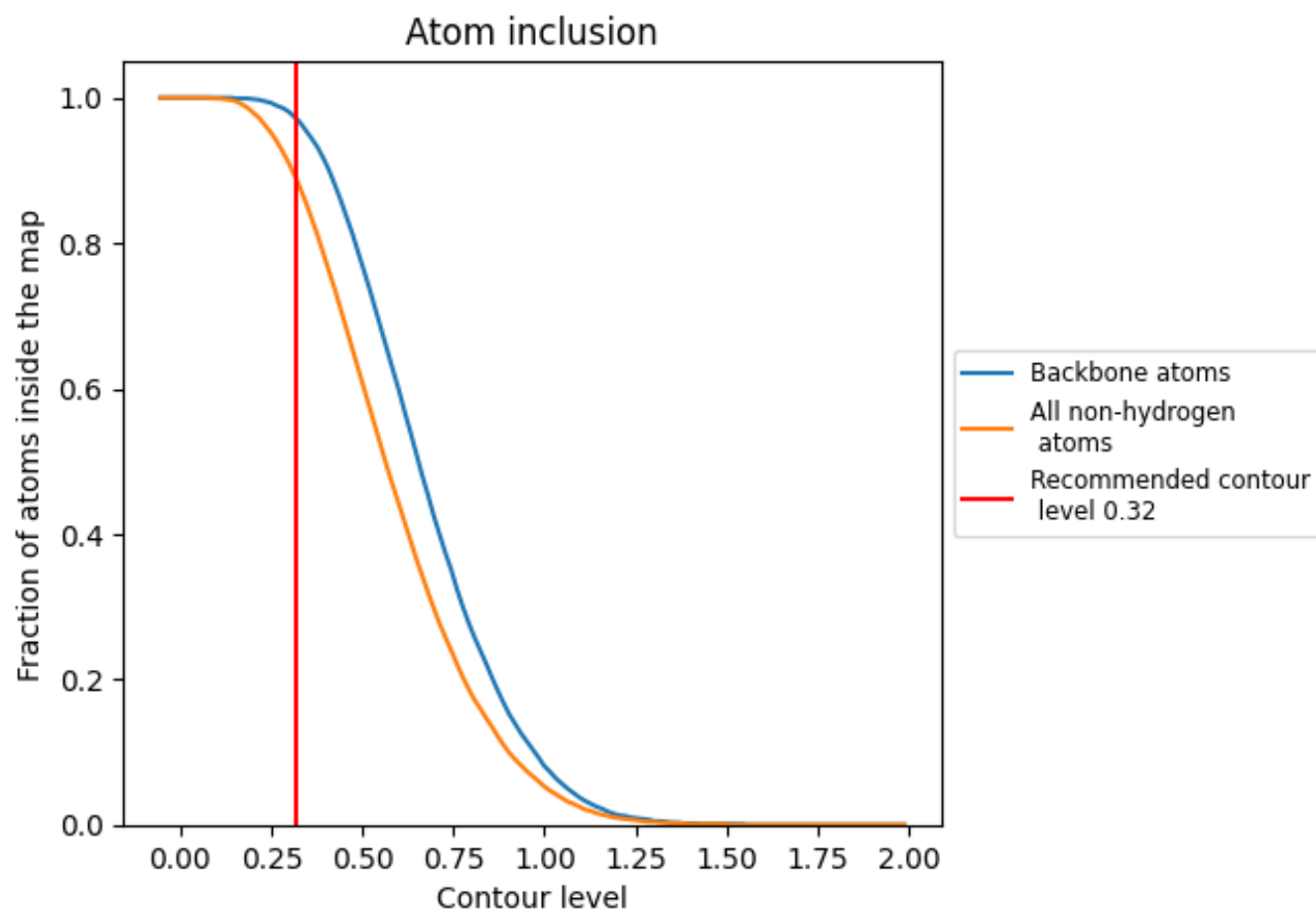
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.32).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 89% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8870	<div></div> 0.3400
A	<div></div> 0.9420	<div></div> 0.3320
B	<div></div> 0.8280	<div></div> 0.3710
C	<div></div> 0.9660	<div></div> 0.3250
D	<div></div> 0.8050	<div></div> 0.3810
E	<div></div> 0.9980	<div></div> 0.3180
F	<div></div> 0.8800	<div></div> 0.3060

