



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 12:57 AM UTC

PDB ID : 5LI2 / pdb_00005li2
EMDB ID : EMD-4051
Title : bacteriophage phi812K1-420 tail sheath and tail tube protein in native tail
Authors : Novacek, J.; Siborova, M.; Benesik, M.; Pantucek, R.; Doskar, J.; Plevka, P.
Deposited on : 2016-07-14
Resolution : 6.20 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

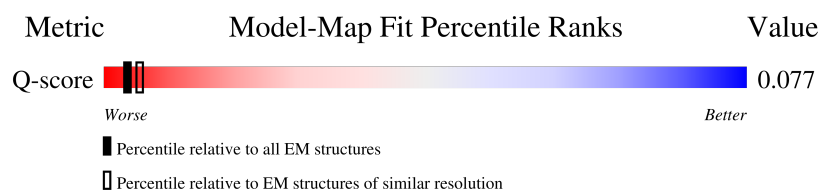
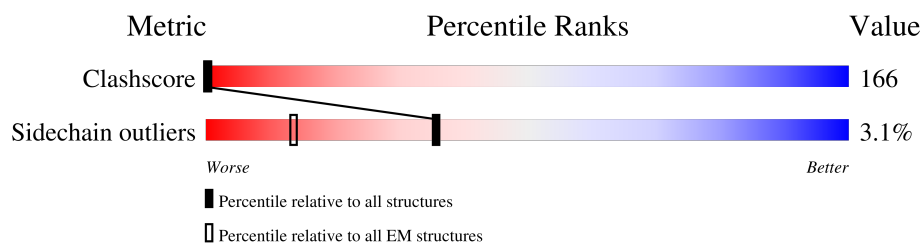
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	537 (5.70 - 6.70)

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	587	22% 15% 40% 17% 27%
1	B	587	24% 15% 40% 18% 27%
1	C	587	26% 15% 40% 18% 27%
1	D	587	27% 15% 40% 18% 27%
1	E	587	28% 15% 40% 17% 27%

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Mol	Chain	Length	Quality of chain
1	F	587	
2	G	155	
2	H	155	
2	I	155	
2	J	155	
2	K	155	
2	L	155	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24732 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 tail sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	427	Total	C	N	O	S	0	0
			3345	2110	567	661	7		
1	B	427	Total	C	N	O	S	0	0
			3345	2110	567	661	7		
1	C	427	Total	C	N	O	S	0	0
			3345	2110	567	661	7		
1	D	427	Total	C	N	O	S	0	0
			3345	2110	567	661	7		
1	E	427	Total	C	N	O	S	0	0
			3345	2110	567	661	7		
1	F	427	Total	C	N	O	S	0	0
			3345	2110	567	661	7		

- Molecule 2 is a protein called Phage-like element PBSX protein XkdM.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	100	Total	C	N	O	S	0	0
			777	489	124	161	3		
2	H	100	Total	C	N	O	S	0	0
			777	489	124	161	3		
2	I	100	Total	C	N	O	S	0	0
			777	489	124	161	3		
2	J	100	Total	C	N	O	S	0	0
			777	489	124	161	3		
2	K	100	Total	C	N	O	S	0	0
			777	489	124	161	3		
2	L	100	Total	C	N	O	S	0	0
			777	489	124	161	3		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	148	LEU	-	expression tag	UNP P54332
G	149	GLU	-	expression tag	UNP P54332

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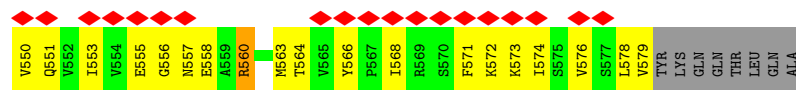
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Chain	Residue	Modelled	Actual	Comment	Reference
G	150	HIS	-	expression tag	UNP P54332
G	151	HIS	-	expression tag	UNP P54332
G	152	HIS	-	expression tag	UNP P54332
G	153	HIS	-	expression tag	UNP P54332
G	154	HIS	-	expression tag	UNP P54332
G	155	HIS	-	expression tag	UNP P54332
H	148	LEU	-	expression tag	UNP P54332
H	149	GLU	-	expression tag	UNP P54332
H	150	HIS	-	expression tag	UNP P54332
H	151	HIS	-	expression tag	UNP P54332
H	152	HIS	-	expression tag	UNP P54332
H	153	HIS	-	expression tag	UNP P54332
H	154	HIS	-	expression tag	UNP P54332
H	155	HIS	-	expression tag	UNP P54332
I	148	LEU	-	expression tag	UNP P54332
I	149	GLU	-	expression tag	UNP P54332
I	150	HIS	-	expression tag	UNP P54332
I	151	HIS	-	expression tag	UNP P54332
I	152	HIS	-	expression tag	UNP P54332
I	153	HIS	-	expression tag	UNP P54332
I	154	HIS	-	expression tag	UNP P54332
I	155	HIS	-	expression tag	UNP P54332
J	148	LEU	-	expression tag	UNP P54332
J	149	GLU	-	expression tag	UNP P54332
J	150	HIS	-	expression tag	UNP P54332
J	151	HIS	-	expression tag	UNP P54332
J	152	HIS	-	expression tag	UNP P54332
J	153	HIS	-	expression tag	UNP P54332
J	154	HIS	-	expression tag	UNP P54332
J	155	HIS	-	expression tag	UNP P54332
K	148	LEU	-	expression tag	UNP P54332
K	149	GLU	-	expression tag	UNP P54332
K	150	HIS	-	expression tag	UNP P54332
K	151	HIS	-	expression tag	UNP P54332
K	152	HIS	-	expression tag	UNP P54332
K	153	HIS	-	expression tag	UNP P54332
K	154	HIS	-	expression tag	UNP P54332
K	155	HIS	-	expression tag	UNP P54332
L	148	LEU	-	expression tag	UNP P54332
L	149	GLU	-	expression tag	UNP P54332
L	150	HIS	-	expression tag	UNP P54332
L	151	HIS	-	expression tag	UNP P54332

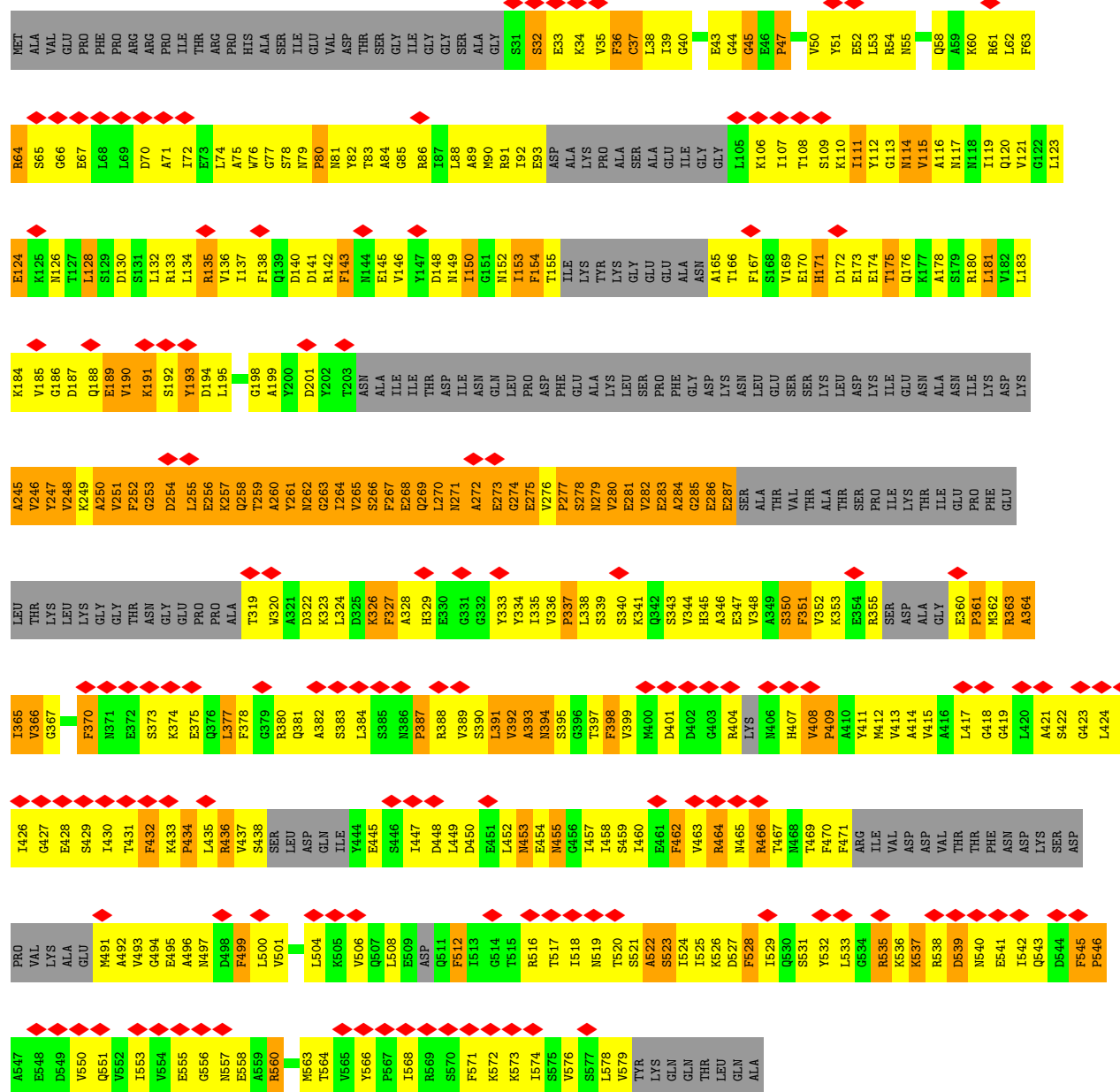
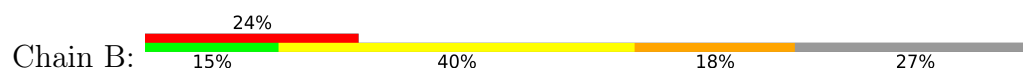
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Chain	Residue	Modelled	Actual	Comment	Reference
L	152	HIS	-	expression tag	UNP P54332
L	153	HIS	-	expression tag	UNP P54332
L	154	HIS	-	expression tag	UNP P54332
L	155	HIS	-	expression tag	UNP P54332



• Molecule 1: tail sheath protein

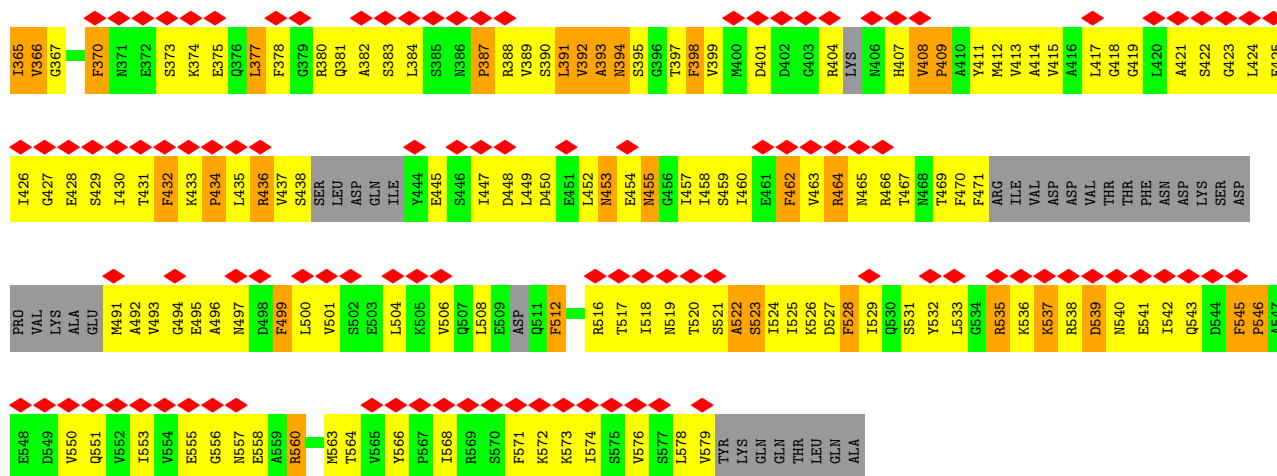


• Molecule 1: tail sheath protein

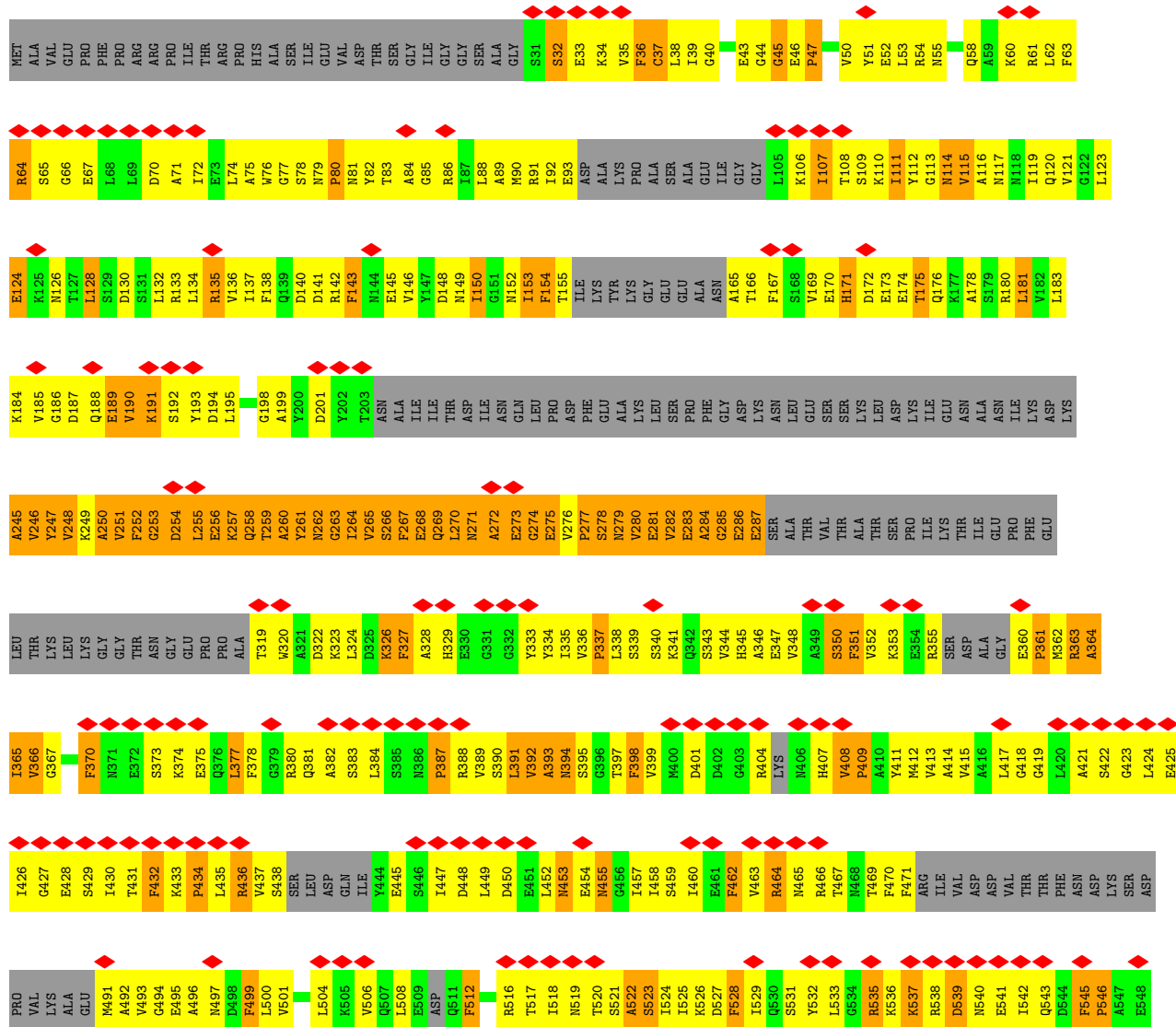


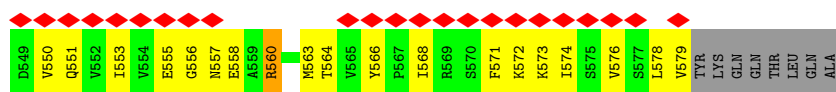
[illegible]



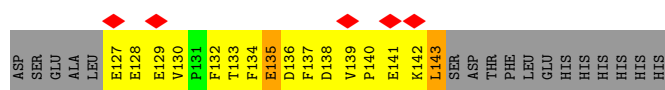
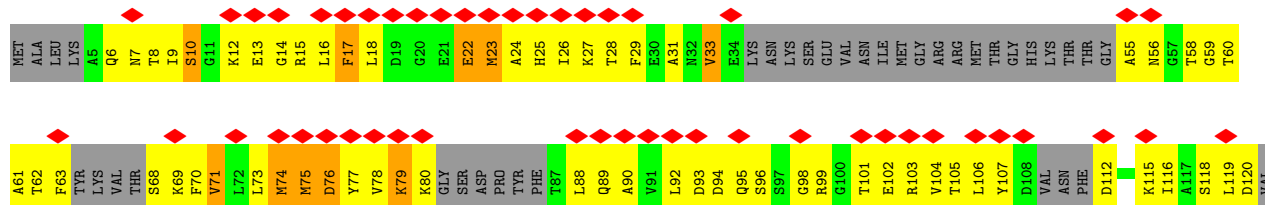


• Molecule 1: tail sheath protein

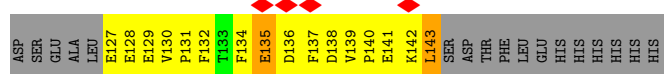
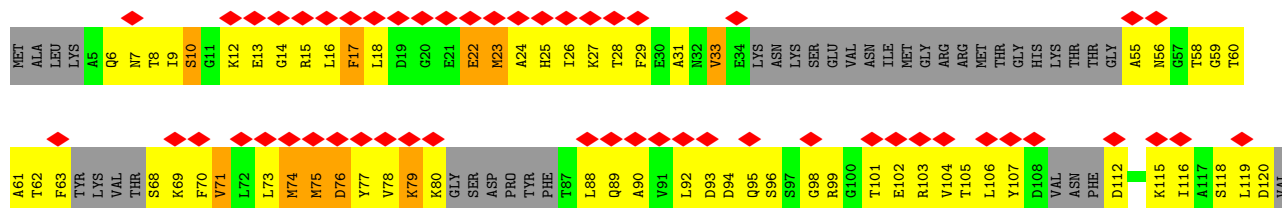




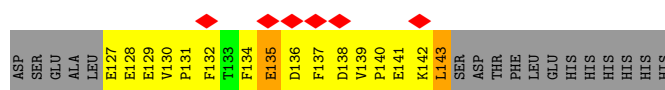
• Molecule 2: Phage-like element PBSX protein XkdM



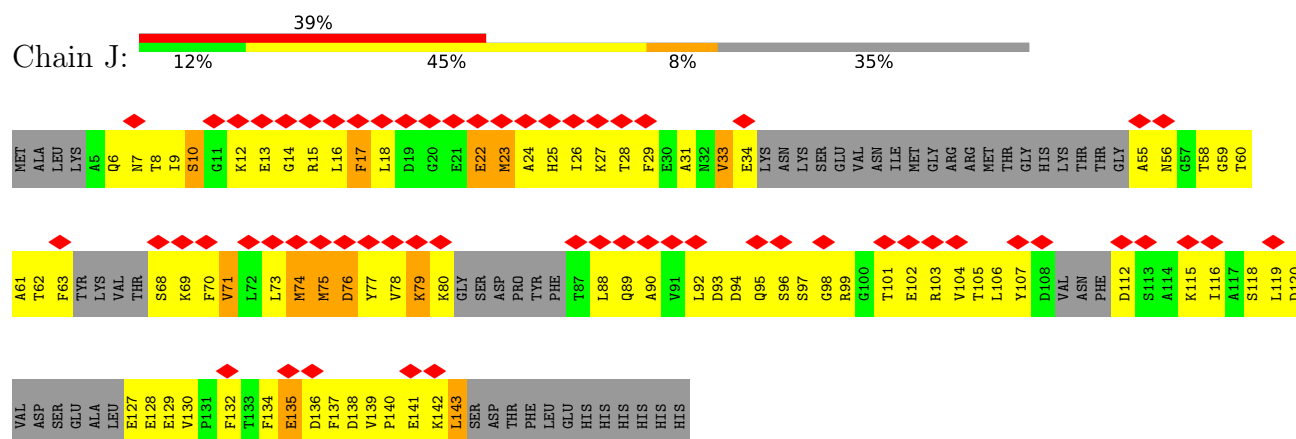
• Molecule 2: Phage-like element PBSX protein XkdM



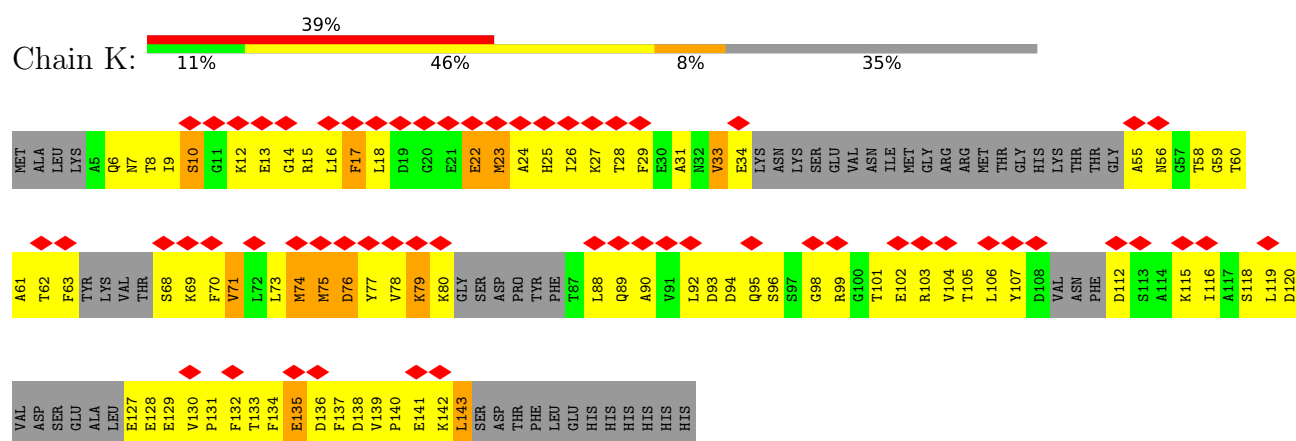
• Molecule 2: Phage-like element PBSX protein XkdM



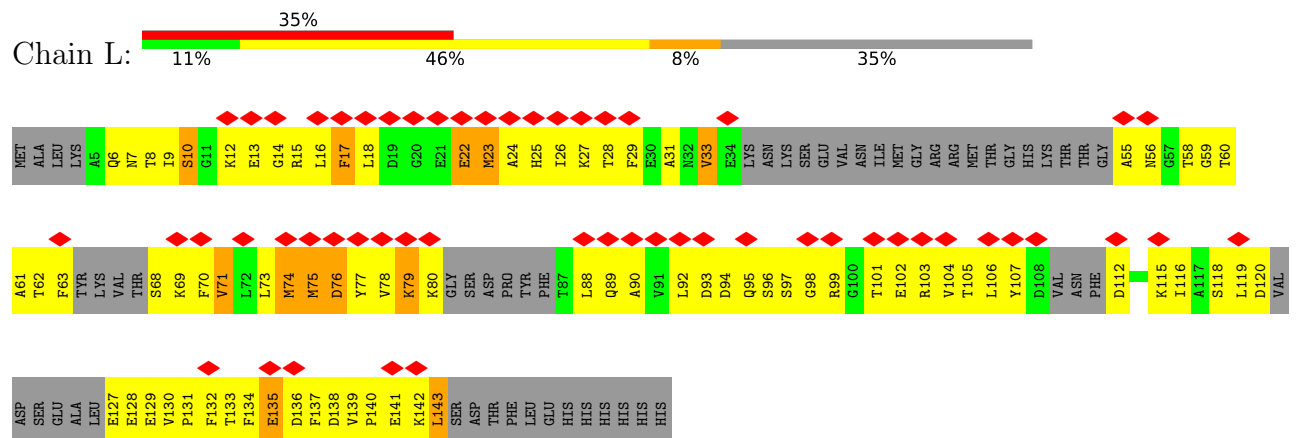
• Molecule 2: Phage-like element PBSX protein XkdM



- Molecule 2: Phage-like element PBSX protein XkdM



- Molecule 2: Phage-like element PBSX protein XkdM



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=21.4°, rise=38.9 Å, axial sym=C6	Depositor
Number of segments used	3628	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 ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	4.589	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.168	Depositor
Map value standard deviation	0.517	Depositor
Recommended contour level	1.6	Depositor
Map size (Å)	282.9, 282.9, 282.9	wwPDB
Map dimensions	205, 205, 205	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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	3.95	247/3387 (7.3%)	2.45	139/4554 (3.1%)
1	B	3.95	247/3387 (7.3%)	2.45	139/4554 (3.1%)
1	C	3.95	247/3387 (7.3%)	2.45	139/4554 (3.1%)
1	D	3.95	246/3387 (7.3%)	2.45	139/4554 (3.1%)
1	E	3.95	246/3387 (7.3%)	2.45	139/4554 (3.1%)
1	F	3.95	247/3387 (7.3%)	2.45	139/4554 (3.1%)
2	G	0.82	5/783 (0.6%)	1.02	2/1046 (0.2%)
2	H	0.82	5/783 (0.6%)	1.02	2/1046 (0.2%)
2	I	0.82	5/783 (0.6%)	1.02	2/1046 (0.2%)
2	J	0.82	5/783 (0.6%)	1.02	2/1046 (0.2%)
2	K	0.82	5/783 (0.6%)	1.02	2/1046 (0.2%)
2	L	0.82	5/783 (0.6%)	1.02	2/1046 (0.2%)
All	All	3.58	1510/25020 (6.0%)	2.25	846/33600 (2.5%)

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	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
All	All	0	18

The worst 5 of 1510 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	546	PRO	N-CD	55.53	2.25	1.47
1	F	546	PRO	N-CD	55.52	2.25	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	546	PRO	N-CD	55.49	2.25	1.47
1	A	546	PRO	N-CD	55.48	2.25	1.47
1	D	546	PRO	N-CD	55.48	2.25	1.47

The worst 5 of 846 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	ARG	N-CA-C	22.13	157.94	110.80
1	C	64	ARG	N-CA-C	22.12	157.92	110.80
1	F	64	ARG	N-CA-C	22.12	157.92	110.80
1	B	64	ARG	N-CA-C	22.10	157.87	110.80
1	E	64	ARG	N-CA-C	22.10	157.87	110.80

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	392	VAL	Peptide
1	A	393	ALA	Peptide
1	A	394	ASN	Peptide
1	B	392	VAL	Peptide
1	B	393	ALA	Peptide

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	3345	0	3267	1044	0
1	B	3345	0	3267	1050	0
1	C	3345	0	3267	1056	0
1	D	3345	0	3267	1069	0
1	E	3345	0	3267	1056	0
1	F	3345	0	3267	1053	0
2	G	777	0	731	458	0
2	H	777	0	731	460	0
2	I	777	0	731	473	0
2	J	777	0	731	480	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	777	0	731	480	0
2	L	777	0	731	471	0
All	All	24732	0	23988	8098	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 166.

The worst 5 of 8098 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:B:320:TRP:CD1	1:B:344:VAL:HG23	1.31	1.65
1:A:252:PHE:CE2	1:A:257:LYS:HG2	1.11	1.63
1:B:252:PHE:CE2	1:B:257:LYS:HG2	1.11	1.63
1:C:320:TRP:CD1	1:C:344:VAL:HG23	1.31	1.63
1:A:320:TRP:CD1	1:A:344:VAL:HG23	1.31	1.63

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	159/495 (32%)	155 (98%)	4 (2%)	42	62
1	B	363/495 (73%)	358 (99%)	5 (1%)	59	72
1	C	363/495 (73%)	358 (99%)	5 (1%)	59	72
1	D	363/495 (73%)	358 (99%)	5 (1%)	59	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	363/495 (73%)	358 (99%)	5 (1%)	59	72
1	F	363/495 (73%)	358 (99%)	5 (1%)	59	72
2	G	84/134 (63%)	76 (90%)	8 (10%)	8	25
2	H	84/134 (63%)	76 (90%)	8 (10%)	8	25
2	I	84/134 (63%)	76 (90%)	8 (10%)	8	25
2	J	84/134 (63%)	76 (90%)	8 (10%)	8	25
2	K	84/134 (63%)	76 (90%)	8 (10%)	8	25
2	L	84/134 (63%)	76 (90%)	8 (10%)	8	25
All	All	2478/3774 (66%)	2401 (97%)	77 (3%)	36	56

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	71	VAL
2	L	33	VAL
2	J	135	GLU
2	K	71	VAL
2	L	135	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	511	GLN
2	L	7	ASN
1	F	557	ASN
2	I	7	ASN
1	D	55	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 [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	9
1	B	9
1	C	9
1	D	9
1	E	9
1	F	9

The worst 5 of 54 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	427:GLY	C	428:GLU	N	15.07
1	B	427:GLY	C	428:GLU	N	15.07
1	C	427:GLY	C	428:GLU	N	15.07
1	D	427:GLY	C	428:GLU	N	15.07
1	E	427:GLY	C	428:GLU	N	15.07

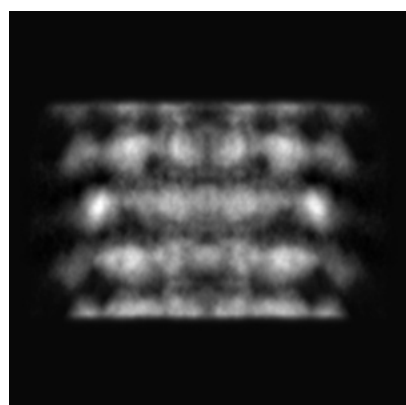
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4051. These allow visual inspection of the internal detail of the map and identification of artifacts.

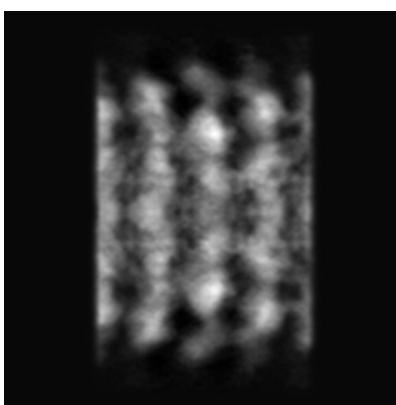
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

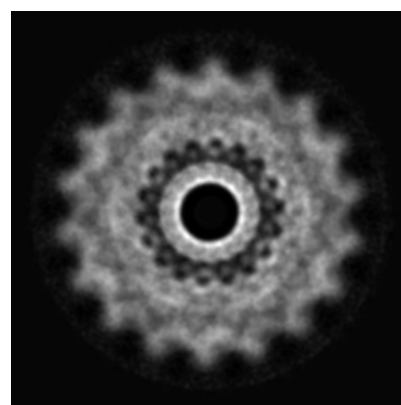
6.1.1 Primary map



X



Y

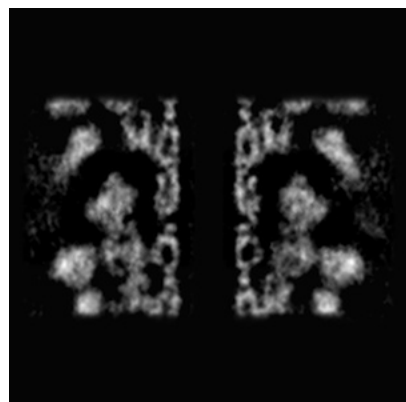


Z

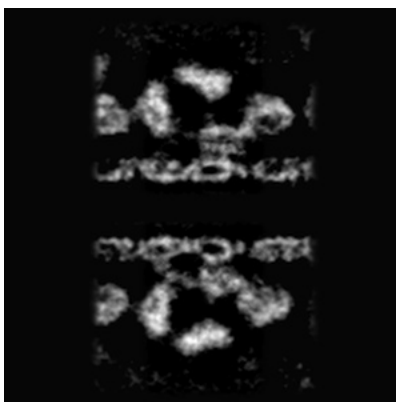
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

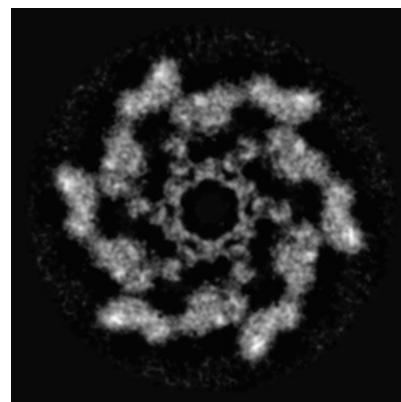
6.2.1 Primary map



X Index: 102



Y Index: 102

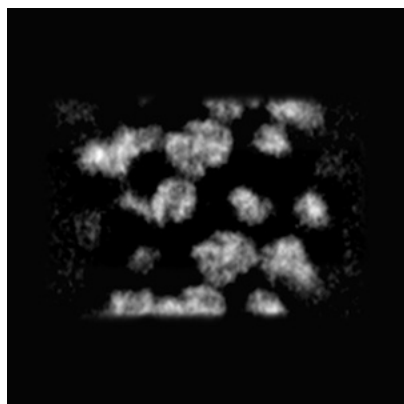


Z Index: 102

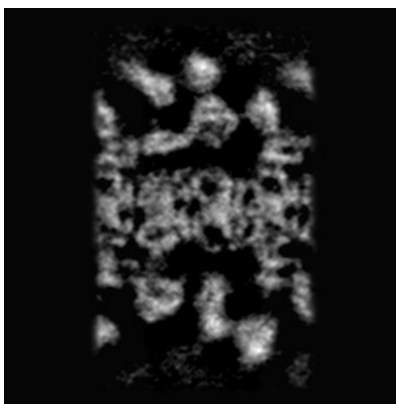
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

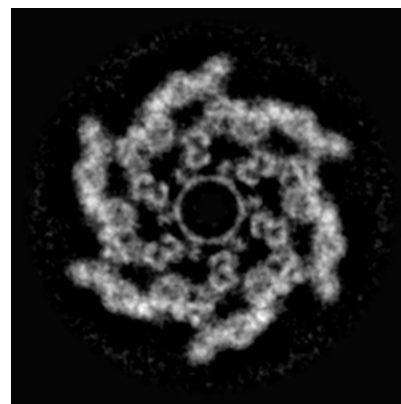
6.3.1 Primary map



X Index: 151



Y Index: 85

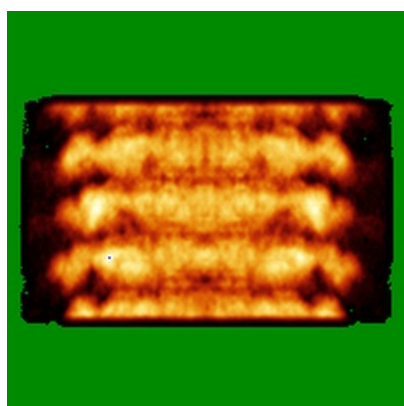


Z Index: 78

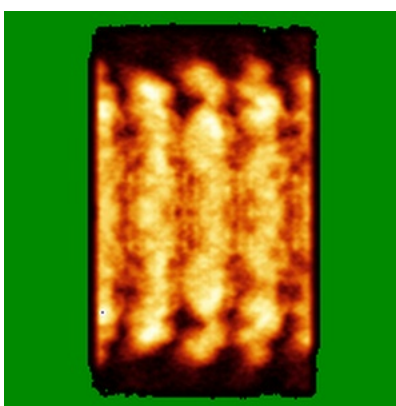
The images above show the largest variance slices of the map in three orthogonal directions.

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

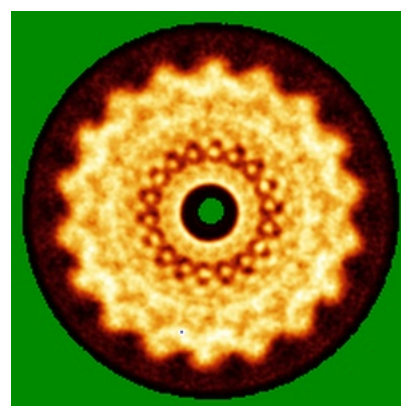
6.4.1 Primary map



X



Y

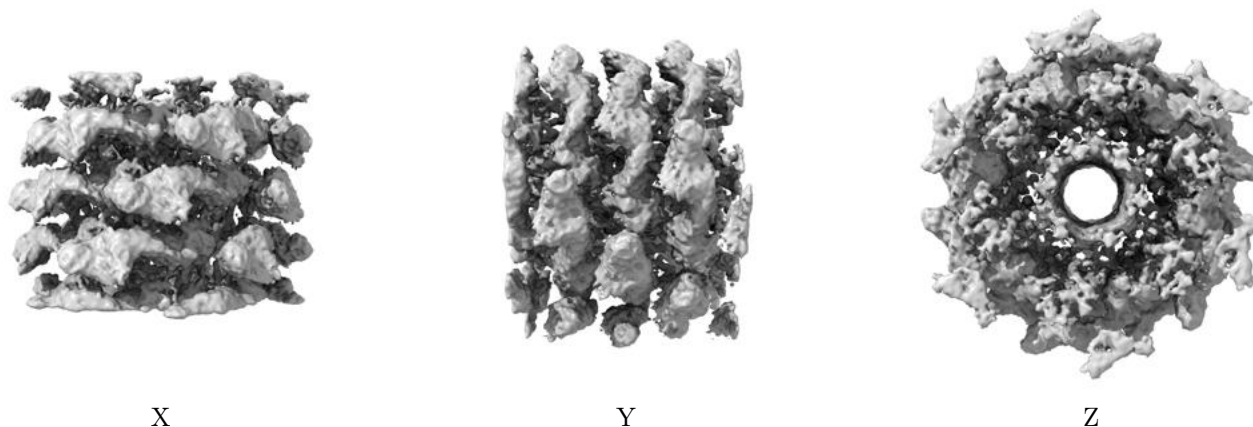


Z

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

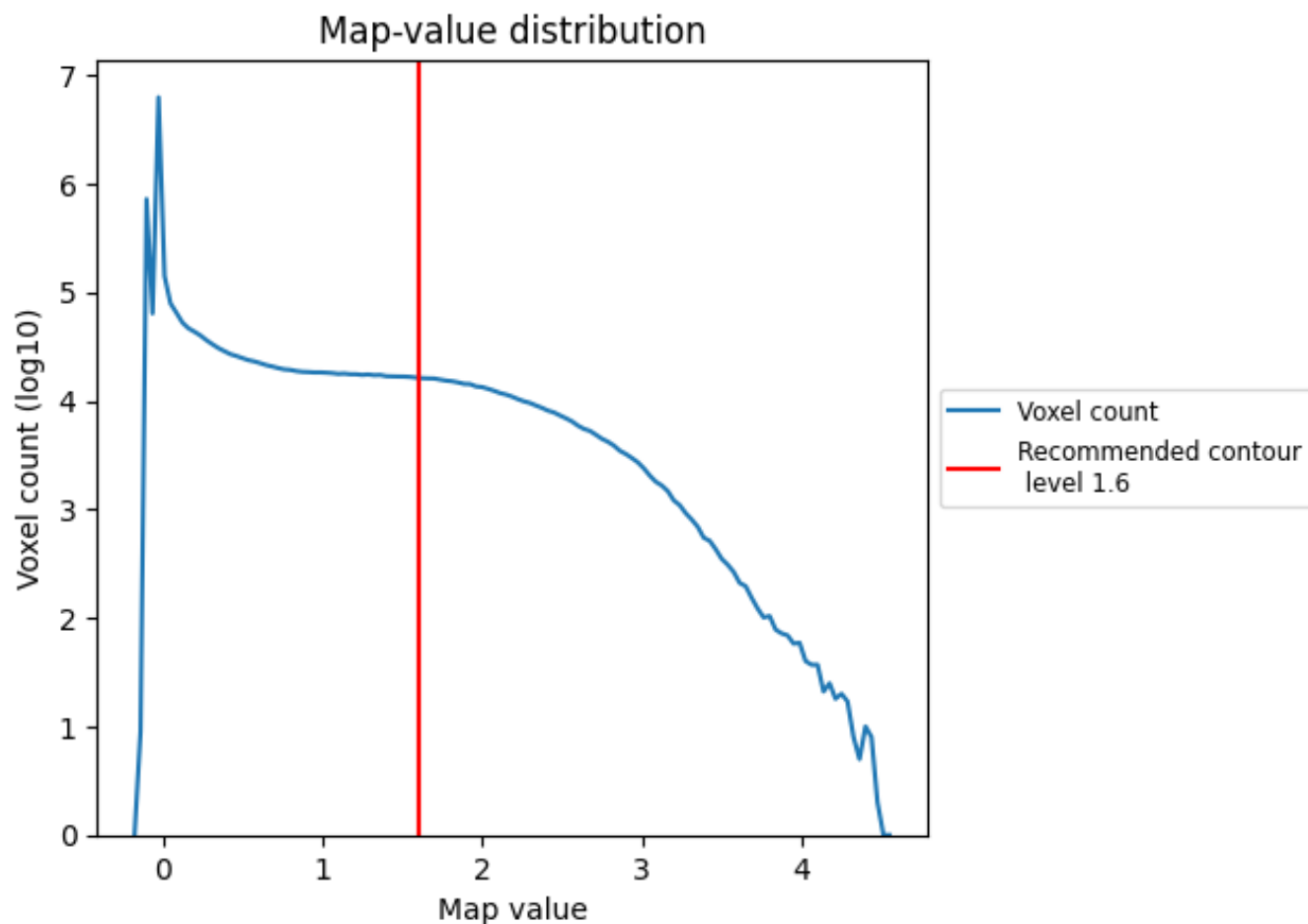
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

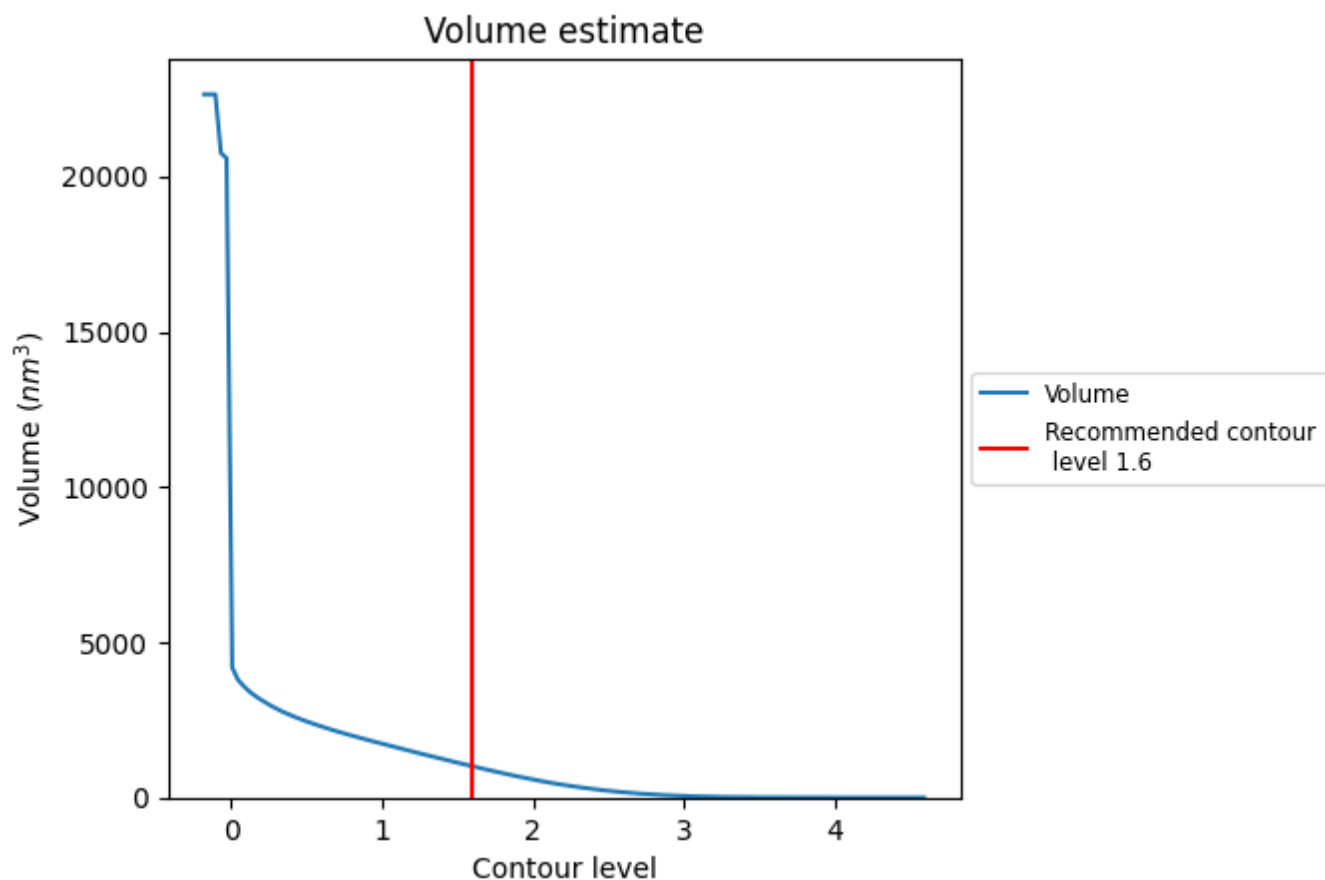
This section contains the results of statistical analysis of the map.

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.

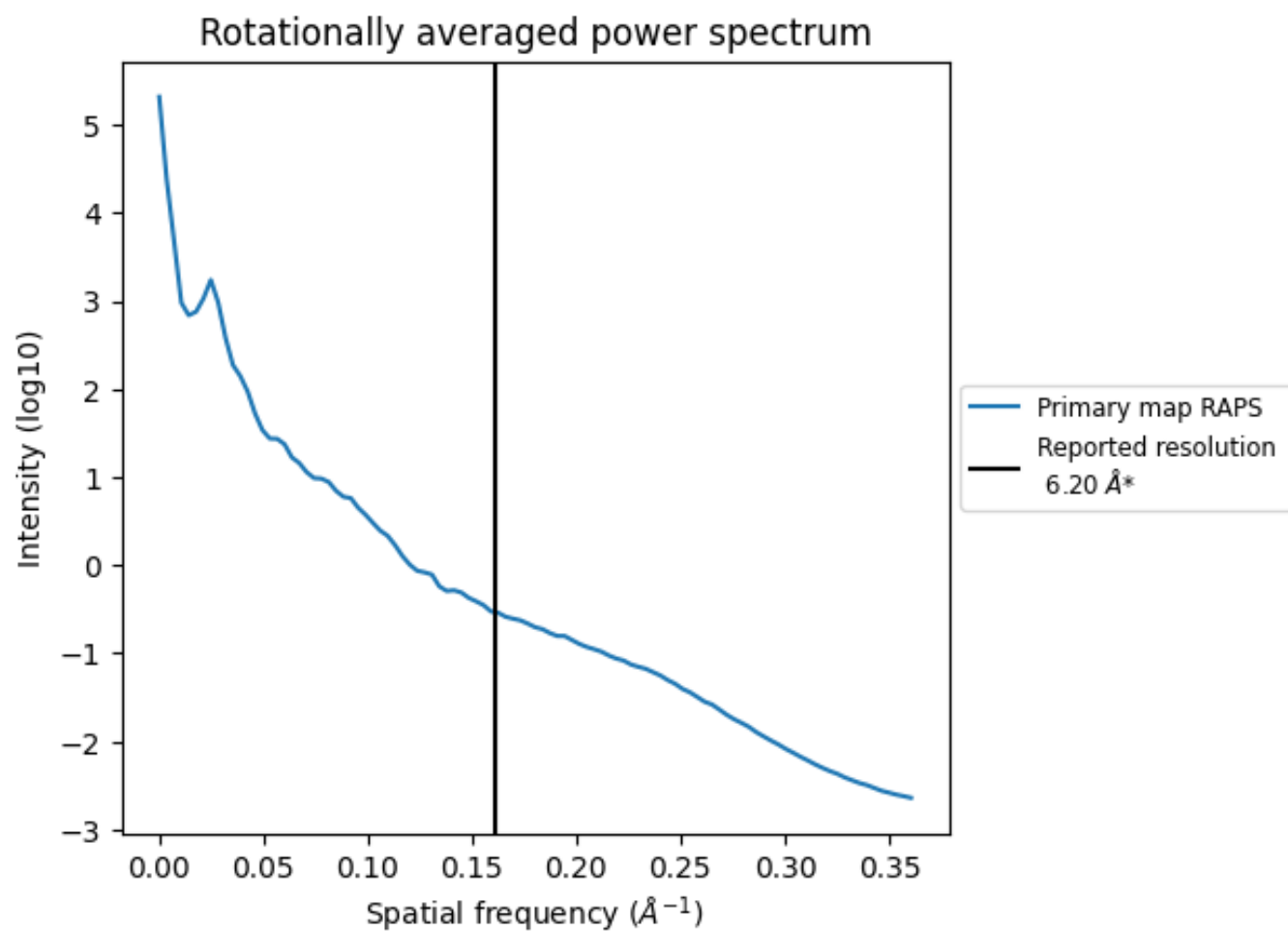
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1007 nm³; this corresponds to an approximate mass of 909 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 0.161 Å⁻¹

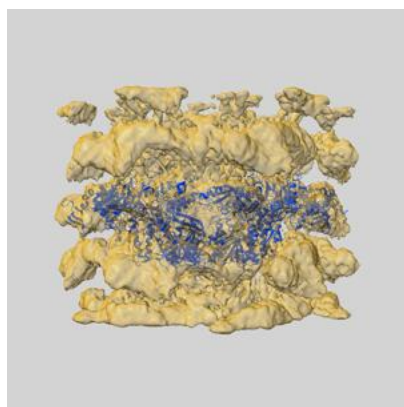
8 Fourier-Shell correlation ⓘ

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

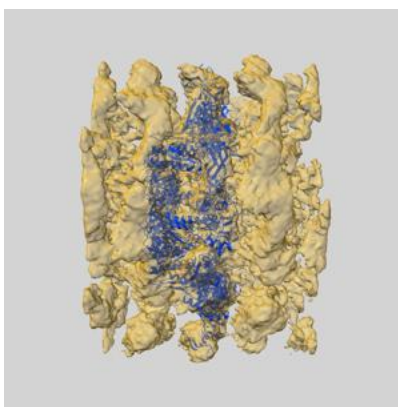
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4051 and PDB model 5LI2. Per-residue inclusion information can be found in section [3](#) on page [7](#).

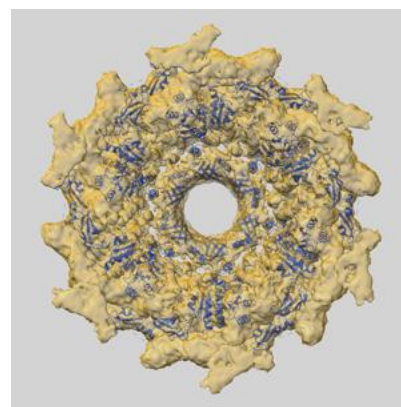
9.1 Map-model overlay [i](#)



X



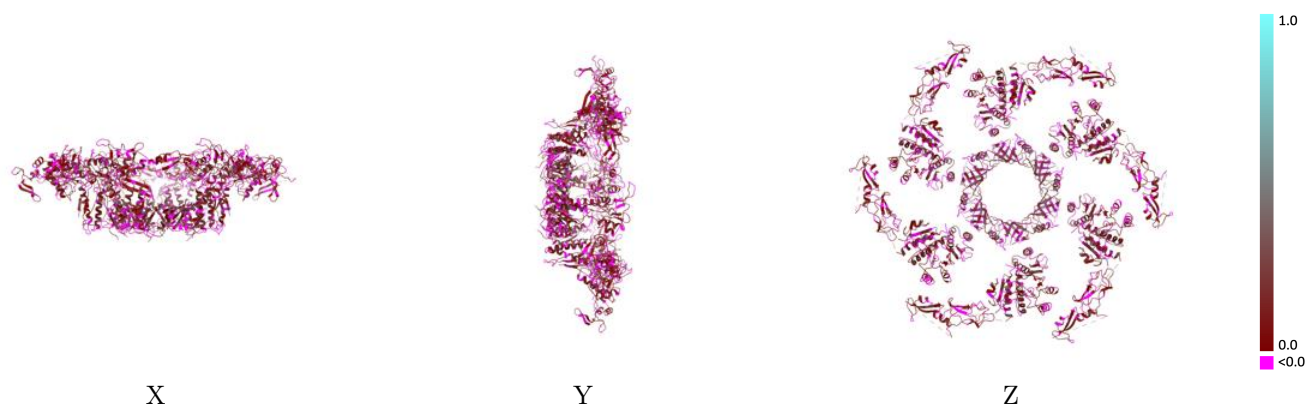
Y



Z

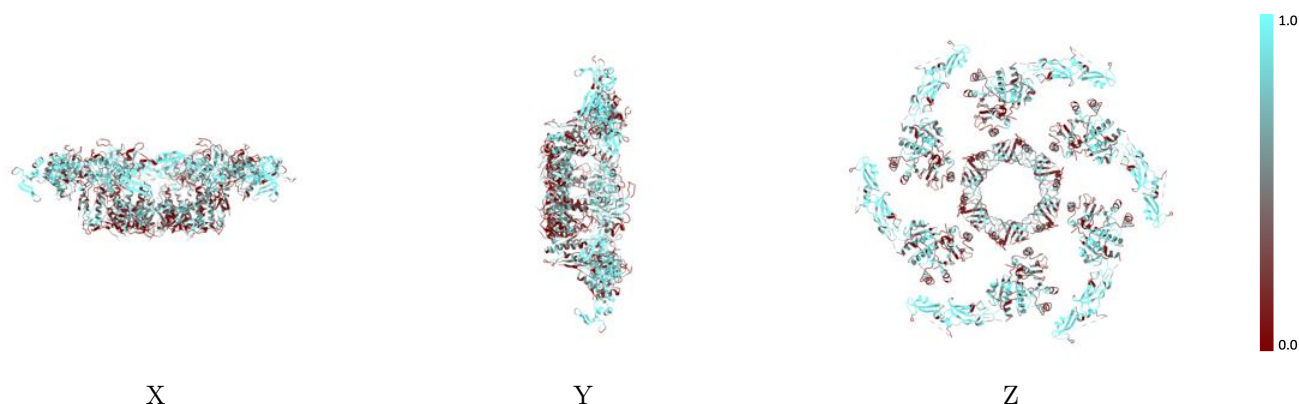
The images above show the 3D surface view of the map at the recommended contour level 1.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



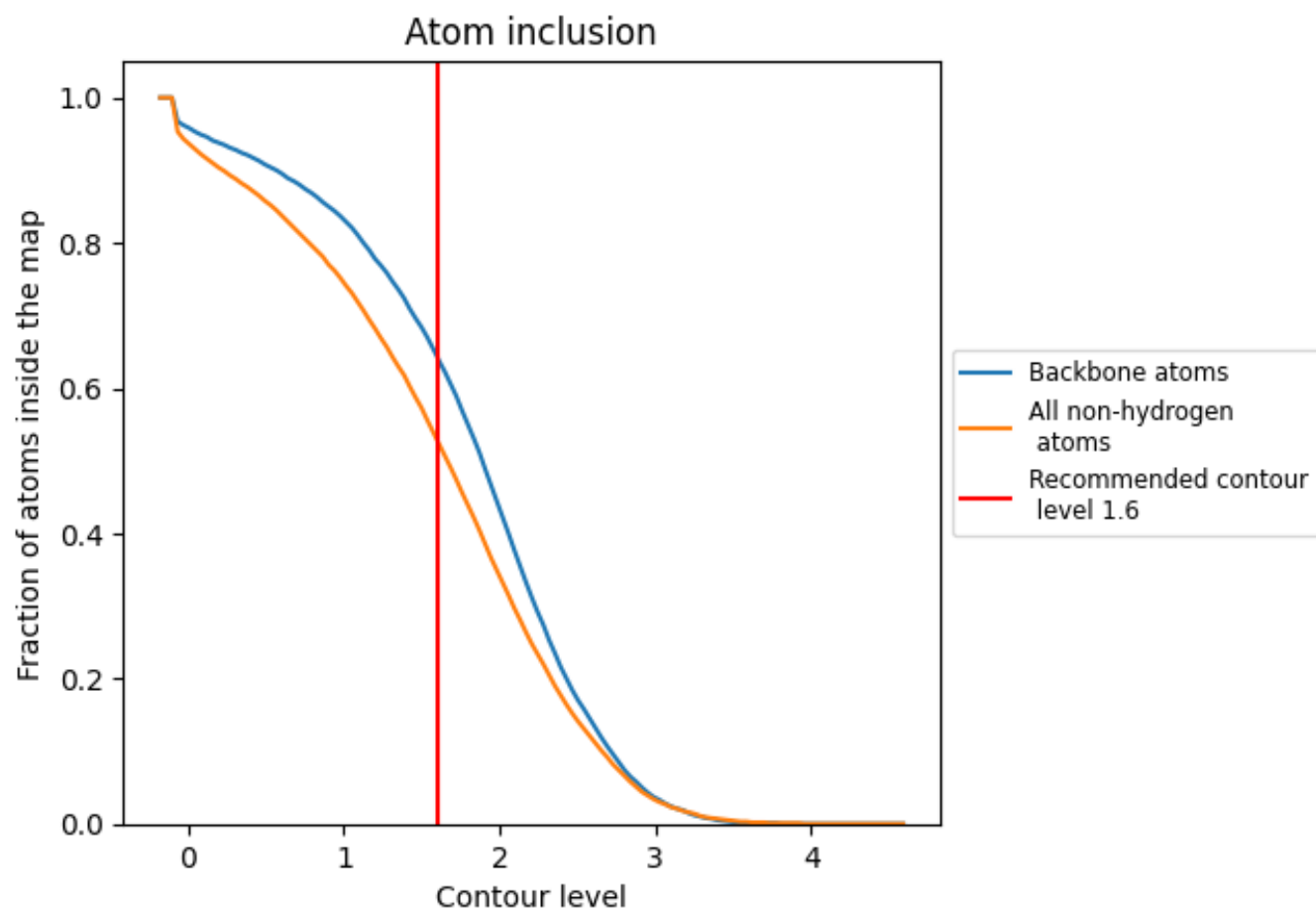
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 53% 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 (1.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5280	0.0770
A	0.6010	0.0850
B	0.5910	0.0810
C	0.5670	0.0750
D	0.5530	0.0730
E	0.5540	0.0720
F	0.5760	0.0790
G	0.3720	0.0880
H	0.3410	0.0830
I	0.3120	0.0670
J	0.3090	0.0630
K	0.3210	0.0780
L	0.3510	0.0770

1.0

0.0

<0.0