



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 12:25 pm GMT

PDB ID : 6SD5
EMDB ID : EMD-10149
Title : Structure of the RBM2 inner ring of Salmonella flagella MS-ring protein FlIF with 22-fold symmetry applied
Authors : Johnson, S.; Fong, Y.H.; Deme, J.C.; Furlong, E.J.; Kuhlen, L.; Lea, S.M.
Deposited on : 2019-07-26
Resolution : 3.10 Å (reported)
Based on initial model : 6SCN

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

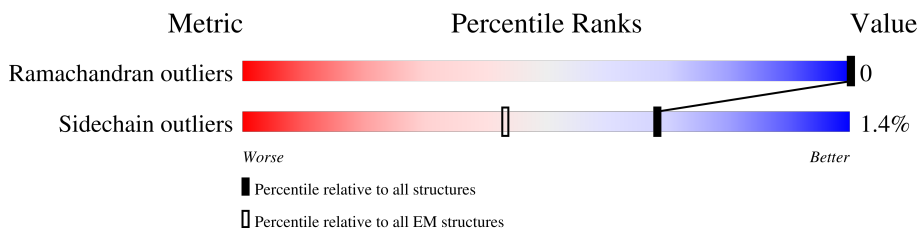
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.








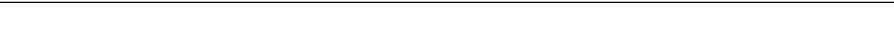

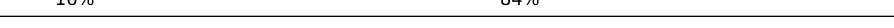
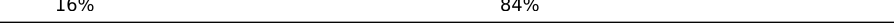




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	A	560	16%	84%
1	C	560	16%	84%
1	D	560	16%	84%
1	F	560	16%	84%
1	G	560	16%	84%
1	I	560	16%	84%
1	J	560	16%	84%
1	L	560	16%	84%
1	M	560	16%	84%

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Mol	Chain	Length	Quality of chain	
1	O	560	 16%	84%
1	P	560	 16%	84%
1	R	560	 16%	84%
1	T	560	 16%	84%
1	U	560	 16%	84%
1	W	560	 16%	84%
1	X	560	 16%	84%
1	Z	560	 16%	84%
1	a	560	 16%	84%
1	c	560	 16%	84%
1	d	560	 16%	84%
1	f	560	 16%	84%
1	g	560	 16%	84%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 14212 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
			Total	C	N	O	S		
1	A	88	646	402	115	128	1	0	0
1	C	88	646	402	115	128	1	0	0
1	D	88	646	402	115	128	1	0	0
1	F	88	646	402	115	128	1	0	0
1	G	88	646	402	115	128	1	0	0
1	I	88	646	402	115	128	1	0	0
1	J	88	646	402	115	128	1	0	0
1	L	88	646	402	115	128	1	0	0
1	M	88	646	402	115	128	1	0	0
1	O	88	646	402	115	128	1	0	0
1	P	88	646	402	115	128	1	0	0
1	R	88	646	402	115	128	1	0	0
1	T	88	646	402	115	128	1	0	0
1	U	88	646	402	115	128	1	0	0
1	W	88	646	402	115	128	1	0	0
1	X	88	646	402	115	128	1	0	0
1	Z	88	646	402	115	128	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	88	Total	C	N	O	S	0	0
			646	402	115	128	1		
1	c	88	Total	C	N	O	S	0	0
			646	402	115	128	1		
1	d	88	Total	C	N	O	S	0	0
			646	402	115	128	1		
1	f	88	Total	C	N	O	S	0	0
			646	402	115	128	1		
1	g	88	Total	C	N	O	S	0	0
			646	402	115	128	1		

PHE	GLY	ILE	SER	THR	GLN	VAL	THR	LYS	GLY	GLU	ASN	GLY	THR	ASP	LEU	ASN	ASN	ASN	ASP	VAL	GLU	SER
Q125	E128	P160	PRO	SER	LEU	PHE	ALA	ASN	ARG	GLN	LYS	S171	D214	Q222	SER	ASN	THR	GLY	ARG	ASP	LEU	ASN
ASN	GLY	ASN	VAL	HIS	ALA	GLN	VAL	THR	ALA	GLN	PRO	SER	LEU	PHE	ASP	ALA	VAL	GLN	LYS	ILE	GLU	ASN
GLN	PRO	ALA	PRO	PRO	ASN	GLY	VAL	GLU	ALA	ILE	ALA	THR	LEU	ASP	PRO	THR	THR	GLN	LYS	THR	ASN	ASN
VAL	GLY	ASP	ILE	GLU	ARG	LEU	VAL	VAL	PRO	TRP	VAL	VAL	ASP	ASN	THR	THR	TYR	LYS	ASN	ASN	VAL	ASN
ALA	VAL	ASP	ASN	THR	GLY	GLY	LEU	VAL	PHE	TRP	GLN	GLN	PHE	THR	THR	GLN	ASN	LYS	THR	GLN	GLY	ASN
GLN	VAL	ARG	GLN	GLU	THR	GLU	ALA	VAL	VAL	GLU	VAL	ARG	LEU	ASN	GLY	LEU	GLN	ASP	ILE	ASP	ARG	ASN
HIS	GLU																					

Molecule 1: Flagellar M-ring protein

Chain D: 16% 84%

MET	SER	ALA	THR	THR	ALA	THR	GLN	VAL	THR	LYS	LEU	LEU	LEU	ILE	ILE	ILE	THR	PRO	GLN	ARG	LEU	ASP
GLN	ASP	GLY	ALA	ILE	VAL	ALA	GLN	GLN	THR	VAL	MET	ASN	ILE	PRO	TYR	PHE	ARG	ALA	ASN	GLY	ALA	LYS
PHE	GLY	ILE	SER	Q125	E128	P160	LYS	GLY	LEU	SER	LEU	PHE	ALA	ASN	ARG	GLN	LYS	S171	D214	Q222	SER	ASN
ASN	GLY	ASN	VAL	HIS	ALA	GLN	VAL	THR	ALA	GLN	VAL	PHE	ALA	ASN	ARG	GLU	GLY	THR	GLY	HIS	TYR	PRO
GLN	PRO	ALA	PRO	PRO	ASN	GLY	VAL	GLU	ALA	ILE	PRO	PRO	THR	THR	ASN	GLN	ASN	ALA	ALA	THR	GLN	THR
VAL	GLY	ASP	ILE	GLU	ARG	LEU	VAL	VAL	PRO	TRP	VAL	VAL	ASP	ASN	TYR	THR	LYS	ASP	THR	THR	THR	THR
ALA	VAL	ASP	ASN	THR	GLY	GLY	LEU	VAL	PHE	TRP	GLN	GLN	PHE	THR	THR	GLN	ASN	LYS	THR	GLN	GLY	ASN
GLN	VAL	ARG	GLN	GLU	THR	ALA	VAL	VAL	PRO	PHE	VAL	VAL	ARG	LEU	LYS	VAL	GLY	ASP	ILE	ASP	ARG	ASP
HIS	GLU																					

Molecule 1: Flagellar M-ring protein

Chain F: 16% 84%

Molecule 1: Flagellar M-ring protein

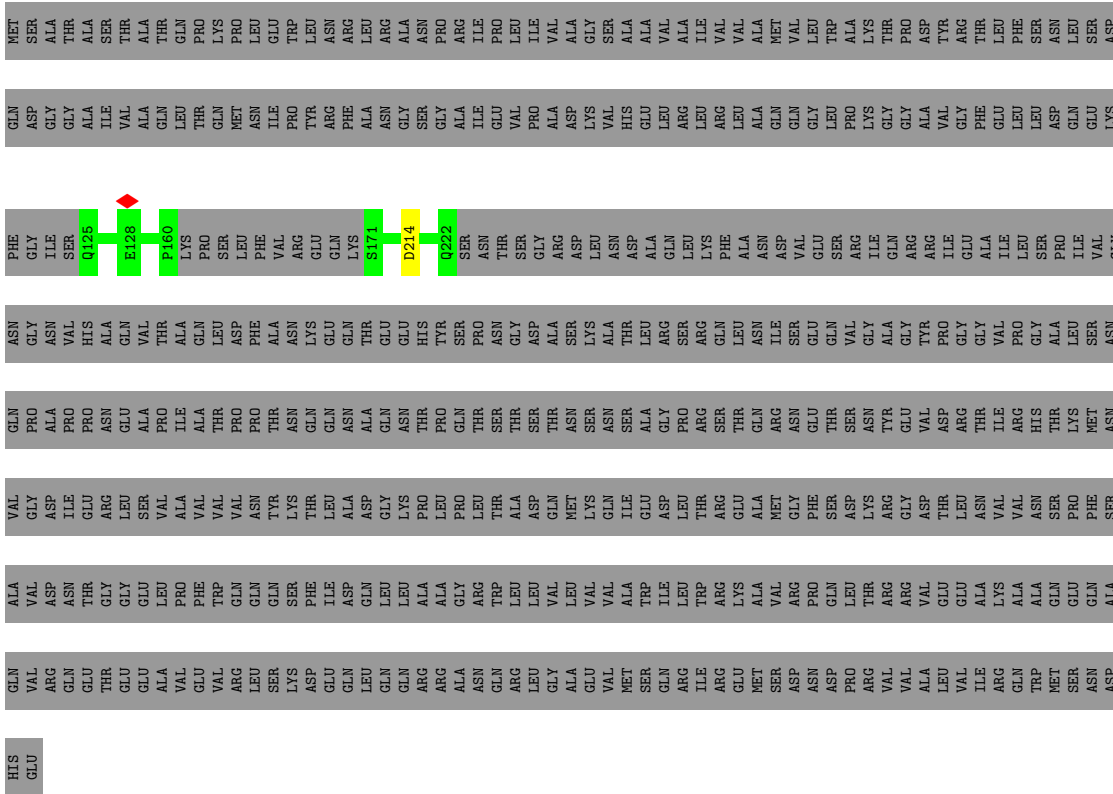
Chain I: 16% 84%

Table of amino acid sequences for Chain I, showing residues MET through ASP with highlighted positions Q125, E128, P160, S173, D214, and Q222.

Molecule 1: Flagellar M-ring protein

Chain J: 16% 84%

Table of amino acid sequences for Chain J, showing residues MET through ASP with highlighted positions Q125, E128, P160, S171, D214, and Q222.



• Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein

Chain Z:  16% 84%

MET	SER	ALA	THR	THR	THR	GLN	PRO	GLN	LYS	PRO	GLU	TRP	LEU	ASN	ARG	LEU	ARG	GLY	SER	ALA	VAL	VAL	GLY	ASP	LEU	TRP	ALA	THR	TYR	ARG	THR	LEU	THR	LEU	ASP
GLN	ASP	GLY	ILE	ALA	VAL	ALA	GLN	THR	LYS	PRO	MET	ASN	ILE	TYR	GLN	PHE	ALA	ASN	GLY	SER	ASN	VAL	VAL	GLY	LEU	TRP	ALA	THR	GLY	GLU	PHE	GLU	VAL	LYS	
PHE	GLY	ILE	Q125	E128	P160	LYS	PRO	THR	LEU	SER	PHE	VAL	ASN	ARG	GLU	GLN	S173	D214	Q222	SER	ASN	THR	THR	GLY	ARG	LEU	ASN	ALA	THR	GLY	ILE	ALA	GLN	ASP	
ASN	GLY	ASN	VAL	HIS	ALA	GLN	THR	VAL	LEU	ASP	PHE	ALA	ASN	ARG	LYS	GLN	THR	GLU	HIS	ASN	THR	THR	TYR	PRO	GLN	THR	ASN	ALA	THR	GLY	VAL	GLN	ASP	ASN	
GLN	PRO	ALA	PRO	ASN	PRO	GLU	ASN	PRO	THR	PRO	PRO	THR	THR	GLN	GLN	ASN	ALA	ALA	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN	
VAL	GLY	ASP	ILE	GLU	ARG	LEU	SER	VAL	VAL	VAL	ASN	TYR	THR	LYS	THR	LEU	ASP	ALA	GLY	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	SER	
ALA	VAL	ASP	ASN	THR	GLY	GLU	LEU	PRO	PHE	VAL	TRP	GLN	GLN	SER	PHE	THR	ILE	GLN	ASP	ALA	GLN	LEU	LEU	TRP	ARG	TRP	ARG	THR	ARG	GLU	GLU	GLU	GLU	ALA	
GLN	VAL	ARG	GLN	THR	THR	VAL	VAL	VAL	VAL	LEU	LEU	SER	LYS	ASP	GLY	GLN	LEU	ALA	ALA	ARG	ARG	ALA	ALA	ASN	ASN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	ASP	
HIS	GLU																																		

- Molecule 1: Flagellar M-ring protein

Chain a:  16% 84%

MET	SER	ALA	THR	THR	THR	GLN	PRO	GLN	LYS	PRO	GLU	TRP	LEU	ASN	ARG	LEU	ARG	GLY	SER	ALA	VAL	VAL	GLY	ASP	LEU	TRP	ALA	THR	TYR	ARG	THR	LEU	THR	LEU	ASP
GLN	ASP	GLY	ILE	ALA	VAL	ALA	GLN	THR	LYS	PRO	MET	ASN	ILE	TYR	GLN	PHE	ALA	ASN	GLY	SER	ASN	VAL	VAL	GLY	LEU	TRP	ALA	THR	GLY	GLU	PHE	GLU	VAL	LYS	
PHE	GLY	ILE	Q125	E128	P160	LYS	PRO	THR	LEU	SER	PHE	VAL	ASN	ARG	GLU	GLN	S171	D214	Q222	SER	ASN	THR	THR	GLY	ARG	LEU	ASN	ALA	THR	GLY	ILE	ALA	GLN	ASP	
ASN	GLY	ASN	VAL	HIS	ALA	GLN	THR	VAL	LEU	ASP	PHE	ALA	ASN	ARG	LYS	GLN	THR	GLU	HIS	ASN	THR	THR	TYR	PRO	GLN	THR	ASN	ALA	THR	GLY	VAL	GLN	ASP	ASN	
GLN	PRO	ALA	PRO	ASN	PRO	GLU	ASN	PRO	THR	PRO	PRO	THR	THR	GLN	GLN	ASN	ALA	ALA	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN
VAL	GLY	ASP	ILE	GLU	ARG	LEU	SER	VAL	VAL	VAL	ASN	TYR	THR	LYS	THR	LEU	ASP	ALA	GLY	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	SER	
ALA	VAL	ASP	ASN	THR	GLY	GLU	LEU	PRO	PHE	VAL	TRP	GLN	GLN	SER	PHE	THR	ILE	GLN	ASP	ALA	GLN	LEU	LEU	TRP	ARG	TRP	ARG	THR	ARG	GLU	GLU	GLU	GLU	ALA	

ASN GLY
GLN PRO
ALA ASN
VAL HIS
THR GLY
ASN ALA
GLU VAL
ALA THR
PRO GLN
ALA GLN
LEU THR
ASP PRO
PHE ALA
ASN ALA
LYS GLN
GLN THR
GLN ASN
GLN THR

GLN PRO
ALA ASN
VAL HIS
THR GLY
ASN ALA
GLU VAL
ALA THR
PRO GLN
ALA GLN
LEU THR
ASP PRO
PHE ALA
ASN ALA
LYS GLN
GLN THR
GLN ASN
GLN THR

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

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

GLN VAL
VAL ARG
GLN GLN
THR GLU
GLU GLU
ALA VAL
GLU VAL
VAL VAL
ARG THR
LEU THR
SER LYS
LYS ASP
GLU THR
GLN THR
LEU THR
GLN THR
GLN THR
VAL THR
VAL THR
MET THR
GLN THR
ILE THR
ARG THR
MET THR
ASP THR
ASN THR
ASP THR
PRO THR
ARG THR
VAL THR
VAL THR
ALA THR
LEU THR
VAL THR
ILE THR
ARG THR
MET THR
SER THR
ASP THR
ASN THR
ASP THR
PRO THR
ARG THR
VAL THR
VAL THR
ALA THR
LEU THR
VAL THR
ILE THR
ARG THR
MET THR
SER THR
ASP THR
ASN THR
ASP THR

HIS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C22	Depositor
Number of particles used	87107	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	0.079	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	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 [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	0.32	0/655	0.49	0/893
1	C	0.32	0/655	0.49	0/893
1	D	0.32	0/655	0.49	0/893
1	F	0.32	0/655	0.49	0/893
1	G	0.32	0/655	0.49	0/893
1	I	0.32	0/655	0.49	0/893
1	J	0.32	0/655	0.49	0/893
1	L	0.32	0/655	0.49	0/893
1	M	0.32	0/655	0.49	0/893
1	O	0.32	0/655	0.49	0/893
1	P	0.32	0/655	0.49	0/893
1	R	0.32	0/655	0.49	0/893
1	T	0.32	0/655	0.49	0/893
1	U	0.32	0/655	0.49	0/893
1	W	0.32	0/655	0.49	0/893
1	X	0.32	0/655	0.49	0/893
1	Z	0.32	0/655	0.49	0/893
1	a	0.32	0/655	0.49	0/893
1	c	0.32	0/655	0.49	0/893
1	d	0.32	0/655	0.49	0/893
1	f	0.32	0/655	0.49	0/893
1	g	0.32	0/655	0.49	0/893
All	All	0.32	0/14410	0.49	0/19646

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](#)

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	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	C	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	D	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	F	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	G	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	I	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	J	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	L	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	M	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	O	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	P	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	R	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	T	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	U	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	W	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	X	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	Z	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	a	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	c	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	d	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	f	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
1	g	84/560 (15%)	77 (92%)	7 (8%)	0	100	100
All	All	1848/12320 (15%)	1694 (92%)	154 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	C	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	D	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	F	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	G	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	I	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	J	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	L	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	M	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	O	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	P	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	R	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	T	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	U	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	W	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	X	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	Z	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	a	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	c	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	d	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	f	72/467 (15%)	71 (99%)	1 (1%)	67	86
1	g	72/467 (15%)	71 (99%)	1 (1%)	67	86
All	All	1584/10274 (15%)	1562 (99%)	22 (1%)	68	86

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	ASP
1	C	214	ASP
1	D	214	ASP
1	F	214	ASP
1	G	214	ASP
1	I	214	ASP
1	J	214	ASP
1	L	214	ASP
1	M	214	ASP
1	O	214	ASP
1	P	214	ASP
1	R	214	ASP
1	T	214	ASP
1	U	214	ASP
1	W	214	ASP
1	X	214	ASP
1	Z	214	ASP
1	a	214	ASP
1	c	214	ASP
1	d	214	ASP
1	f	214	ASP
1	g	214	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
1	C	196	HIS
1	D	196	HIS
1	F	196	HIS
1	G	196	HIS
1	I	196	HIS
1	J	196	HIS
1	L	196	HIS
1	M	196	HIS
1	O	196	HIS
1	P	196	HIS
1	R	196	HIS
1	T	196	HIS
1	U	196	HIS
1	W	196	HIS
1	X	196	HIS
1	Z	196	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	196	HIS
1	c	196	HIS
1	d	196	HIS
1	f	196	HIS
1	g	196	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

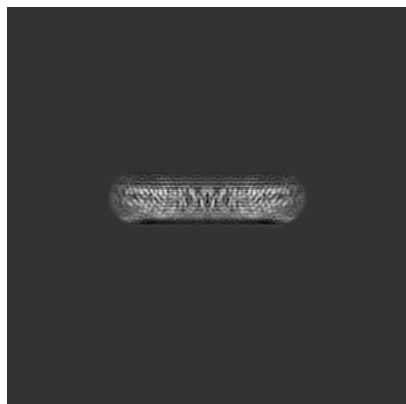
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10149. These allow visual inspection of the internal detail of the map and identification of artifacts.

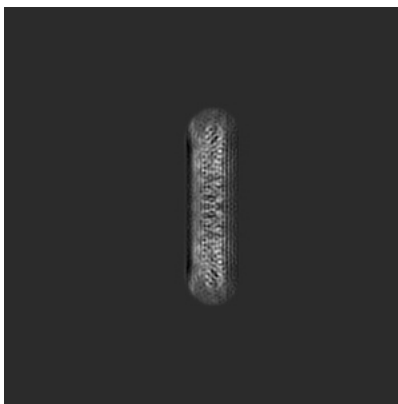
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

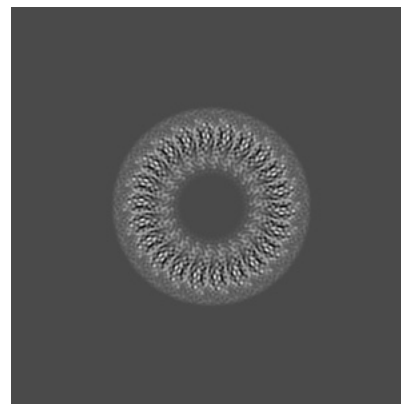
6.1.1 Primary map



X

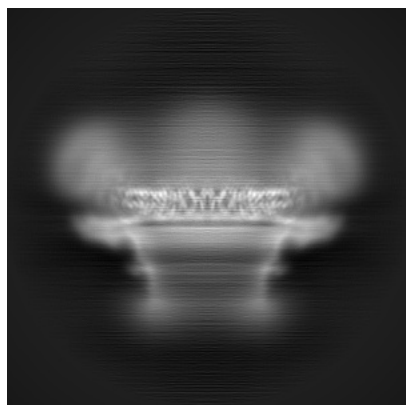


Y

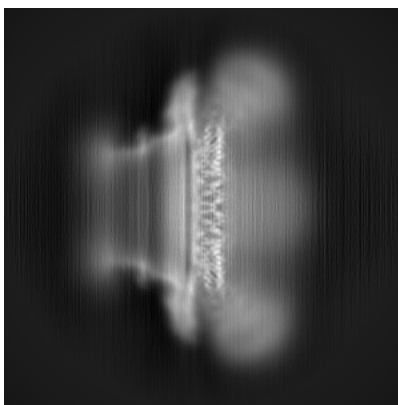


Z

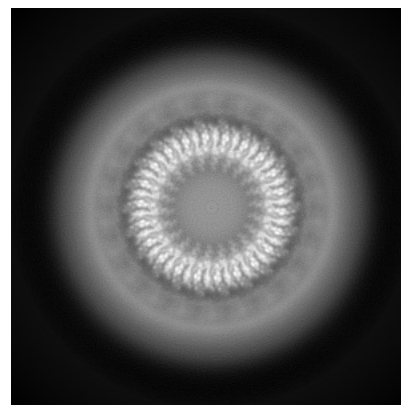
6.1.2 Raw map



X



Y



Z

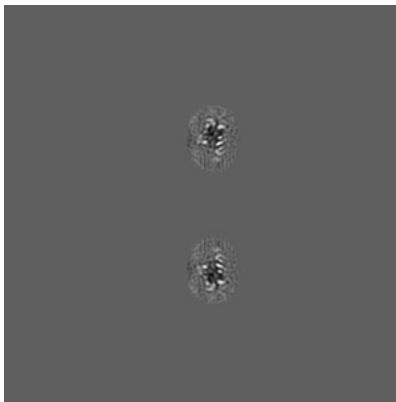
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

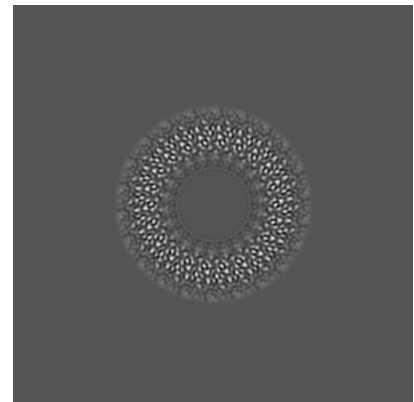
6.2.1 Primary map



X Index: 216

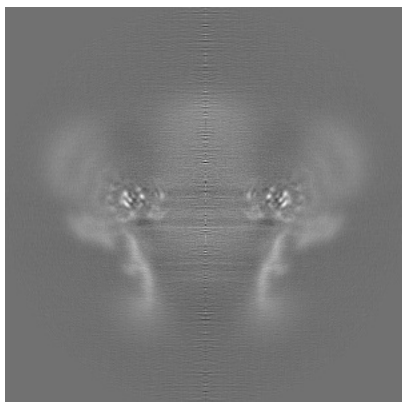


Y Index: 216

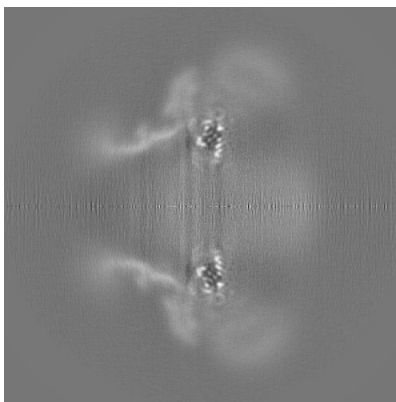


Z Index: 216

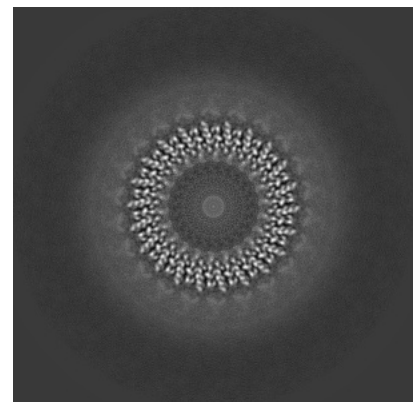
6.2.2 Raw map



X Index: 216



Y Index: 216

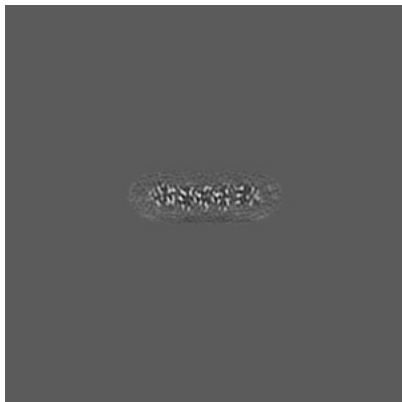


Z Index: 216

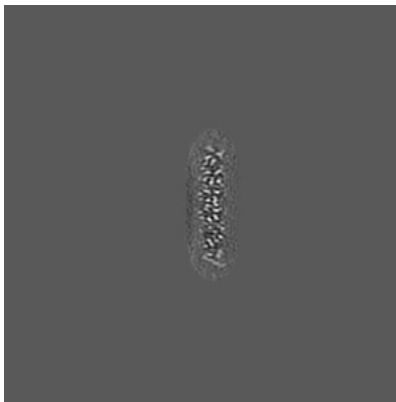
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

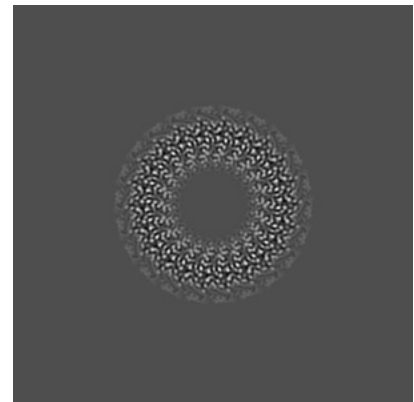
6.3.1 Primary map



X Index: 149

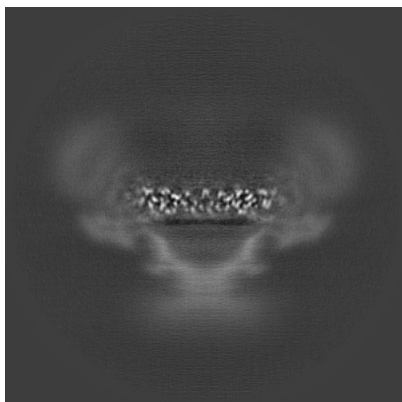


Y Index: 285

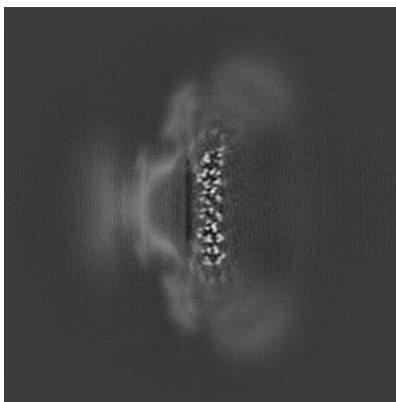


Z Index: 230

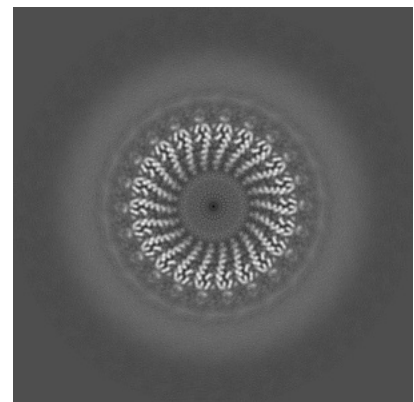
6.3.2 Raw map



X Index: 277



Y Index: 151

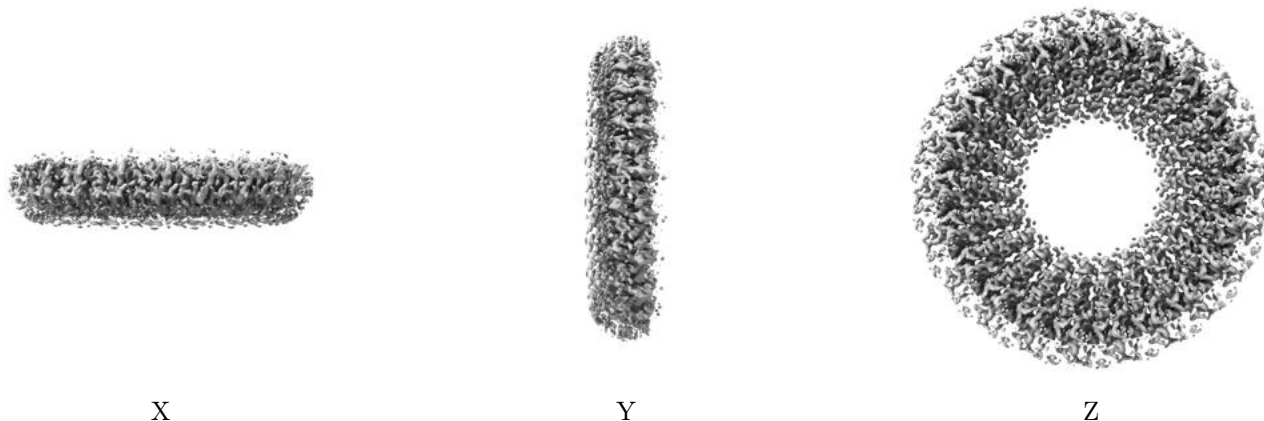


Z Index: 232

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

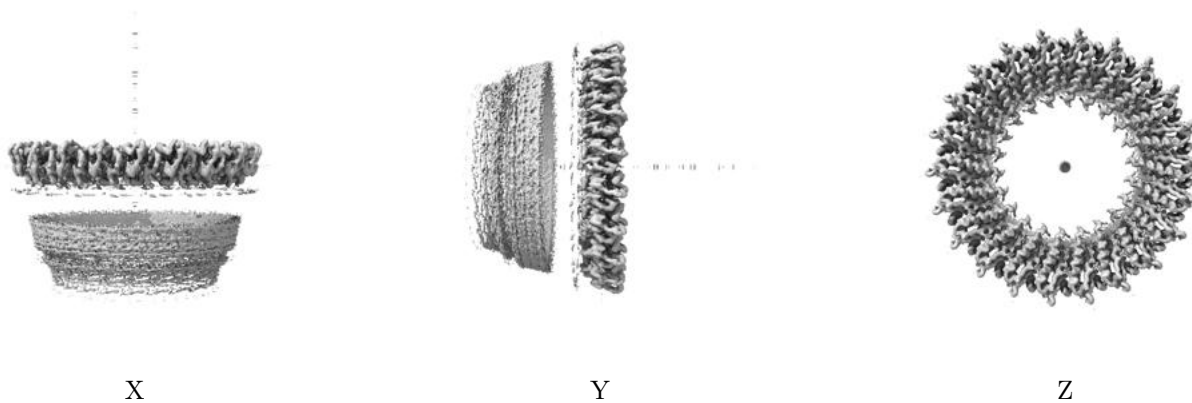
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

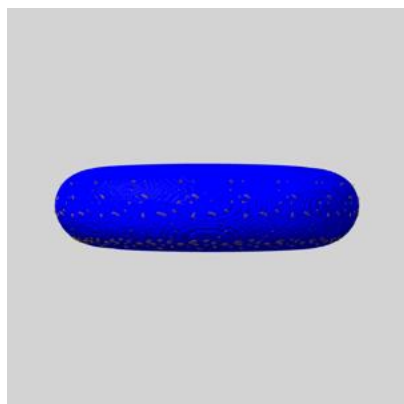
6.5 Mask visualisation [i](#)

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

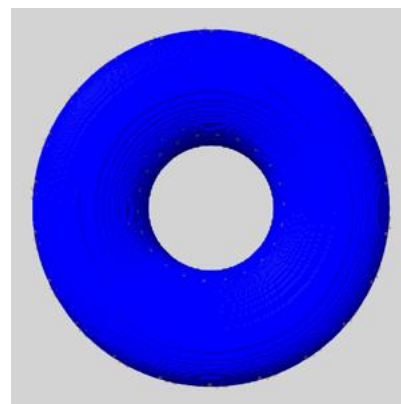
6.5.1 emd_10149_msk_1.map [i](#)



X



Y

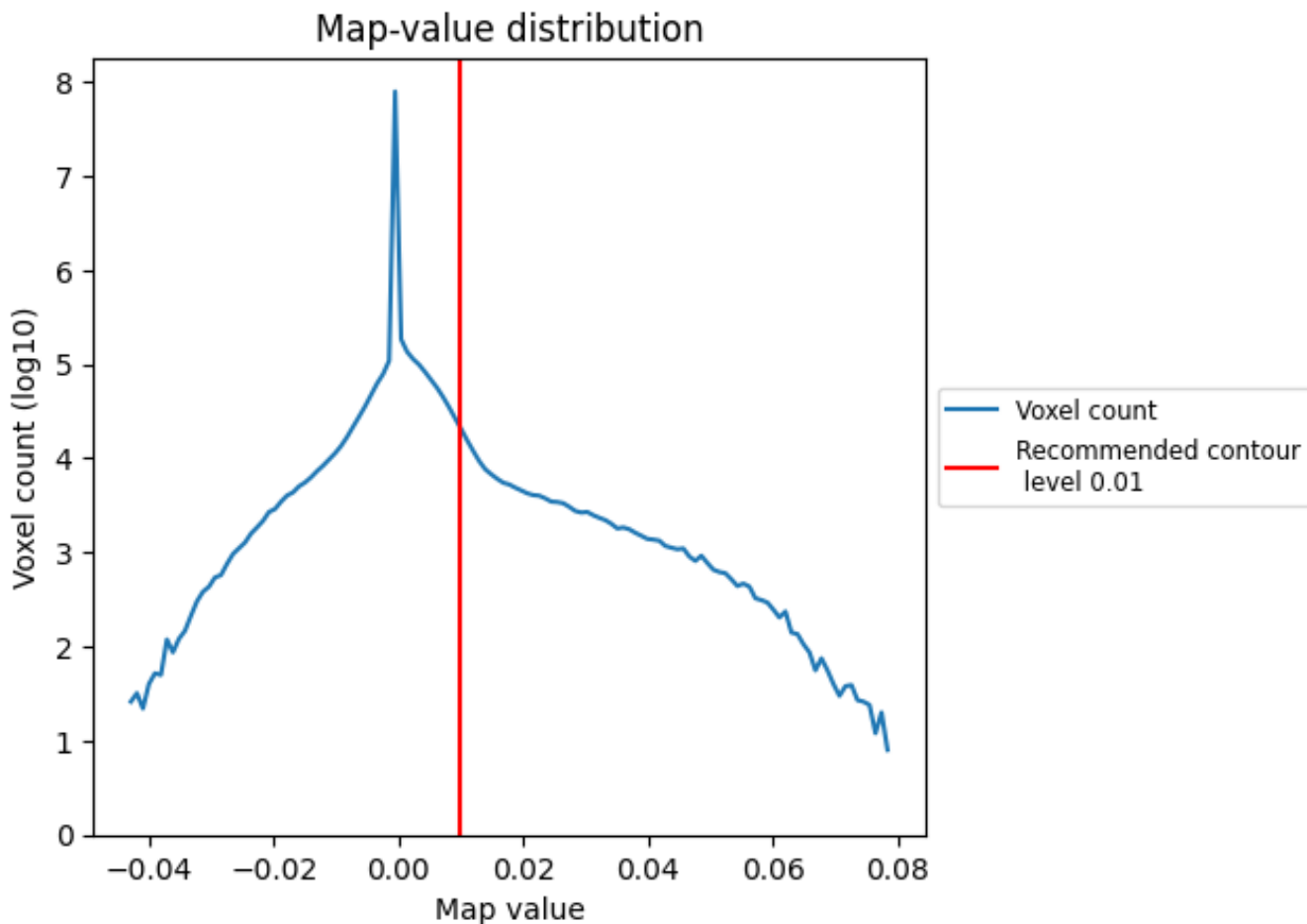


Z

7 Map analysis [i](#)

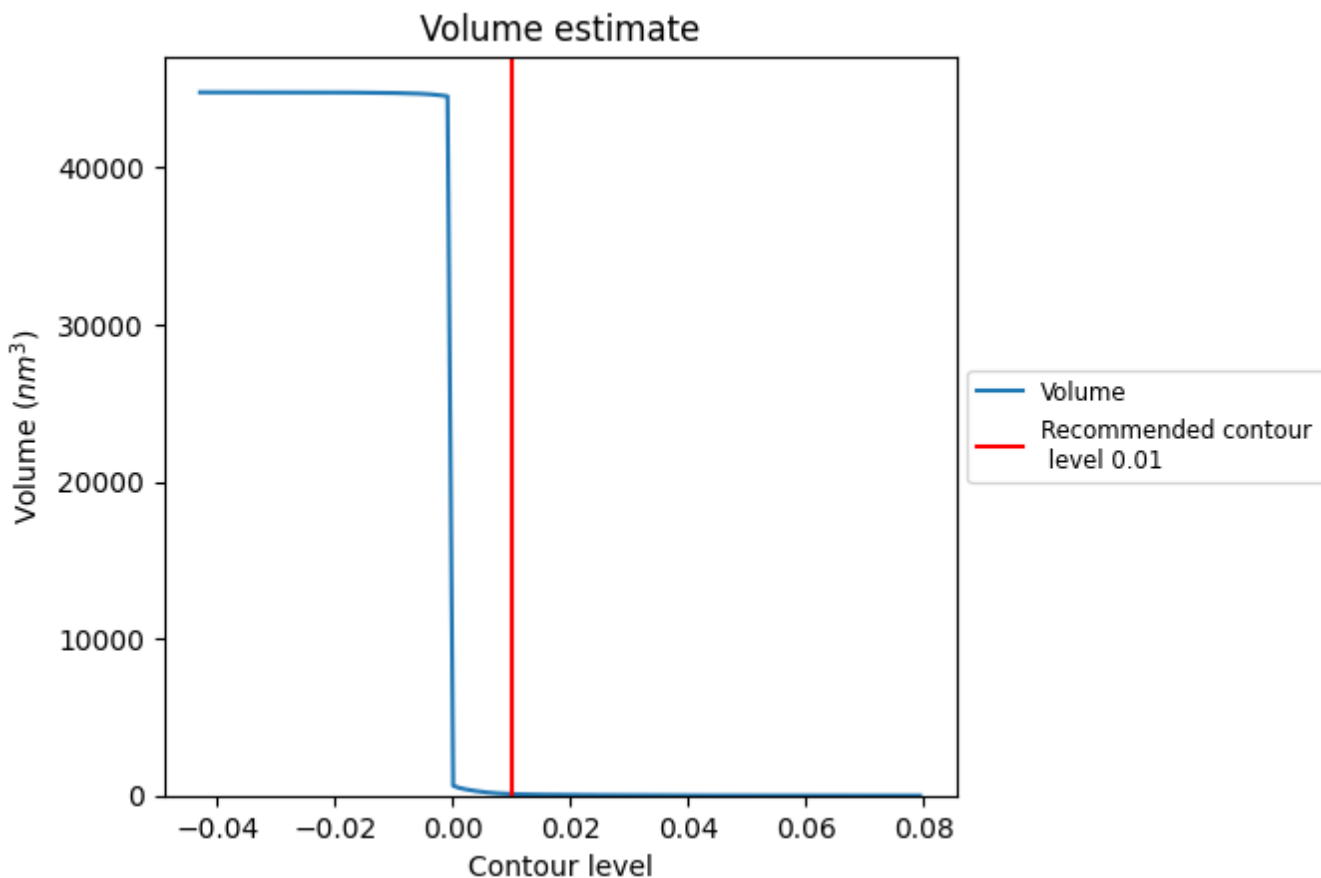
This section contains the results of statistical analysis of the map.

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.

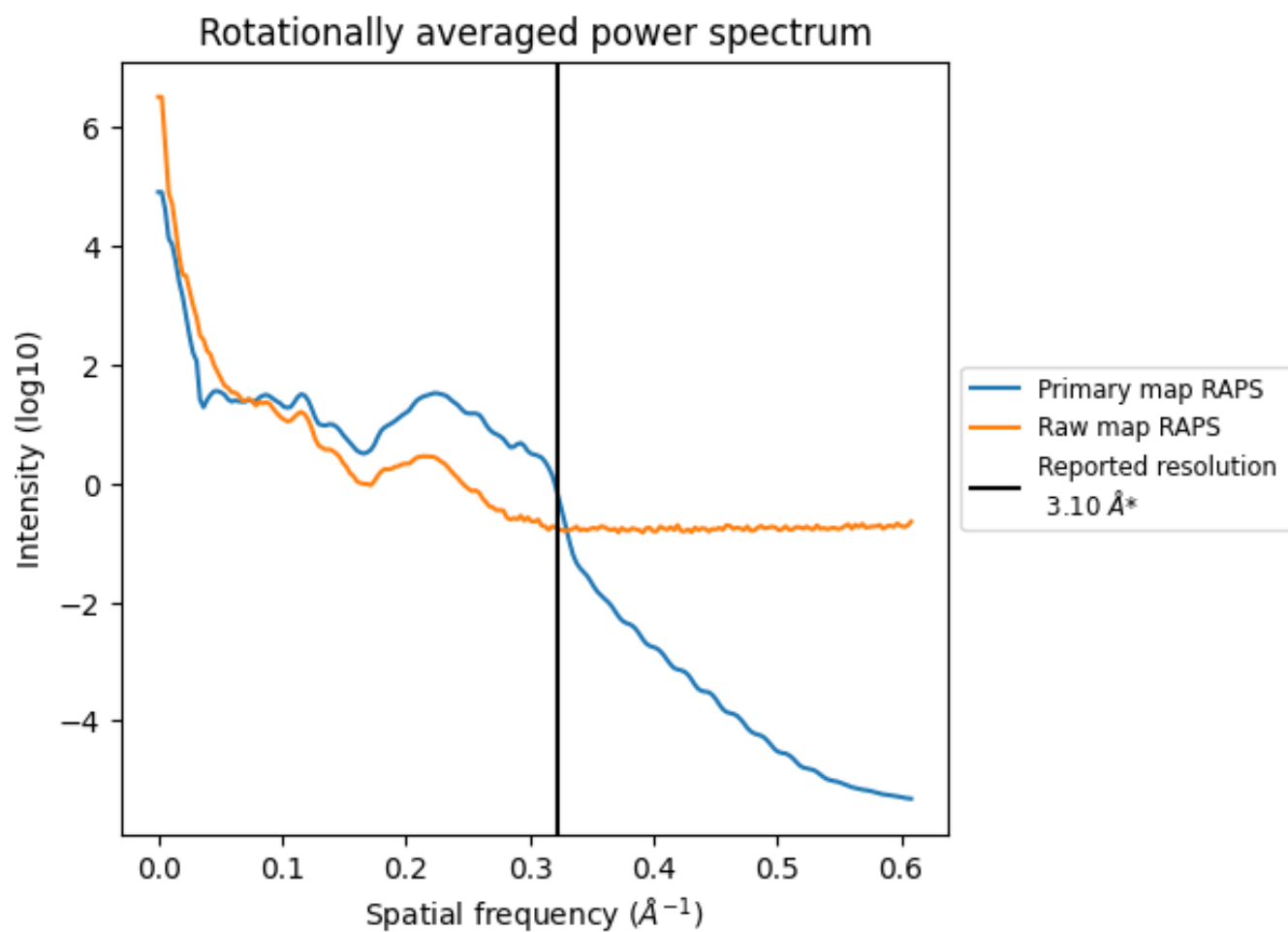
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm³; this corresponds to an approximate mass of 87 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

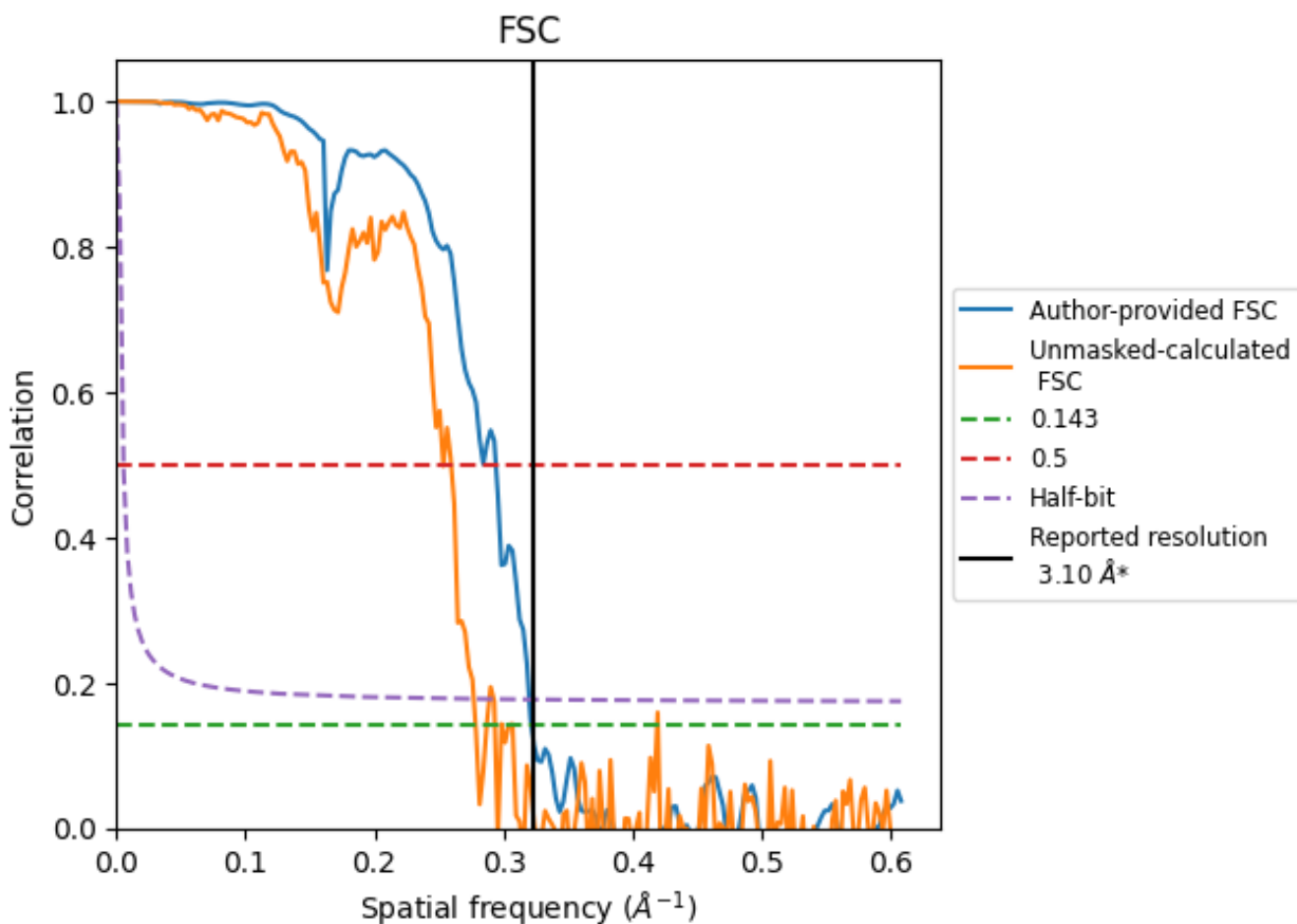


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

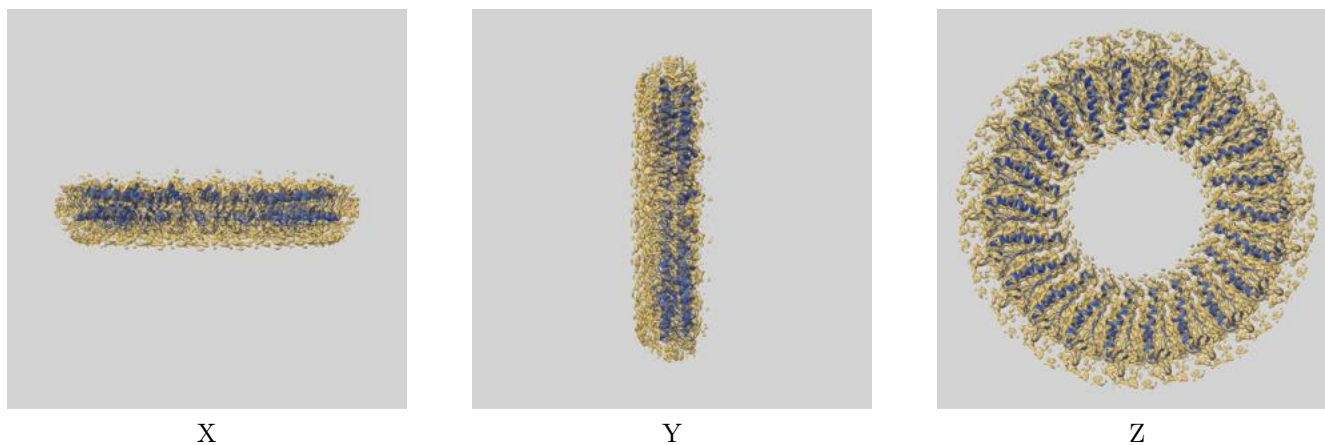
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.40	3.12
Unmasked-calculated*	3.59	3.95	3.61

*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 3.59 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

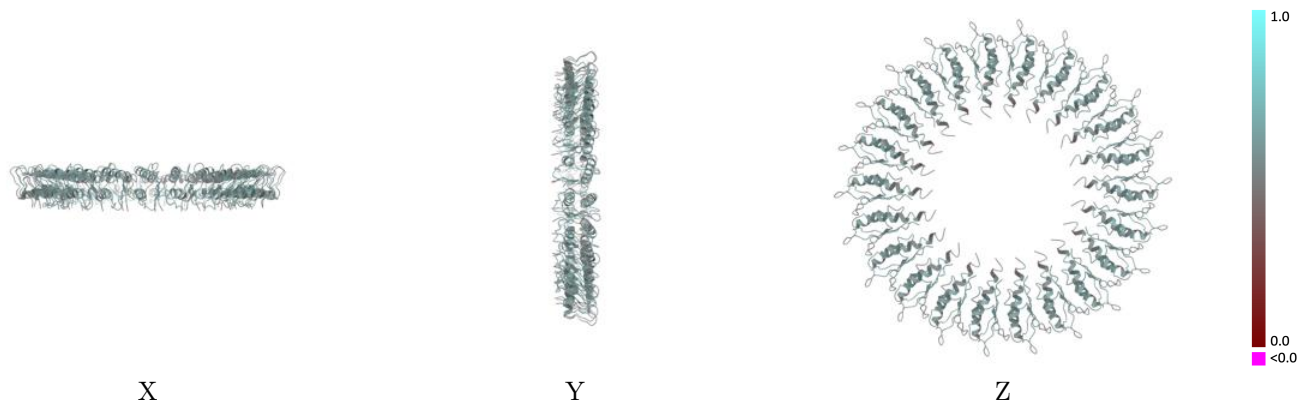
This section contains information regarding the fit between EMDB map EMD-10149 and PDB model 6SD5. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



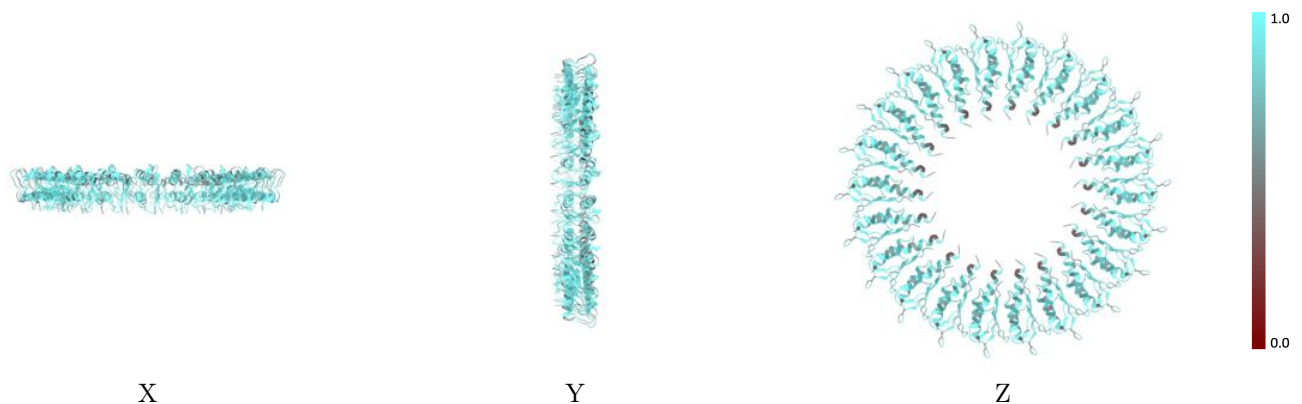
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



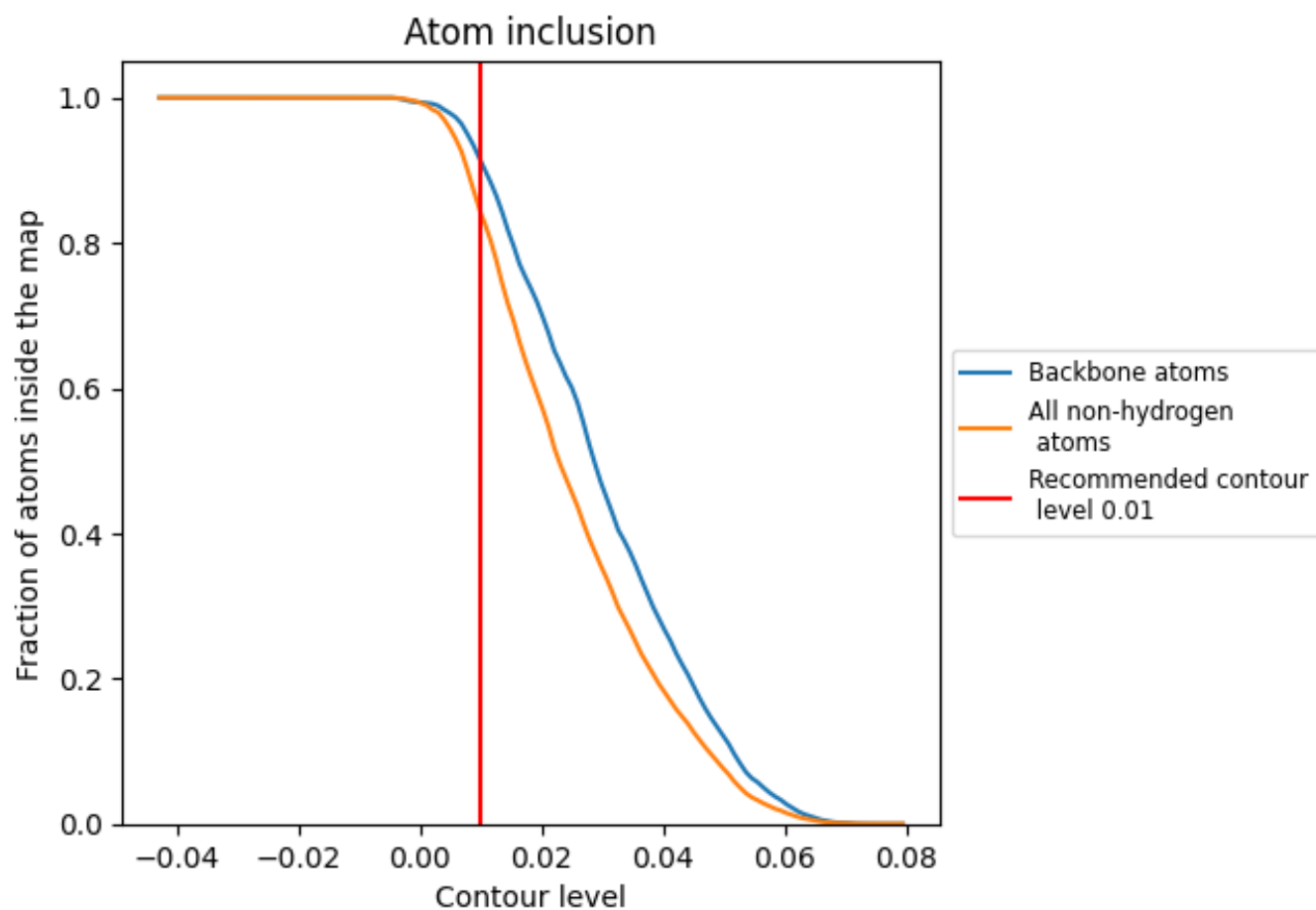
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 84% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8394	 0.5510
A	 0.8367	 0.5520
C	 0.8462	 0.5510
D	 0.8399	 0.5520
F	 0.8367	 0.5510
G	 0.8352	 0.5510
I	 0.8352	 0.5500
J	 0.8383	 0.5490
L	 0.8430	 0.5490
M	 0.8367	 0.5510
O	 0.8430	 0.5500
P	 0.8383	 0.5500
R	 0.8352	 0.5500
T	 0.8414	 0.5500
U	 0.8493	 0.5520
W	 0.8383	 0.5530
X	 0.8367	 0.5520
Z	 0.8352	 0.5520
a	 0.8430	 0.5520
c	 0.8446	 0.5520
d	 0.8399	 0.5520
f	 0.8414	 0.5500
g	 0.8336	 0.5500

