



## wwPDB EM Validation Summary Report ⓘ

May 12, 2024 – 02:53 pm BST

PDB ID : 6SD3  
EMDB ID : EMD-10147  
Title : 34mer structure of the Salmonella flagella MS-ring protein FljF  
Authors : Johnson, S.; Fong, Y.H.; Deme, J.C.; Furlong, E.J.; Kuhlen, L.; Lea, S.M.  
Deposited on : 2019-07-26  
Resolution : 3.30 Å(reported)  
Based on initial model : 6SCN

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:

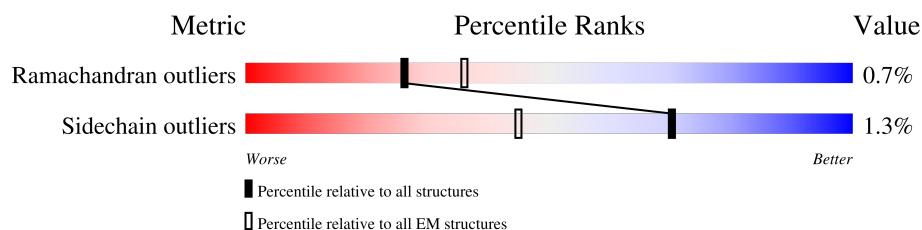
EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 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 3.30 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.





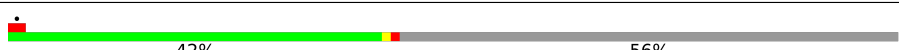


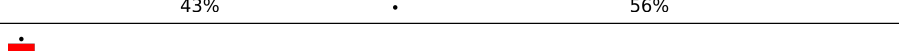
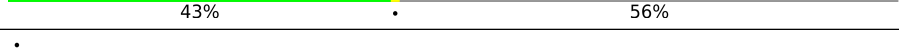





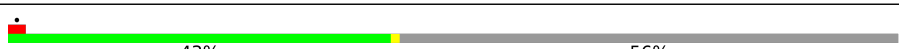


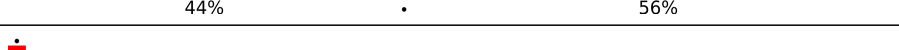








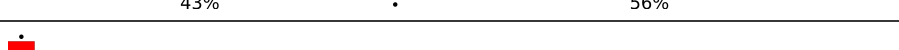
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	A	560	
1	B	560	
1	C	560	
1	D	560	
1	E	560	
1	F	560	
1	G	560	
1	H	560	
1	I	560	

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Mol	Chain	Length	Quality of chain
1	J	560	
1	K	560	
1	L	560	
1	M	560	
1	N	560	
1	O	560	
1	P	560	
1	Q	560	
1	R	560	
1	S	560	
1	T	560	
1	U	560	
1	V	560	
1	W	560	
1	X	560	
1	Y	560	
1	Z	560	
1	a	560	
1	b	560	
1	c	560	
1	d	560	
1	e	560	
1	f	560	
1	g	560	
1	h	560	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 63144 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 Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	B	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	C	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	D	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	E	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	F	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	G	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	H	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	I	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	J	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	K	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	L	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	M	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	N	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	O	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	P	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	Q	154	Total	C	N	O	S	0	0
			1220	742	229	246	3		

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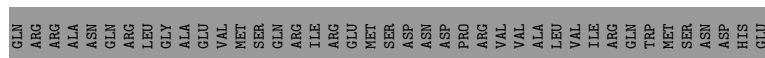
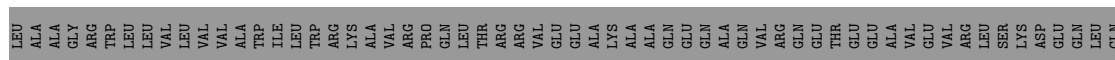
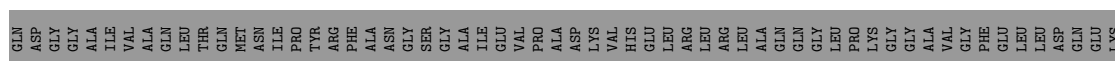
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	S	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	T	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	U	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	V	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	W	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	X	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	Y	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	Z	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	a	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	b	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	c	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	d	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	e	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	f	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	g	247	Total	C	N	O	S	0	0
			1897	1160	350	383	4		
1	h	154	Total	C	N	O	S	0	0
			1220	742	229	246	3		

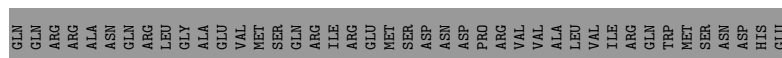




Chain C:  43% 56%



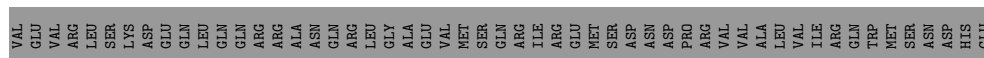
Chain D:  43% 56%



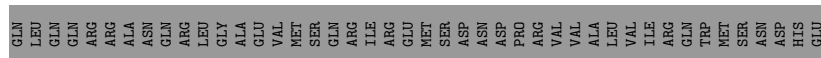
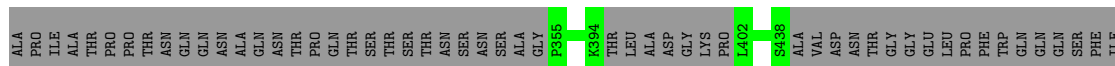


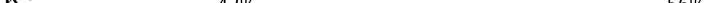


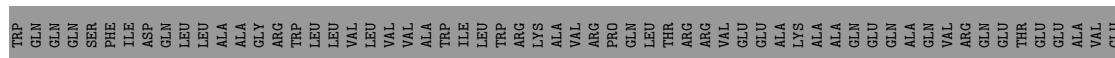
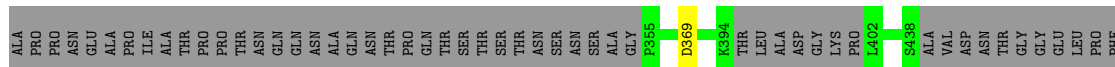
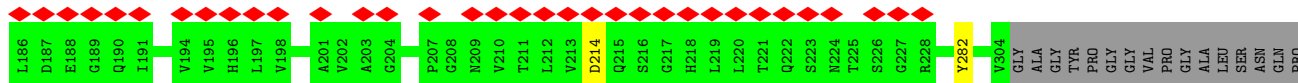
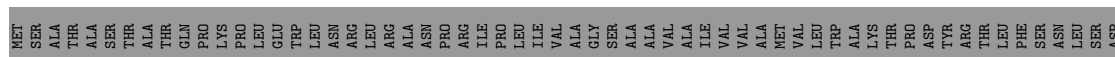




Chain J:  43% 56%



Chain K: 



VAL	ARG	GLN	ASP	GLU	GLN	LEU	GLN	GLN	ARG	ARG	ALA	ASN	GLN	ARG	GLY	ALA	GLU	MET	ASN	GLN	ARG	GLY	ASP	ASN	GLU	HIS	GLU
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• Molecule 1: Flagellar M-ring protein



MET	SER	THR	ALA	GLY	THR	ASP	GLN	PRO	THR	LEU	PRO	LEU	GLN	ARG	ASN	LEU	ARG	LEU	ALA	GLY	ASP	ASN	GLU	ASP	THR	PRO	ASP	TYR	THR	THR	THR	GLY	LEU	ASP	GLN	LEU	GLY	SER	ASP
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GLN	ASP	GLY	THR	ILE	VAL	ALA	GLN	THR	THR	GLN	PRO	LEU	GLN	ARG	ASN	LEU	ARG	LEU	ALA	GLY	ASP	ASN	GLU	ASP	THR	PRO	ASP	TYR	THR	THR	THR	GLY	LEU	ASP	GLN	LEU	GLY	SER	ASP
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PHE	GLY	ILE	Q125	M159	P160	LYS	THR	LEU	PRO	THR	LEU	GLN	ARG	ASN	LEU	ARG	LEU	ALA	GLY	ASP	ASN	GLU	ASP	THR	PRO	ASP	TYR	THR	THR	THR	GLY	LEU	ASP	GLN	LEU	GLY	SER	ASP	GLN	LEU	GLY	SER	ASP
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PRO	ALA	PRO	PRO	ASN	GLU	ALA	PRO	ILE	THR	THR	PRO	LEU	GLN	ARG	ASN	LEU	ARG	LEU	ALA	GLY	ASP	ASN	GLU	ASP	THR	PRO	ASP	TYR	THR	THR	THR	GLY	LEU	ASP	GLN	LEU	GLY	SER	ASP	GLN	LEU	GLY	SER	ASP
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GLN	GLN	SER	PHE	ASP	GLN	LEU	GLN	ALA	GLY	ARG	THR	LEU	GLN	ARG	ASN	LEU	ARG	LEU	ALA	GLY	ASP	ASN	GLU	ASP	THR	PRO	ASP	TYR	THR	THR	THR	GLY	LEU	ASP	GLN	LEU	GLY	SER	ASP	GLN	LEU	GLY	SER	ASP
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ARG	LEU	SER	LYS	ASP	GLU	GLN	LEU	GLN	ARG	ALA	GLY	ARG	ASN	LEU	ARG	LEU	ALA	GLY	ASP	ASN	GLU	ASP	THR	PRO	ASP	TYR	THR	THR	THR	GLY	LEU	ASP	GLN	LEU	GLY	SER	ASP	GLN	LEU	GLY	SER	ASP
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• Molecule 1: Flagellar M-ring protein



MET	SER	THR	ALA	GLY	THR	ASP	GLN	PRO	THR	LEU	PRO	LEU	GLN	ARG	ASN	LEU	ARG	LEU	ALA	GLY	ASP	ASN	GLU	ASP	THR	PRO	ASP	TYR	THR	THR	THR	GLY	LEU	ASP	GLN	LEU	GLY	SER	ASP	GLN	LEU	GLY	SER	ASP
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GLN	ASP	GLY	THR	ILE	VAL	ALA	GLN	THR	THR	PRO	LEU	GLN	ARG	ASN	LEU	ARG	LEU	ALA	GLY	ASP	ASN	GLU	ASP	THR	PRO	ASP	TYR	THR	THR	THR	GLY	LEU	ASP	GLN	LEU	GLY	SER	ASP	GLN	LEU	GLY	SER	ASP
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PHE	GLY	ILE	Q125	F126	L157	M159	P160	LYS	THR	LEU	PRO	LEU	GLN	ARG	ASN	LEU	ARG	LEU	ALA	GLY	ASP	ASN	GLU	ASP	THR	PRO	ASP	TYR	THR	THR	THR	GLY	LEU	ASP	GLN	LEU	GLY	SER	ASP	GLN	LEU	GLY	SER	ASP
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PRO	ASN	GLU	ALA	ILE	THR	PRO	PRO	ASN	GLN	GLN	ASN	LEU	GLN	ARG	ASN	LEU	ARG	LEU	ALA	GLY	ASP	ASN	GLU	ASP	THR	PRO	ASP	TYR	THR	THR	THR	GLY	LEU	ASP	GLN	LEU	GLY	SER	ASP	GLN	LEU	GLY	SER	ASP
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SER	PHE	ILE	ASP	GLN	LEU	GLN	ALA	THR	THR	PRO	LEU	GLN	ARG	ASN	LEU	ARG	LEU	ALA	GLY	ASP	ASN	GLU	ASP	THR	PRO	ASP	TYR	THR	THR	THR	GLY	LEU	ASP	GLN	LEU	GLY	SER	ASP	GLN	LEU	GLY	SER	ASP
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LYS	ASP	GLU	GLN	GLN	ARG	ALA	GLY	THR	THR	PRO	LEU	GLN	ARG	ASN	LEU	ARG	LEU	ALA	GLY	ASP	ASN	GLU	ASP	THR	PRO	ASP	TYR	THR	THR	THR	GLY	LEU	ASP	GLN	LEU	GLY	SER	ASP	GLN	LEU	GLY	SER	ASP
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• Molecule 1: Flagellar M-ring protein

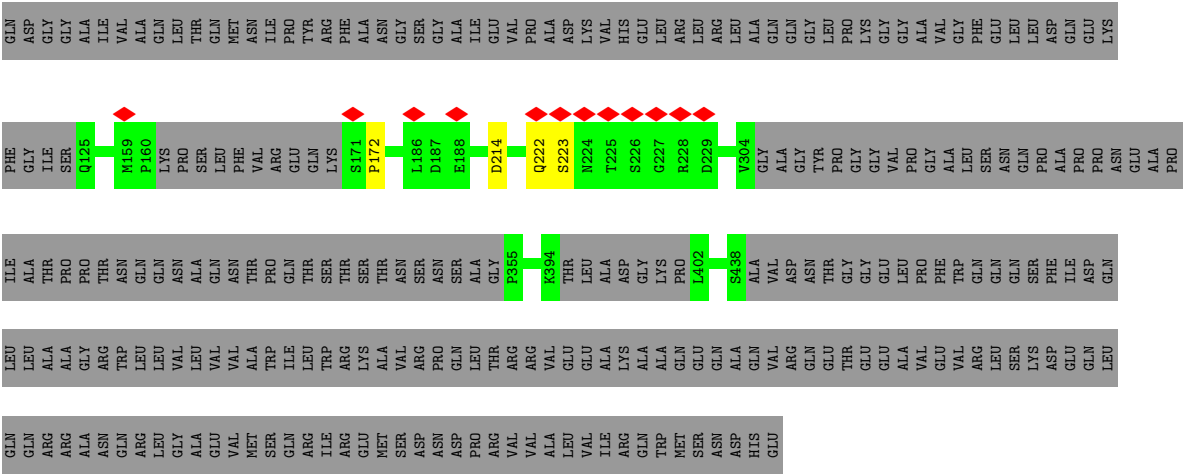


MET	SER	THR	ALA	GLY	THR	ASP	GLN	PRO	THR	LEU	PRO	LEU	GLN	ARG	ASN	LEU	ARG	LEU	ALA	GLY	ASP	ASN	GLU	ASP	THR	PRO	ASP	TYR	THR	THR	THR	GLY	LEU	ASP	GLN	LEU	GLY	SER	ASP	GLN	LEU	GLY	SER	ASP
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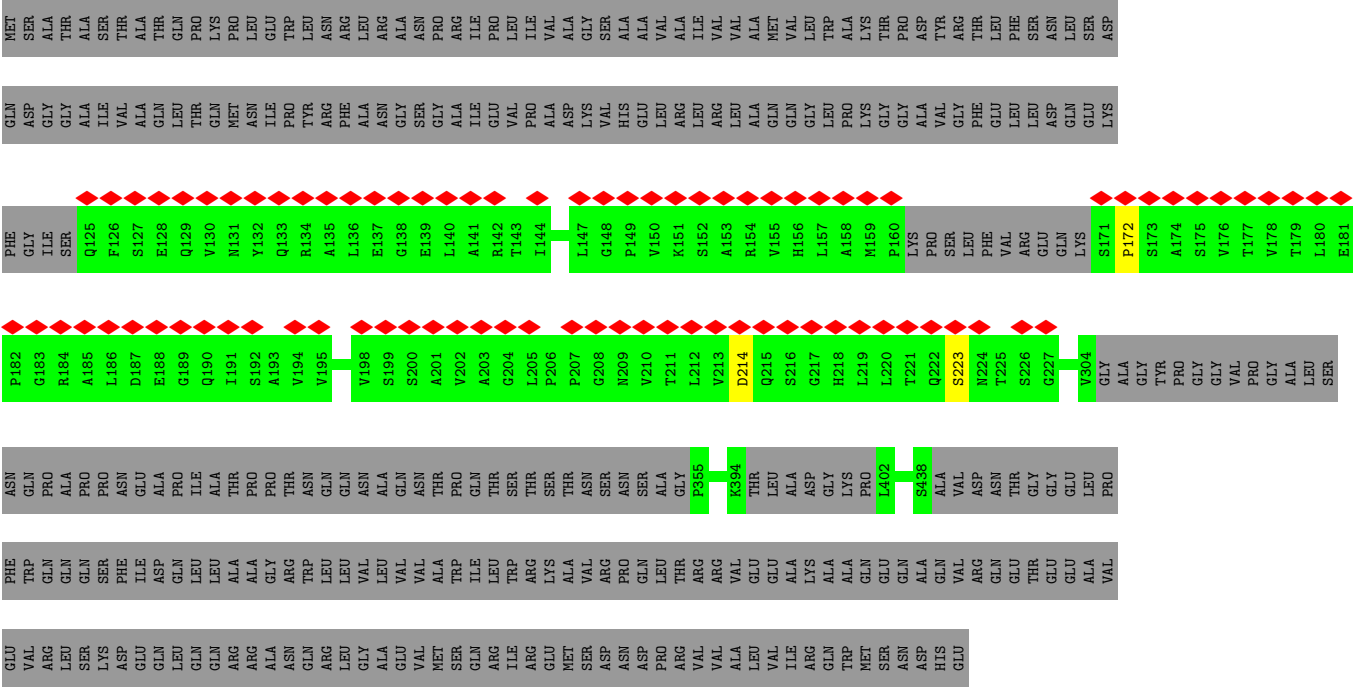




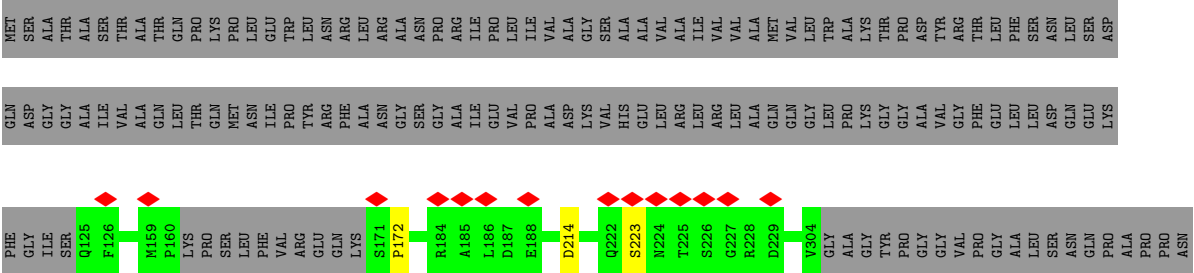
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• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein



GLU  
GLN  
LEU  
LEU  
GLN  
GLN  
ARG  
ARG  
ALA  
ASN  
GLN  
ARG  
LEU  
GLY  
ALA  
GLU  
VAL  
MET  
SER  
GLN  
ARG  
ILE  
ARG  
GLU  
MET  
SER  
ASP  
ASN  
ASP  
PRO  
ARG  
VAL  
VAL  
ALA  
LEU  
LEU  
VAL  
ILE  
ARG  
GLN  
TRP  
MET  
SER  
ASN  
ASP  
HIS  
GLU

- Molecule 1: Flagellar M-ring protein



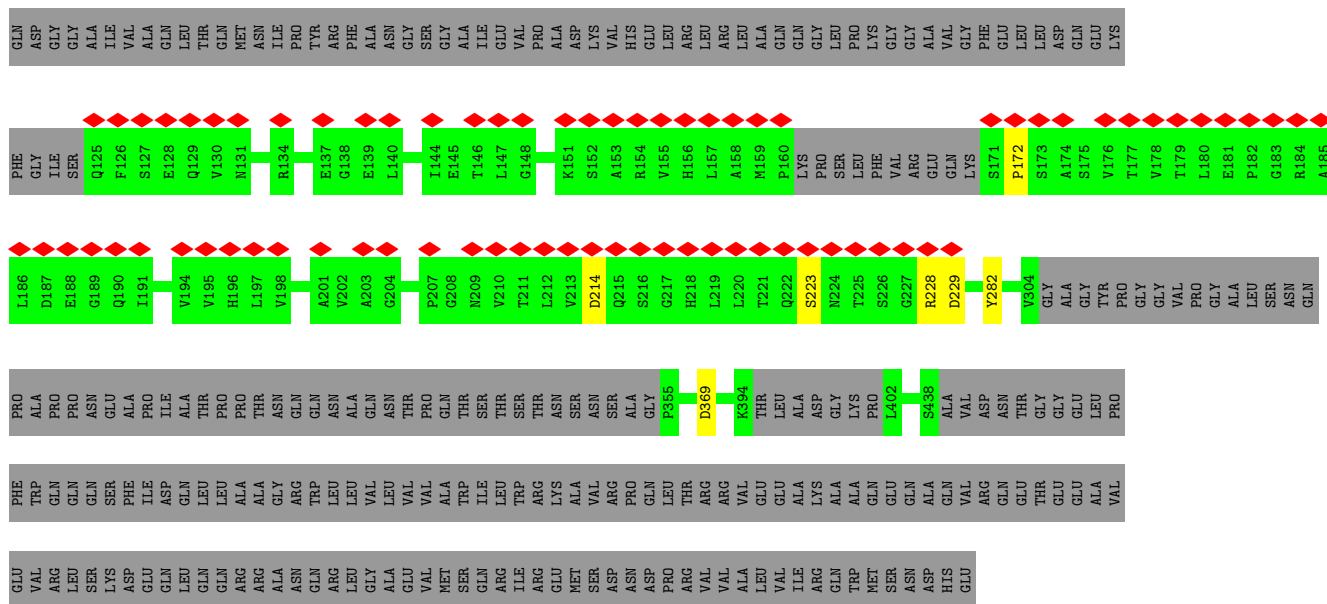
LYS ASP GLN LEU GLN ARG ARG ASN GLN LEU GLY ALA GLU VAL MET SER SER ASP ASP ASP PRO ARG VAL VAL ALA LEU VAL ILE ARG GLN TRP MET SER ASN ASP HIS GLU

- Molecule 1: Flagellar M-ring protein

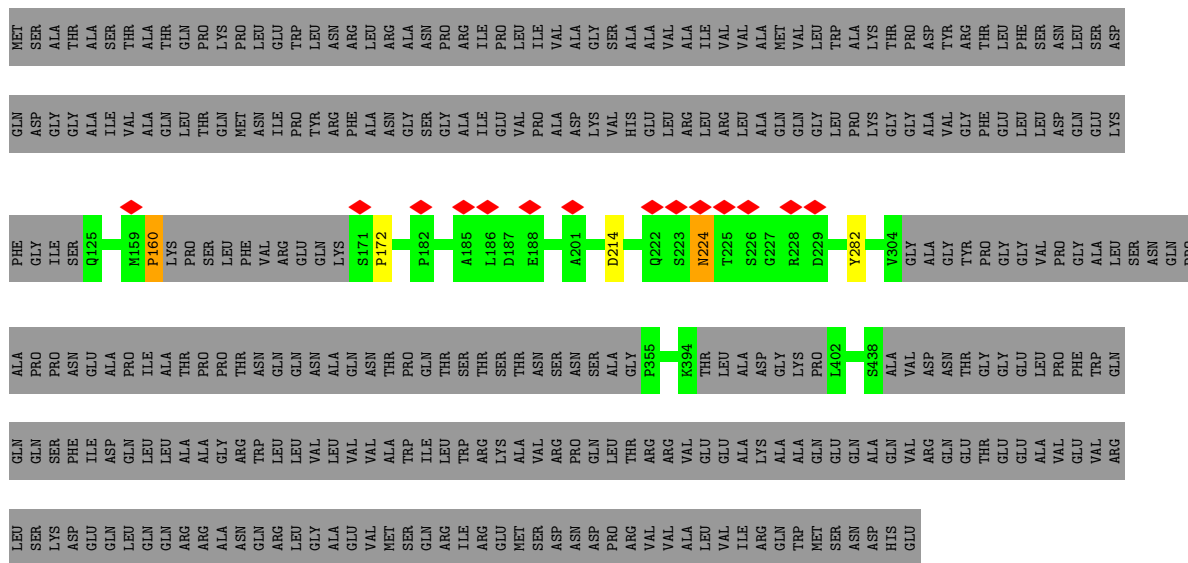
[illegible]



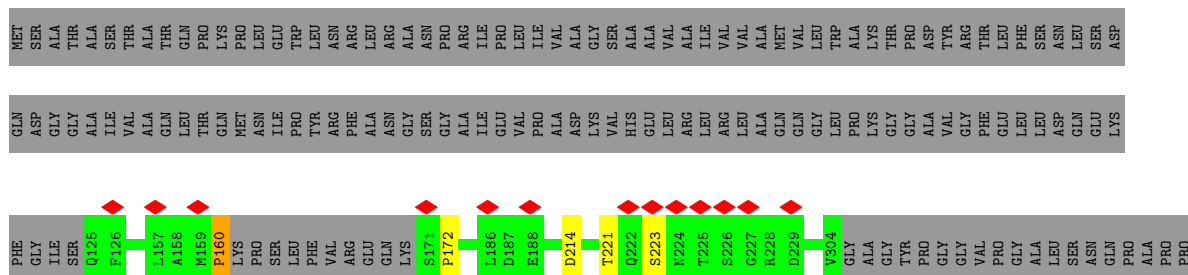




- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	140606	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 ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.009	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	355.104, 355.104, 355.104	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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	0.40	0/1919	0.50	0/2598
1	B	0.40	0/1919	0.51	1/2598 (0.0%)
1	C	0.39	0/1919	0.51	1/2598 (0.0%)
1	D	0.40	0/1919	0.50	0/2598
1	E	0.40	0/1919	0.51	0/2598
1	F	0.40	0/1919	0.51	0/2598
1	G	0.41	0/1919	0.63	8/2598 (0.3%)
1	H	0.40	0/1919	0.50	0/2598
1	I	0.41	0/1919	0.54	2/2598 (0.1%)
1	J	0.39	0/1919	0.51	0/2598
1	K	0.40	0/1919	0.52	1/2598 (0.0%)
1	L	0.41	0/1919	0.55	3/2598 (0.1%)
1	M	0.42	0/1919	0.56	2/2598 (0.1%)
1	N	0.40	0/1919	0.51	1/2598 (0.0%)
1	O	0.42	0/1919	0.54	2/2598 (0.1%)
1	P	0.39	0/1919	0.51	0/2598
1	Q	0.42	0/1232	0.50	0/1660
1	R	0.40	0/1919	0.51	0/2598
1	S	0.40	0/1919	0.51	1/2598 (0.0%)
1	T	0.40	0/1919	0.51	1/2598 (0.0%)
1	U	0.40	0/1919	0.50	0/2598
1	V	0.41	0/1919	0.51	0/2598
1	W	0.40	0/1919	0.50	0/2598
1	X	0.41	0/1919	0.53	2/2598 (0.1%)
1	Y	0.40	0/1919	0.50	0/2598
1	Z	0.41	0/1919	0.55	2/2598 (0.1%)
1	a	0.46	2/1919 (0.1%)	0.58	3/2598 (0.1%)
1	b	0.40	0/1919	0.52	1/2598 (0.0%)
1	c	0.41	0/1918	0.53	2/2595 (0.1%)
1	d	0.43	0/1919	0.53	1/2598 (0.0%)
1	e	0.39	0/1919	0.51	1/2598 (0.0%)
1	f	0.42	0/1919	0.57	3/2598 (0.1%)
1	g	0.39	0/1919	0.50	0/2598
1	h	0.42	0/1232	0.51	0/1660

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.41	2/63871 (0.0%)	0.52	38/86453 (0.0%)

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	G	0	1
1	I	0	1
1	L	0	2
1	f	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	160	PRO	N-CA	6.36	1.58	1.47
1	a	171	SER	N-CA	5.51	1.57	1.46

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	160	PRO	N-CA-CB	-9.35	92.08	103.30
1	G	222	GLN	CA-C-N	-8.31	98.91	117.20
1	f	160	PRO	N-CA-CB	-7.62	94.16	103.30
1	f	282	TYR	C-N-CA	-7.42	103.15	121.70
1	O	282	TYR	C-N-CA	-7.41	103.17	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	222	GLN	Mainchain
1	I	221	THR	Mainchain
1	L	227	GLY	Mainchain
1	L	228	ARG	Sidechain
1	f	159	MET	Mainchain

## 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	A	239/560 (43%)	213 (89%)	25 (10%)	1 (0%)	34	66
1	B	239/560 (43%)	214 (90%)	24 (10%)	1 (0%)	34	66
1	C	239/560 (43%)	212 (89%)	26 (11%)	1 (0%)	34	66
1	D	239/560 (43%)	210 (88%)	28 (12%)	1 (0%)	34	66
1	E	239/560 (43%)	210 (88%)	28 (12%)	1 (0%)	34	66
1	F	239/560 (43%)	212 (89%)	27 (11%)	0	100	100
1	G	239/560 (43%)	213 (89%)	24 (10%)	2 (1%)	19	51
1	H	239/560 (43%)	213 (89%)	24 (10%)	2 (1%)	19	51
1	I	239/560 (43%)	213 (89%)	23 (10%)	3 (1%)	12	40
1	J	239/560 (43%)	216 (90%)	22 (9%)	1 (0%)	34	66
1	K	239/560 (43%)	211 (88%)	27 (11%)	1 (0%)	34	66
1	L	239/560 (43%)	205 (86%)	28 (12%)	6 (2%)	5	27
1	M	239/560 (43%)	205 (86%)	31 (13%)	3 (1%)	12	40
1	N	239/560 (43%)	210 (88%)	26 (11%)	3 (1%)	12	40
1	O	239/560 (43%)	209 (87%)	27 (11%)	3 (1%)	12	40
1	P	239/560 (43%)	215 (90%)	24 (10%)	0	100	100
1	Q	148/560 (26%)	133 (90%)	14 (10%)	1 (1%)	22	54
1	R	239/560 (43%)	211 (88%)	27 (11%)	1 (0%)	34	66
1	S	239/560 (43%)	215 (90%)	23 (10%)	1 (0%)	34	66
1	T	239/560 (43%)	212 (89%)	26 (11%)	1 (0%)	34	66
1	U	239/560 (43%)	209 (87%)	29 (12%)	1 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	239/560 (43%)	211 (88%)	27 (11%)	1 (0%)	34	66
1	W	239/560 (43%)	212 (89%)	26 (11%)	1 (0%)	34	66
1	X	239/560 (43%)	212 (89%)	24 (10%)	3 (1%)	12	40
1	Y	239/560 (43%)	212 (89%)	25 (10%)	2 (1%)	19	51
1	Z	239/560 (43%)	213 (89%)	24 (10%)	2 (1%)	19	51
1	a	239/560 (43%)	213 (89%)	23 (10%)	3 (1%)	12	40
1	b	239/560 (43%)	210 (88%)	27 (11%)	2 (1%)	19	51
1	c	237/560 (42%)	210 (89%)	25 (10%)	2 (1%)	19	51
1	d	239/560 (43%)	210 (88%)	27 (11%)	2 (1%)	19	51
1	e	239/560 (43%)	209 (87%)	28 (12%)	2 (1%)	19	51
1	f	239/560 (43%)	208 (87%)	28 (12%)	3 (1%)	12	40
1	g	239/560 (43%)	212 (89%)	27 (11%)	0	100	100
1	h	148/560 (26%)	133 (90%)	14 (10%)	1 (1%)	22	54
All	All	7942/19040 (42%)	7026 (88%)	858 (11%)	58 (1%)	26	54

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	172	PRO
1	G	223	SER
1	I	223	SER
1	L	172	PRO
1	L	228	ARG

### 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	213/467 (46%)	211 (99%)	2 (1%)	78	87
1	B	213/467 (46%)	211 (99%)	2 (1%)	78	87
1	C	213/467 (46%)	210 (99%)	3 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	213/467 (46%)	209 (98%)	4 (2%)	57	77
1	E	213/467 (46%)	211 (99%)	2 (1%)	78	87
1	F	213/467 (46%)	211 (99%)	2 (1%)	78	87
1	G	213/467 (46%)	210 (99%)	3 (1%)	67	82
1	H	213/467 (46%)	210 (99%)	3 (1%)	67	82
1	I	213/467 (46%)	210 (99%)	3 (1%)	67	82
1	J	213/467 (46%)	210 (99%)	3 (1%)	67	82
1	K	213/467 (46%)	211 (99%)	2 (1%)	78	87
1	L	213/467 (46%)	207 (97%)	6 (3%)	43	70
1	M	213/467 (46%)	209 (98%)	4 (2%)	57	77
1	N	213/467 (46%)	211 (99%)	2 (1%)	78	87
1	O	213/467 (46%)	210 (99%)	3 (1%)	67	82
1	P	213/467 (46%)	210 (99%)	3 (1%)	67	82
1	Q	137/467 (29%)	136 (99%)	1 (1%)	84	90
1	R	213/467 (46%)	211 (99%)	2 (1%)	78	87
1	S	213/467 (46%)	211 (99%)	2 (1%)	78	87
1	T	213/467 (46%)	210 (99%)	3 (1%)	67	82
1	U	213/467 (46%)	210 (99%)	3 (1%)	67	82
1	V	213/467 (46%)	211 (99%)	2 (1%)	78	87
1	W	213/467 (46%)	211 (99%)	2 (1%)	78	87
1	X	213/467 (46%)	211 (99%)	2 (1%)	78	87
1	Y	213/467 (46%)	210 (99%)	3 (1%)	67	82
1	Z	213/467 (46%)	210 (99%)	3 (1%)	67	82
1	a	213/467 (46%)	210 (99%)	3 (1%)	67	82
1	b	213/467 (46%)	209 (98%)	4 (2%)	57	77
1	c	213/467 (46%)	210 (99%)	3 (1%)	67	82
1	d	213/467 (46%)	209 (98%)	4 (2%)	57	77
1	e	213/467 (46%)	211 (99%)	2 (1%)	78	87
1	f	213/467 (46%)	209 (98%)	4 (2%)	57	77
1	g	213/467 (46%)	209 (98%)	4 (2%)	57	77
1	h	137/467 (29%)	136 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	7090/15878 (45%)	6995 (99%)	95 (1%)	70	82

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	223	SER
1	a	214	ASP
1	V	223	SER
1	Y	223	SER
1	b	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 185 such sidechains are listed below:

Mol	Chain	Res	Type
1	V	365	ASN
1	a	365	ASN
1	W	274	ASN
1	Y	299	ASN
1	b	365	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	c	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c	228:ARG	C	229:ASP	N	5.41

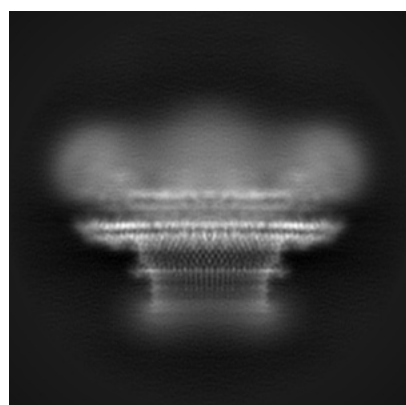
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10147. These allow visual inspection of the internal detail of the map and identification of artifacts.

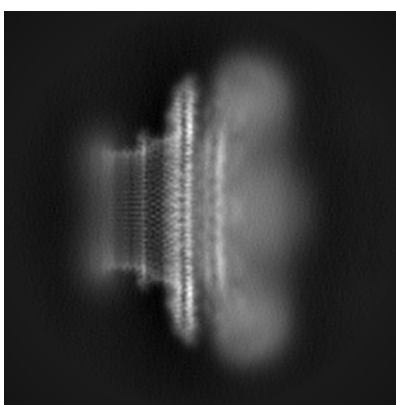
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

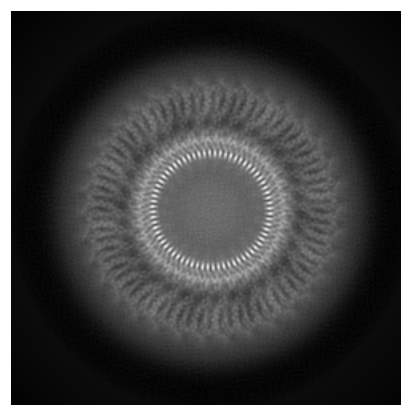
#### 6.1.1 Primary map



X



Y

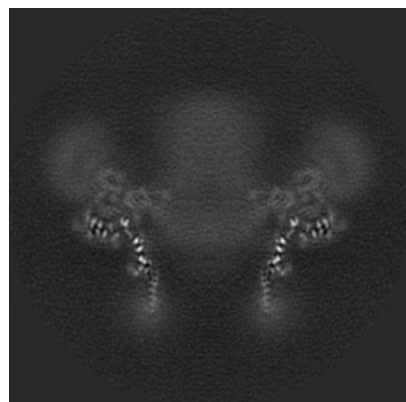


Z

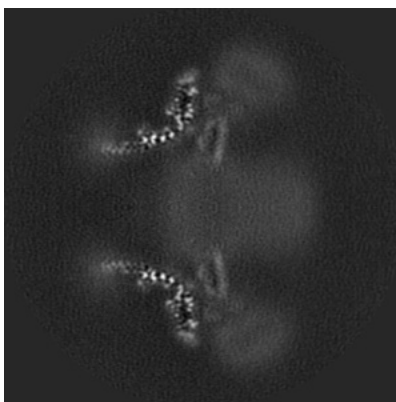
The images above show the map projected in three orthogonal directions.

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

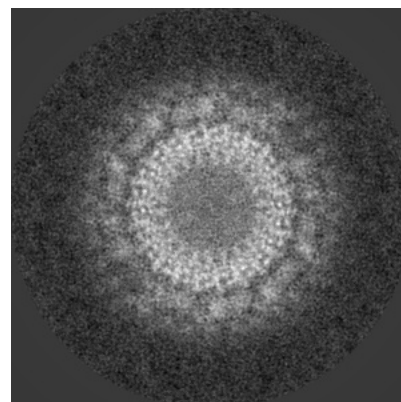
#### 6.2.1 Primary map



X Index: 216



Y Index: 216

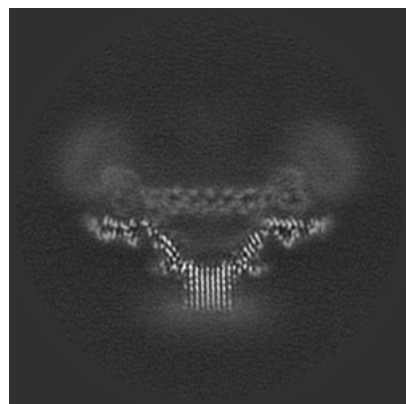


Z Index: 216

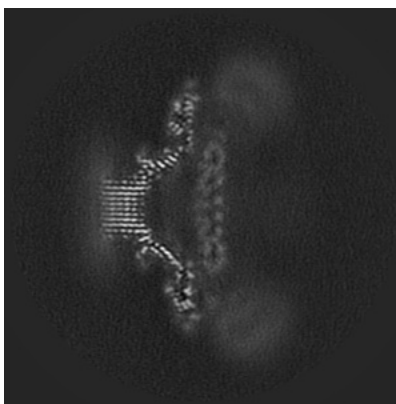
The images above show central slices of the map in three orthogonal directions.

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

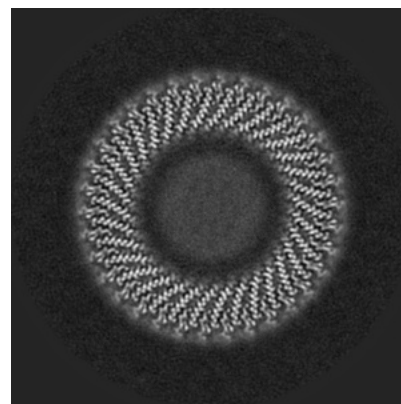
### 6.3.1 Primary map



X Index: 154



Y Index: 275

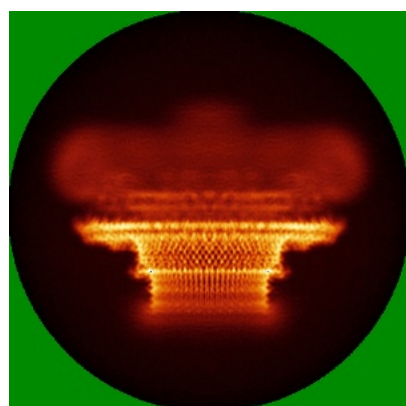


Z Index: 199

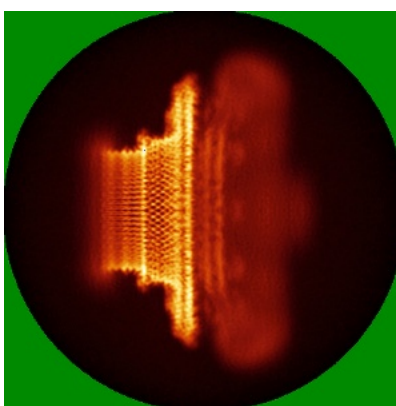
The images above show the largest variance slices of the map in three orthogonal directions.

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

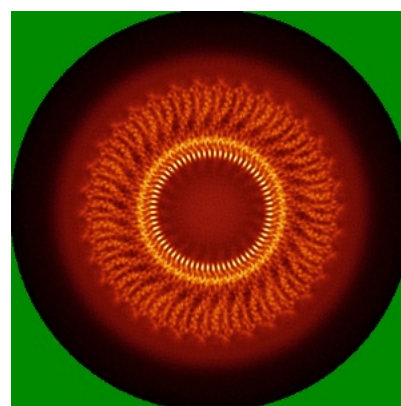
### 6.4.1 Primary map



X



Y

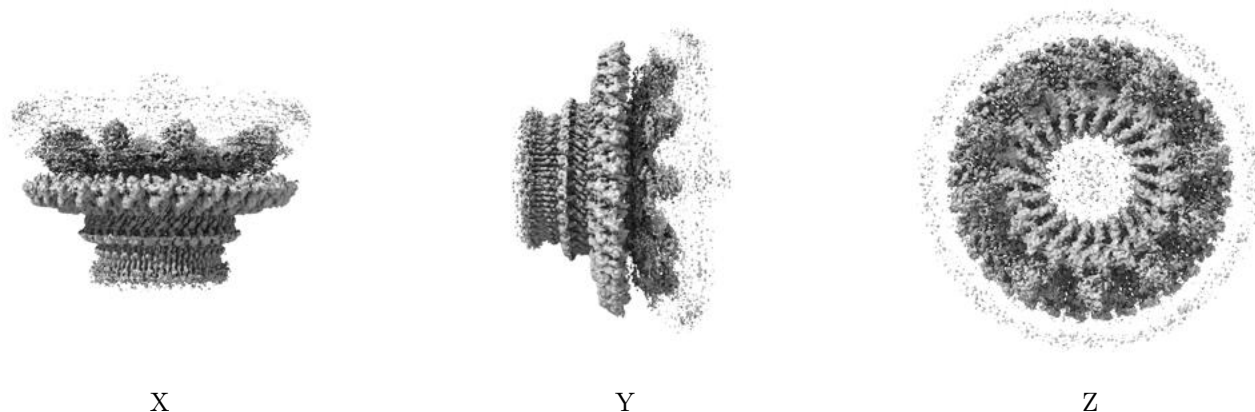


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

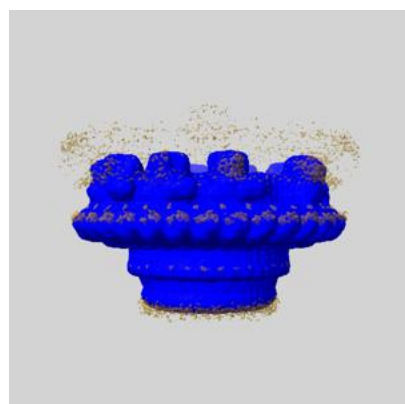
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

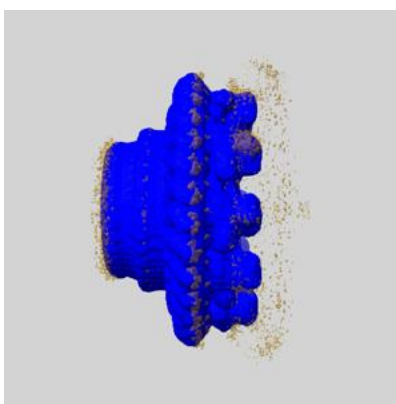
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

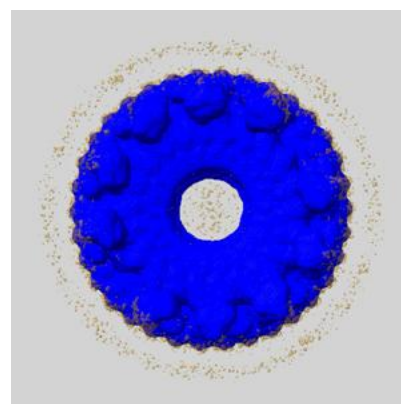
### 6.6.1 emd\_10147\_msk\_1.map [i](#)



X



Y



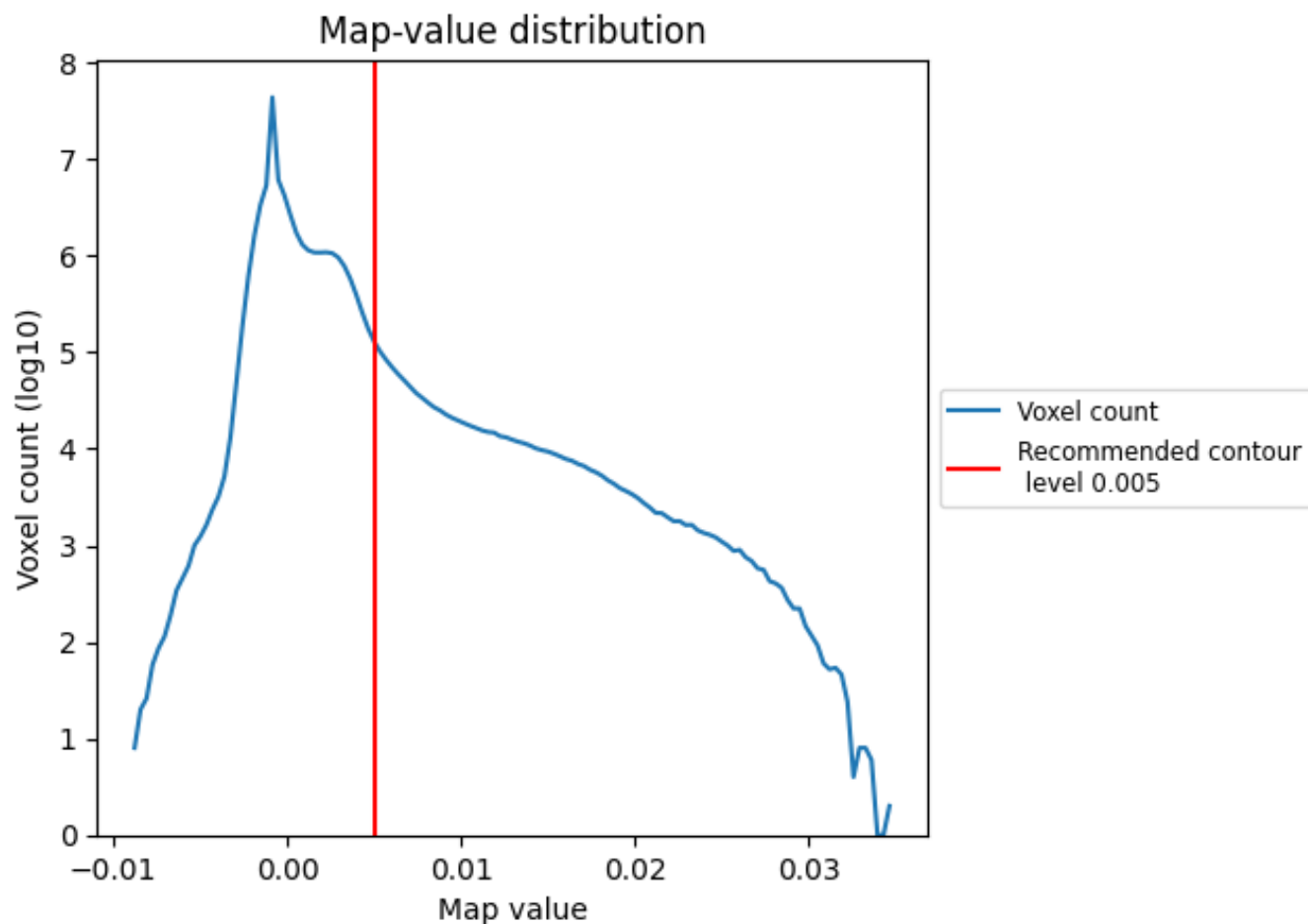
Z



## 7 Map analysis [i](#)

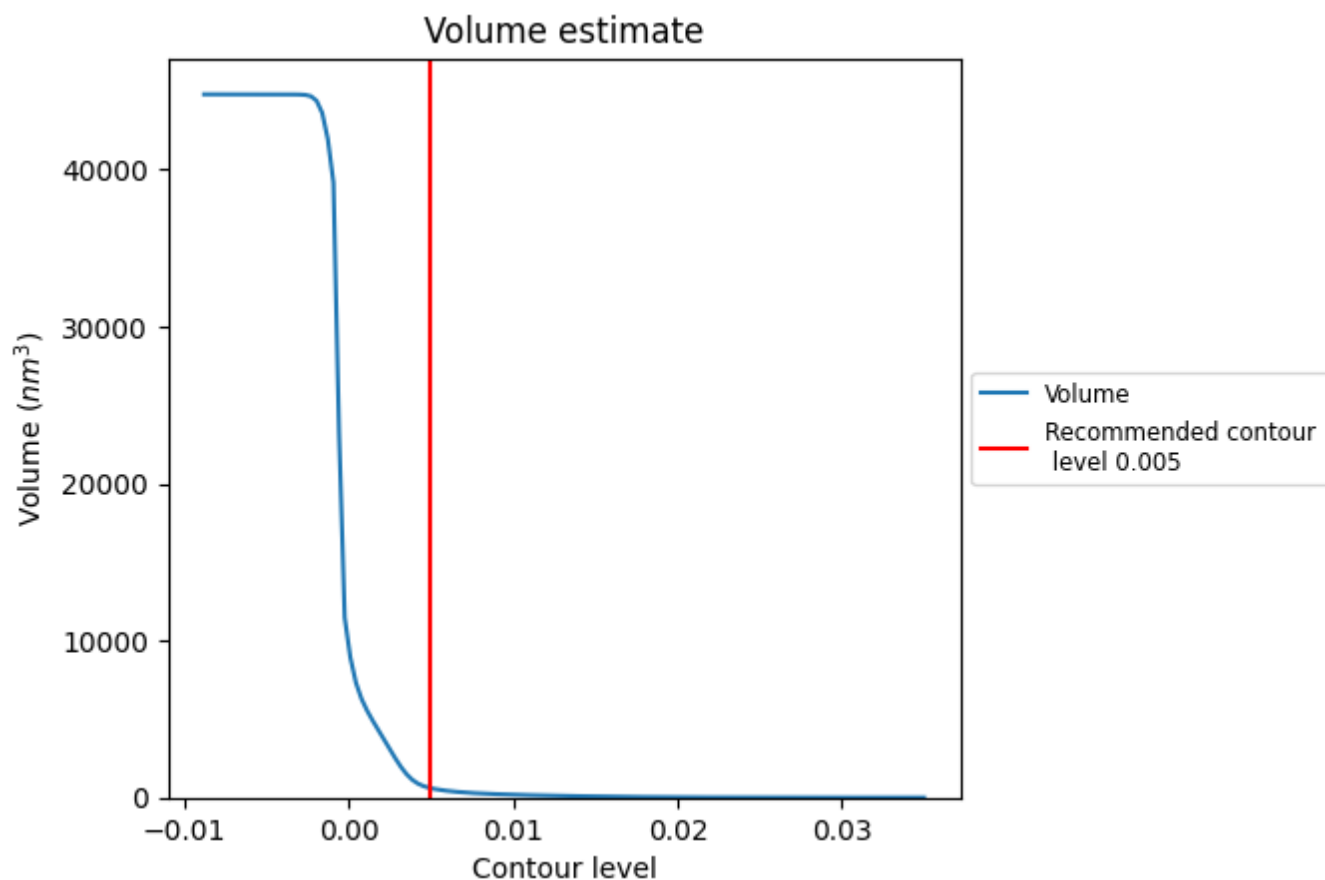
This section contains the results of statistical analysis of the map.

### 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.

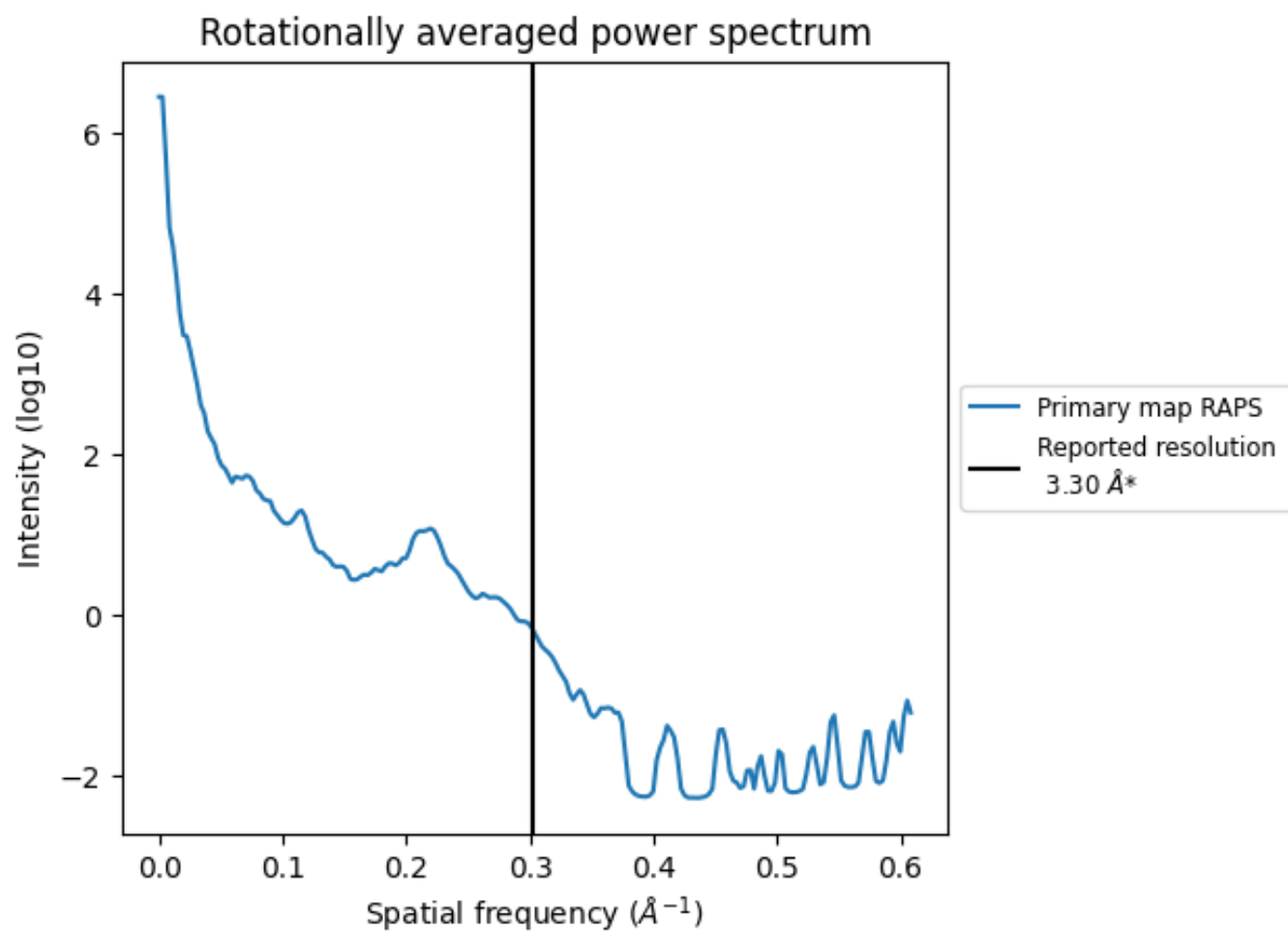
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 600 nm<sup>3</sup>; this corresponds to an approximate mass of 542 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 ⓘ

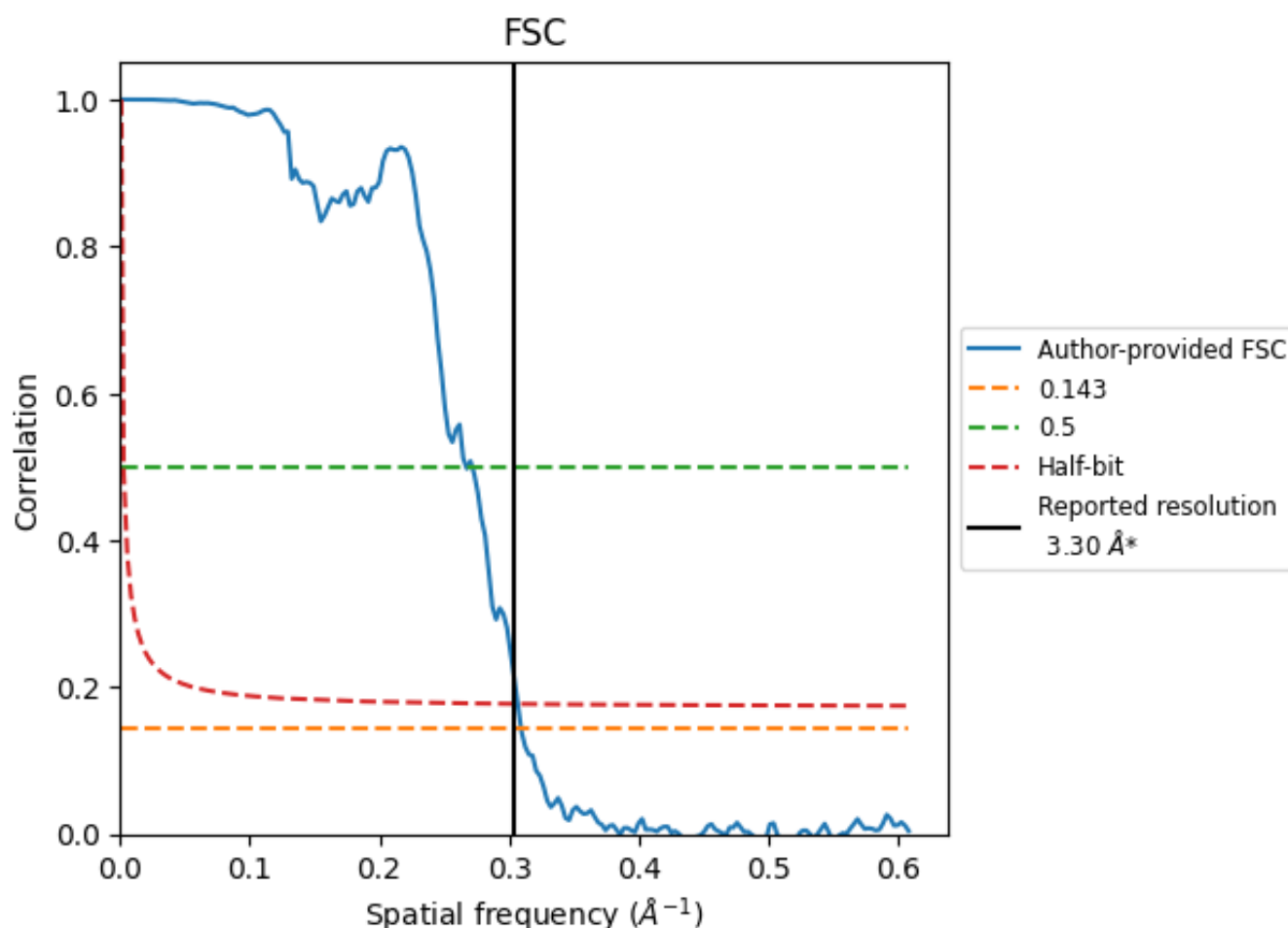


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

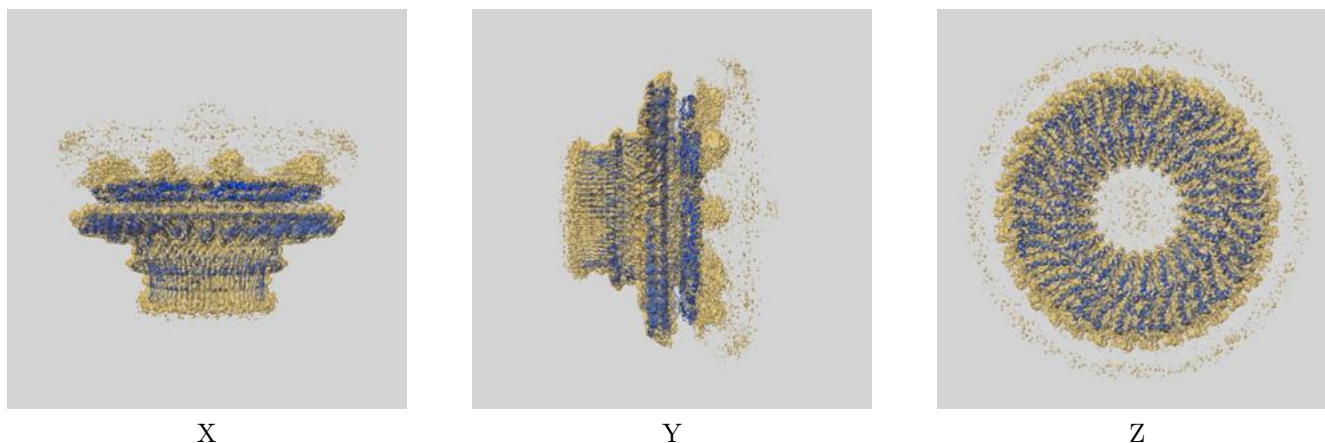
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.23	3.75	3.26
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

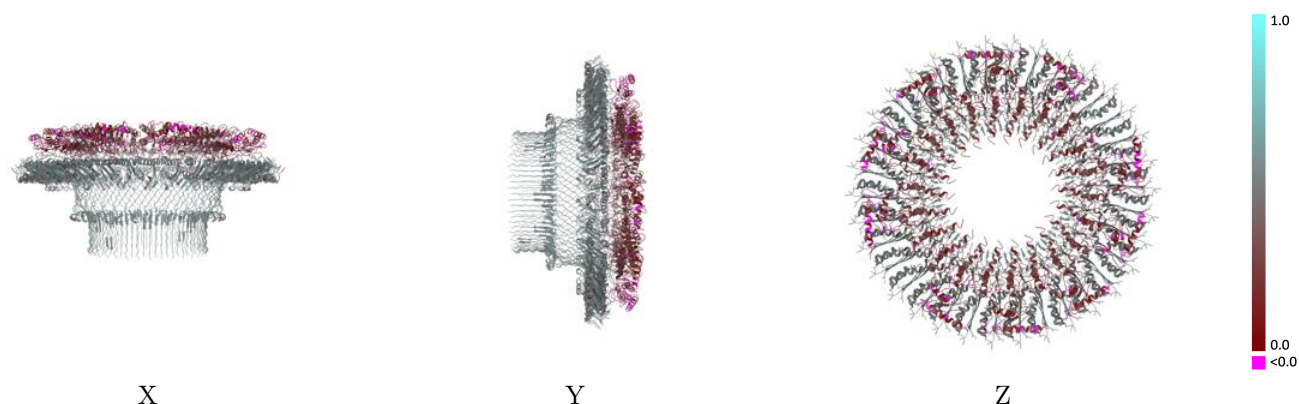
This section contains information regarding the fit between EMDB map EMD-10147 and PDB model 6SD3. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



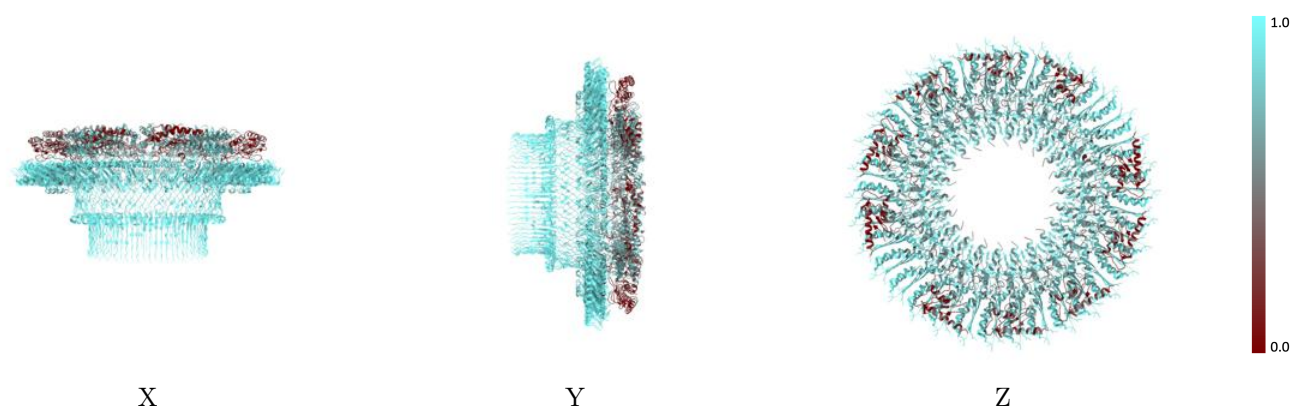
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



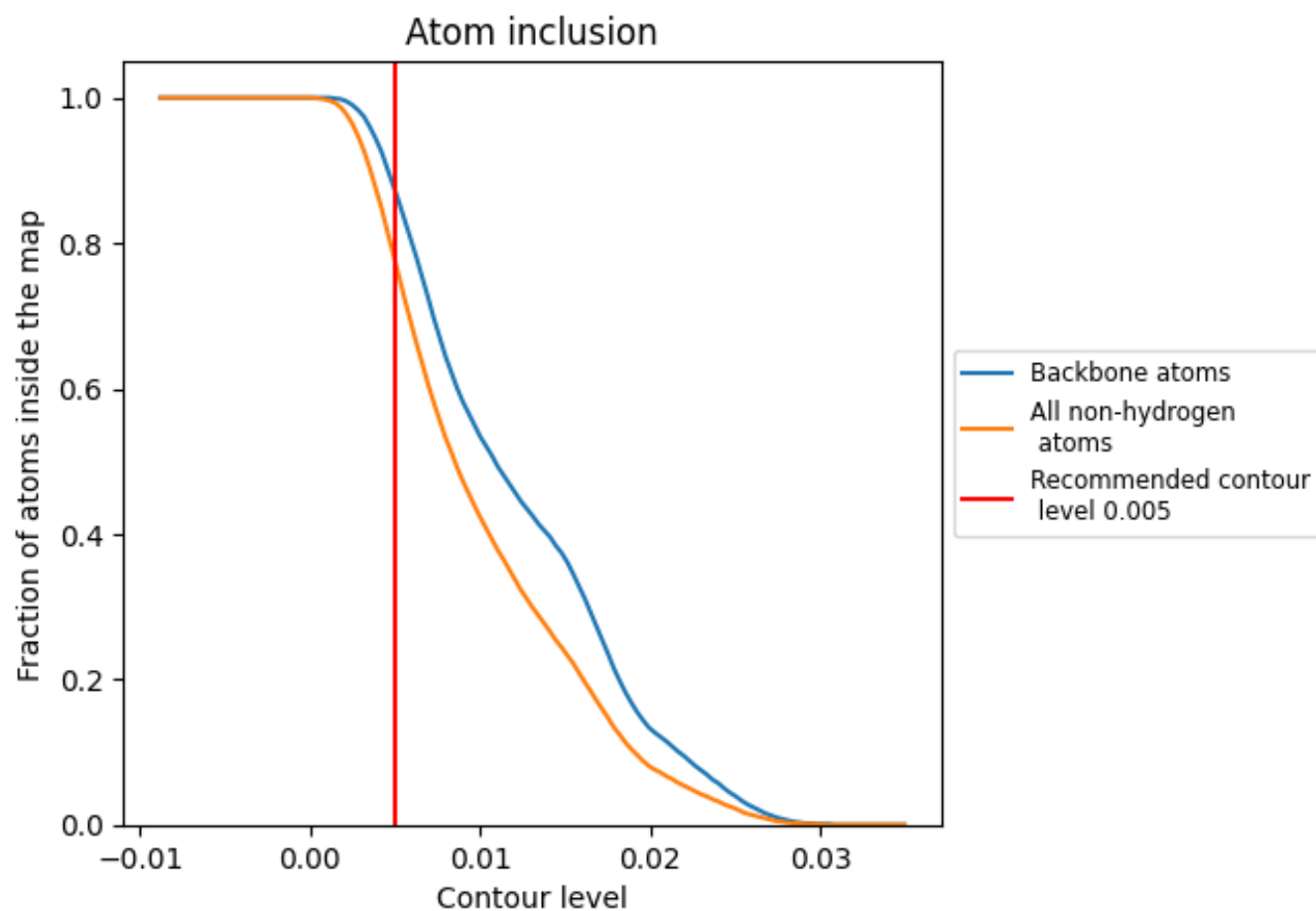
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.4150
A	 0.8220	 0.4200
B	 0.6220	 0.3750
C	 0.8240	 0.4290
D	 0.8190	 0.4300
E	 0.6500	 0.3670
F	 0.8240	 0.4310
G	 0.8310	 0.4350
H	 0.6760	 0.3890
I	 0.8120	 0.4210
J	 0.8180	 0.4190
K	 0.6850	 0.3910
L	 0.8250	 0.4230
M	 0.8180	 0.4150
N	 0.6420	 0.3820
O	 0.8210	 0.4190
P	 0.8340	 0.4240
Q	 0.9290	 0.5090
R	 0.8230	 0.4190
S	 0.6210	 0.3770
T	 0.8270	 0.4310
U	 0.8230	 0.4300
V	 0.6510	 0.3670
W	 0.8240	 0.4320
X	 0.8320	 0.4350
Y	 0.6790	 0.3890
Z	 0.8100	 0.4200
a	 0.8150	 0.4180
b	 0.6840	 0.3930
c	 0.8260	 0.4240
d	 0.8240	 0.4210
e	 0.6450	 0.3830
f	 0.8230	 0.4220
g	 0.8290	 0.4230
h	 0.9290	 0.5110

