



## wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 06:43 PM EST

PDB ID : 6W6M  
EMDB ID : EMD-21559  
Title : Single particle cryoEM structure of V. cholerae Type IV competence pilus secretin PilQ  
Authors : Sazinsky, M.H.; Weaver, S.J.  
Deposited on : 2020-03-17  
Resolution : 2.70 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](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.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) : 2.31.2

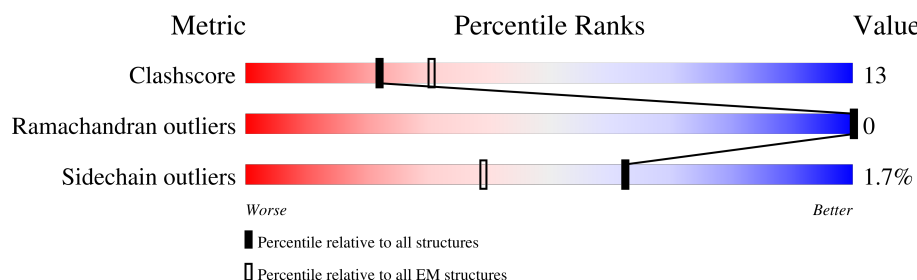
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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.



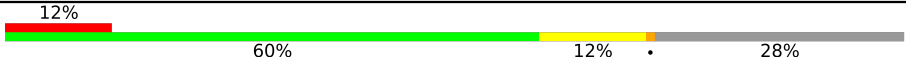

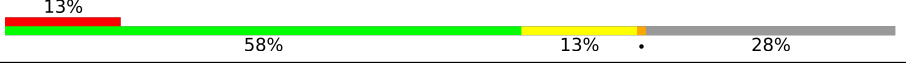


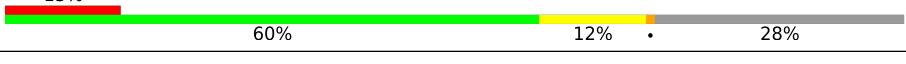
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	571	<div> <div>13%</div> <div>60%</div> <div>12%</div> <div>28%</div> </div>
1	B	571	<div> <div>13%</div> <div>59%</div> <div>12%</div> <div>28%</div> </div>
1	C	571	<div> <div>13%</div> <div>60%</div> <div>12%</div> <div>28%</div> </div>
1	D	571	<div> <div>12%</div> <div>59%</div> <div>13%</div> <div>28%</div> </div>
1	E	571	<div> <div>12%</div> <div>60%</div> <div>11%</div> <div>28%</div> </div>
1	F	571	<div> <div>13%</div> <div>59%</div> <div>12%</div> <div>28%</div> </div>
1	G	571	<div> <div>12%</div> <div>59%</div> <div>13%</div> <div>28%</div> </div>
1	H	571	<div> <div>12%</div> <div>60%</div> <div>12%</div> <div>28%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	571	
1	J	571	
1	K	571	
1	L	571	
1	M	571	
1	N	571	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 43638 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 Type IV pilus secretin PilQ family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	412	Total 3117	C 1962	N 531	O 620	S 4	0	0
1	B	412	Total 3117	C 1962	N 531	O 620	S 4	0	0
1	C	412	Total 3117	C 1962	N 531	O 620	S 4	0	0
1	D	412	Total 3117	C 1962	N 531	O 620	S 4	0	0
1	E	412	Total 3117	C 1962	N 531	O 620	S 4	0	0
1	F	412	Total 3117	C 1962	N 531	O 620	S 4	0	0
1	G	412	Total 3117	C 1962	N 531	O 620	S 4	0	0
1	H	412	Total 3117	C 1962	N 531	O 620	S 4	0	0
1	I	412	Total 3117	C 1962	N 531	O 620	S 4	0	0
1	J	412	Total 3117	C 1962	N 531	O 620	S 4	0	0
1	K	412	Total 3117	C 1962	N 531	O 620	S 4	0	0
1	L	412	Total 3117	C 1962	N 531	O 620	S 4	0	0
1	M	412	Total 3117	C 1962	N 531	O 620	S 4	0	0
1	N	412	Total 3117	C 1962	N 531	O 620	S 4	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ARG	LYS	conflict	UNP A0A2V4P274
A	27	THR	MET	conflict	UNP A0A2V4P274

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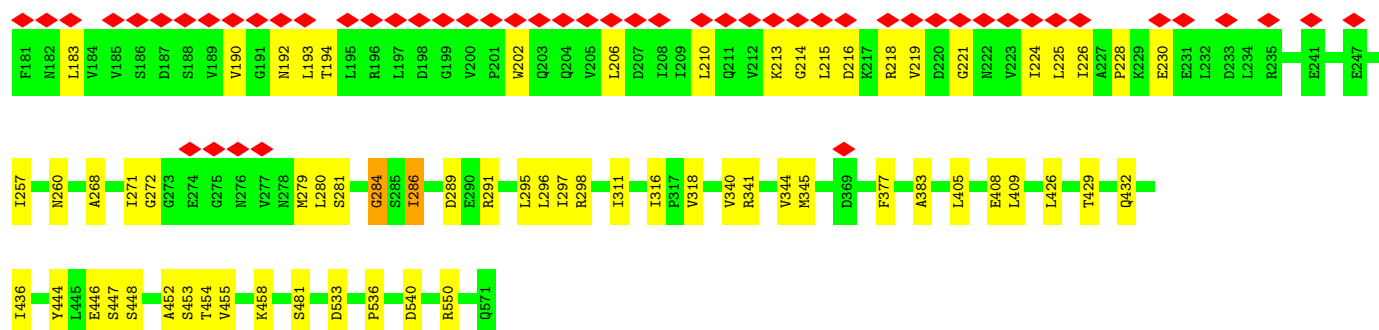
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	PHE	SER	conflict	UNP A0A2V4P274
A	36	THR	ALA	conflict	UNP A0A2V4P274
A	75	ASN	SER	conflict	UNP A0A2V4P274
A	109	ALA	GLU	conflict	UNP A0A2V4P274
B	2	ARG	LYS	conflict	UNP A0A2V4P274
B	27	THR	MET	conflict	UNP A0A2V4P274
B	33	PHE	SER	conflict	UNP A0A2V4P274
B	36	THR	ALA	conflict	UNP A0A2V4P274
B	75	ASN	SER	conflict	UNP A0A2V4P274
B	109	ALA	GLU	conflict	UNP A0A2V4P274
C	2	ARG	LYS	conflict	UNP A0A2V4P274
C	27	THR	MET	conflict	UNP A0A2V4P274
C	33	PHE	SER	conflict	UNP A0A2V4P274
C	36	THR	ALA	conflict	UNP A0A2V4P274
C	75	ASN	SER	conflict	UNP A0A2V4P274
C	109	ALA	GLU	conflict	UNP A0A2V4P274
D	2	ARG	LYS	conflict	UNP A0A2V4P274
D	27	THR	MET	conflict	UNP A0A2V4P274
D	33	PHE	SER	conflict	UNP A0A2V4P274
D	36	THR	ALA	conflict	UNP A0A2V4P274
D	75	ASN	SER	conflict	UNP A0A2V4P274
D	109	ALA	GLU	conflict	UNP A0A2V4P274
E	2	ARG	LYS	conflict	UNP A0A2V4P274
E	27	THR	MET	conflict	UNP A0A2V4P274
E	33	PHE	SER	conflict	UNP A0A2V4P274
E	36	THR	ALA	conflict	UNP A0A2V4P274
E	75	ASN	SER	conflict	UNP A0A2V4P274
E	109	ALA	GLU	conflict	UNP A0A2V4P274
F	2	ARG	LYS	conflict	UNP A0A2V4P274
F	27	THR	MET	conflict	UNP A0A2V4P274
F	33	PHE	SER	conflict	UNP A0A2V4P274
F	36	THR	ALA	conflict	UNP A0A2V4P274
F	75	ASN	SER	conflict	UNP A0A2V4P274
F	109	ALA	GLU	conflict	UNP A0A2V4P274
G	2	ARG	LYS	conflict	UNP A0A2V4P274
G	27	THR	MET	conflict	UNP A0A2V4P274
G	33	PHE	SER	conflict	UNP A0A2V4P274
G	36	THR	ALA	conflict	UNP A0A2V4P274
G	75	ASN	SER	conflict	UNP A0A2V4P274
G	109	ALA	GLU	conflict	UNP A0A2V4P274
H	2	ARG	LYS	conflict	UNP A0A2V4P274
H	27	THR	MET	conflict	UNP A0A2V4P274

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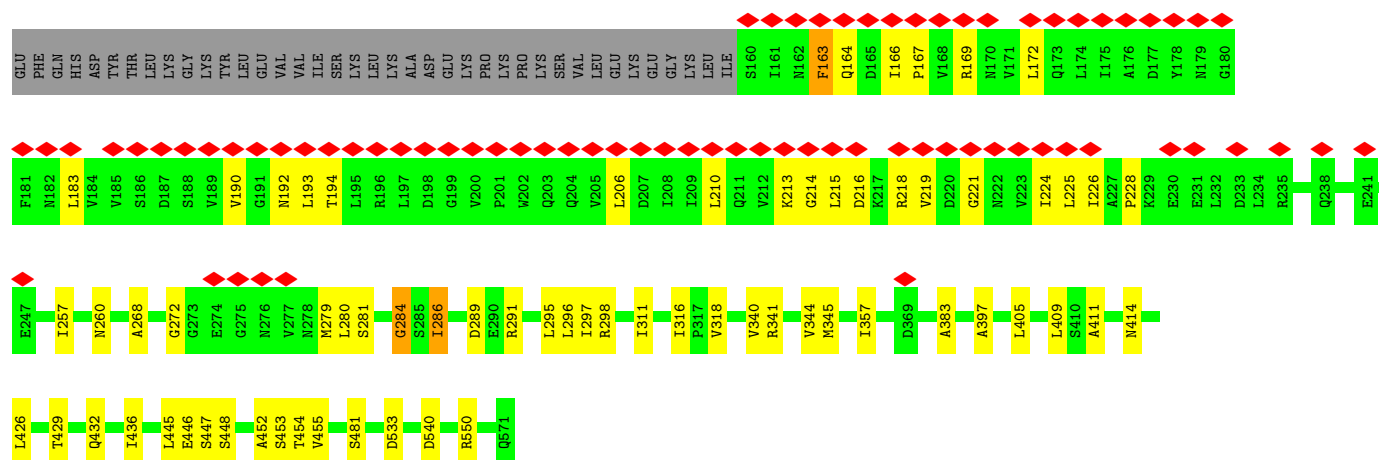
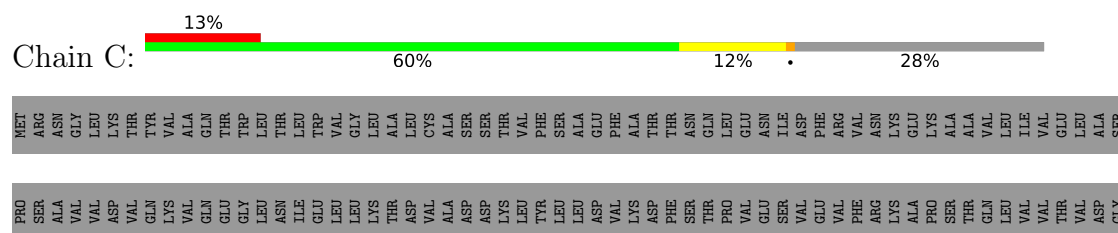
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Chain	Residue	Modelled	Actual	Comment	Reference
H	33	PHE	SER	conflict	UNP A0A2V4P274
H	36	THR	ALA	conflict	UNP A0A2V4P274
H	75	ASN	SER	conflict	UNP A0A2V4P274
H	109	ALA	GLU	conflict	UNP A0A2V4P274
I	2	ARG	LYS	conflict	UNP A0A2V4P274
I	27	THR	MET	conflict	UNP A0A2V4P274
I	33	PHE	SER	conflict	UNP A0A2V4P274
I	36	THR	ALA	conflict	UNP A0A2V4P274
I	75	ASN	SER	conflict	UNP A0A2V4P274
I	109	ALA	GLU	conflict	UNP A0A2V4P274
J	2	ARG	LYS	conflict	UNP A0A2V4P274
J	27	THR	MET	conflict	UNP A0A2V4P274
J	33	PHE	SER	conflict	UNP A0A2V4P274
J	36	THR	ALA	conflict	UNP A0A2V4P274
J	75	ASN	SER	conflict	UNP A0A2V4P274
J	109	ALA	GLU	conflict	UNP A0A2V4P274
K	2	ARG	LYS	conflict	UNP A0A2V4P274
K	27	THR	MET	conflict	UNP A0A2V4P274
K	33	PHE	SER	conflict	UNP A0A2V4P274
K	36	THR	ALA	conflict	UNP A0A2V4P274
K	75	ASN	SER	conflict	UNP A0A2V4P274
K	109	ALA	GLU	conflict	UNP A0A2V4P274
L	2	ARG	LYS	conflict	UNP A0A2V4P274
L	27	THR	MET	conflict	UNP A0A2V4P274
L	33	PHE	SER	conflict	UNP A0A2V4P274
L	36	THR	ALA	conflict	UNP A0A2V4P274
L	75	ASN	SER	conflict	UNP A0A2V4P274
L	109	ALA	GLU	conflict	UNP A0A2V4P274
M	2	ARG	LYS	conflict	UNP A0A2V4P274
M	27	THR	MET	conflict	UNP A0A2V4P274
M	33	PHE	SER	conflict	UNP A0A2V4P274
M	36	THR	ALA	conflict	UNP A0A2V4P274
M	75	ASN	SER	conflict	UNP A0A2V4P274
M	109	ALA	GLU	conflict	UNP A0A2V4P274
N	2	ARG	LYS	conflict	UNP A0A2V4P274
N	27	THR	MET	conflict	UNP A0A2V4P274
N	33	PHE	SER	conflict	UNP A0A2V4P274
N	36	THR	ALA	conflict	UNP A0A2V4P274
N	75	ASN	SER	conflict	UNP A0A2V4P274
N	109	ALA	GLU	conflict	UNP A0A2V4P274

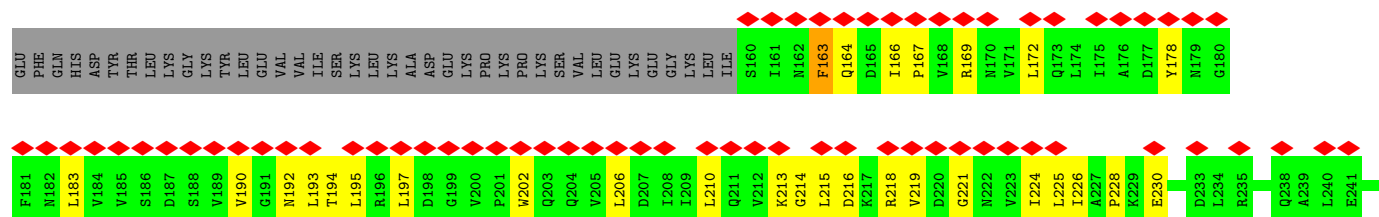
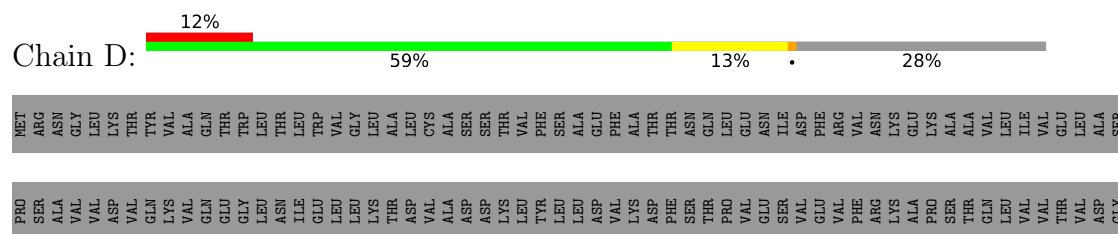




- Molecule 1: Type IV pilus secretin PilQ family protein



- Molecule 1: Type IV pilus secretin PilQ family protein











MET	ARG	ASN	GLY	LEU	LYS	THR	TTR	VAL	ALA	GLN	THR	TRP	LEU	THR	THR	ILE	TRP	VAL	GLY	LEU	LEU	ALA	CYS	ASP	VAL	ASP	SER	THR	VAL	PHE	THR	THR	ASN	GLN	LEU	GLU	GLU	ASN	ILE	ASP	PHE	ARG	VAL	ASN	LYS	GLU	LYS	ALA	ALA	VAL	LEU	ILE	VAL	GLU	LEU	ALA	SER
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PRO	SER	ALA	VAL	ASP	VAL	VAL	GLN	VAL	GLN	GLN	GLY	LEU	LEU	ASN	VAL	ILE	GLU	TRP	VAL	LEU	LEU	LYS	THR	ASP	VAL	ASP	ASP	LYS	LYS	VAL	TYR	THR	SER	LEU	LEU	ASP	VAL	VAL	LEU	VAL	GLU	SER	ILE	ASP	VAL	PHE	ARG	LYS	ALA	PRO	SER	THR	THR	VAL	GLN	VAL	VAL	THR	VAL	ASP	GLY
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GLU	PHE	GLN	HIS	ASP	TYR	THR	LEU	LYS	GLY	LYS	TYR	LEU	LEU	GLU	VAL	VAL	VAL	ILE	SER	LYS	LEU	LYS	LEU	ALA	ASP	GLU	LYS	PRO	LYS	PRO	PRO	LYS	SER	VAL	LEU	LEU	ILE	S160	I161	N162	F163	Q164	D165	I166	P167	V168	R169	L172	Q173	L174	I175	A176	D177	Y178	N179	G180	F181
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M182	L183	V184	V185	S186	D187	S188	V189	V190	G191	M192	T193	T194	L195	R196	L197	D198	V200	P201	W202	Q203	Q204	V205	L206	D207	I208	I209	L210	Q211	V212	K213	G214	L215	D216	K217	R218	V219	D220	G221	N222	V223	I224	L225	I226	A227	P228	R229	E230	E231	L232	D233	L234	R235	E236	E247	I257
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N260	A268	A269	M270	I271	G272	G273	E274	G275	N276	V277	N278	M279	L280	S281	G284	S285	I286	D289	F290	R291	L296	L297	R298	I311	I316	P317	V318	K319	Q320	V340	R341	V344	M345	A383	L405	L409	S410	A411	L426	T429	Q432	P433	A436
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E446	S447	S448	A452	S453	T454	V455	S481	Q504	D533	P536	D540	R550	Q571
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- Molecule 1: Type IV pilus secretin PilQ family protein



MET	ARG	ASN	GLY	LEU	LYS	THR	TYR	VAL	ALA	GLN	THR	TRP	LEU	THR	THR	ILE	TRP	VAL	GLY	LEU	LEU	ALA	CYS	ASP	VAL	ASP	SER	THR	VAL	PHE	THR	THR	ASN	GLN	LEU	GLU	GLU	ASN	ILE	ASP	PHE	ARG	VAL	ASN	LYS	GLU	LYS	ALA	ALA	VAL	LEU	ILE	VAL	GLU	LEU	ALA	SER
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PRO	SER	ALA	VAL	ASP	VAL	VAL	GLN	VAL	GLN	GLN	GLY	LEU	LEU	ASN	VAL	ILE	GLU	TRP	VAL	LEU	LEU	LYS	THR	ASP	VAL	ASP	ASP	LYS	LYS	VAL	TYR	THR	SER	LEU	LEU	ASP	VAL	ASP	PRO	LYS	PRO	PRO	LYS	THR	PHE	THR	ASN	GLN	LEU	VAL	GLU	GLU	ASN	ILE	ASP	VAL	PHE	ARG	VAL	ASN	LYS	GLU	LYS	ALA	PRO	SER	THR	THR	GLN	VAL	VAL	THR	VAL	ASP	ALA	GLY
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GLU	PHE	GLN	HIS	ASP	TYR	THR	LEU	LYS	GLY	LYS	TYR	LEU	LEU	GLU	VAL	VAL	VAL	ILE	SER	LYS	LEU	LYS	LEU	ALA	ASP	GLU	LYS	PRO	LYS	PRO	PRO	LYS	SER	VAL	LEU	LEU	ILE	S160	I161	N162	F163	Q164	D165	I166	P167	V168	R169	N170	V171	L172	Q173	L174	I175	A176	D177	Y178	N179	G180
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F181	M182	L183	V184	V185	S186	D187	S188	V189	V190	G191	M192	L193	T194	L195	R196	L197	D198	G199	V200	P201	W202	Q203	Q204	V205	L206	D207	I208	I209	L210	Q211	V212	K213	G214	L215	D216	K217	R218	V219	D220	G221	N222	V223	I224	L225	I226	A227	P228	R229	E230	E231	L232	D233	L234	R235	E241	E247
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I257	N260	A268	G272	G273	E274	G275	N276	V277	N278	M279	L280	S281	G284	S285	I286	D289	F290	R291	L296	L297	R298	I311	I316	P317	V318	V340	R341	V344	M345	A383	L405	L409	S410	A411	L426	T429	Q432	P433	I436	E437	Q438
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E446	S447	S448	A452	S453	T454	V455	S481	D533	P536	D540	R550	Q571
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- Molecule 1: Type IV pilus secretin PilQ family protein

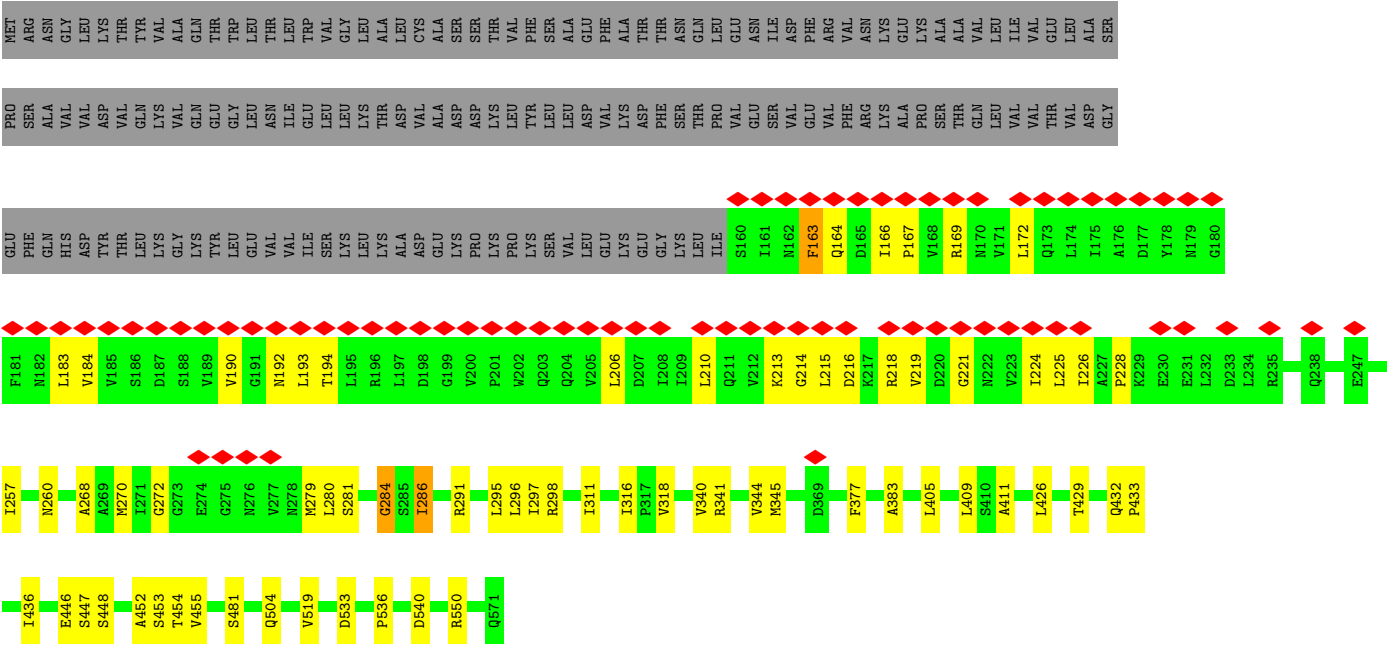


MET	ARG	ASN	GLY	LEU	LYS	THR	TYR	VAL	ALA	GLN	THR	TRP	LEU	THR	THR	ILE	TRP	VAL	GLY	LEU	LEU	ALA	CYS	ASP	VAL	ASP	SER	THR	VAL	PHE	THR	THR	ASN	GLN	LEU	GLU	GLU	ASN	ILE	ASP	PHE	ARG	VAL	ASN	LYS	GLU	LYS	ALA	ALA	VAL	VAL	ILE	VAL	GLU	LEU	ALA	SER
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● Molecule 1: Type IV pilus secretin PilQ family protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C14	Depositor
Number of particles used	100543	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; First whole micrograph correction with CtfFind4. Then per particle CTF Refinement in Relion.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.5	Depositor
Minimum defocus (nm)	10000	Depositor
Maximum defocus (nm)	30000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.217	Depositor
Minimum map value	-0.103	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.017	Depositor
Map size ( $\text{\AA}$ )	441.59998, 441.59998, 441.59998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.104, 1.104, 1.104	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	0.38	0/3152	0.55	0/4279
1	B	0.38	0/3152	0.55	0/4279
1	C	0.38	0/3152	0.55	0/4279
1	D	0.38	0/3152	0.55	0/4279
1	E	0.38	0/3152	0.55	0/4279
1	F	0.39	0/3152	0.55	0/4279
1	G	0.38	0/3152	0.55	0/4279
1	H	0.38	0/3152	0.55	0/4279
1	I	0.38	0/3152	0.55	0/4279
1	J	0.38	0/3152	0.55	0/4279
1	K	0.38	0/3152	0.55	0/4279
1	L	0.38	0/3152	0.55	0/4279
1	M	0.38	0/3152	0.55	0/4279
1	N	0.38	0/3152	0.55	0/4279
All	All	0.38	0/44128	0.55	0/59906

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
1	M	0	1
1	N	0	1
All	All	0	14

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	GLY	Peptide
1	B	284	GLY	Peptide
1	C	284	GLY	Peptide
1	D	284	GLY	Peptide
1	E	284	GLY	Peptide

## 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	3117	0	3181	95	0
1	B	3117	0	3181	99	0
1	C	3117	0	3181	93	0
1	D	3117	0	3181	100	0
1	E	3117	0	3181	90	0
1	F	3117	0	3181	99	0
1	G	3117	0	3181	109	0
1	H	3117	0	3181	92	0
1	I	3117	0	3181	97	0
1	J	3117	0	3181	97	0
1	K	3117	0	3181	111	0
1	L	3117	0	3181	95	0
1	M	3117	0	3181	94	0
1	N	3117	0	3181	97	0
All	All	43638	0	44534	1130	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 13.

The worst 5 of 1130 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:452:ALA:C	1:G:448:SER:OG	1.95	1.05
1:F:453:SER:C	1:G:448:SER:HB2	1.78	1.03
1:C:448:SER:HB2	1:E:453:SER:C	1.81	1.00
1:M:453:SER:C	1:N:448:SER:HB2	1.83	0.99
1:G:453:SER:C	1:K:448:SER:HB2	1.82	0.98

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	410/571 (72%)	378 (92%)	32 (8%)	0	100	100
1	B	410/571 (72%)	378 (92%)	32 (8%)	0	100	100
1	C	410/571 (72%)	378 (92%)	32 (8%)	0	100	100
1	D	410/571 (72%)	379 (92%)	31 (8%)	0	100	100
1	E	410/571 (72%)	378 (92%)	32 (8%)	0	100	100
1	F	410/571 (72%)	378 (92%)	32 (8%)	0	100	100
1	G	410/571 (72%)	378 (92%)	32 (8%)	0	100	100
1	H	410/571 (72%)	378 (92%)	32 (8%)	0	100	100
1	I	410/571 (72%)	377 (92%)	33 (8%)	0	100	100
1	J	410/571 (72%)	378 (92%)	32 (8%)	0	100	100
1	K	410/571 (72%)	379 (92%)	31 (8%)	0	100	100
1	L	410/571 (72%)	378 (92%)	32 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	410/571 (72%)	377 (92%)	33 (8%)	0	100	100
1	N	410/571 (72%)	378 (92%)	32 (8%)	0	100	100
All	All	5740/7994 (72%)	5292 (92%)	448 (8%)	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	A	349/497 (70%)	343 (98%)	6 (2%)	60	84
1	B	349/497 (70%)	343 (98%)	6 (2%)	60	84
1	C	349/497 (70%)	343 (98%)	6 (2%)	60	84
1	D	349/497 (70%)	343 (98%)	6 (2%)	60	84
1	E	349/497 (70%)	343 (98%)	6 (2%)	60	84
1	F	349/497 (70%)	343 (98%)	6 (2%)	60	84
1	G	349/497 (70%)	343 (98%)	6 (2%)	60	84
1	H	349/497 (70%)	343 (98%)	6 (2%)	60	84
1	I	349/497 (70%)	343 (98%)	6 (2%)	60	84
1	J	349/497 (70%)	343 (98%)	6 (2%)	60	84
1	K	349/497 (70%)	343 (98%)	6 (2%)	60	84
1	L	349/497 (70%)	343 (98%)	6 (2%)	60	84
1	M	349/497 (70%)	343 (98%)	6 (2%)	60	84
1	N	349/497 (70%)	343 (98%)	6 (2%)	60	84
All	All	4886/6958 (70%)	4802 (98%)	84 (2%)	62	84

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	286	ILE

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Mol	Chain	Res	Type
1	L	540	ASP
1	J	540	ASP
1	K	540	ASP
1	M	286	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	484	GLN
1	M	525	GLN
1	I	203	GLN
1	M	484	GLN
1	N	484	GLN

### 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.

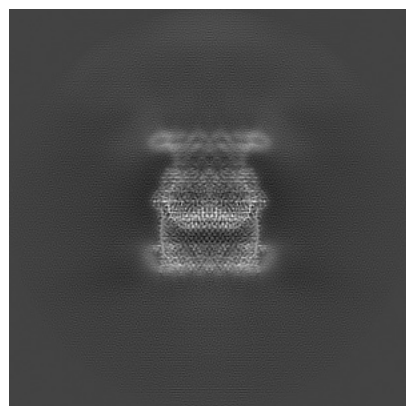
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21559. These allow visual inspection of the internal detail of the map and identification of artifacts.

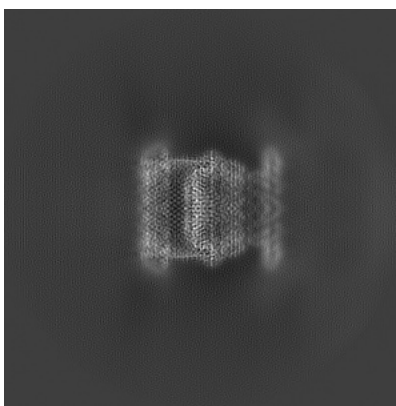
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

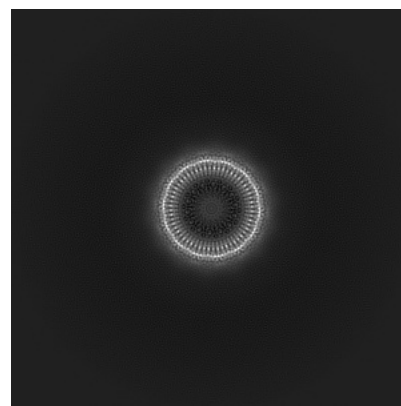
#### 6.1.1 Primary map



X

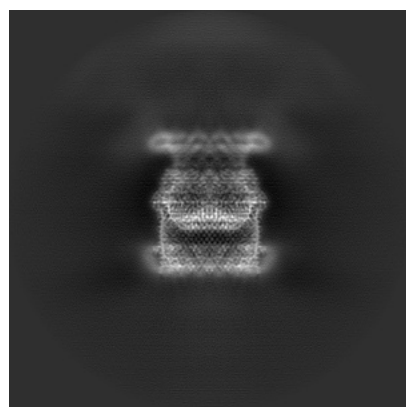


Y

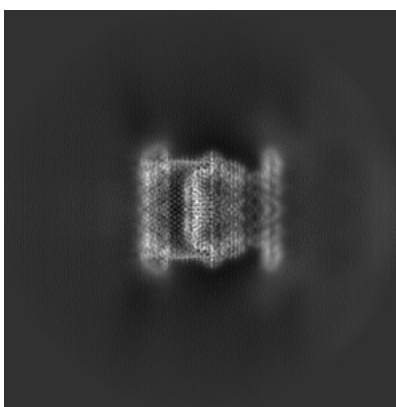


Z

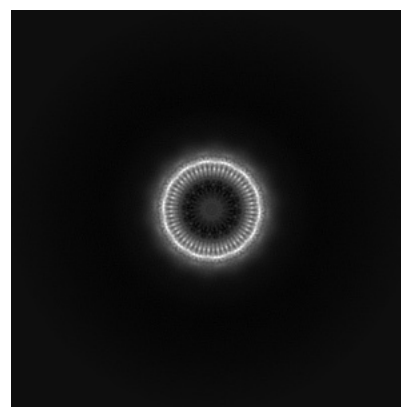
#### 6.1.2 Raw map



X



Y

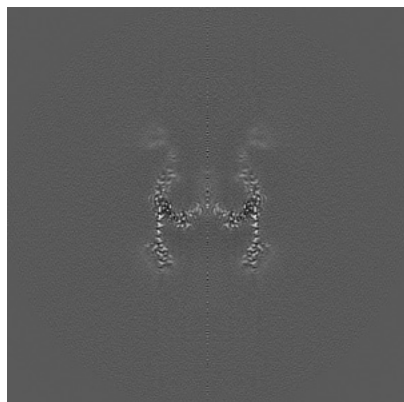


Z

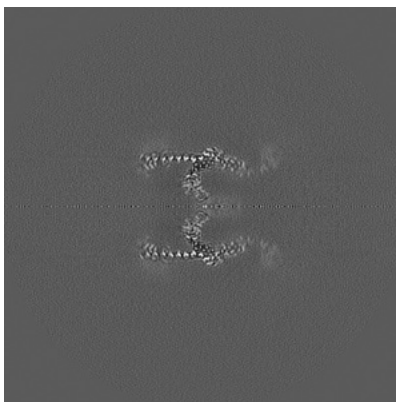
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

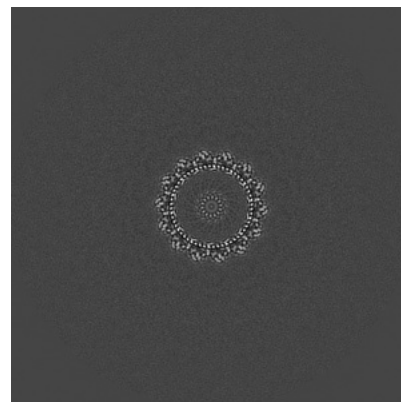
### 6.2.1 Primary map



X Index: 200

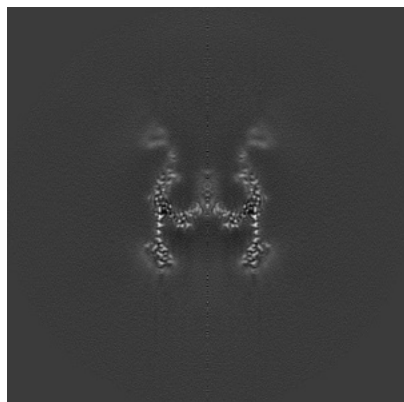


Y Index: 200

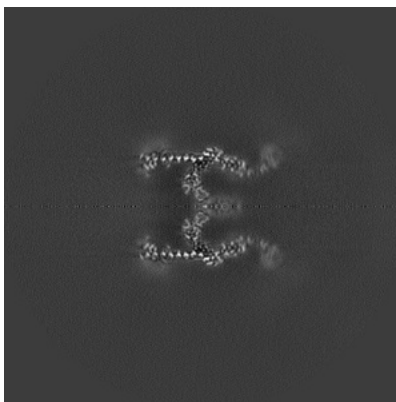


Z Index: 200

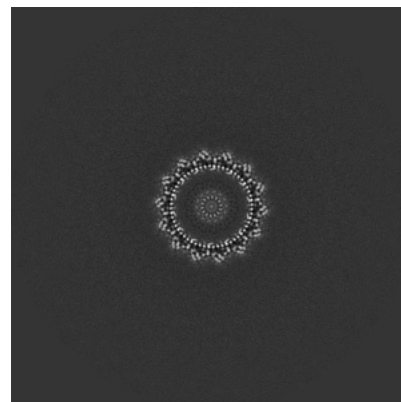
### 6.2.2 Raw map



X Index: 200



Y Index: 200

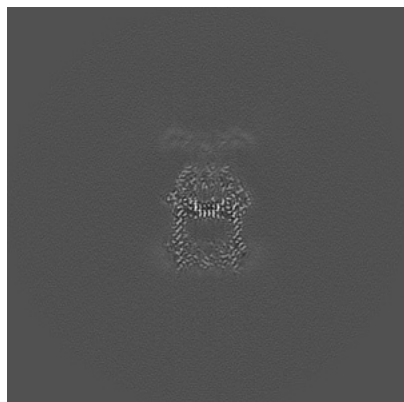


Z Index: 200

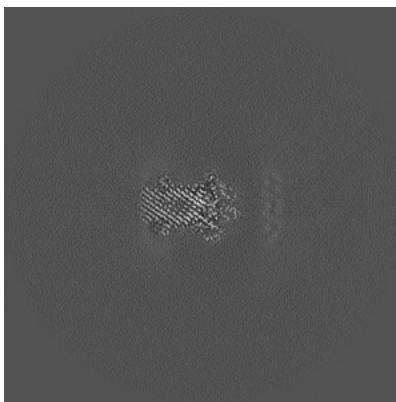
The images above show central slices of the map in three orthogonal directions.

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

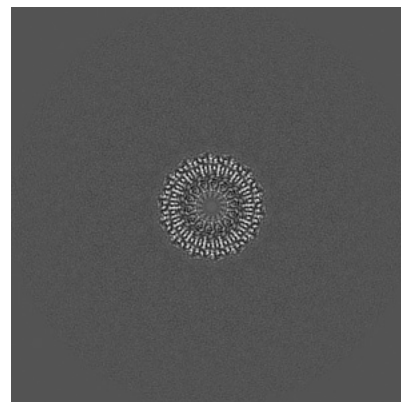
### 6.3.1 Primary map



X Index: 239

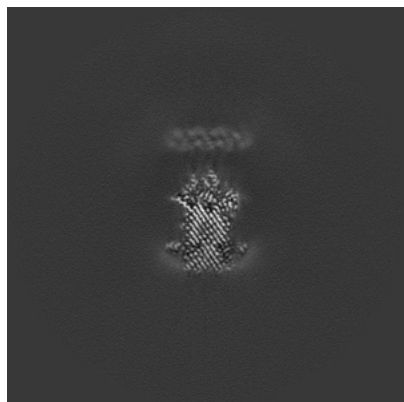


Y Index: 247

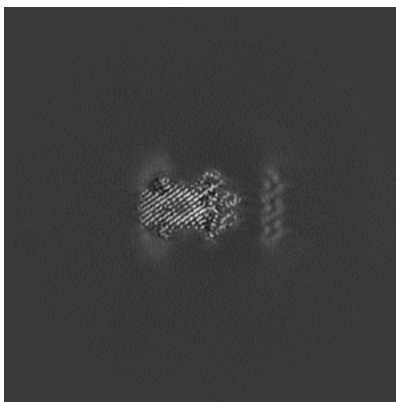


Z Index: 191

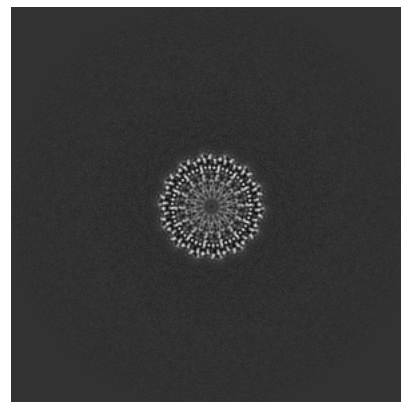
### 6.3.2 Raw map



X Index: 153



Y Index: 153

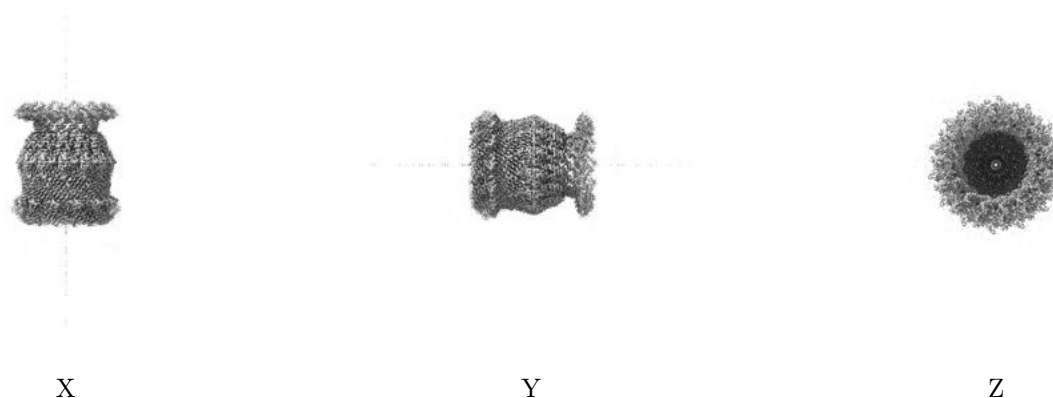


Z Index: 192

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

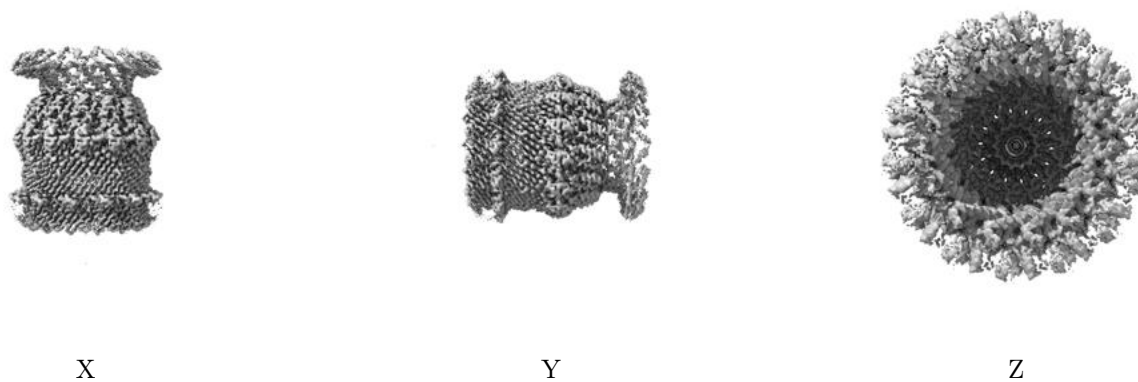
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. 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.



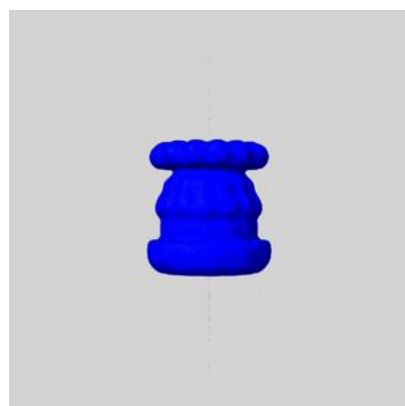
## 6.5 Mask visualisation [i](#)

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

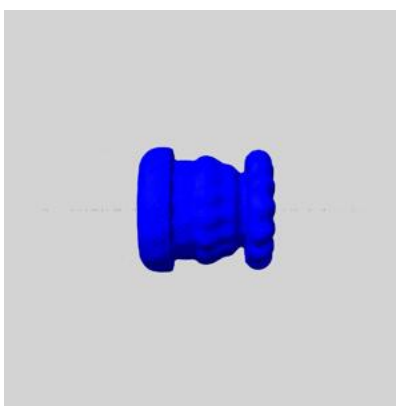
A mask typically either:

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

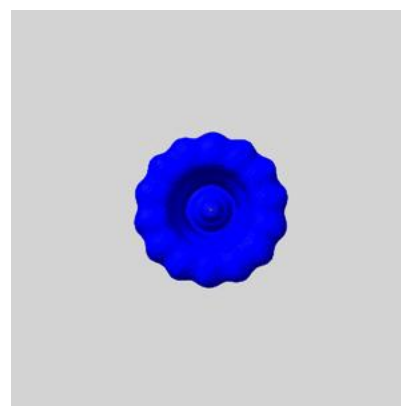
### 6.5.1 emd\_21559\_msk\_1.map [i](#)



X



Y



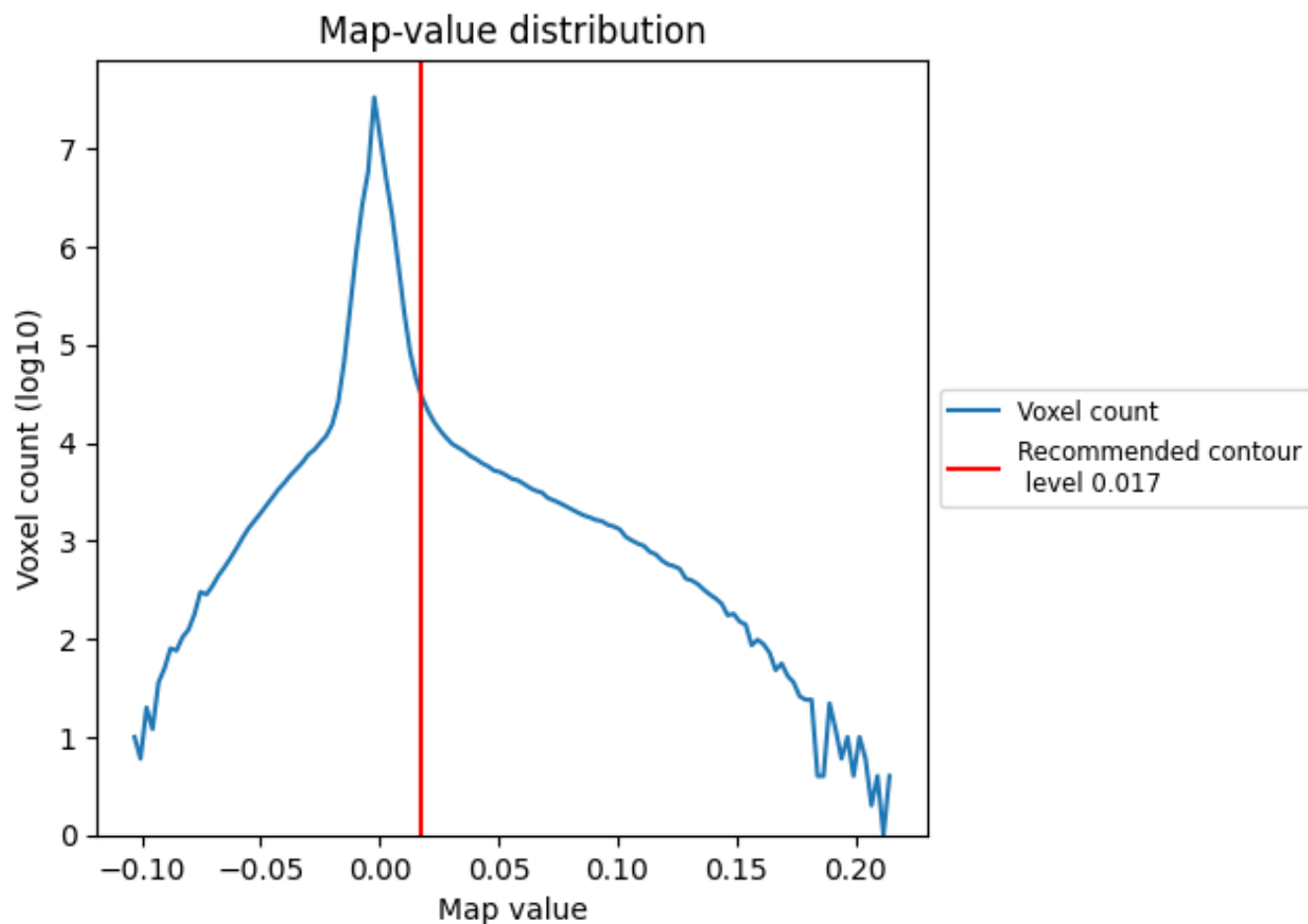
Z



## 7 Map analysis [i](#)

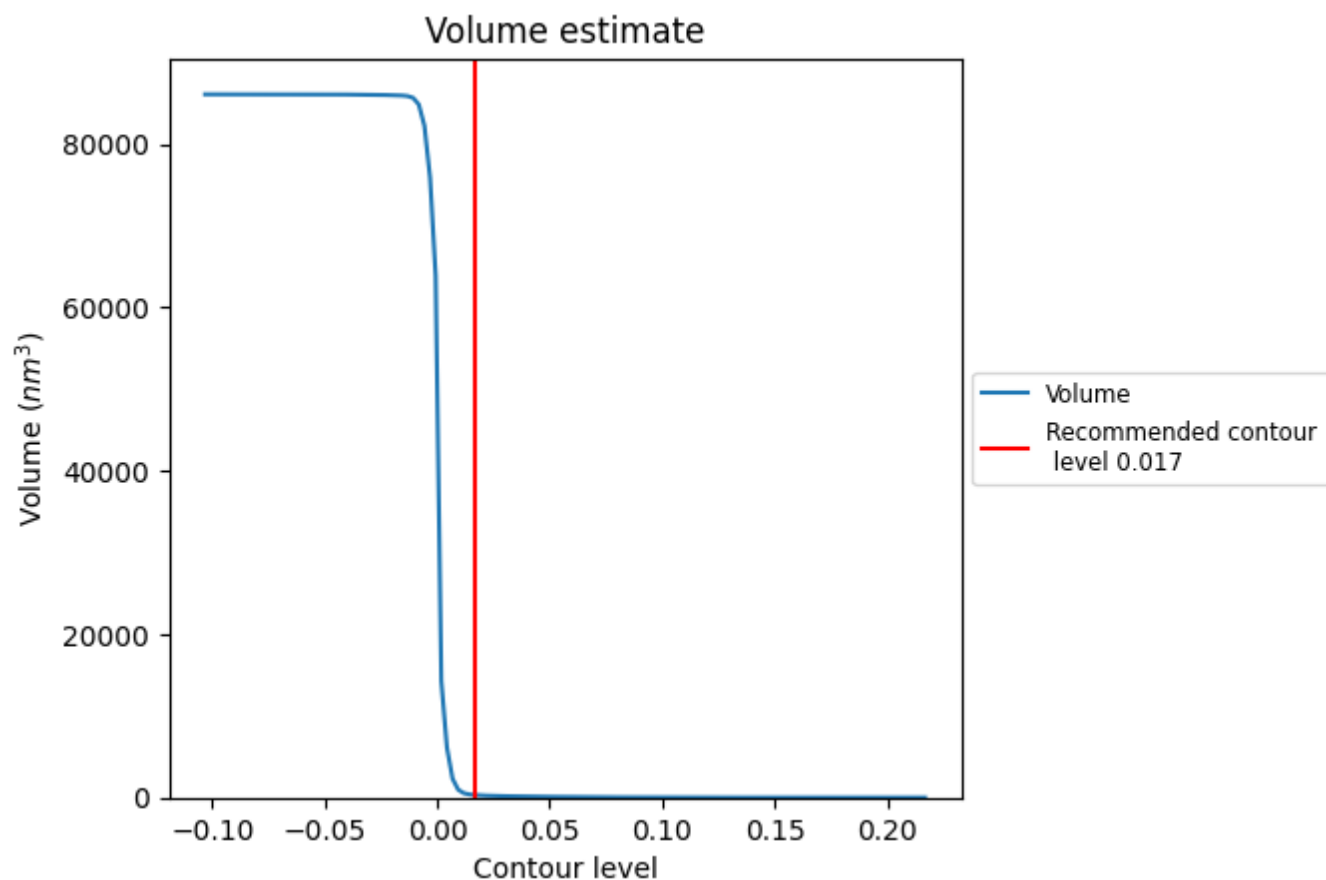
This section contains the results of statistical analysis of the map.

### 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.

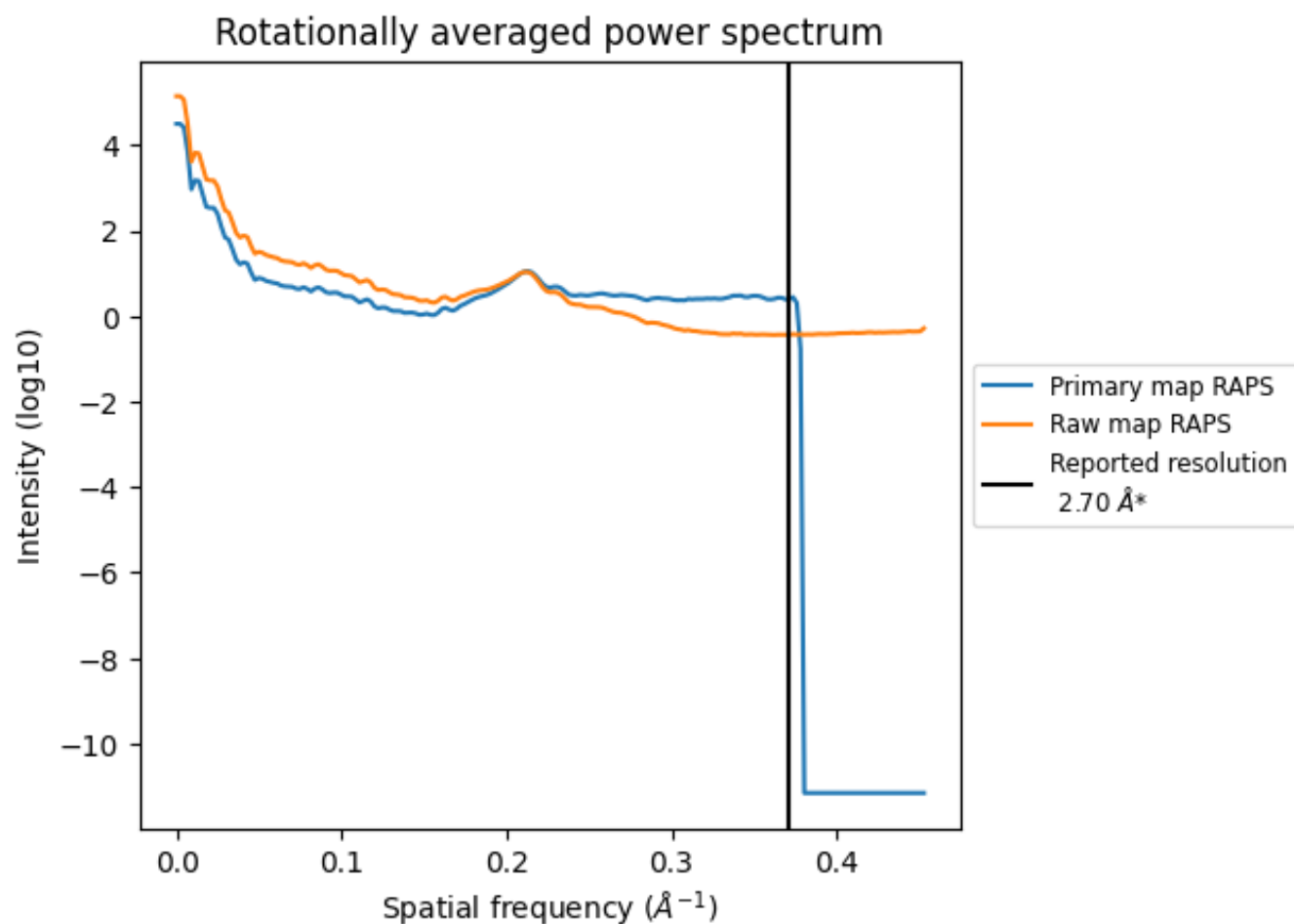
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 309 nm<sup>3</sup>; this corresponds to an approximate mass of 279 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 ⓘ

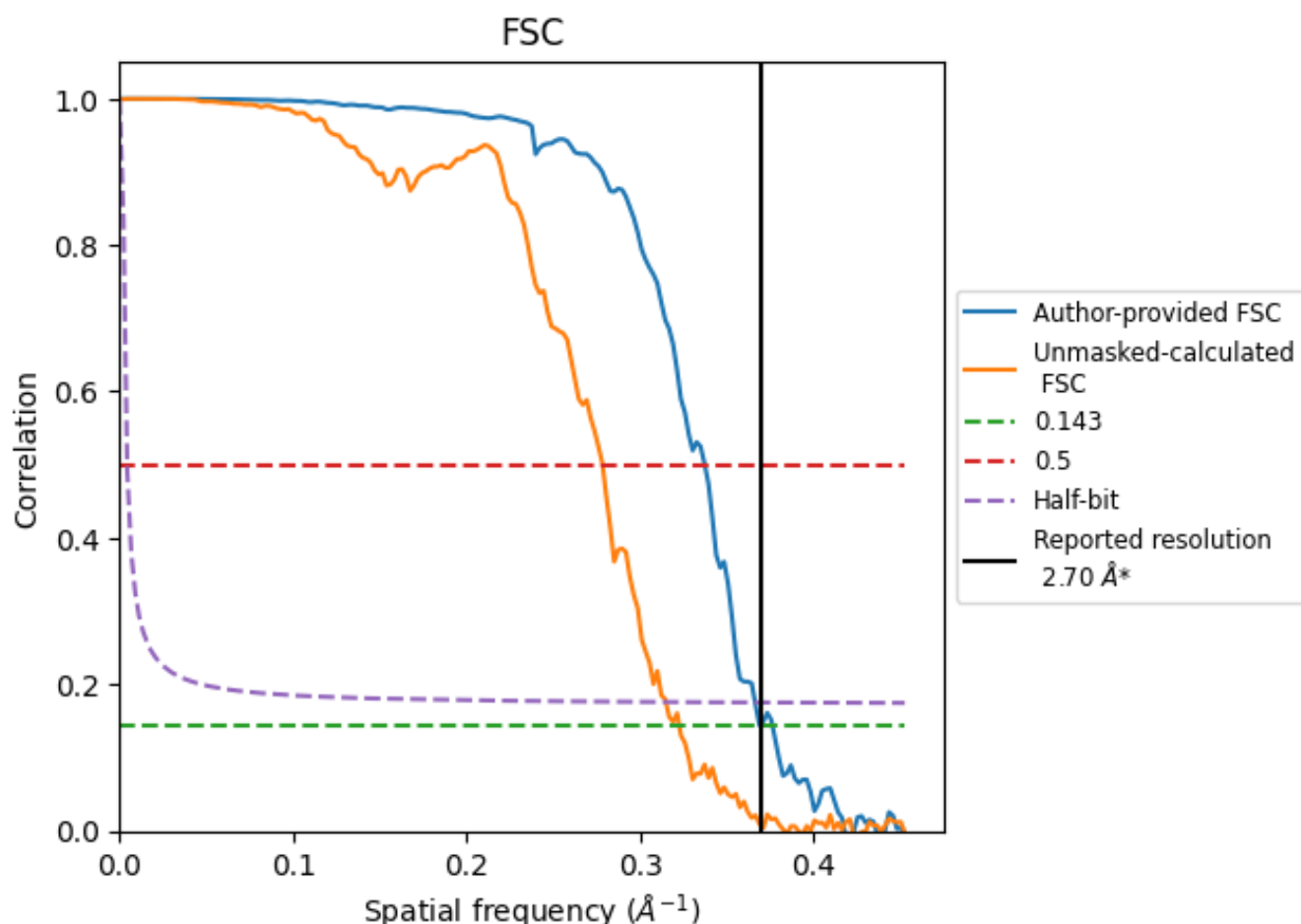


\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

## 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 0.370 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

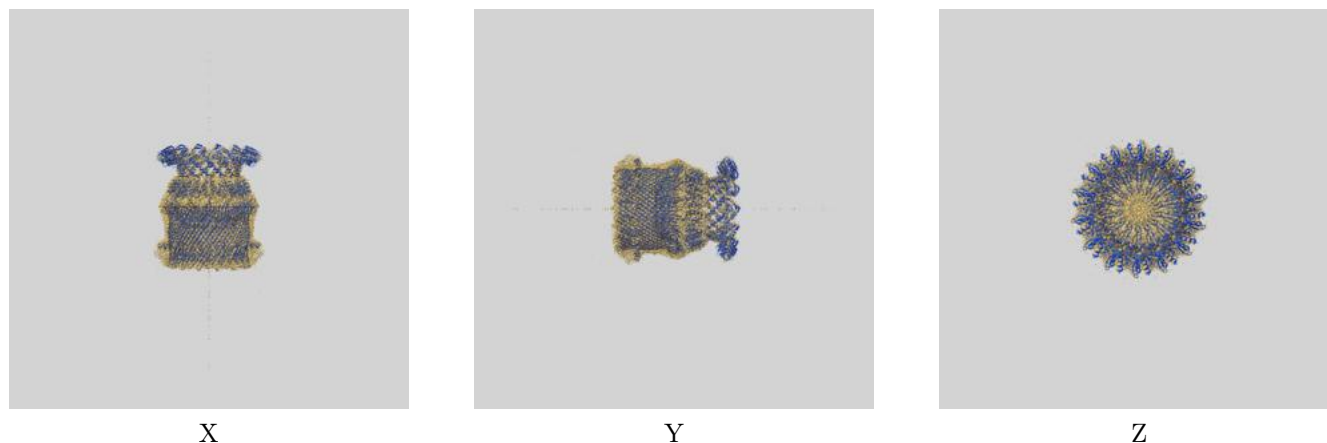
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.66	2.96	2.73
Unmasked-calculated*	3.10	3.59	3.17

\*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 3.10 differs from the reported value 2.7 by more than 10 %

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

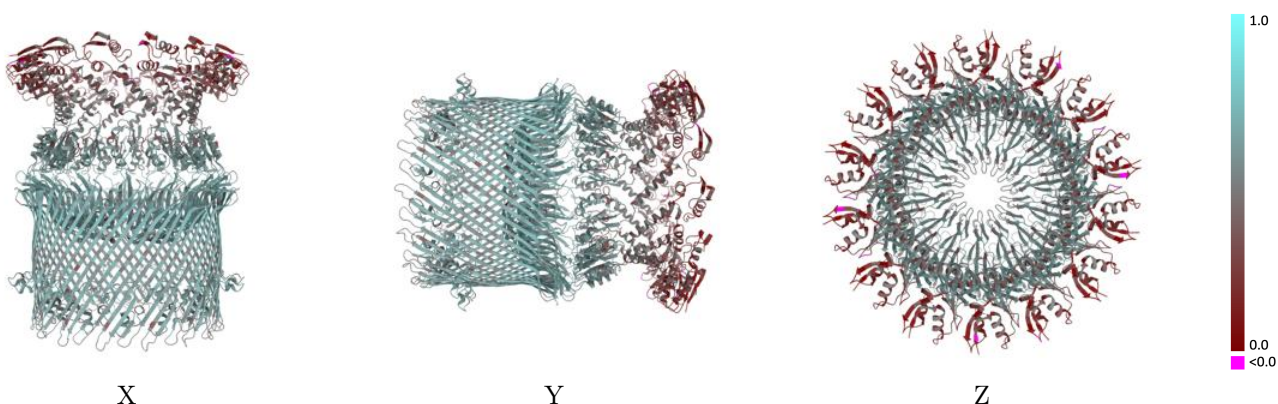
This section contains information regarding the fit between EMDB map EMD-21559 and PDB model 6W6M. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



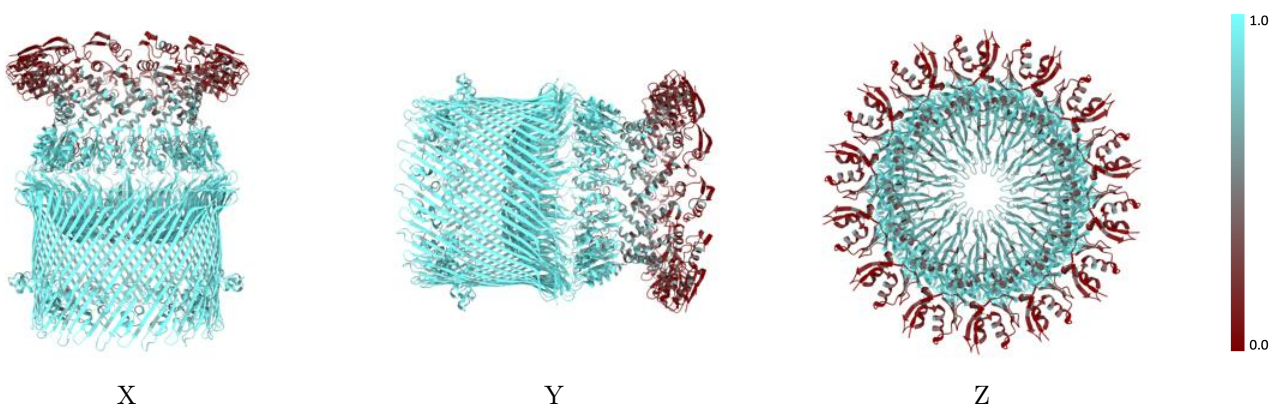
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



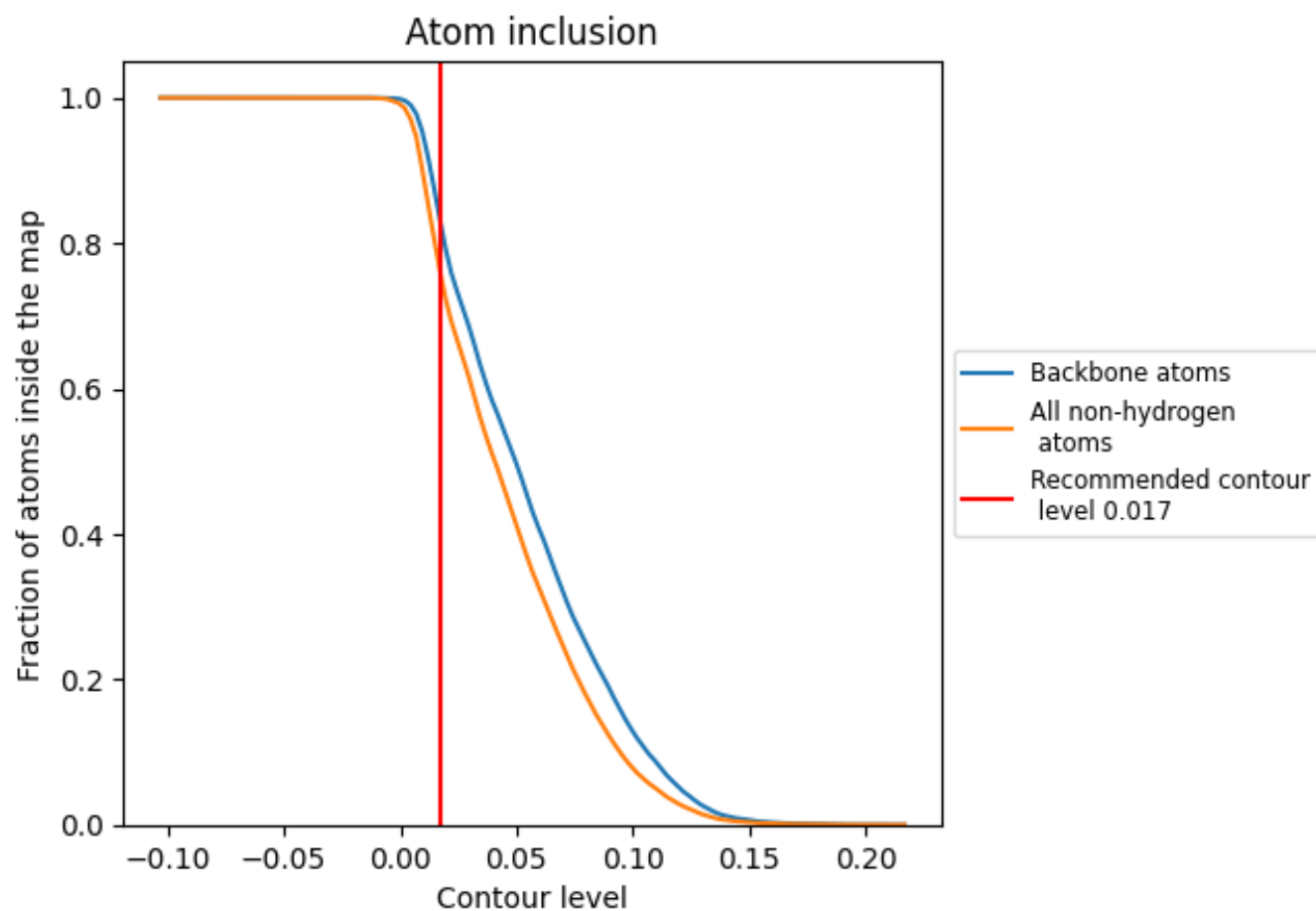
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7633	<div></div> 0.5130
A	<div></div> 0.7661	<div></div> 0.5140
B	<div></div> 0.7671	<div></div> 0.5160
C	<div></div> 0.7609	<div></div> 0.5110
D	<div></div> 0.7570	<div></div> 0.5010
E	<div></div> 0.7700	<div></div> 0.5150
F	<div></div> 0.7580	<div></div> 0.5130
G	<div></div> 0.7638	<div></div> 0.5150
H	<div></div> 0.7628	<div></div> 0.5180
I	<div></div> 0.7658	<div></div> 0.5160
J	<div></div> 0.7635	<div></div> 0.5150
K	<div></div> 0.7648	<div></div> 0.5110
L	<div></div> 0.7641	<div></div> 0.5130
M	<div></div> 0.7622	<div></div> 0.5150
N	<div></div> 0.7602	<div></div> 0.5150

