



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:49 PM UTC

PDB ID : 7Y1C / pdb_00007y1c
EMDB ID : EMD-33560
Title : CryoEM structure of Klebsiella phage Kp9 tail complex applied with C6 symmetry
Authors : Huang, L.; Xiang, Y.
Deposited on : 2022-06-08
Resolution : 3.13 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

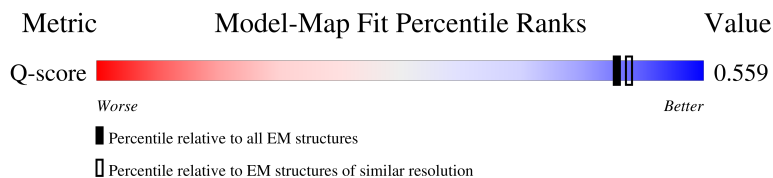
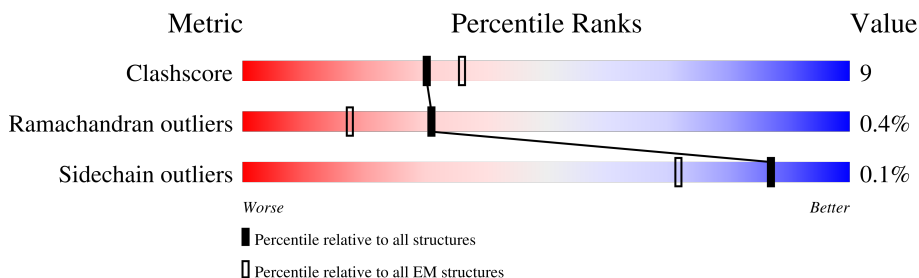
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 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	14478 (2.63 - 3.63)

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	535	
1	L	535	
2	W	192	
2	X	192	

Continued on next page...

Mol	Chain	Length	Quality of chain
3	Y	791	 74%25%
4	e	777	 16%80%
4	f	777	 16%80%
4	g	777	 15%5%80%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20697 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 phage connector protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	506	Total	C	N	O	S	0	0
			3887	2442	646	778	21		
1	L	506	Total	C	N	O	S	0	0
			3887	2442	646	778	21		

- Molecule 2 is a protein called phage tail tubular protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	192	Total	C	N	O	S	0	0
			1498	933	253	302	10		
2	X	192	Total	C	N	O	S	0	0
			1498	933	253	302	10		

- Molecule 3 is a protein called phage tail tubular protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Y	790	Total	C	N	O	S	0	0
			6281	3972	1077	1215	17		

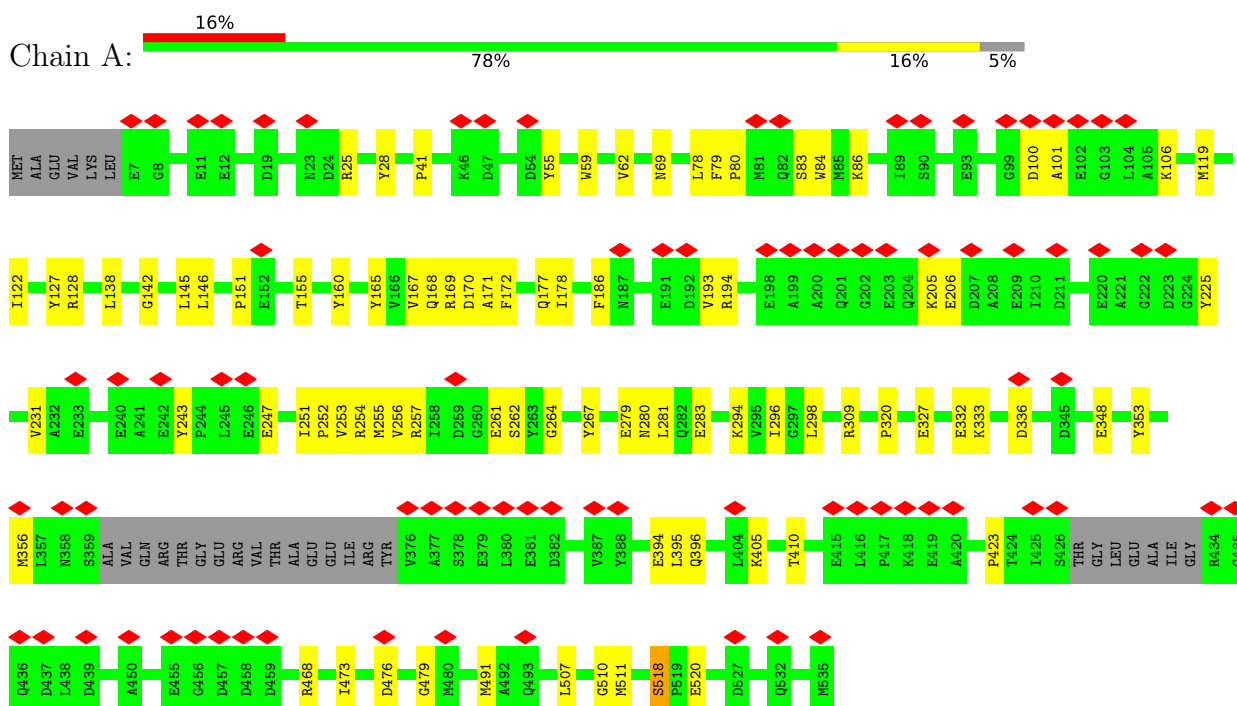
- Molecule 4 is a protein called phage type I tail fiber.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	153	Total	C	N	O	S	0	0
			1208	748	219	240	1		
4	f	156	Total	C	N	O	S	0	0
			1229	760	222	245	2		
4	g	155	Total	C	N	O	S	0	0
			1209	749	220	239	1		

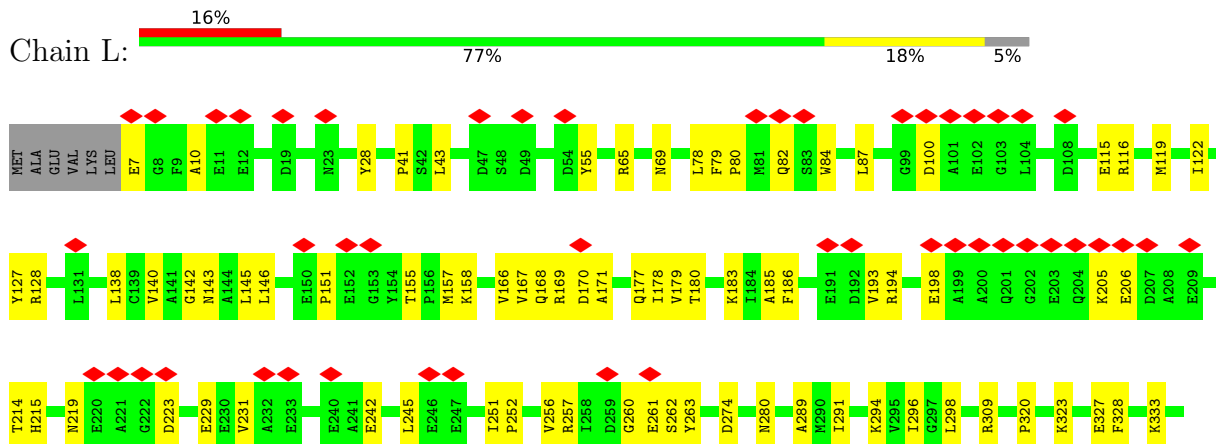
3 Residue-property plots

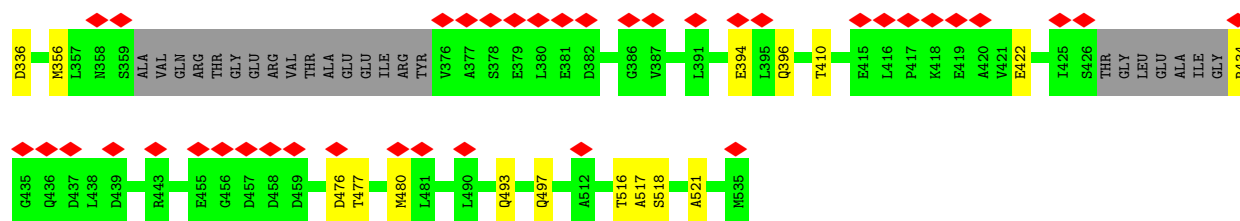
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: phage connector protein

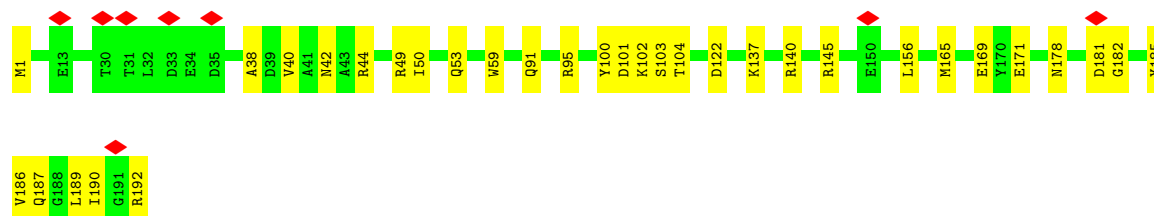
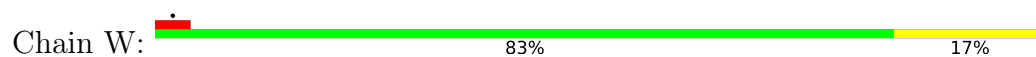


- Molecule 1: phage connector protein

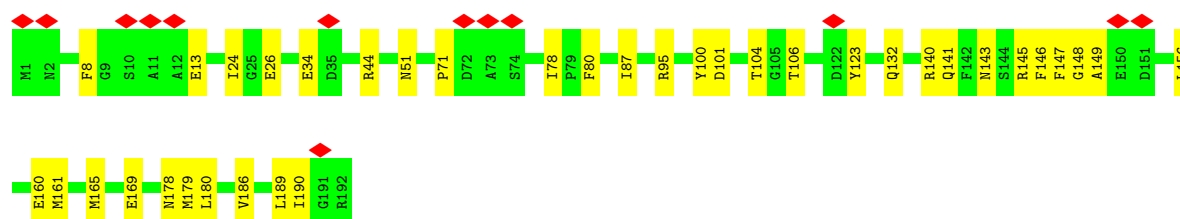
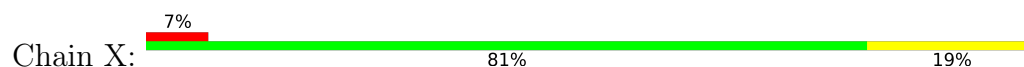




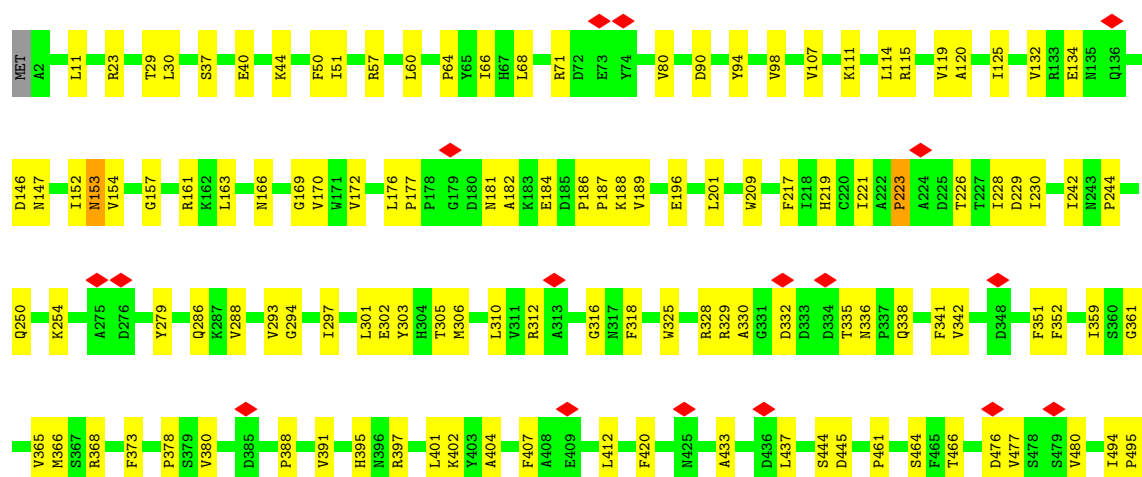
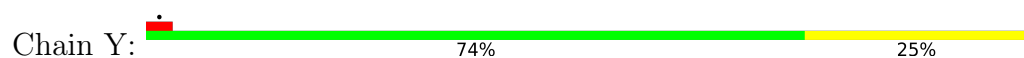
- Molecule 2: phage tail tubular protein A



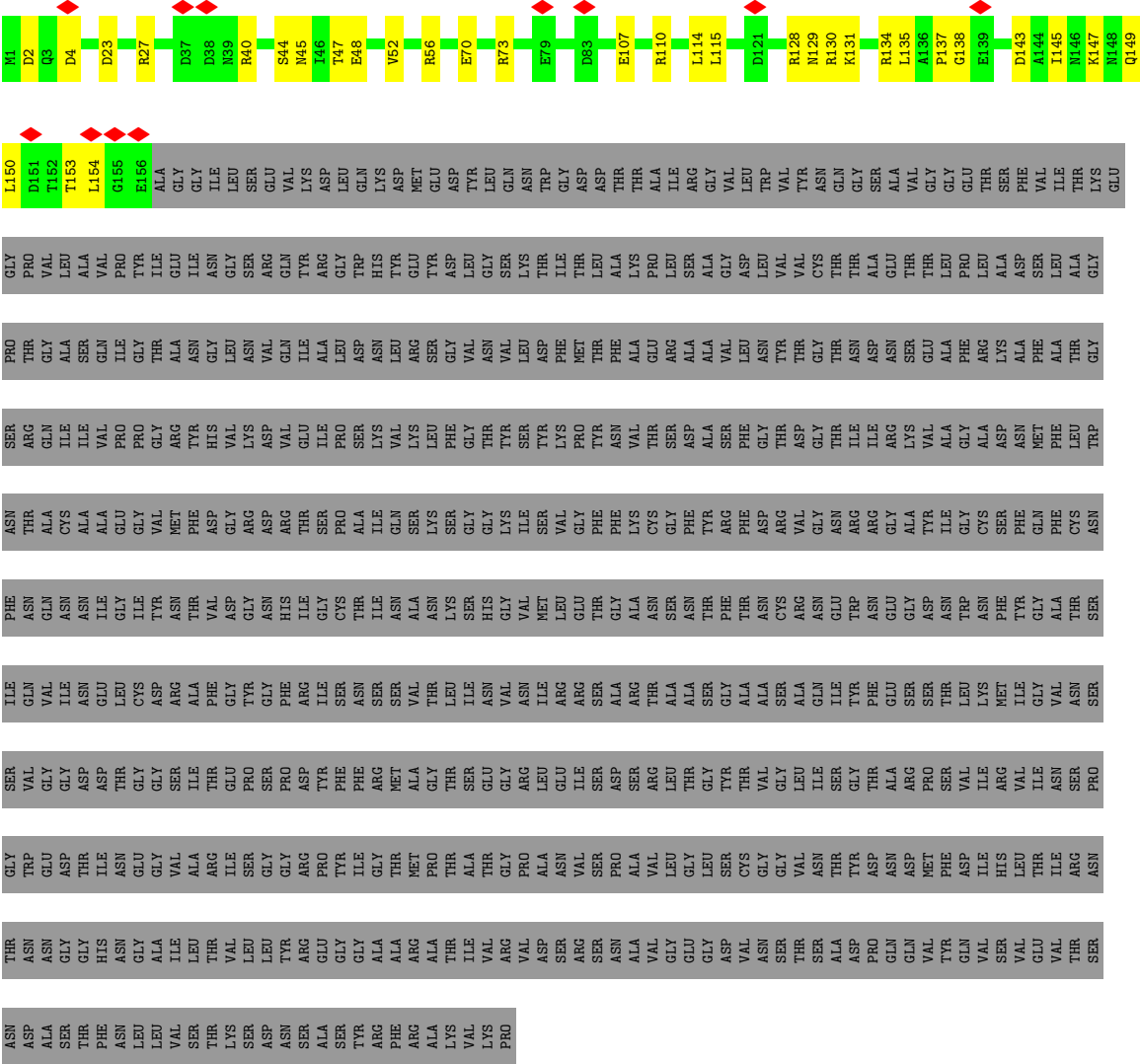
- Molecule 2: phage tail tubular protein A



- Molecule 3: phage tail tubular protein B







ASN	GLY	VAL	ALA	ASN	ASP	GLY
THR	THR	GLY	SER	SER	ARG	THR
SER	VAL	LEU	ALA	ASP	VAL	ASP
ALA	ASN	ILE	GLN	GLN	GLY	GLY
ASP	THR	SER	ILE	ASN	THR	ILE
PRO	ASP	THR	PHE	ASN	ARG	ILE
GLN	ASN	ALA	GLU	GLY	GLY	ARG
VAL	ASP	ARG	SER	SER	ALA	LYS
GLN	MET	PRO	MET	THR	TYR	VAL
THR	PHE	SER	THR	ASN	ILE	ALA
GLN	ASP	VAL	LEU	THR	GLY	GLY
VAL	ILE	ILE	LYS	ASN	THR	ALA
SER	THR	ARG	LEU	THR	CYS	LEU
SER	THR	THR	LEU	ASN	THR	TRP
ASN	THR	GLY	SER	SER	ASN	ASN
ASP	ASN	PRO	SER	ILE	PHE	THR
ALA	ASN	TRP	VAL	GLN	ASN	THR
ALA	ASN	GLU	GLY	VAL	GLN	ALA
SER	GLY	ASP	GLY	GLY	ASN	CYS
THR	GLY	THR	ASP	GLY	ASN	ALA
PHE	HIS	ILE	ASP	GLU	ILE	ALA
ASN	ASN	ASN	THR	LEU	GLY	GLU
LEU	GLY	GLU	GLY	GLY	ILE	VAL
LEU	ALA	GLY	GLY	ASP	TYR	VAL
VAL	ILE	VAL	SER	ARG	ASN	MET
SER	LEU	ALA	ILE	ILE	THR	PHE
THR	THR	ARG	THR	PHE	VAL	ASP
LYS	VAL	ILE	GLU	GLY	GLY	ASP
SER	LEU	TYR	PHE	SER	THR	PRO
ASP	LEU	GLY	GLY	GLY	ILE	ILE
ASN	TYR	GLY	PRO	PHE	HIS	ARG
SER	ARG	GLY	ASP	ARG	ILE	THR
ALA	GLU	PRO	TYR	ILE	GLY	SER
SER	GLY	TYR	PHE	SER	CYS	PRO
TYR	GLY	ILE	PHE	ALA	THR	ALA
ARG	ALA	GLY	ARG	SER	ILE	ILE
PHE	ALA	THR	MET	SER	ASN	GLN
ARG	ARG	MET	ALA	VAL	ALA	SER
ALA	ALA	PRO	GLY	THR	ASN	LYS
LYS	THR	THR	THR	LEU	LYS	SER
VAL	ILE	ALA	SER	ILE	SER	GLY
LYS	VAL	THR	GLU	ASN	HIS	GLY
PRO	ARG	GLY	GLY	VAL	GLY	LYS
	VAL	PRO	ARG	ASN	VAL	ILE
	ASP	ALA	LEU	ILE	MET	SER
	SER	ASN	GLU	ARG	LEU	VAL
	ARG	VAL	ILE	ARG	GLY	VAL
	SER	SER	SER	SER	THR	PHE
	ASN	PRO	ASP	ALA	GLY	PHE
	ALA	ALA	SER	ARG	ALA	LYS
	VAL	VAL	ARG	THR	ASN	CYS
	GLY	LEU	LEU	GLY	SER	GLY
	GLU	GLY	THR	ALA	ASN	PHE
	GLY	LEU	GLY	SER	THR	THR
	ASP	SER	TYR	GLY	PHE	THR
	VAL	CYS	THR	ALA	THR	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	41926	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)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	1074.2001, 1074.2001, 1074.2001	wwPDB
Map dimensions	1000, 1000, 1000	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	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	0.15	0/3944	0.27	0/5341
1	L	0.14	0/3944	0.27	0/5341
2	W	0.15	0/1526	0.27	0/2067
2	X	0.16	0/1526	0.30	0/2067
3	Y	0.15	0/6436	0.33	0/8752
4	e	0.14	0/1222	0.28	0/1654
4	f	0.15	0/1243	0.33	0/1681
4	g	0.14	0/1223	0.34	0/1654
All	All	0.15	0/21064	0.30	0/28557

There are no bond length outliers.

There are no bond angle outliers.

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	3887	0	3858	61	0
1	L	3887	0	3858	60	0
2	W	1498	0	1417	23	0
2	X	1498	0	1417	23	0
3	Y	6281	0	6022	138	0
4	e	1208	0	1207	43	0
4	f	1229	0	1228	29	0
4	g	1209	0	1211	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20697	0	20218	367	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 9.

The worst 5 of 367 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:e:147:LYS:CG	4:g:141:GLY:HA2	1.49	1.41
4:e:147:LYS:HG3	4:g:141:GLY:CA	1.90	1.02
4:e:147:LYS:HG3	4:g:141:GLY:HA2	1.02	1.00
1:A:146:LEU:HD11	1:A:251:ILE:HD11	1.43	1.00
4:e:147:LYS:CG	4:g:141:GLY:CA	2.45	0.89

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	500/535 (94%)	476 (95%)	22 (4%)	2 (0%)	30	59
1	L	500/535 (94%)	475 (95%)	23 (5%)	2 (0%)	30	59
2	W	190/192 (99%)	181 (95%)	9 (5%)	0	100	100
2	X	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
3	Y	788/791 (100%)	713 (90%)	70 (9%)	5 (1%)	21	50
4	e	151/777 (19%)	145 (96%)	5 (3%)	1 (1%)	18	47
4	f	154/777 (20%)	148 (96%)	5 (3%)	1 (1%)	21	50
4	g	153/777 (20%)	144 (94%)	9 (6%)	0	100	100
All	All	2626/4576 (57%)	2465 (94%)	150 (6%)	11 (0%)	31	59

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Y	656	ILE
4	f	2	ASP
1	A	518	SER
1	L	518	SER
3	Y	657	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/435 (95%)	413 (100%)	0	100	100
1	L	413/435 (95%)	412 (100%)	1 (0%)	87	87
2	W	157/157 (100%)	157 (100%)	0	100	100
2	X	157/157 (100%)	157 (100%)	0	100	100
3	Y	680/681 (100%)	679 (100%)	1 (0%)	88	89
4	e	133/636 (21%)	133 (100%)	0	100	100
4	f	135/636 (21%)	135 (100%)	0	100	100
4	g	131/636 (21%)	131 (100%)	0	100	100
All	All	2219/3773 (59%)	2217 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	493	GLN
3	Y	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
4	f	10	GLN
4	f	149	GLN
3	Y	492	ASN

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Mol	Chain	Res	Type
3	Y	535	GLN
3	Y	553	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 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.

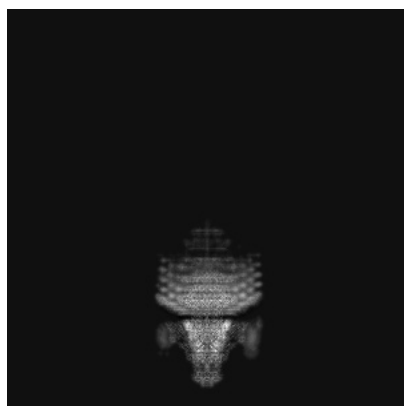
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33560. These allow visual inspection of the internal detail of the map and identification of artifacts.

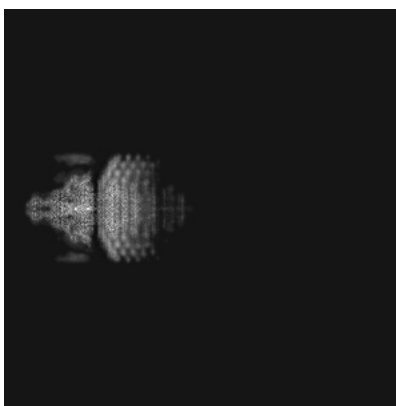
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

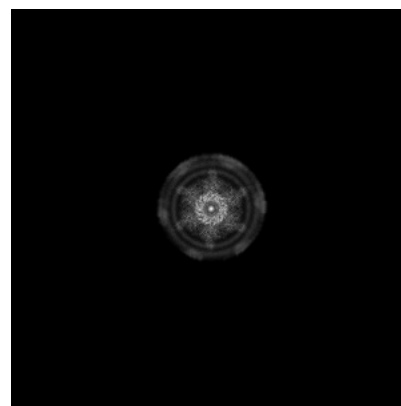
6.1.1 Primary map



X

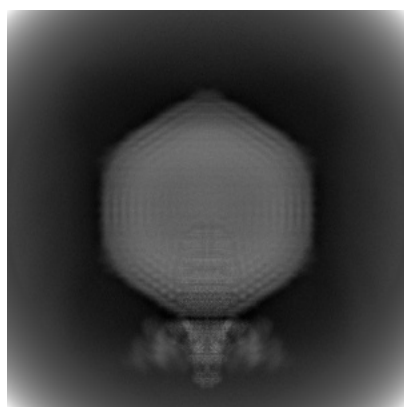


Y

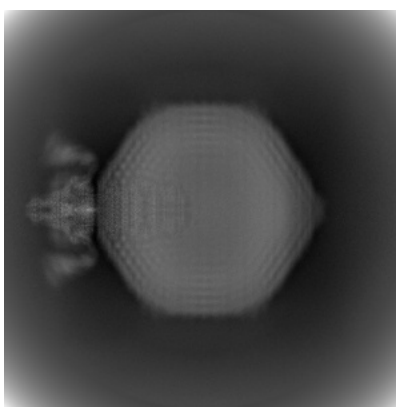


Z

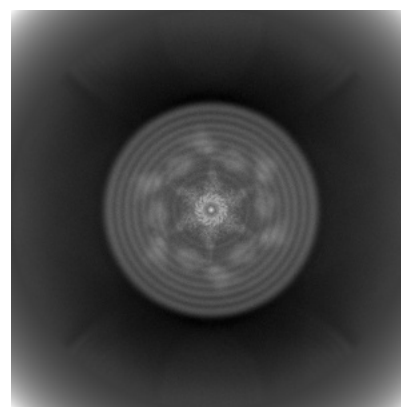
6.1.2 Raw map



X



Y

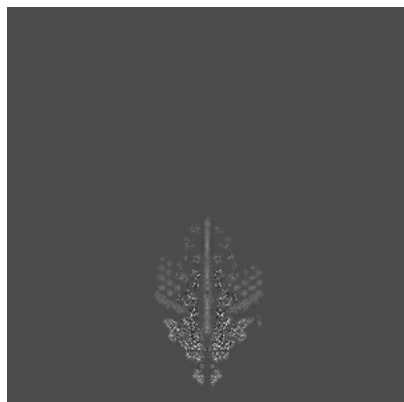


Z

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

6.2 Central slices [i](#)

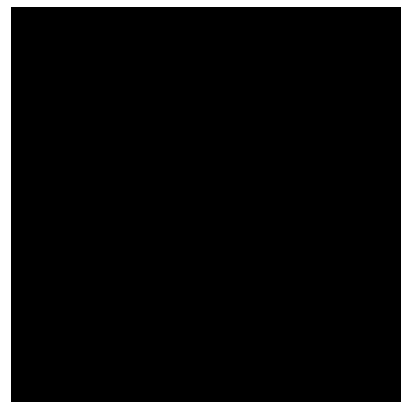
6.2.1 Primary map



X Index: 500

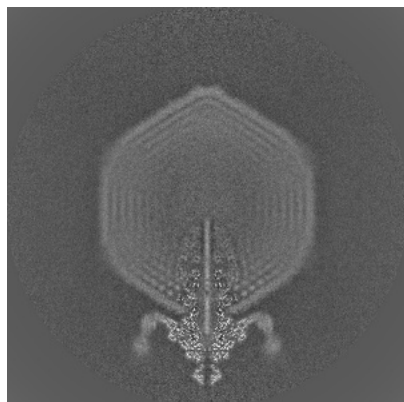


Y Index: 500

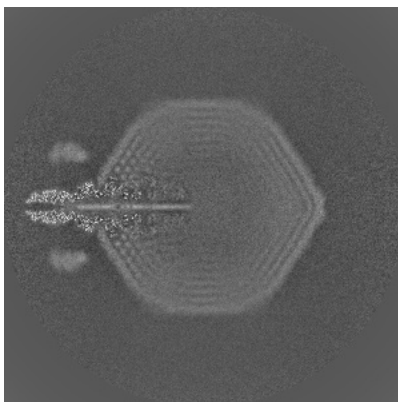


Z Index: 500

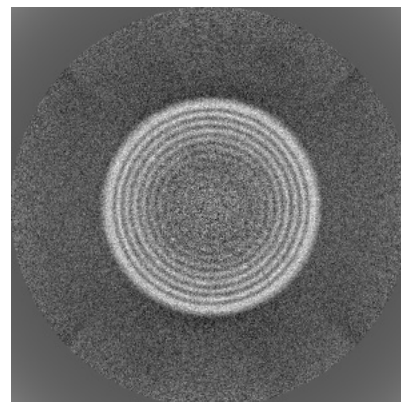
6.2.2 Raw map



X Index: 500



Y Index: 500

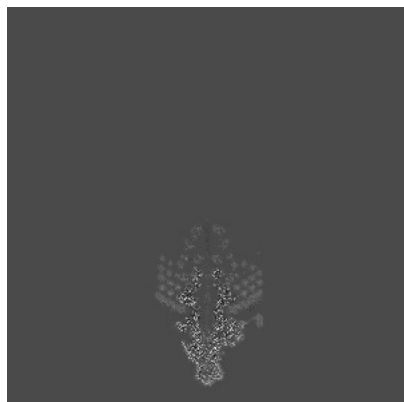


Z Index: 500

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

6.3 Largest variance slices [i](#)

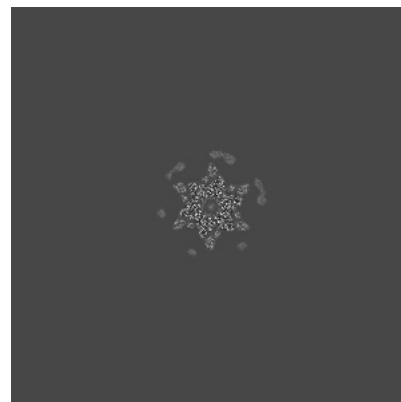
6.3.1 Primary map



X Index: 512

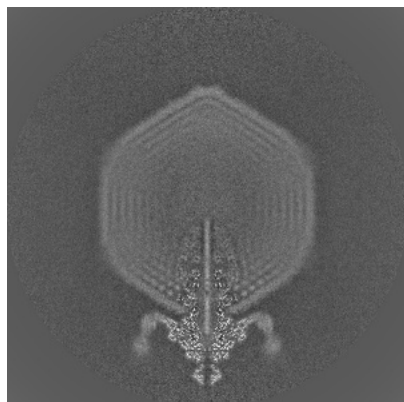


Y Index: 524

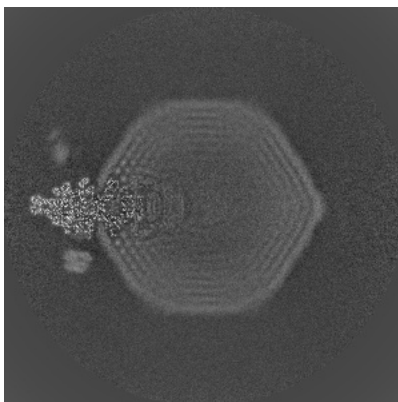


Z Index: 209

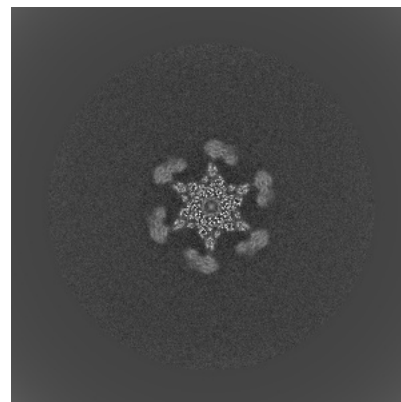
6.3.2 Raw map



X Index: 500



Y Index: 476

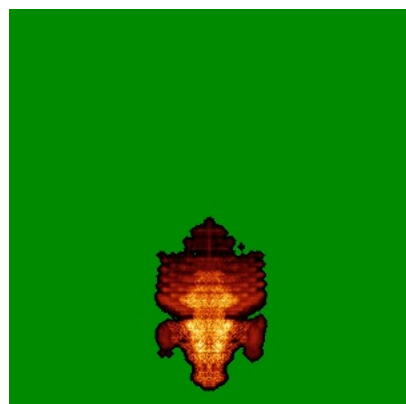


Z Index: 209

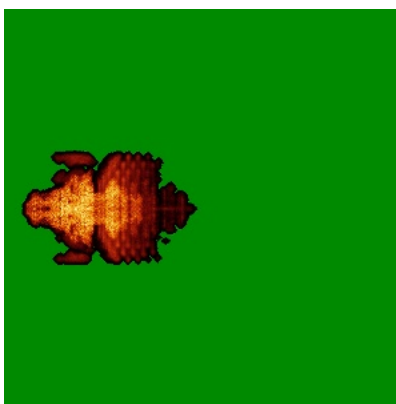
The images above show the largest variance slices of the map in three orthogonal directions.

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

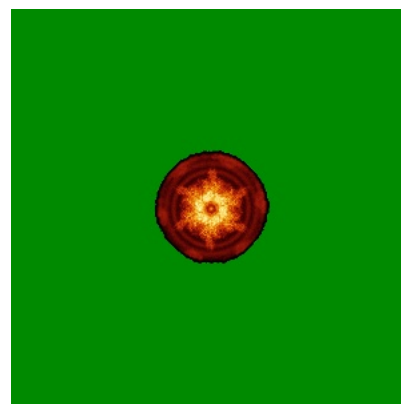
6.4.1 Primary map



X

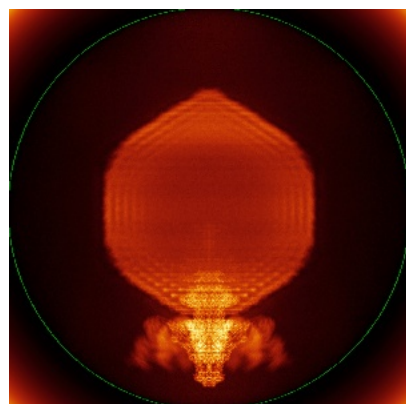


Y

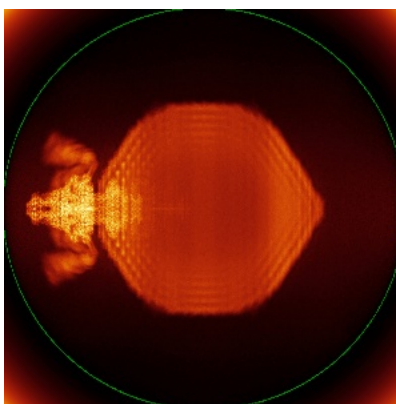


Z

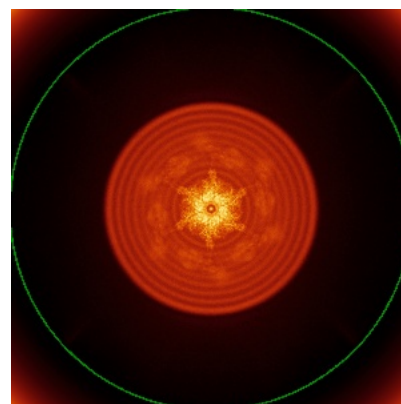
6.4.2 Raw map



X



Y

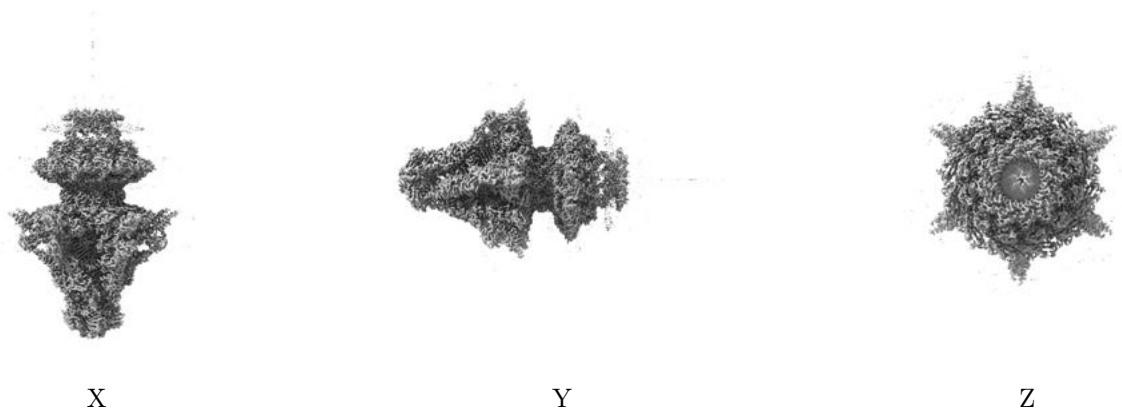


Z

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.

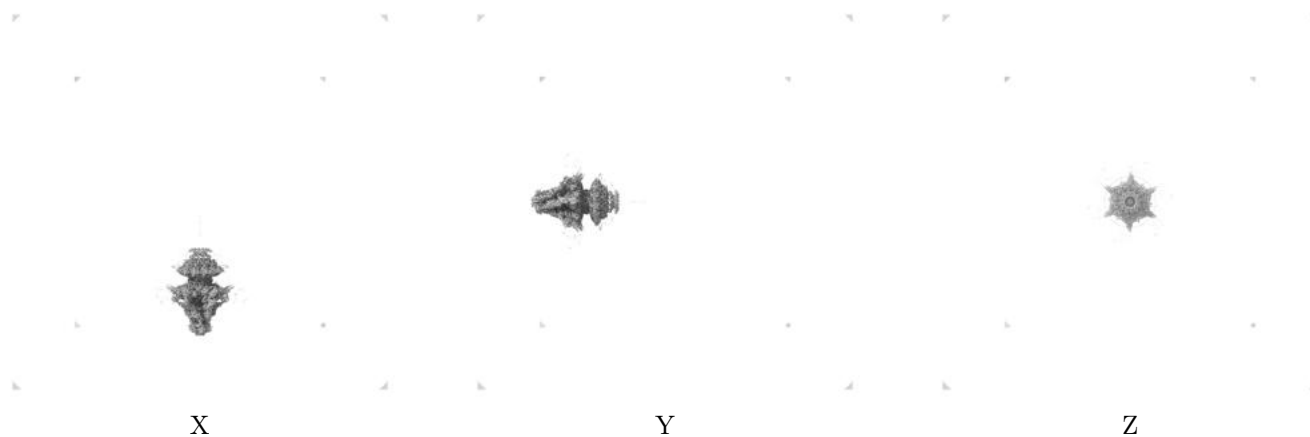
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

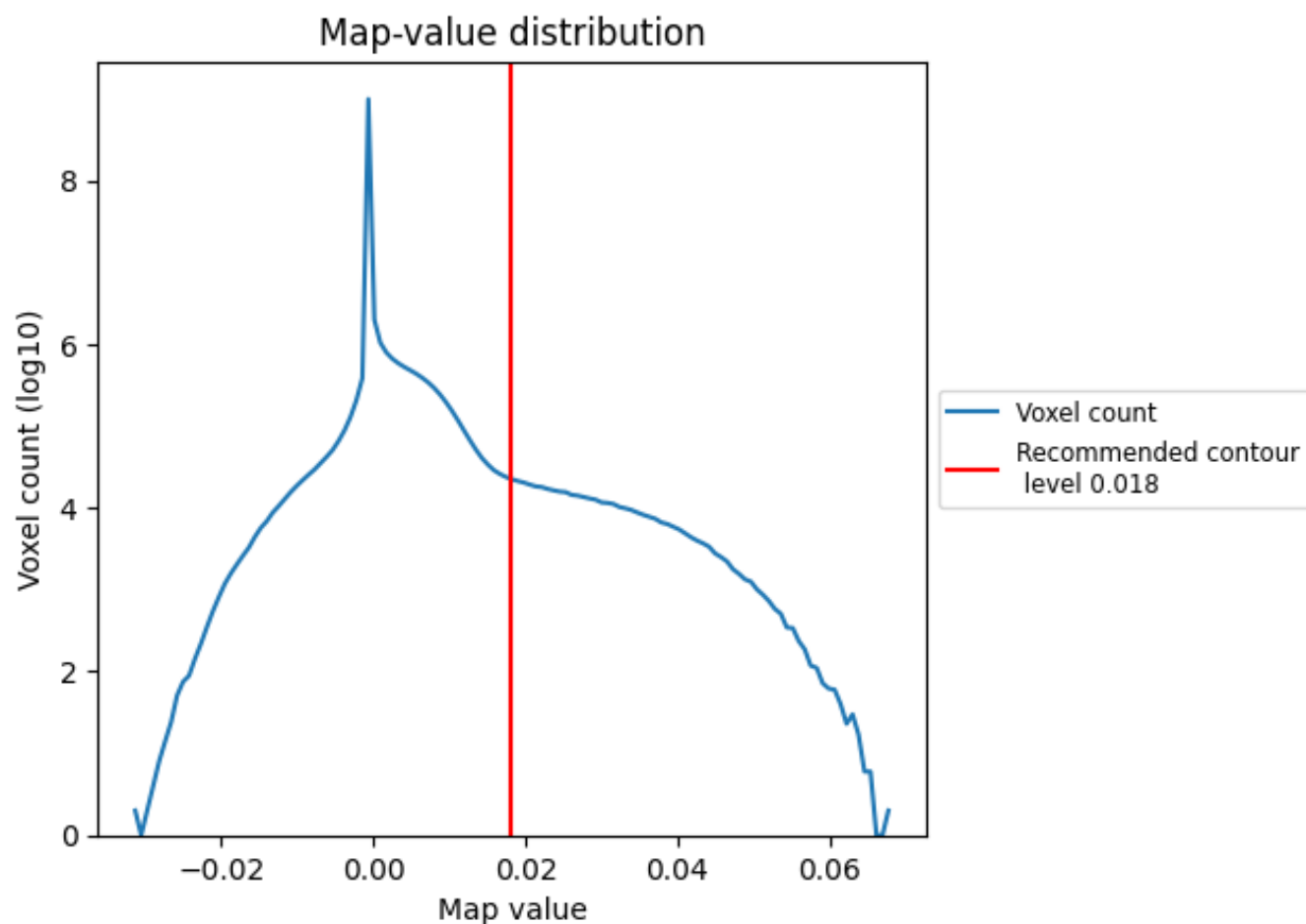
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

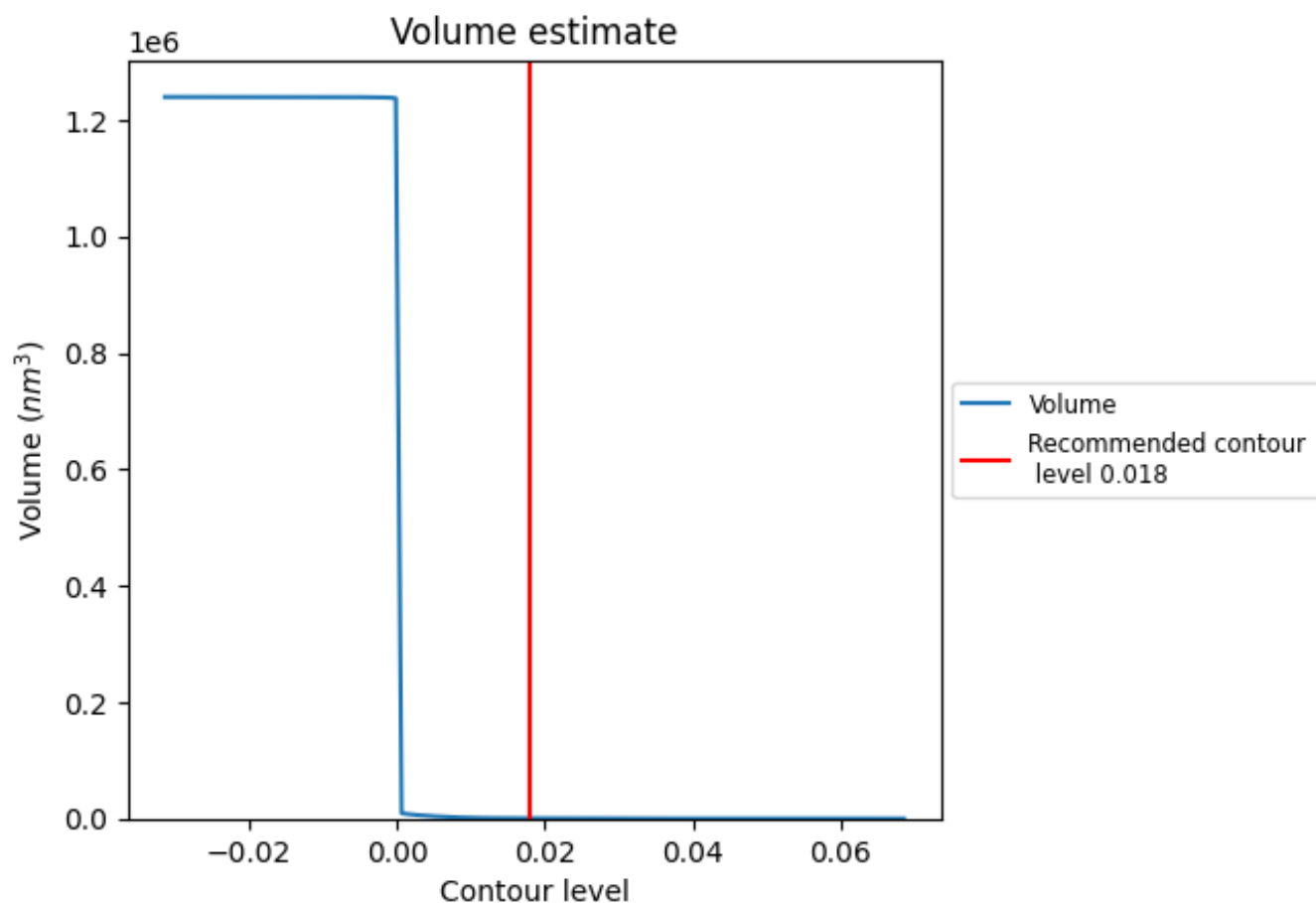
This section contains the results of statistical analysis of the map.

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.

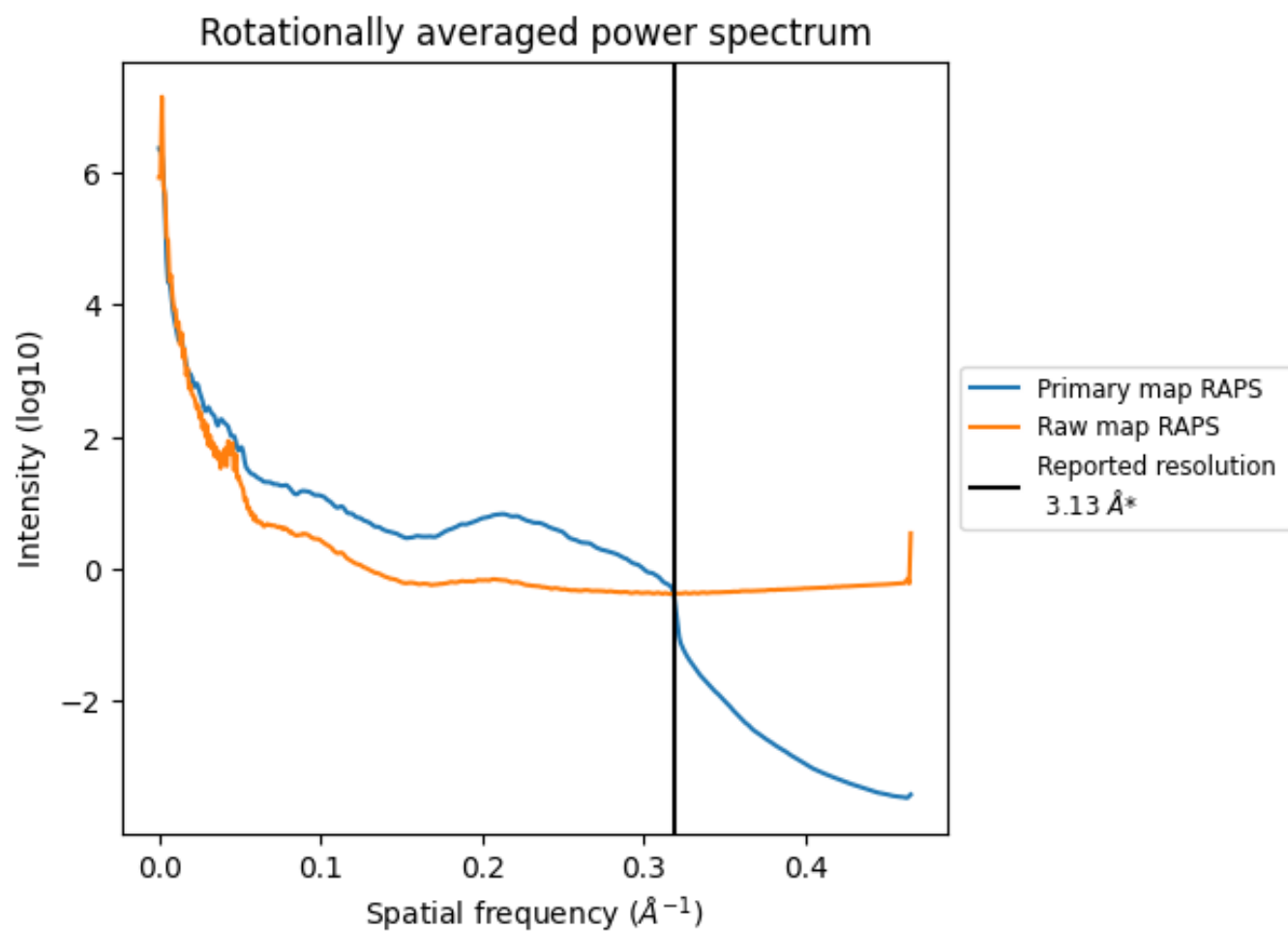
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 518 nm^3 ; this corresponds to an approximate mass of 468 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 ⓘ

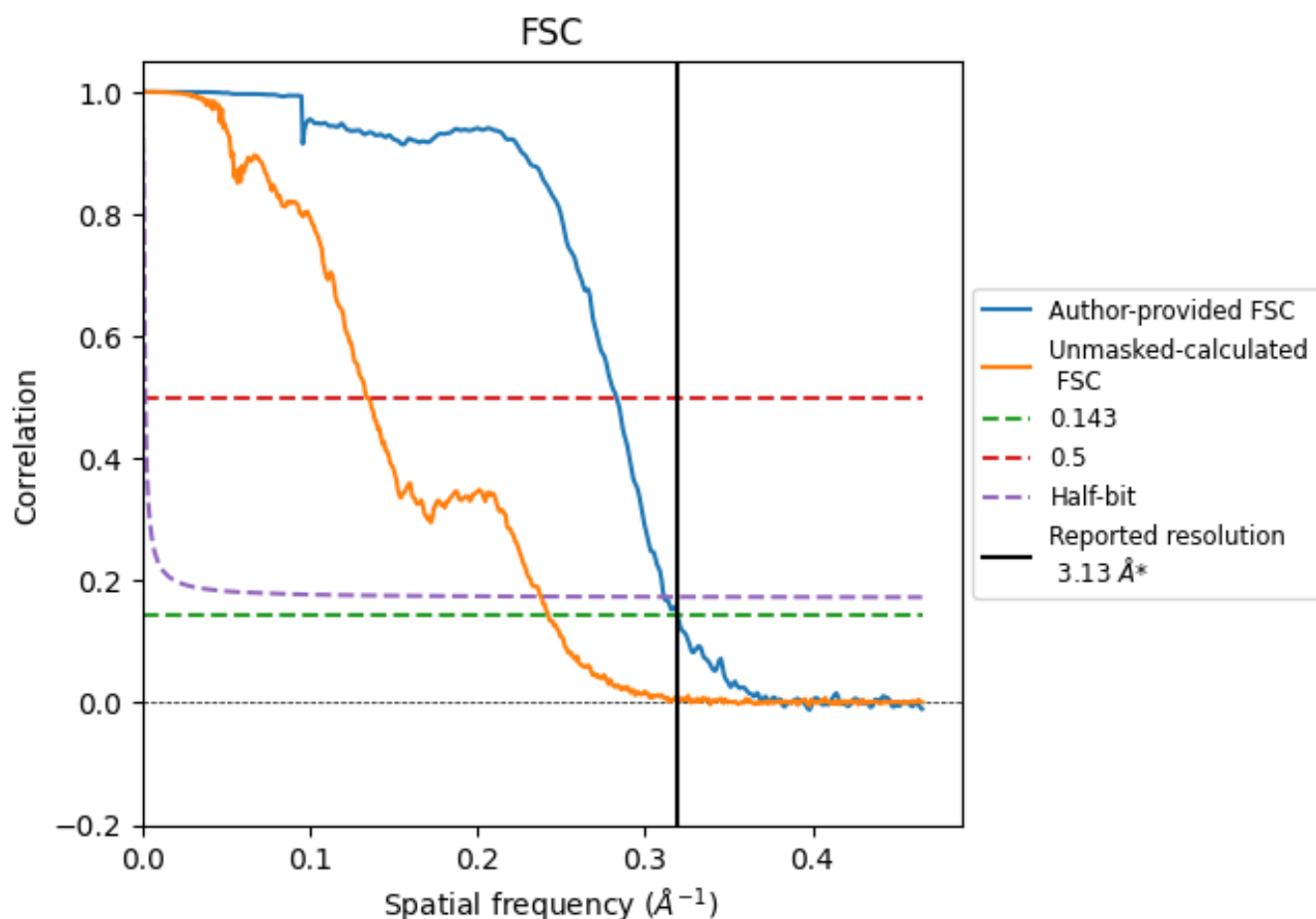


*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.13	3.53	3.21
Unmasked-calculated*	4.13	7.47	4.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.13 differs from the reported value 3.13 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33560 and PDB model 7Y1C. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

This section was not generated.

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

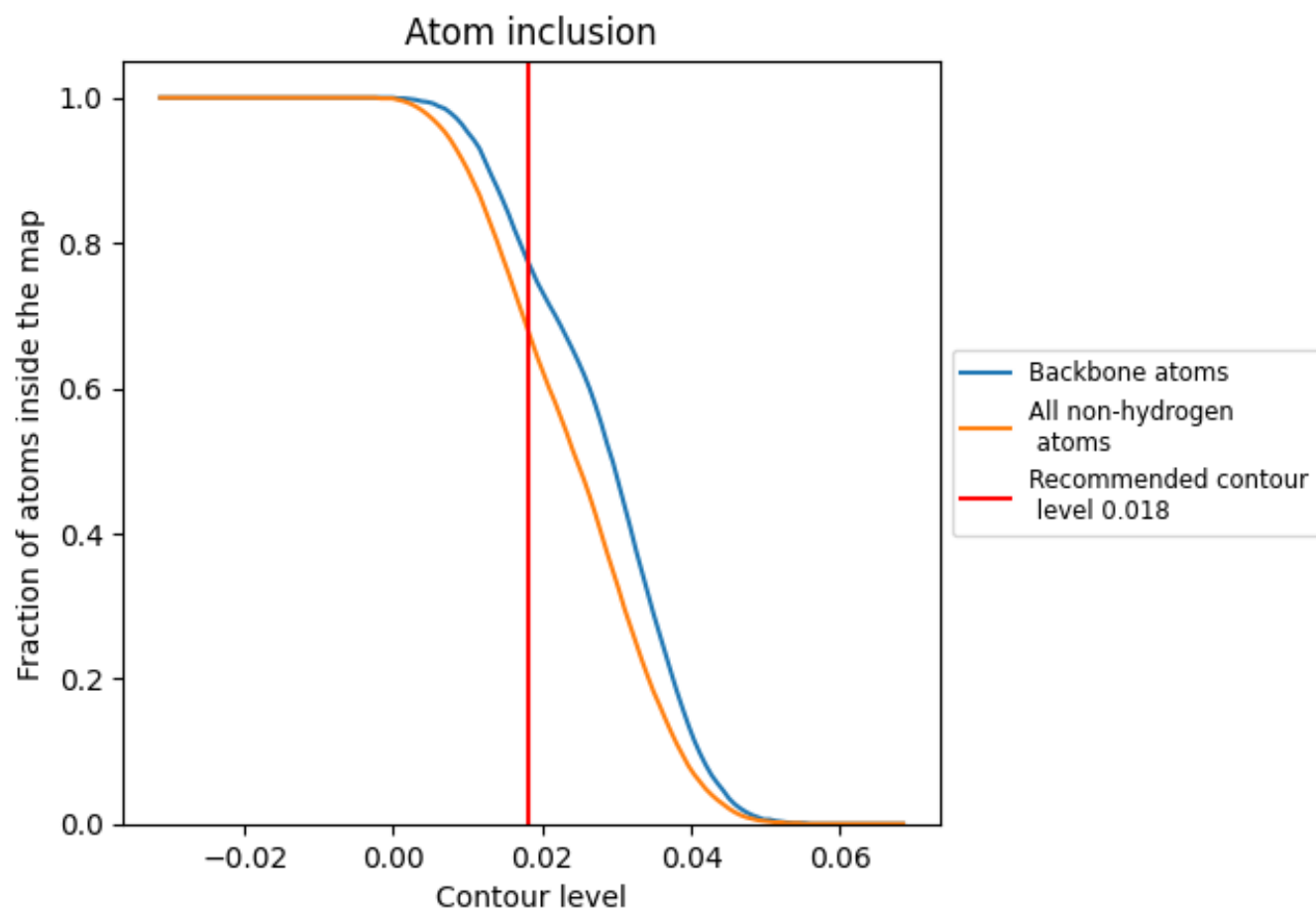


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 78% of all backbone atoms, 68% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.5590
A	0.5980	0.5620
L	0.5940	0.5590
W	0.7370	0.5710
X	0.7330	0.5700
Y	0.7680	0.5550
e	0.6860	0.5640
f	0.6900	0.5650
g	0.6600	0.5390

1.0

0.0

<0.0