



## wwPDB EM Validation Summary Report ⓘ

Feb 12, 2025 – 12:43 am GMT

PDB ID : 8QEK  
EMDB ID : EMD-18369  
Title : Neck and tail of phage 812 after tail contraction (composite)  
Authors : Cienikova, Z.; Siborova, M.; Fuzik, T.; Plevka, P.  
Deposited on : 2023-08-31  
Resolution : 3.60 Å (reported)  
Based on initial models : 8Q7D, 8Q1I, 8Q01

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

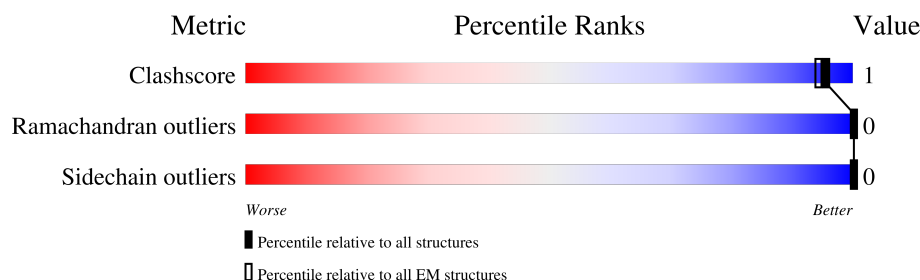
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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.





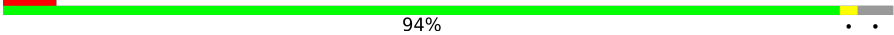
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	D	563	
1	p	563	
2	Y	120	
3	Z	120	
4	A	142	
4	G	142	
5	M	278	
6	S	292	

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Mol	Chain	Length	Quality of chain
7	b	302	 86%14%
7	c	302	 85%14%
8	B	587	 58%40%
8	I	587	 61%37%
8	O	587	 6%94%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 32480 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	441	Total	C	N	O	S	0	0
			3567	2249	622	681	15		
1	D	441	Total	C	N	O	S	0	0
			3567	2249	622	681	15		

- Molecule 2 is a DNA chain called Anchor DNA forward strand (120-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0
			2400	1164	384	732	120		

- Molecule 3 is a DNA chain called Anchor DNA reverse strand (120-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Z	120	Total	C	N	O	P	0	0
			2520	1200	492	708	120		

- Molecule 4 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
4	G	140	Total	C	N	O	S	0	0
			1102	691	187	220	4		

- Molecule 5 is a protein called Baseplate hub assembly protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	277	Total	C	N	O	S	0	0
			2230	1417	357	450	6		

- Molecule 6 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	227	Total	C	N	O	S	0	0
			1887	1212	313	352	10		

- Molecule 7 is a protein called Putative neck protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	259	Total	C	N	O	S	0	0
			2083	1342	347	385	9		
7	c	259	Total	C	N	O	S	0	0
			2083	1342	347	385	9		

- Molecule 8 is a protein called Major tail sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	352	Total	C	N	O	S	0	0
			2719	1708	472	532	7		
8	I	367	Total	C	N	O	S	0	0
			2848	1789	492	560	7		
8	O	563	Total	C	N	O	S	0	0
			4380	2757	745	871	7		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	S	1	Total	Zn	0
			1	1	
9	b	1	Total	Zn	0
			1	1	
9	c	1	Total	Zn	0
			1	1	





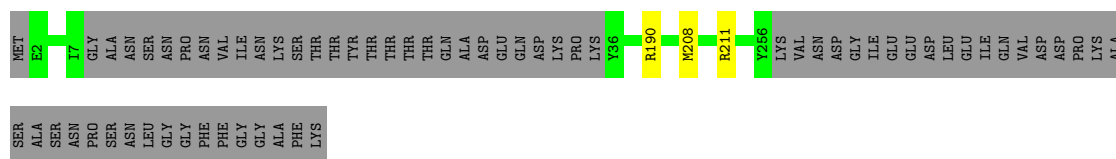
- Molecule 4: Capsid protein



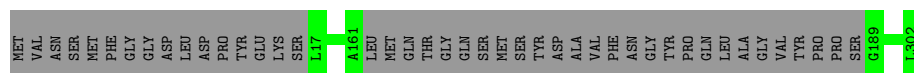
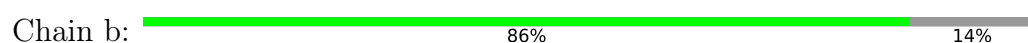
- Molecule 5: Baseplate hub assembly protein



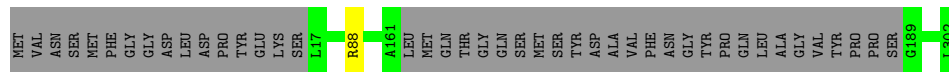
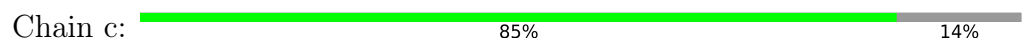
- Molecule 6: Capsid protein



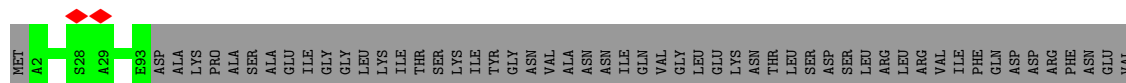
- Molecule 7: Putative neck protein



- Molecule 7: Putative neck protein



- Molecule 8: Major tail sheath protein







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17304	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	15.413	Depositor
Minimum map value	-4.105	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.2	Depositor
Map size (Å)	304.41602, 304.41602, 549.64	wwPDB
Map dimensions	288, 288, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.057, 1.057, 1.057	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	D	0.26	0/3630	0.55	0/4873
1	p	0.26	0/3630	0.55	0/4873
2	Y	0.56	0/2675	0.96	0/4112
3	Z	0.49	0/2843	0.87	0/4400
4	A	0.31	0/1107	0.57	0/1496
4	G	0.27	0/1118	0.56	0/1510
5	M	0.30	0/2267	0.53	0/3059
6	S	0.31	0/1927	0.58	0/2606
7	b	0.29	0/2140	0.53	0/2906
7	c	0.29	0/2140	0.53	0/2906
8	B	0.26	0/2765	0.57	0/3731
8	I	0.26	0/2898	0.57	0/3916
8	O	0.26	0/4453	0.56	0/6015
All	All	0.33	0/33593	0.64	0/46403

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
7	c	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	c	88	ARG	Sidechain

## 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	D	3567	0	3537	4	0
1	p	3567	0	3537	0	0
2	Y	2400	0	1369	0	0
3	Z	2520	0	1357	0	0
4	A	1091	0	1081	10	0
4	G	1102	0	1094	2	0
5	M	2230	0	2189	12	0
6	S	1887	0	1897	2	0
7	b	2083	0	2028	0	0
7	c	2083	0	2028	0	0
8	B	2719	0	2675	14	0
8	I	2848	0	2811	5	0
8	O	4380	0	4336	6	0
9	S	1	0	0	0	0
9	b	1	0	0	0	0
9	c	1	0	0	0	0
All	All	32480	0	29939	41	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 1.

The worst 5 of 41 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:A:94:LEU:CD1	8:B:524:ILE:HD11	1.74	1.17
4:A:94:LEU:CD1	8:B:524:ILE:CD1	2.34	1.05
4:A:94:LEU:HD11	8:B:524:ILE:HD11	1.41	1.01
5:M:136:LYS:HB2	8:B:548:GLU:HG3	1.43	1.01
4:A:94:LEU:HD13	8:B:524:ILE:CD1	1.97	0.95

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	D	437/563 (78%)	432 (99%)	5 (1%)	0	100	100
1	p	437/563 (78%)	432 (99%)	5 (1%)	0	100	100
4	A	137/142 (96%)	137 (100%)	0	0	100	100
4	G	138/142 (97%)	138 (100%)	0	0	100	100
5	M	275/278 (99%)	274 (100%)	1 (0%)	0	100	100
6	S	223/292 (76%)	218 (98%)	5 (2%)	0	100	100
7	b	255/302 (84%)	251 (98%)	4 (2%)	0	100	100
7	c	255/302 (84%)	252 (99%)	3 (1%)	0	100	100
8	B	344/587 (59%)	339 (98%)	5 (2%)	0	100	100
8	I	363/587 (62%)	363 (100%)	0	0	100	100
8	O	559/587 (95%)	552 (99%)	7 (1%)	0	100	100
All	All	3423/4345 (79%)	3388 (99%)	35 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	D	389/492 (79%)	389 (100%)	0	100	100
1	p	389/492 (79%)	389 (100%)	0	100	100
4	A	119/122 (98%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	120/122 (98%)	120 (100%)	0	100	100
5	M	252/253 (100%)	252 (100%)	0	100	100
6	S	212/266 (80%)	212 (100%)	0	100	100
7	b	218/254 (86%)	218 (100%)	0	100	100
7	c	218/254 (86%)	218 (100%)	0	100	100
8	B	293/495 (59%)	293 (100%)	0	100	100
8	I	309/495 (62%)	309 (100%)	0	100	100
8	O	477/495 (96%)	477 (100%)	0	100	100
All	All	2996/3740 (80%)	2996 (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. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	484	GLN

### 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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

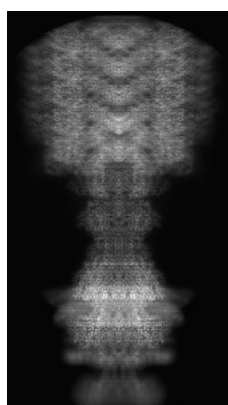
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18369. These allow visual inspection of the internal detail of the map and identification of artifacts.

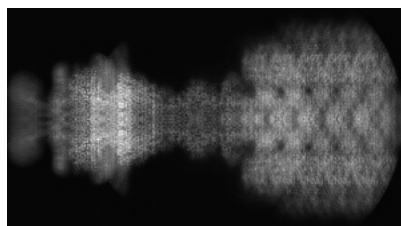
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

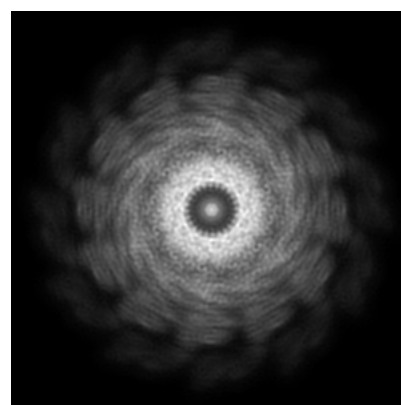
#### 6.1.1 Primary map



X



Y

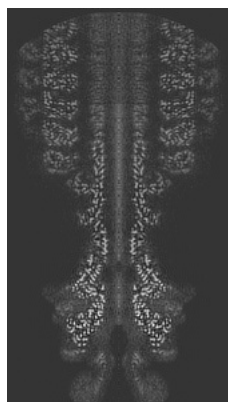


Z

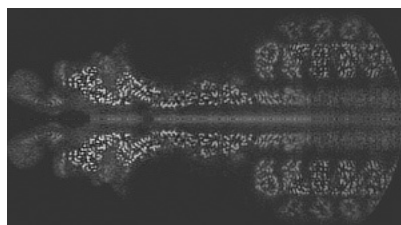
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 144



Y Index: 144

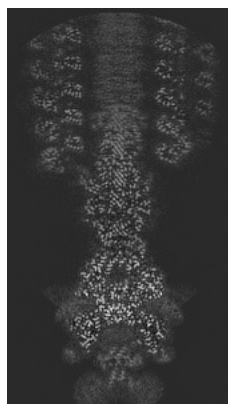


Z Index: 260

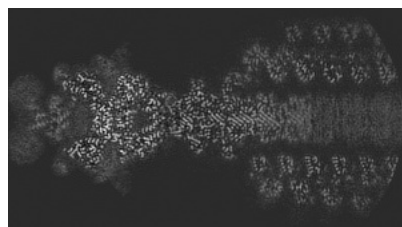
The images above show central slices of the map in three orthogonal directions.

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

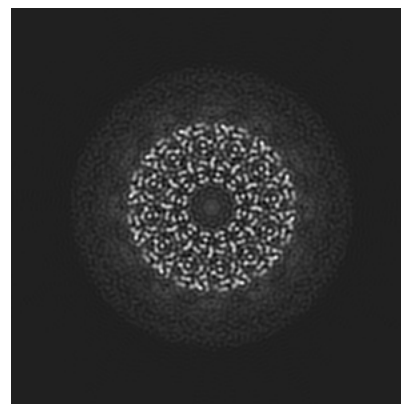
### 6.3.1 Primary map



X Index: 122



Y Index: 166

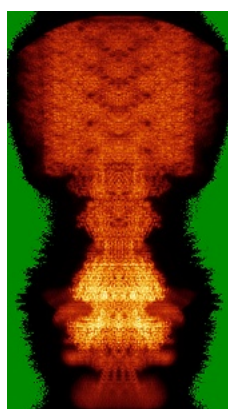


Z Index: 148

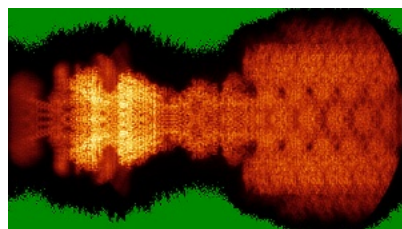
The images above show the largest variance slices of the map in three orthogonal directions.

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

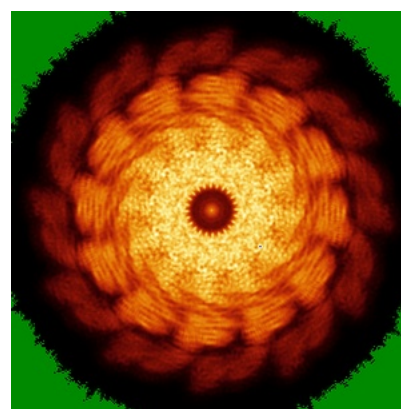
### 6.4.1 Primary map



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.

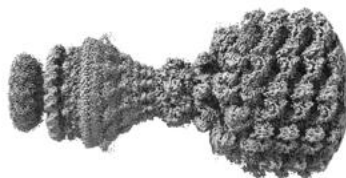


## 6.5 Orthogonal surface views [i](#)

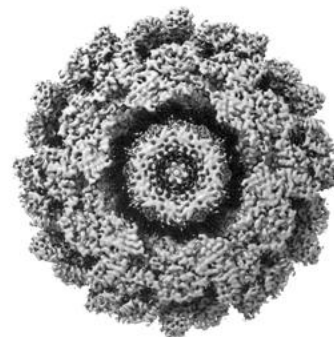
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

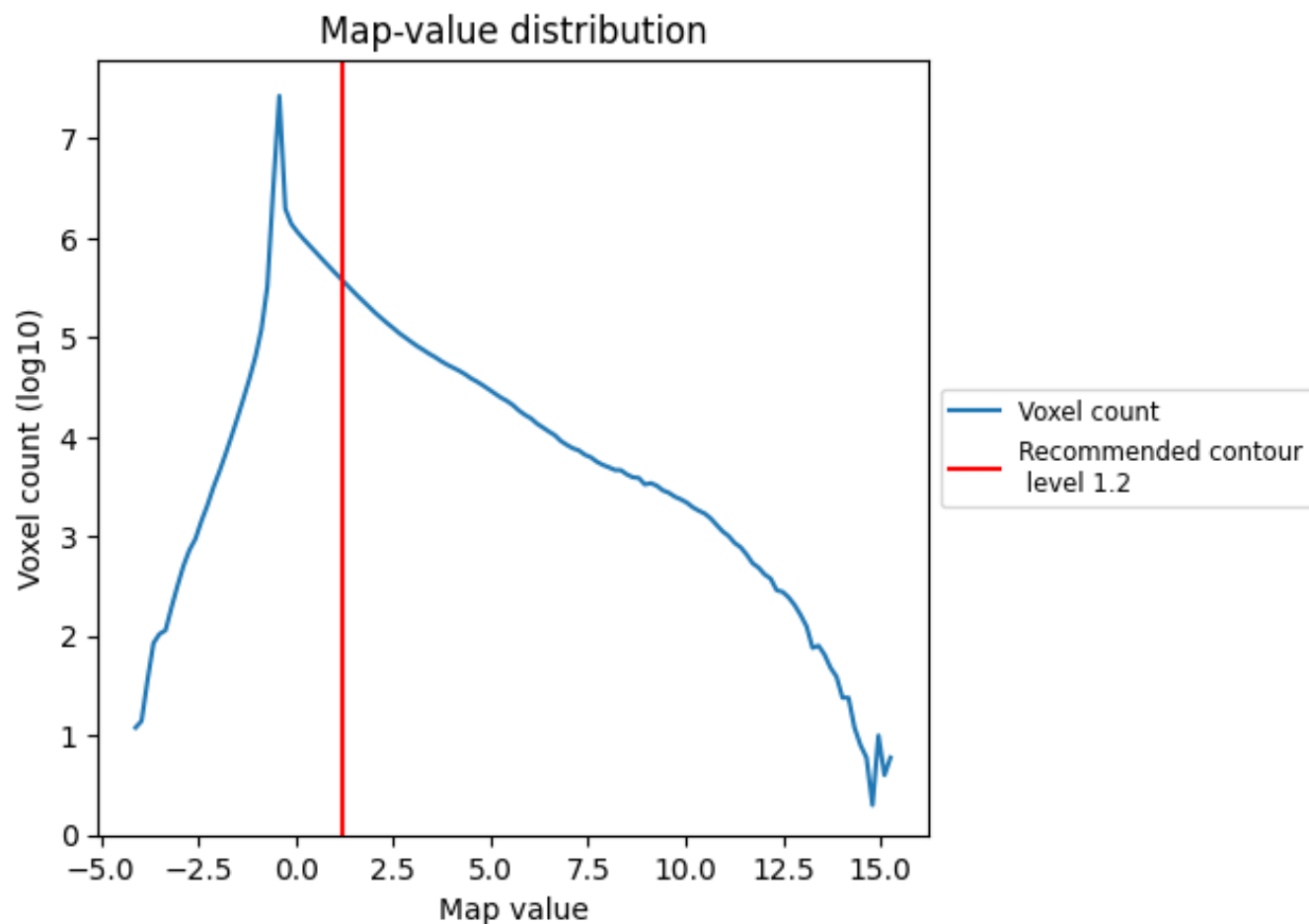
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

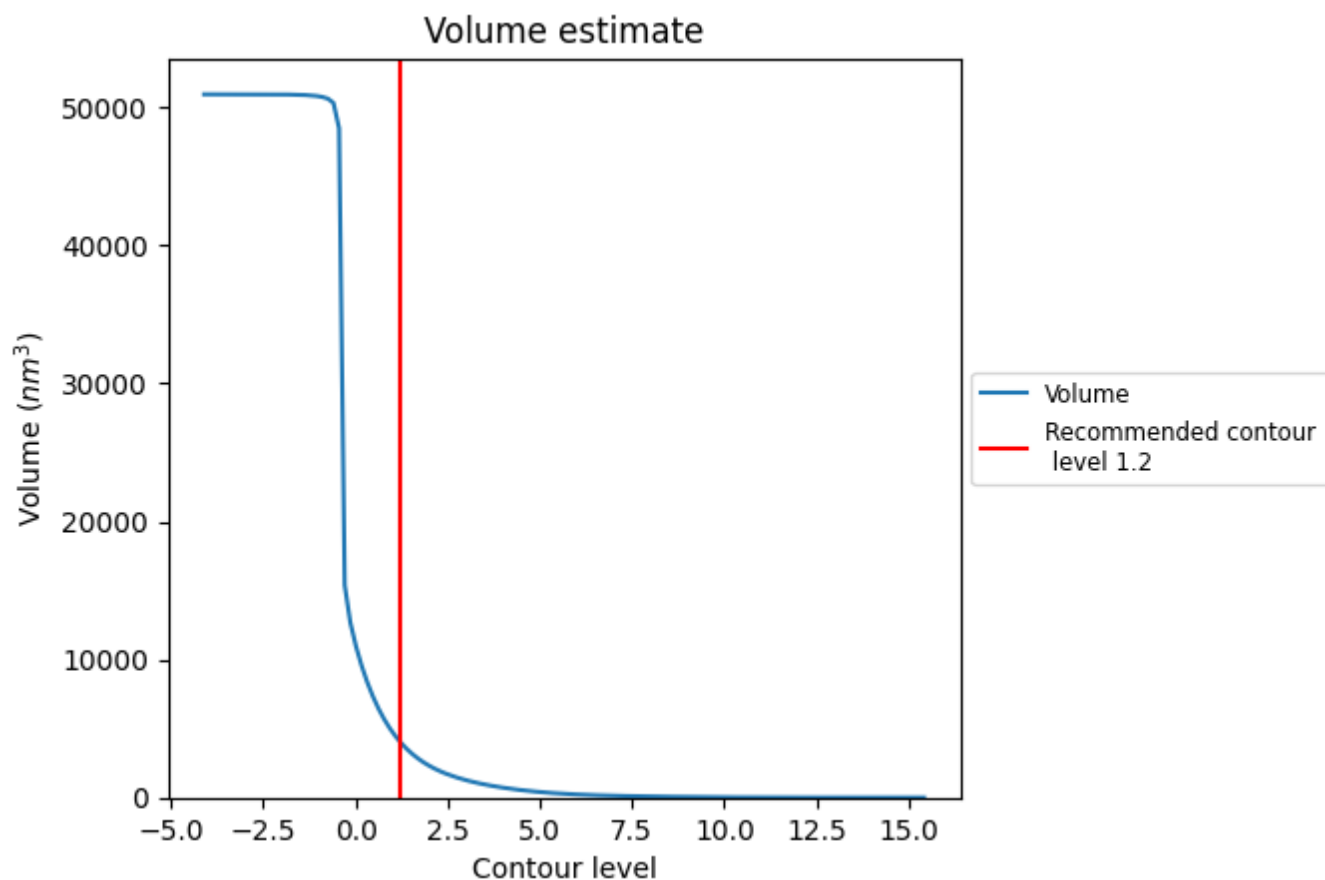
This section contains the results of statistical analysis of the map.

### 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 4069 nm<sup>3</sup>; this corresponds to an approximate mass of 3676 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 8 Fourier-Shell correlation ⓘ

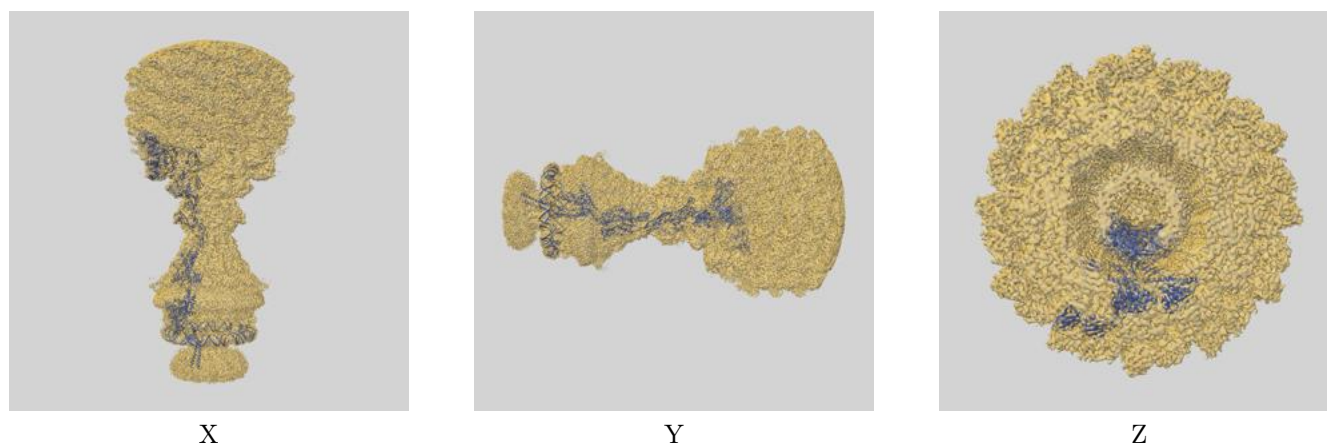
This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

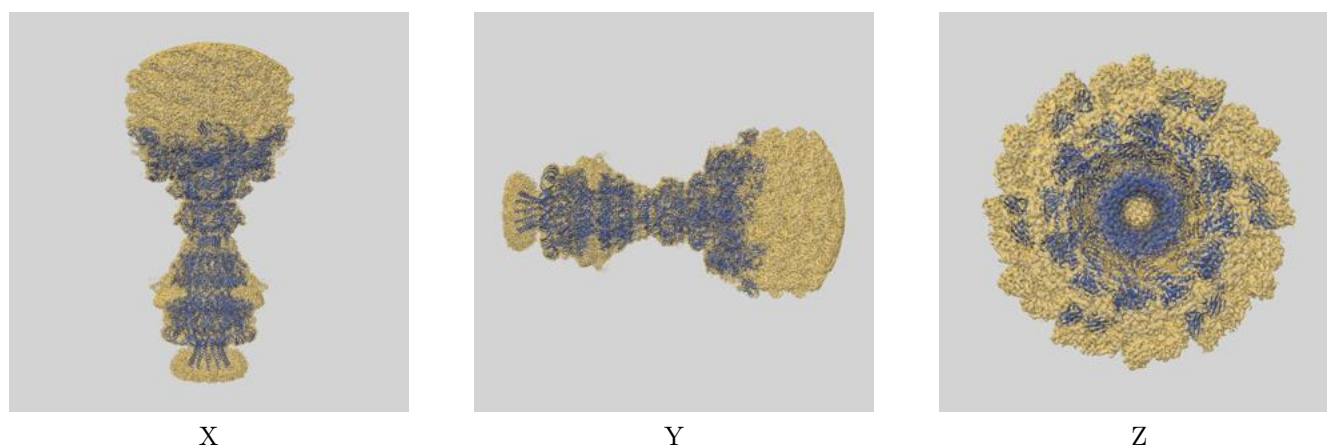
This section contains information regarding the fit between EMDB map EMD-18369 and PDB model 8QEK. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)

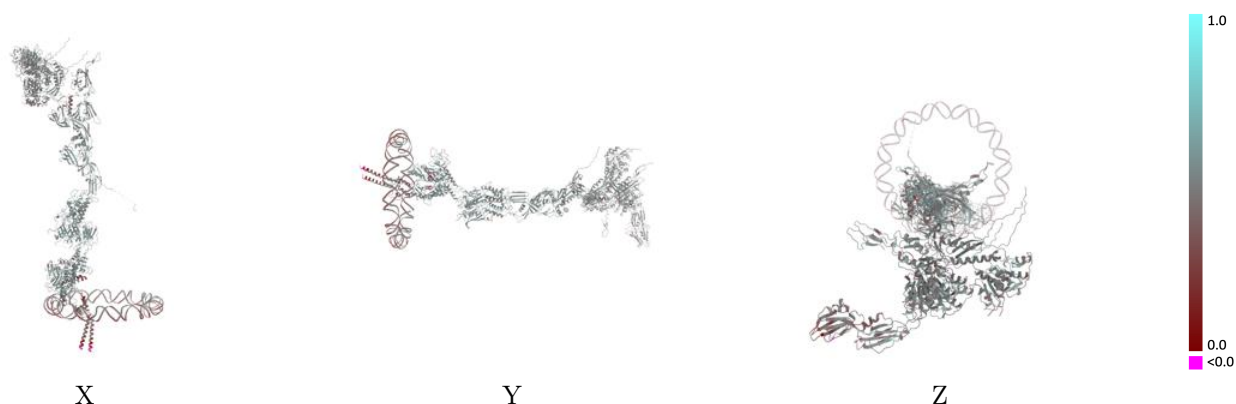


#### 9.1.2 Map-model assembly overlay [i](#)



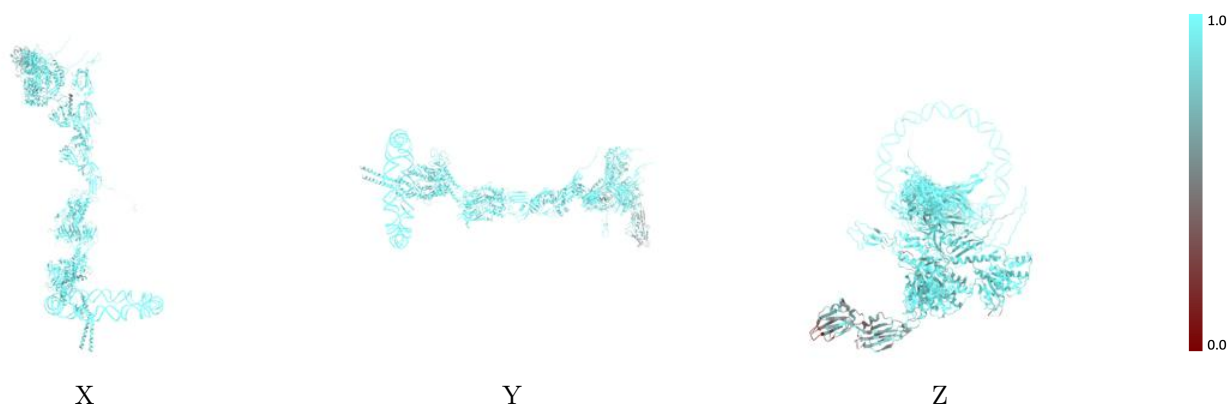
The images above show the 3D surface view of the map at the recommended contour level 1.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



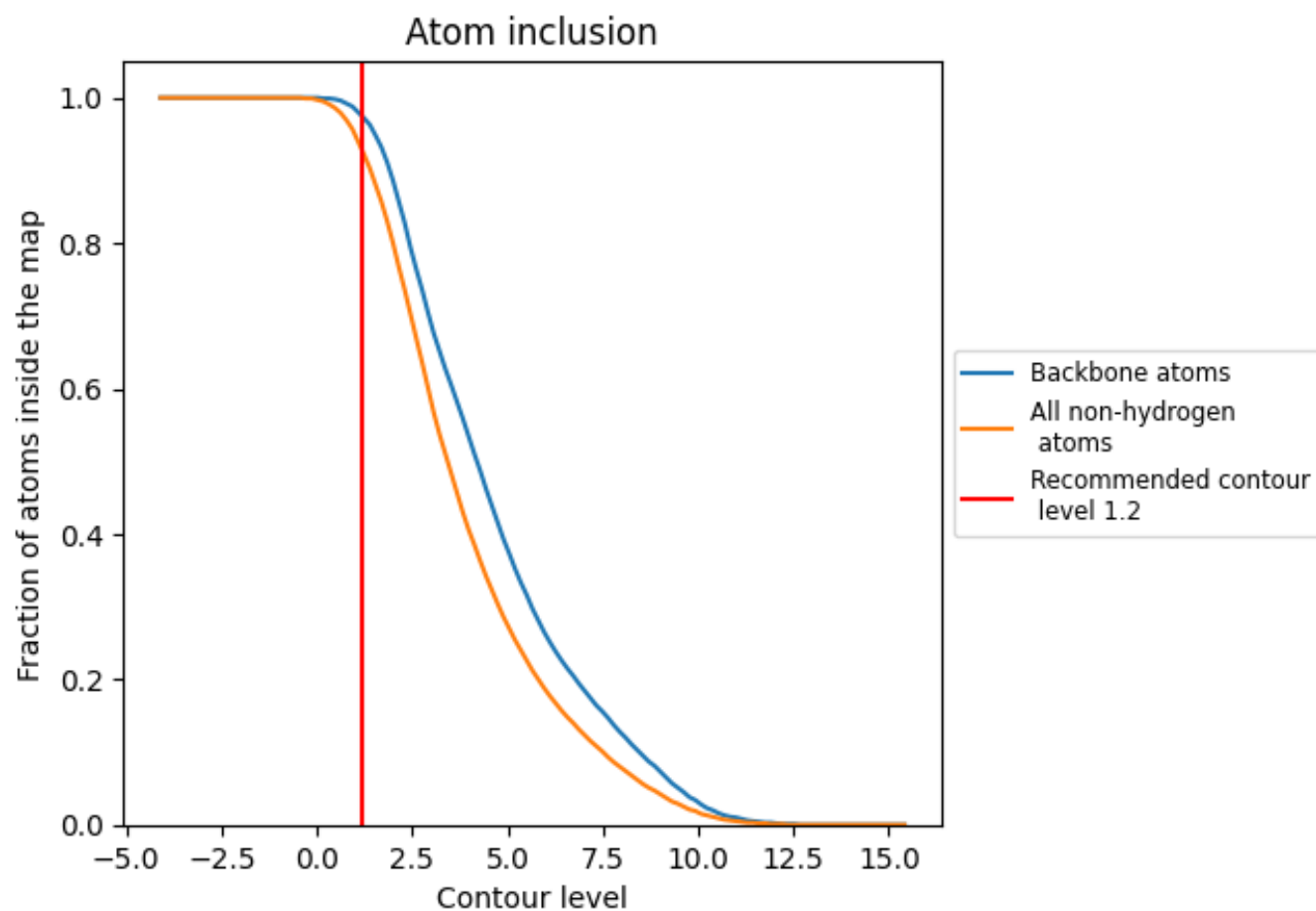
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.2).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9260	 0.4680
A	 0.9500	 0.5100
B	 0.8830	 0.4550
D	 0.9440	 0.4750
G	 0.9330	 0.4730
I	 0.9310	 0.4830
M	 0.9190	 0.4910
O	 0.7980	 0.4670
S	 0.9520	 0.5070
Y	 0.9750	 0.3750
Z	 0.9790	 0.3830
b	 0.9820	 0.5180
c	 0.9820	 0.5170
p	 0.9420	 0.4740

