



wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 10:28 am GMT

PDB ID : 7AE0
EMDB ID : EMD-11735
Title : Cryo-EM structure of an extracellular contractile injection system in marine bacterium *Algoriphagus machipongonensis*, the sheath-tube module in extended state.
Authors : Xu, J.; Ericson, C.; Feldmueller, M.; Lien, Y.W.; Pilhofer, M.
Deposited on : 2020-09-17
Resolution : 2.40 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

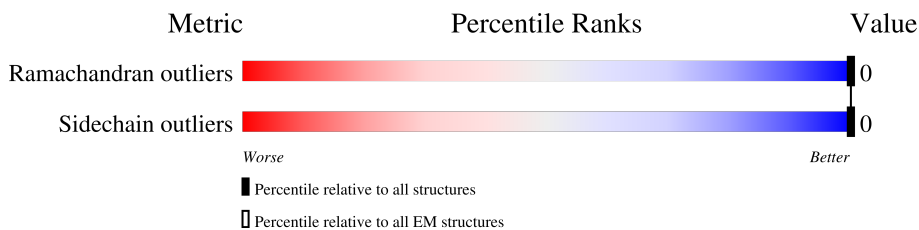
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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)
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	3A	692	 14% 73% • 26%
1	3B	692	 14% 73% • 26%
1	3C	692	 14% 73% • 26%
1	3D	692	 14% 73% • 26%
1	3E	692	 14% 73% • 26%
1	3F	692	 14% 73% • 26%
1	4A	692	 13% 73% • 26%
1	4B	692	 14% 73% • 26%
1	4C	692	 13% 73% • 26%

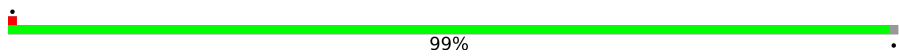
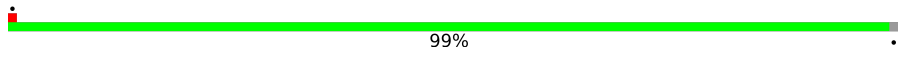
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Mol	Chain	Length	Quality of chain
1	4D	692	 13% 73% 26%
1	4E	692	 14% 73% 26%
1	4F	692	 13% 73% 26%
1	5A	692	 14% 73% 26%
1	5B	692	 14% 73% 26%
1	5C	692	 14% 73% 26%
1	5D	692	 14% 73% 26%
1	5E	692	 14% 73% 26%
1	5F	692	 14% 73% 26%
2	3a	142	 99%
2	3b	142	 99%
2	3c	142	 99%
2	3d	142	 99%
2	3e	142	 99%
2	3f	142	 99%
2	4a	142	 99%
2	4b	142	 99%
2	4c	142	 99%
2	4d	142	 99%
2	4e	142	 99%
2	4f	142	 99%
2	5a	142	 99%
2	5b	142	 99%
2	5c	142	 99%
2	5d	142	 99%

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Mol	Chain	Length	Quality of chain
2	5e	142	 99%
2	5f	142	 99%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 92718 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 Putative phage tail sheath protein FI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	3A	511	4006	2549	660	785	12	0	0
1	3B	511	4006	2549	660	785	12	0	0
1	3C	511	4006	2549	660	785	12	0	0
1	3D	511	4006	2549	660	785	12	0	0
1	3E	511	4006	2549	660	785	12	0	0
1	3F	511	4006	2549	660	785	12	0	0
1	4A	511	4006	2549	660	785	12	0	0
1	4B	511	4006	2549	660	785	12	0	0
1	4C	511	4006	2549	660	785	12	0	0
1	4D	511	4006	2549	660	785	12	0	0
1	4E	511	4006	2549	660	785	12	0	0
1	4F	511	4006	2549	660	785	12	0	0
1	5A	511	4006	2549	660	785	12	0	0
1	5B	511	4006	2549	660	785	12	0	0
1	5C	511	4006	2549	660	785	12	0	0
1	5D	511	4006	2549	660	785	12	0	0
1	5E	511	4006	2549	660	785	12	0	0

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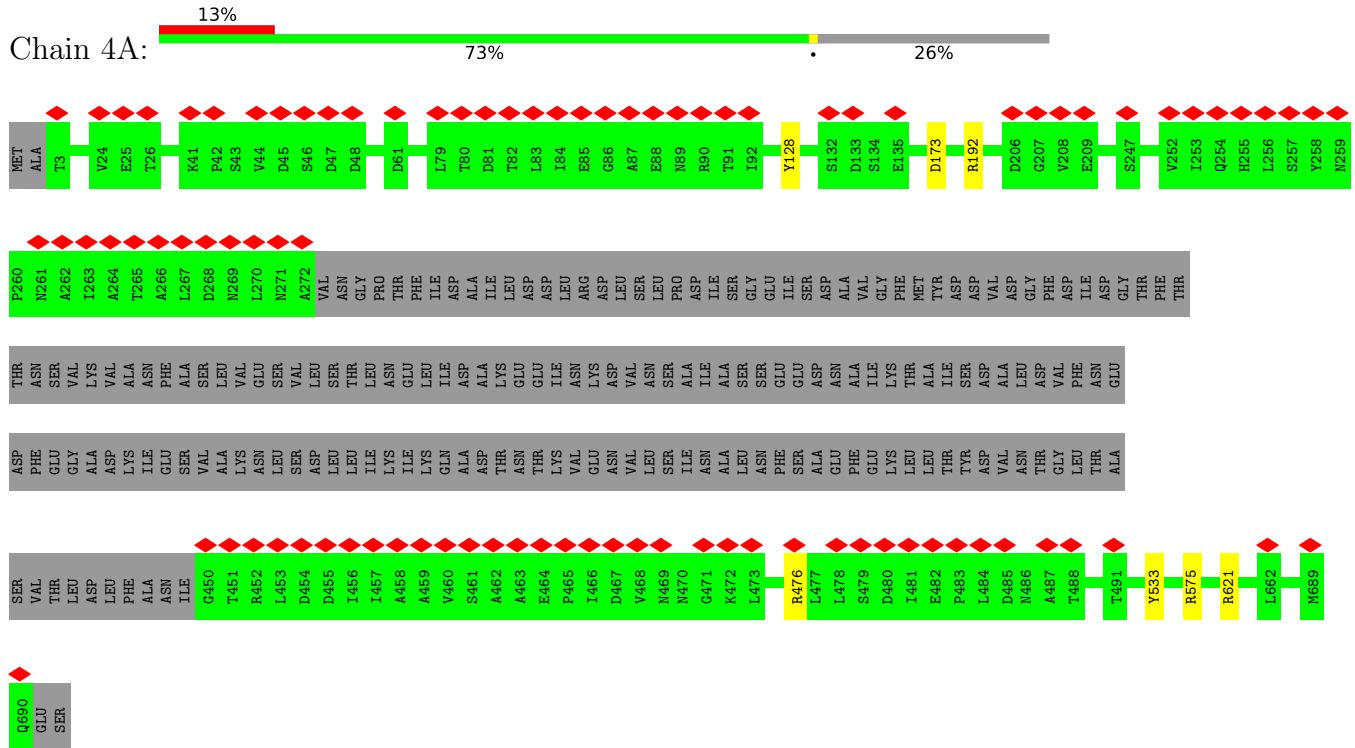
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	5F	511	4006	2549	660	785	12	0	0

- Molecule 2 is a protein called Phage tail protein.

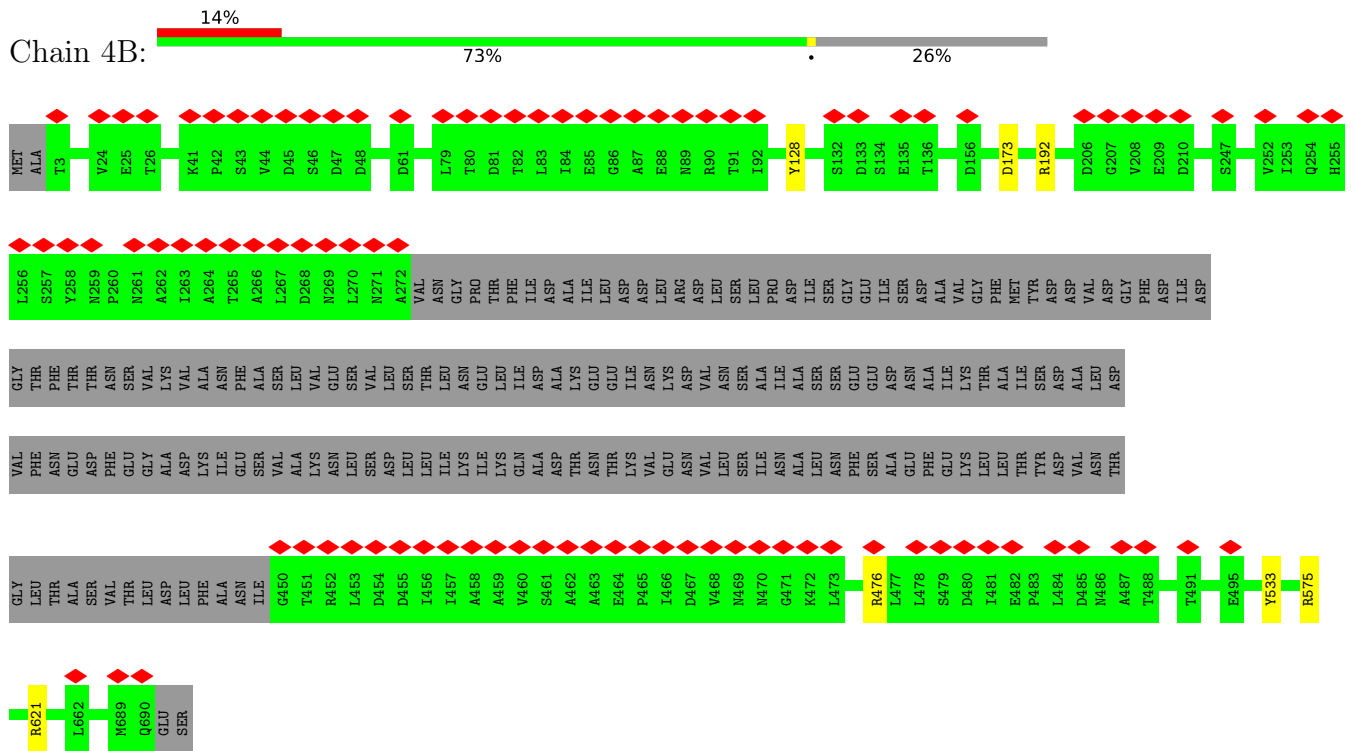
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3a	141	1145	731	190	221	3	0	0
2	3b	141	1145	731	190	221	3	0	0
2	3c	141	1145	731	190	221	3	0	0
2	3d	141	1145	731	190	221	3	0	0
2	3e	141	1145	731	190	221	3	0	0
2	3f	141	1145	731	190	221	3	0	0
2	4a	141	1145	731	190	221	3	0	0
2	4b	141	1145	731	190	221	3	0	0
2	4c	141	1145	731	190	221	3	0	0
2	4d	141	1145	731	190	221	3	0	0
2	4e	141	1145	731	190	221	3	0	0
2	4f	141	1145	731	190	221	3	0	0
2	5a	141	1145	731	190	221	3	0	0
2	5b	141	1145	731	190	221	3	0	0
2	5c	141	1145	731	190	221	3	0	0
2	5d	141	1145	731	190	221	3	0	0
2	5e	141	1145	731	190	221	3	0	0
2	5f	141	1145	731	190	221	3	0	0

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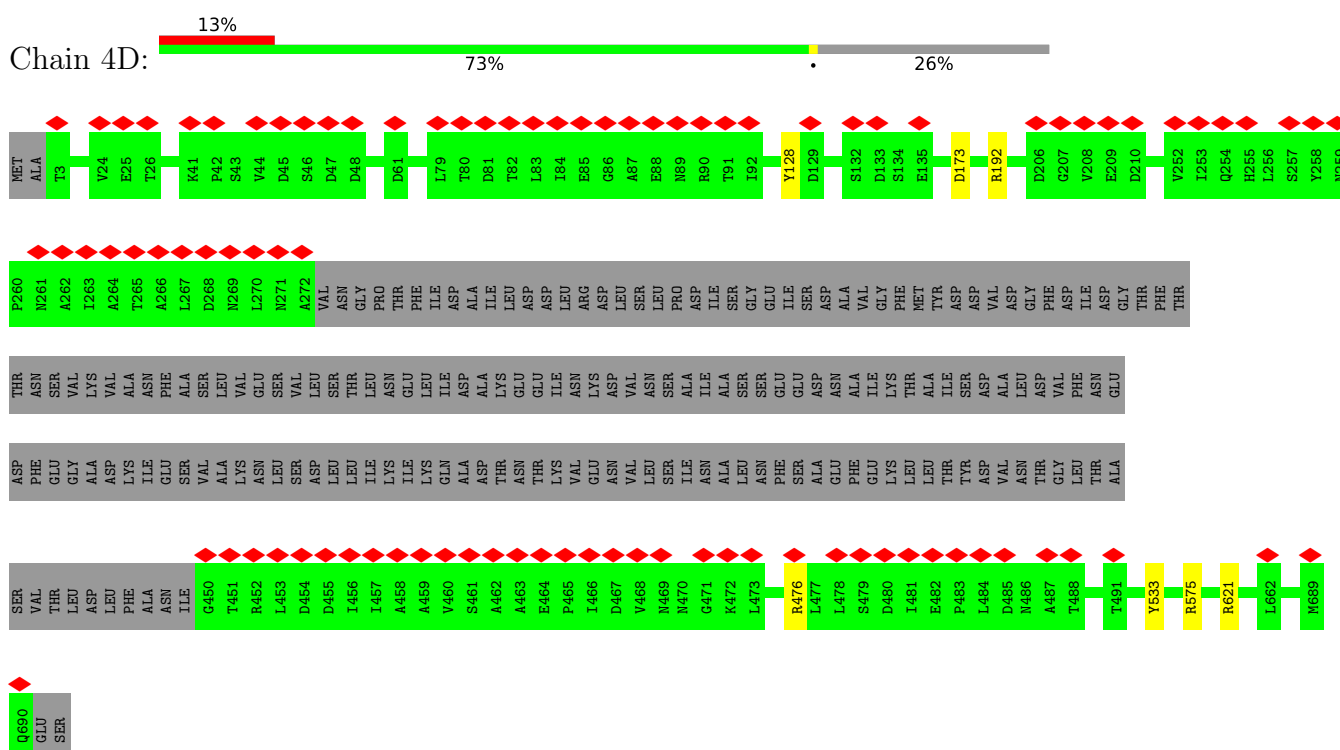
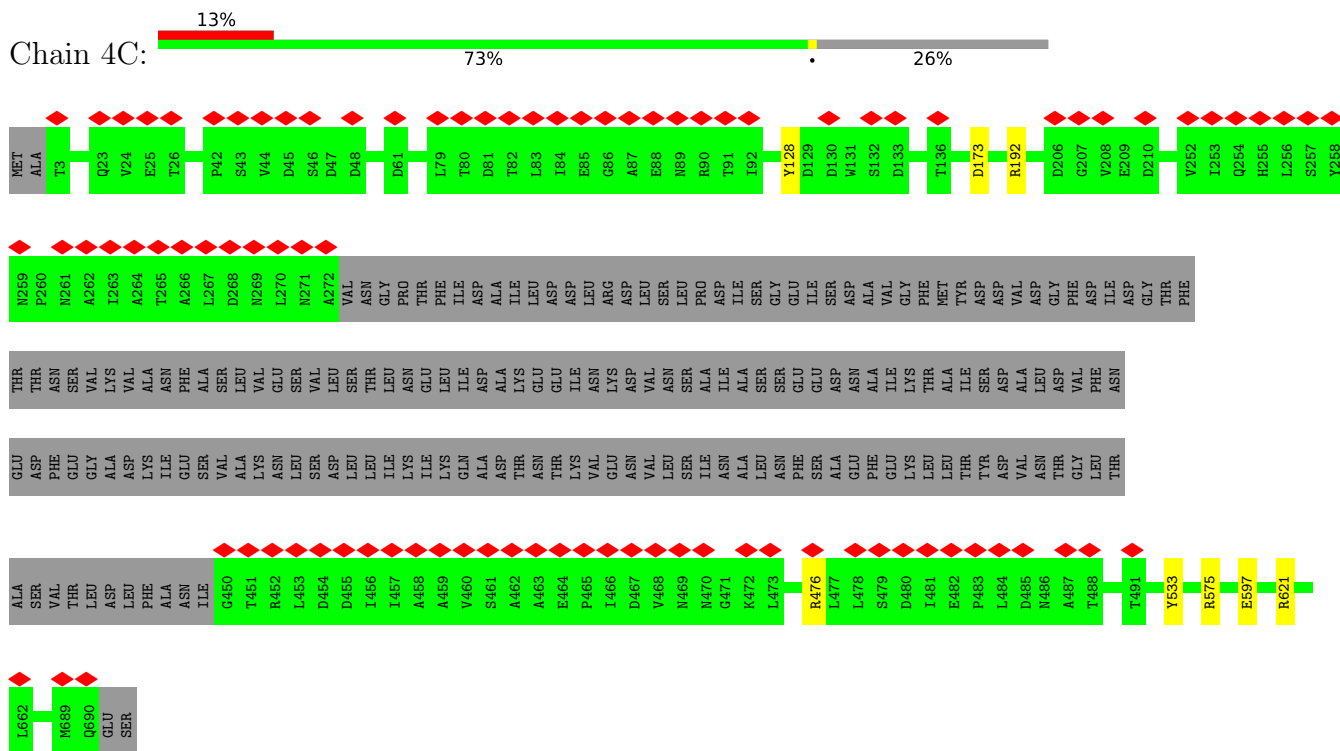
• Molecule 1: Putative phage tail sheath protein FI



• Molecule 1: Putative phage tail sheath protein FI



• Molecule 1: Putative phage tail sheath protein FI



Chain 3c:  99%



- Molecule 2: Phage tail protein

Chain 3d:  99%



- Molecule 2: Phage tail protein

Chain 3e:  99%



- Molecule 2: Phage tail protein

Chain 3f:  99%



- Molecule 2: Phage tail protein

Chain 4a:  99%



- Molecule 2: Phage tail protein

Chain 4b:  99%



- Molecule 2: Phage tail protein

Chain 4c:  99%



- Molecule 2: Phage tail protein

Chain 4d:  99%



- Molecule 2: Phage tail protein

Chain 4e:  99%



- Molecule 2: Phage tail protein

Chain 4f:  99%



- Molecule 2: Phage tail protein

Chain 5a:  99%



- Molecule 2: Phage tail protein

Chain 5b:  99%



- Molecule 2: Phage tail protein

Chain 5c:  99%



- Molecule 2: Phage tail protein

Chain 5d:  99%



- Molecule 2: Phage tail protein

Chain 5e:  99%



- Molecule 2: Phage tail protein

Chain 5f:  99%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=20.54°, rise=40.80 Å, axial sym=C6	Depositor
Number of segments used	225305	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 ($e^-/\text{Å}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.321	Depositor
Minimum map value	-0.200	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	3A	0.87	0/4097	0.88	9/5583 (0.2%)
1	3B	0.88	0/4097	0.88	9/5583 (0.2%)
1	3C	0.88	1/4097 (0.0%)	0.88	9/5583 (0.2%)
1	3D	0.87	0/4097	0.88	9/5583 (0.2%)
1	3E	0.87	0/4097	0.88	9/5583 (0.2%)
1	3F	0.87	0/4097	0.88	9/5583 (0.2%)
1	4A	0.87	0/4097	0.88	9/5583 (0.2%)
1	4B	0.88	0/4097	0.88	9/5583 (0.2%)
1	4C	0.88	1/4097 (0.0%)	0.88	9/5583 (0.2%)
1	4D	0.87	0/4097	0.88	9/5583 (0.2%)
1	4E	0.88	0/4097	0.88	9/5583 (0.2%)
1	4F	0.87	0/4097	0.88	10/5583 (0.2%)
1	5A	0.87	0/4097	0.88	9/5583 (0.2%)
1	5B	0.88	0/4097	0.88	9/5583 (0.2%)
1	5C	0.88	1/4097 (0.0%)	0.88	9/5583 (0.2%)
1	5D	0.87	0/4097	0.88	10/5583 (0.2%)
1	5E	0.88	0/4097	0.88	9/5583 (0.2%)
1	5F	0.87	0/4097	0.88	10/5583 (0.2%)
2	3a	0.76	0/1172	0.80	0/1584
2	3b	0.76	0/1172	0.80	0/1584
2	3c	0.76	0/1172	0.80	0/1584
2	3d	0.76	0/1172	0.80	0/1584
2	3e	0.76	0/1172	0.80	0/1584
2	3f	0.76	0/1172	0.80	0/1584
2	4a	0.76	0/1172	0.80	0/1584
2	4b	0.76	0/1172	0.80	0/1584
2	4c	0.76	0/1172	0.80	0/1584
2	4d	0.76	0/1172	0.80	0/1584
2	4e	0.76	0/1172	0.80	0/1584
2	4f	0.76	0/1172	0.80	0/1584
2	5a	0.76	0/1172	0.80	0/1584
2	5b	0.76	0/1172	0.80	0/1584
2	5c	0.76	0/1172	0.80	0/1584
2	5d	0.76	0/1172	0.80	0/1584

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	5e	0.76	0/1172	0.80	0/1584
2	5f	0.76	0/1172	0.80	0/1584
All	All	0.85	3/94842 (0.0%)	0.86	165/129006 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5C	597	GLU	CD-OE1	-5.12	1.20	1.25
1	4C	597	GLU	CD-OE1	-5.09	1.20	1.25
1	3C	597	GLU	CD-OE1	-5.06	1.20	1.25

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5E	192	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	4A	192	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	4F	192	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	5A	192	ARG	NE-CZ-NH2	-10.75	114.93	120.30
1	4E	192	ARG	NE-CZ-NH2	-10.75	114.93	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	3A	507/692 (73%)	500 (99%)	7 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3B	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	3C	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	3D	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	3E	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	3F	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	4A	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	4B	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	4C	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	4D	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	4E	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	4F	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	5A	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	5B	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	5C	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	5D	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	5E	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
1	5F	507/692 (73%)	500 (99%)	7 (1%)	0	100	100
2	3a	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	3b	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	3c	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	3d	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	3e	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	3f	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	4a	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	4b	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	4c	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	4d	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	4e	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	4f	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	5a	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	5b	139/142 (98%)	137 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	5c	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	5d	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	5e	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
2	5f	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
All	All	11628/15012 (78%)	11466 (99%)	162 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	3A	437/593 (74%)	437 (100%)	0	100	100
1	3B	437/593 (74%)	437 (100%)	0	100	100
1	3C	437/593 (74%)	437 (100%)	0	100	100
1	3D	437/593 (74%)	437 (100%)	0	100	100
1	3E	437/593 (74%)	437 (100%)	0	100	100
1	3F	437/593 (74%)	437 (100%)	0	100	100
1	4A	437/593 (74%)	437 (100%)	0	100	100
1	4B	437/593 (74%)	437 (100%)	0	100	100
1	4C	437/593 (74%)	437 (100%)	0	100	100
1	4D	437/593 (74%)	437 (100%)	0	100	100
1	4E	437/593 (74%)	437 (100%)	0	100	100
1	4F	437/593 (74%)	437 (100%)	0	100	100
1	5A	437/593 (74%)	437 (100%)	0	100	100
1	5B	437/593 (74%)	437 (100%)	0	100	100
1	5C	437/593 (74%)	437 (100%)	0	100	100
1	5D	437/593 (74%)	437 (100%)	0	100	100
1	5E	437/593 (74%)	437 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5F	437/593 (74%)	437 (100%)	0	100	100
2	3a	127/128 (99%)	127 (100%)	0	100	100
2	3b	127/128 (99%)	127 (100%)	0	100	100
2	3c	127/128 (99%)	127 (100%)	0	100	100
2	3d	127/128 (99%)	127 (100%)	0	100	100
2	3e	127/128 (99%)	127 (100%)	0	100	100
2	3f	127/128 (99%)	127 (100%)	0	100	100
2	4a	127/128 (99%)	127 (100%)	0	100	100
2	4b	127/128 (99%)	127 (100%)	0	100	100
2	4c	127/128 (99%)	127 (100%)	0	100	100
2	4d	127/128 (99%)	127 (100%)	0	100	100
2	4e	127/128 (99%)	127 (100%)	0	100	100
2	4f	127/128 (99%)	127 (100%)	0	100	100
2	5a	127/128 (99%)	127 (100%)	0	100	100
2	5b	127/128 (99%)	127 (100%)	0	100	100
2	5c	127/128 (99%)	127 (100%)	0	100	100
2	5d	127/128 (99%)	127 (100%)	0	100	100
2	5e	127/128 (99%)	127 (100%)	0	100	100
2	5f	127/128 (99%)	127 (100%)	0	100	100
All	All	10152/12978 (78%)	10152 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	4B	580	ASN
1	4C	580	ASN
1	4F	580	ASN
1	4E	490	ASN
1	4E	580	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.

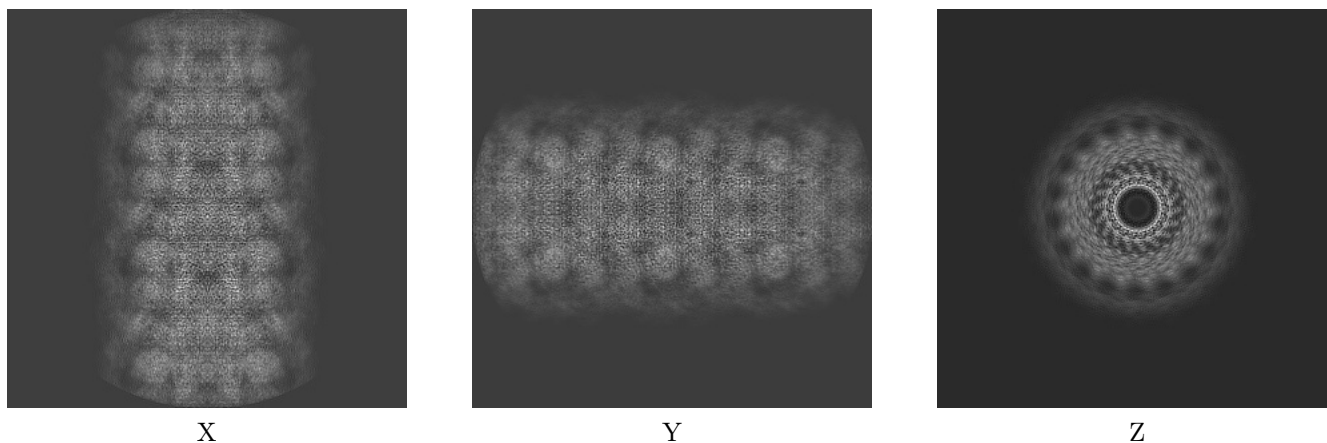
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11735. 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](#)

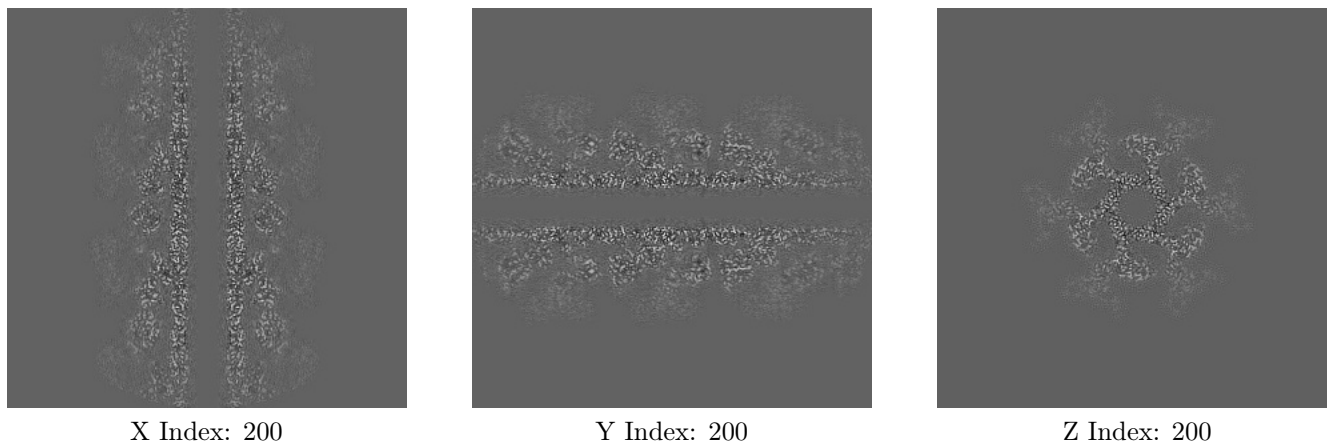
6.1.1 Primary map



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

6.2 Central slices [i](#)

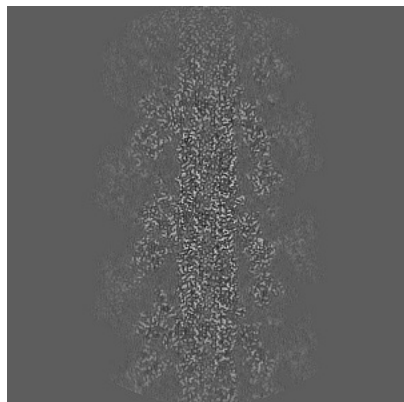
6.2.1 Primary map



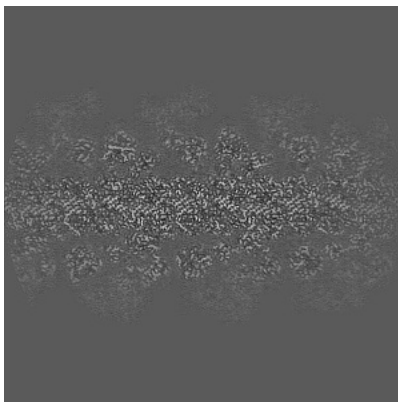
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

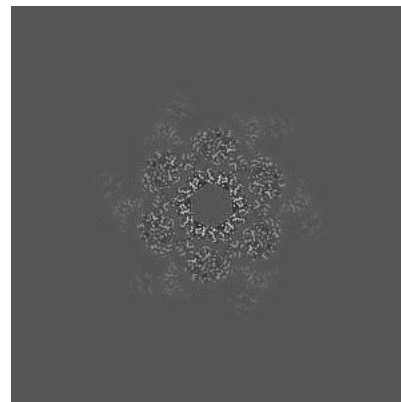
6.3.1 Primary map



X Index: 179



Y Index: 177

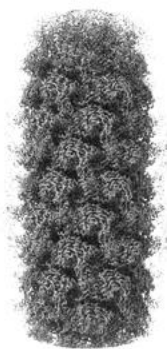


Z Index: 191

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

6.4 Orthogonal surface views [i](#)

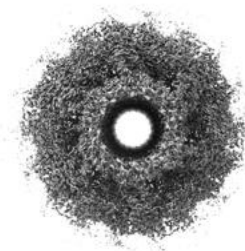
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

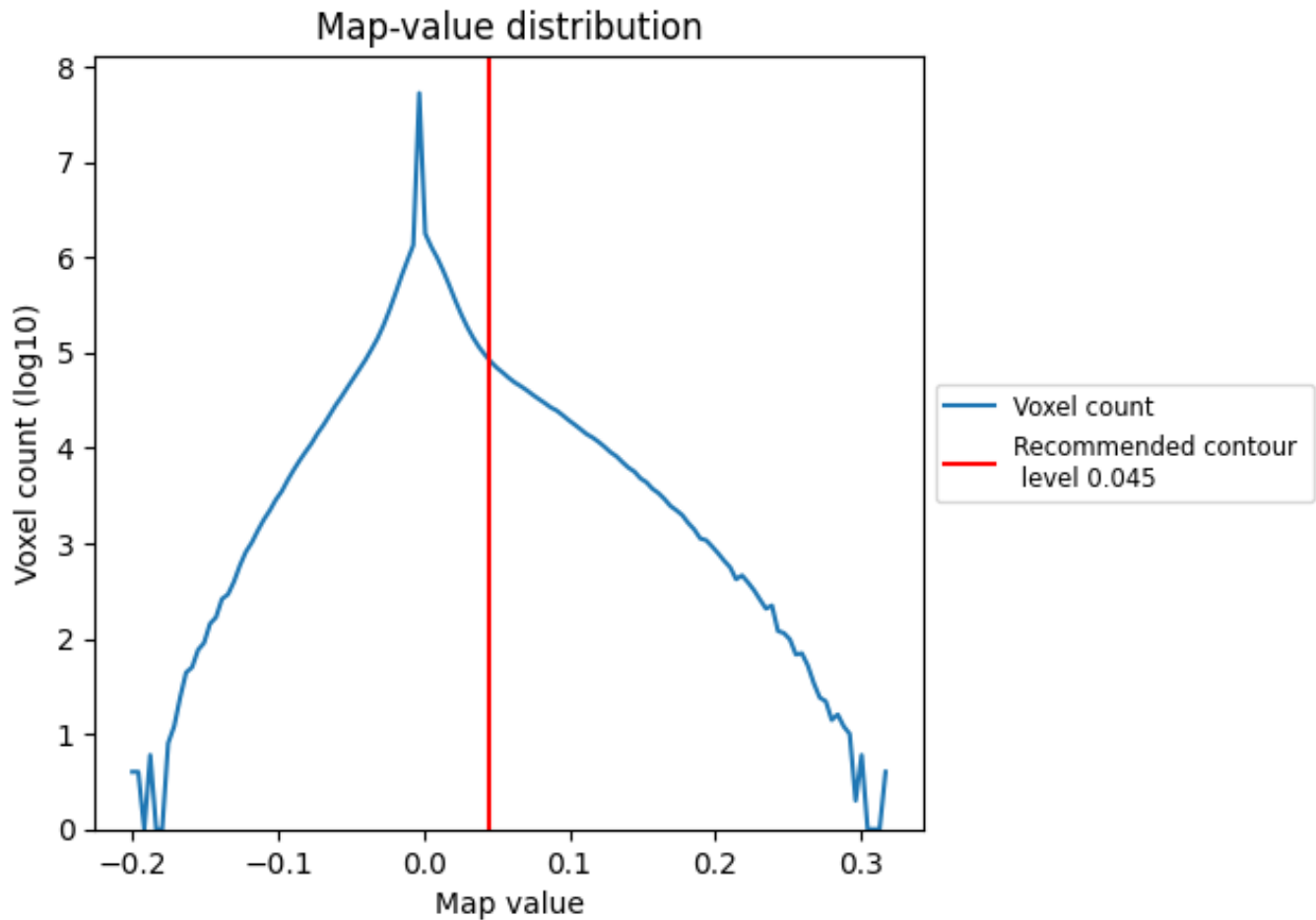
6.5 Mask visualisation

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

7 Map analysis [i](#)

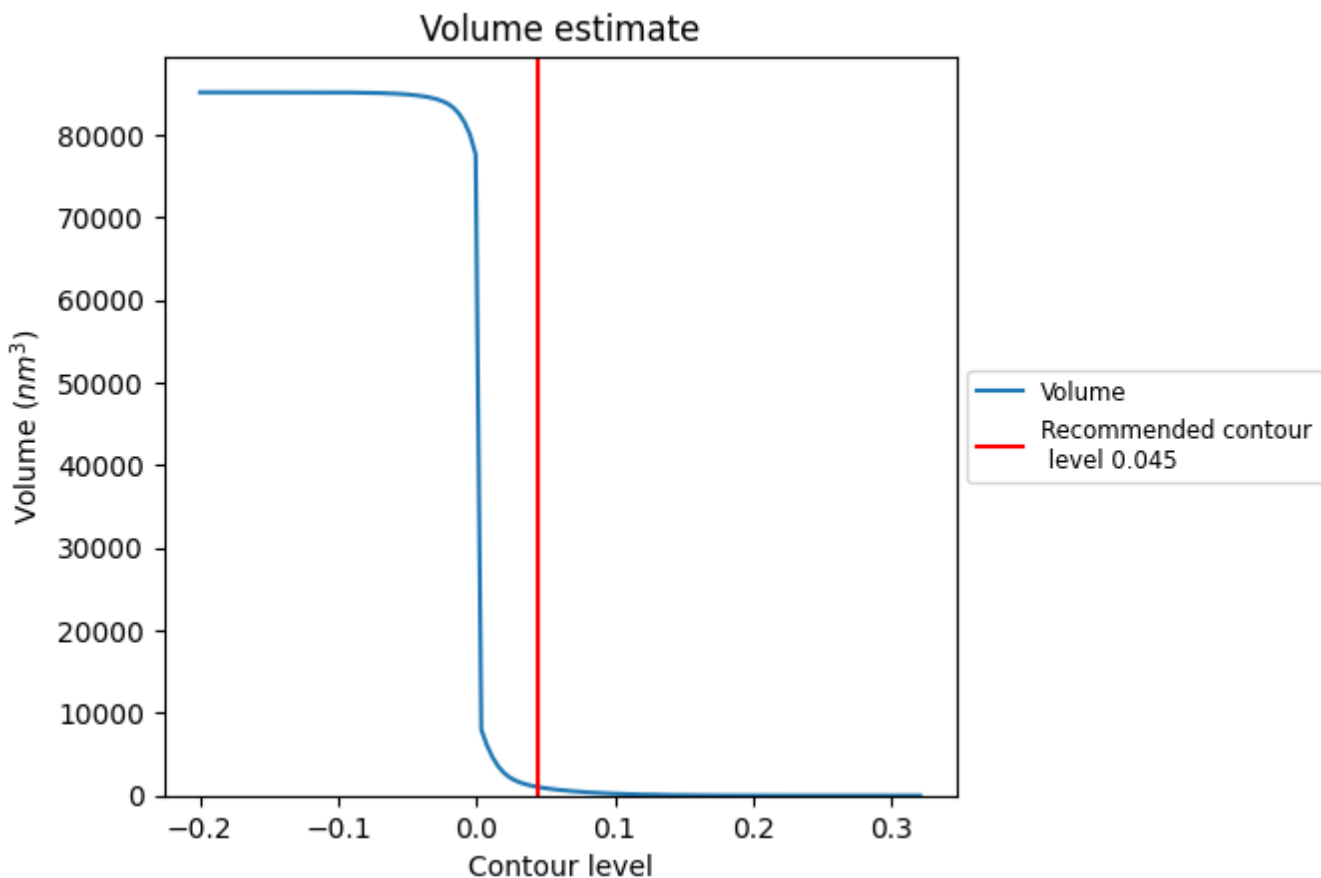
This section contains the results of statistical analysis of the map.

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.

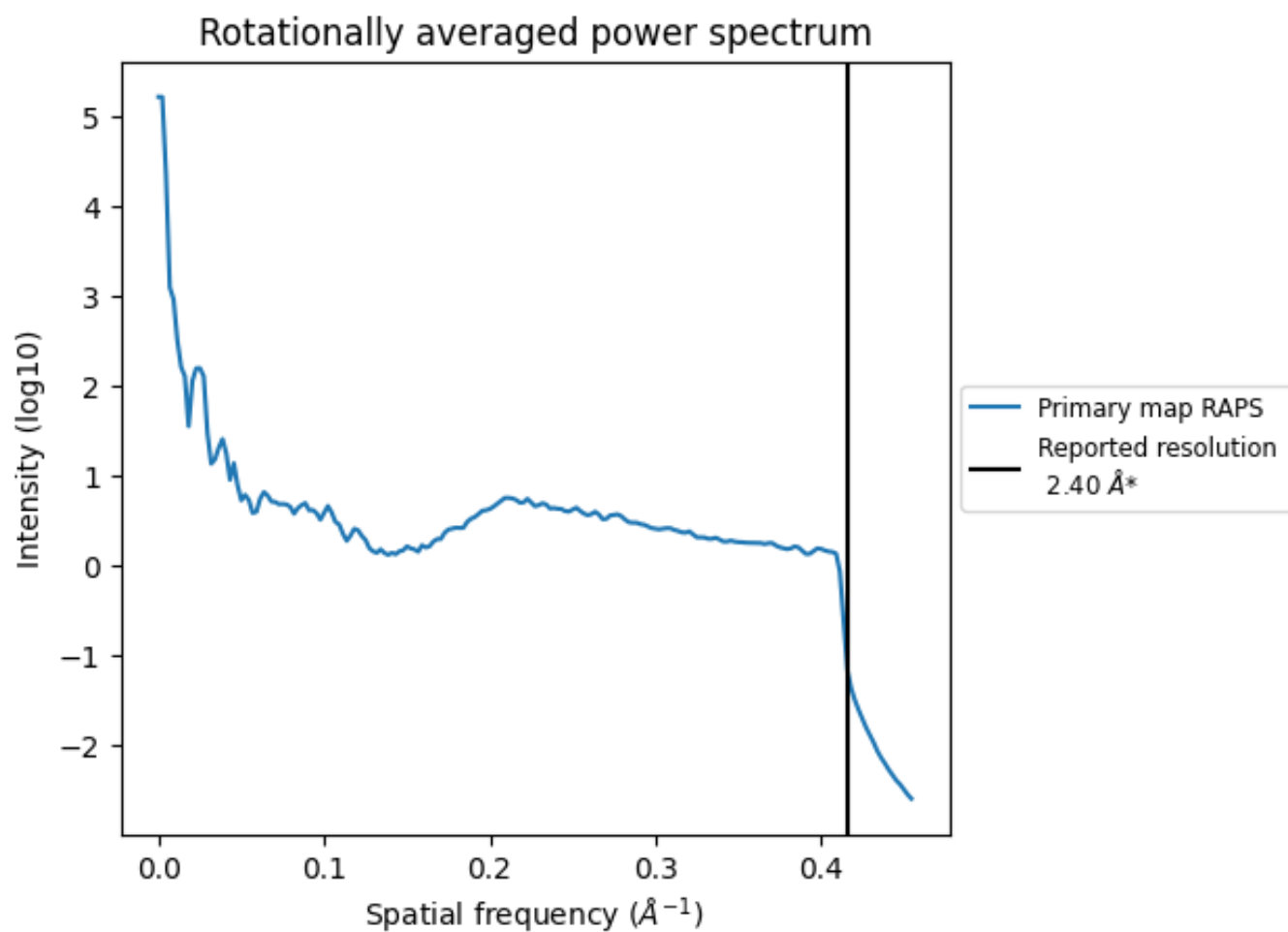
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1019 nm^3 ; this corresponds to an approximate mass of 921 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 0.417 Å⁻¹

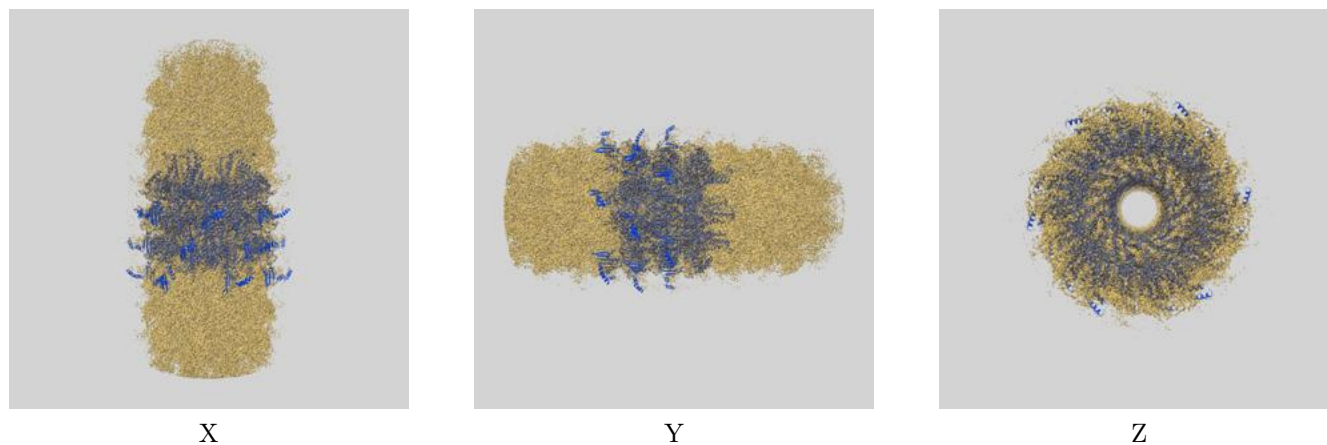
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

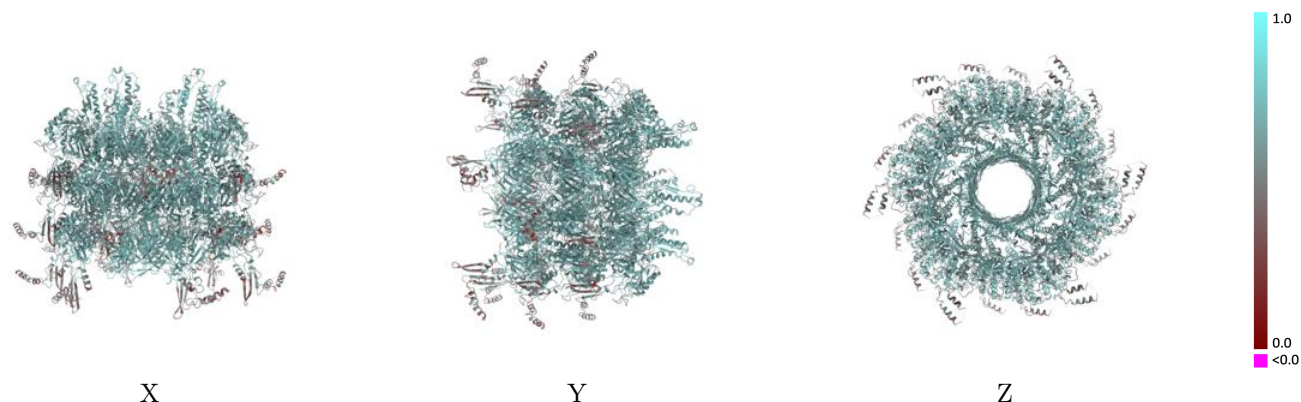
This section contains information regarding the fit between EMDB map EMD-11735 and PDB model 7AE0. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



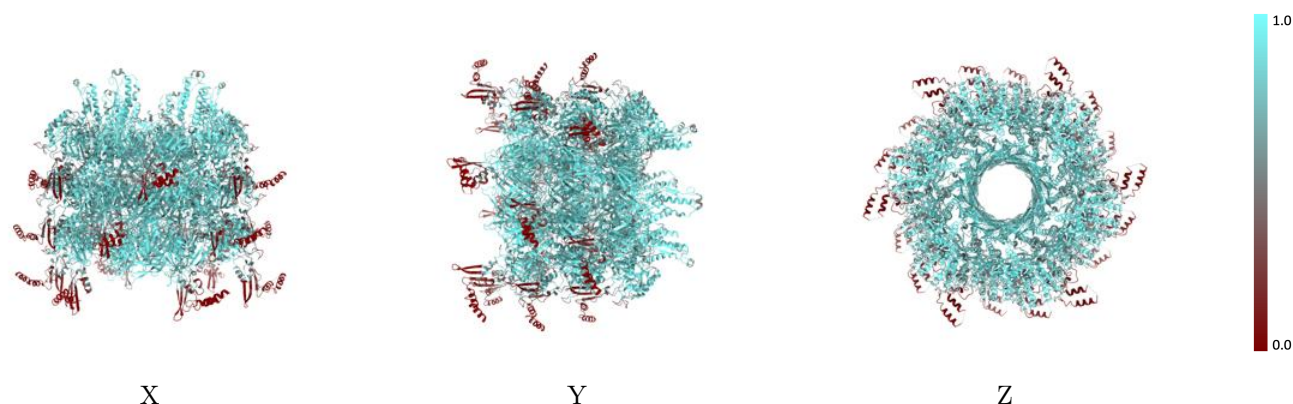
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



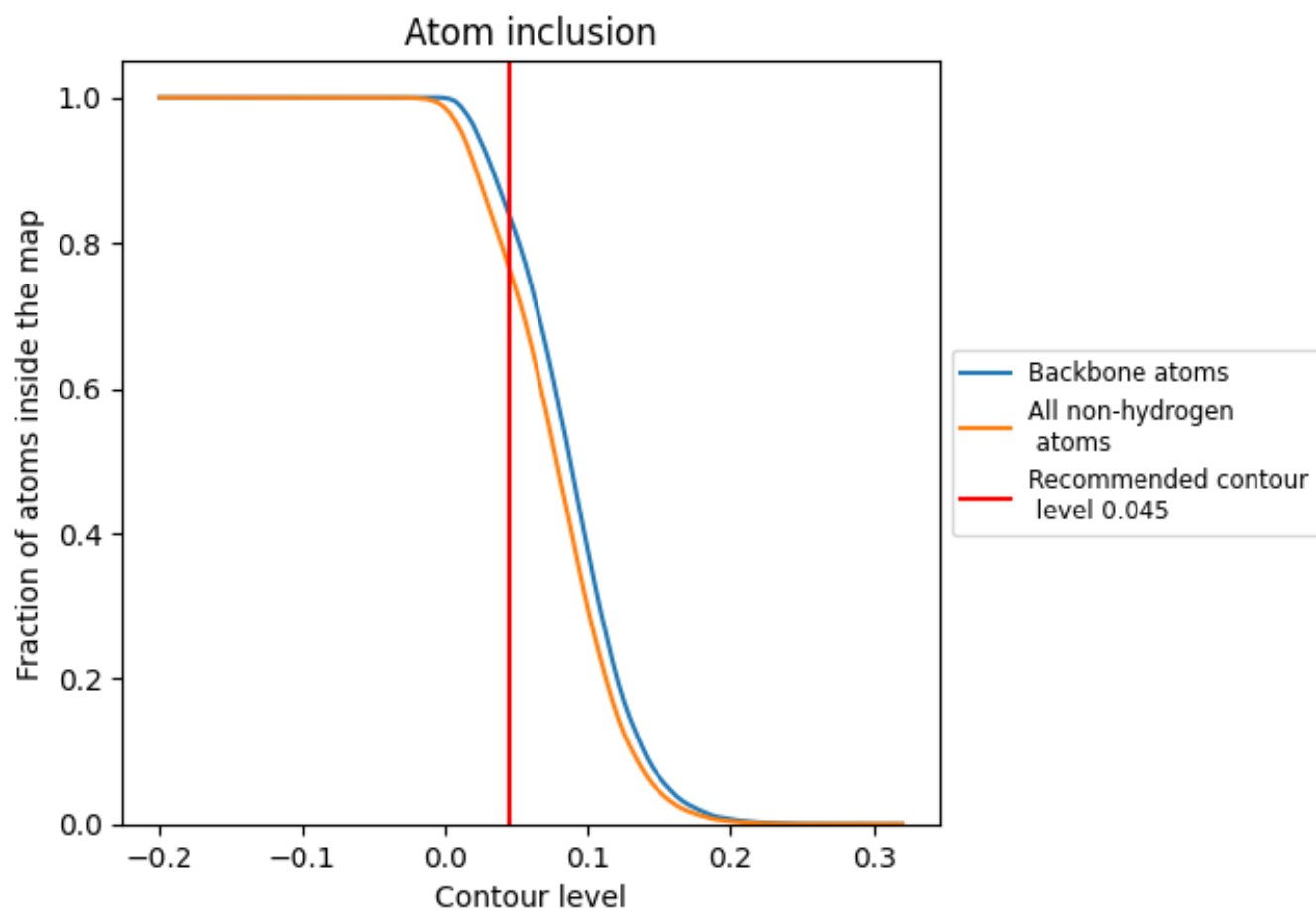
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 77% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7656	 0.6250
3A	 0.7233	 0.6100
3B	 0.7210	 0.6090
3C	 0.7203	 0.6080
3D	 0.7228	 0.6110
3E	 0.7195	 0.6100
3F	 0.7200	 0.6090
3a	 0.9273	 0.6880
3b	 0.9238	 0.6840
3c	 0.9246	 0.6860
3d	 0.9273	 0.6860
3e	 0.9246	 0.6840
3f	 0.9246	 0.6870
4A	 0.7256	 0.6070
4B	 0.7231	 0.6080
4C	 0.7254	 0.6070
4D	 0.7256	 0.6080
4E	 0.7236	 0.6090
4F	 0.7243	 0.6070
4a	 0.9246	 0.6850
4b	 0.9255	 0.6820
4c	 0.9229	 0.6810
4d	 0.9255	 0.6840
4e	 0.9264	 0.6840
4f	 0.9229	 0.6830
5A	 0.7177	 0.6050
5B	 0.7114	 0.6050
5C	 0.7149	 0.6050
5D	 0.7160	 0.6070
5E	 0.7109	 0.6060
5F	 0.7157	 0.6040
5a	 0.9246	 0.6820
5b	 0.9238	 0.6820
5c	 0.9211	 0.6820
5d	 0.9246	 0.6830



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Chain	Atom inclusion	Q-score
5e	 0.9246	 0.6850
5f	 0.9211	 0.6830