



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 02:25 AM EST

PDB ID : 6VE2
EMDB ID : EMD-21152
Title : Tetradecameric PilQ bound by TsaP heptamer from *Pseudomonas aeruginosa*
Authors : McCallum, M.; Tammam, S.; Rubinstein, J.L.; Burrows, L.L.; Howell, P.L.
Deposited on : 2019-12-28
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

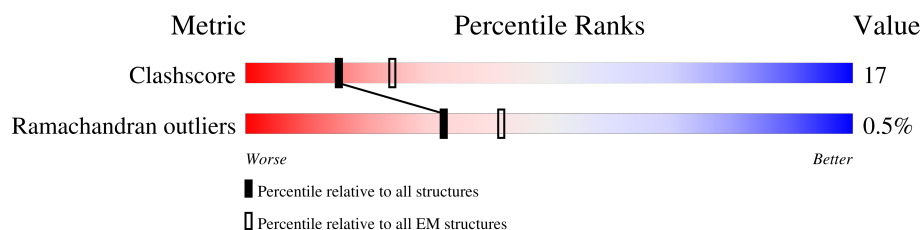
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	731	
1	B	731	
1	C	731	
1	D	731	
1	E	731	
1	F	731	
1	G	731	
1	H	731	
1	I	731	

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Mol	Chain	Length	Quality of chain
1	J	731	
1	K	731	
1	L	731	
1	M	731	
1	N	731	
2	O	341	
2	P	341	
2	Q	341	
2	R	341	
2	S	341	
2	T	341	
2	U	341	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 30198 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 Fimbrial assembly protein PilQ.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	327	Total	C	N	O	0	0
			1606	952	327	327		
1	B	327	Total	C	N	O	0	0
			1606	952	327	327		
1	C	327	Total	C	N	O	0	0
			1606	952	327	327		
1	D	327	Total	C	N	O	0	0
			1606	952	327	327		
1	E	327	Total	C	N	O	0	0
			1606	952	327	327		
1	F	327	Total	C	N	O	0	0
			1606	952	327	327		
1	G	327	Total	C	N	O	0	0
			1606	952	327	327		
1	H	327	Total	C	N	O	0	0
			1606	952	327	327		
1	I	327	Total	C	N	O	0	0
			1606	952	327	327		
1	J	327	Total	C	N	O	0	0
			1606	952	327	327		
1	K	327	Total	C	N	O	0	0
			1606	952	327	327		
1	L	327	Total	C	N	O	0	0
			1606	952	327	327		
1	M	327	Total	C	N	O	0	0
			1606	952	327	327		
1	N	327	Total	C	N	O	0	0
			1606	952	327	327		

There are 238 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-256	HIS	-	insertion	UNP P34750
A	-255	HIS	-	insertion	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-254	HIS	-	insertion	UNP P34750
A	-253	HIS	-	insertion	UNP P34750
A	-252	HIS	-	insertion	UNP P34750
A	-251	HIS	-	insertion	UNP P34750
A	-250	HIS	-	insertion	UNP P34750
A	-249	HIS	-	insertion	UNP P34750
A	330	GLY	-	expression tag	UNP P34750
A	331	HIS	-	expression tag	UNP P34750
A	332	HIS	-	expression tag	UNP P34750
A	333	HIS	-	expression tag	UNP P34750
A	334	HIS	-	expression tag	UNP P34750
A	335	HIS	-	expression tag	UNP P34750
A	336	HIS	-	expression tag	UNP P34750
A	337	HIS	-	expression tag	UNP P34750
A	338	HIS	-	expression tag	UNP P34750
B	-256	HIS	-	insertion	UNP P34750
B	-255	HIS	-	insertion	UNP P34750
B	-254	HIS	-	insertion	UNP P34750
B	-253	HIS	-	insertion	UNP P34750
B	-252	HIS	-	insertion	UNP P34750
B	-251	HIS	-	insertion	UNP P34750
B	-250	HIS	-	insertion	UNP P34750
B	-249	HIS	-	insertion	UNP P34750
B	330	GLY	-	expression tag	UNP P34750
B	331	HIS	-	expression tag	UNP P34750
B	332	HIS	-	expression tag	UNP P34750
B	333	HIS	-	expression tag	UNP P34750
B	334	HIS	-	expression tag	UNP P34750
B	335	HIS	-	expression tag	UNP P34750
B	336	HIS	-	expression tag	UNP P34750
B	337	HIS	-	expression tag	UNP P34750
B	338	HIS	-	expression tag	UNP P34750
C	-256	HIS	-	insertion	UNP P34750
C	-255	HIS	-	insertion	UNP P34750
C	-254	HIS	-	insertion	UNP P34750
C	-253	HIS	-	insertion	UNP P34750
C	-252	HIS	-	insertion	UNP P34750
C	-251	HIS	-	insertion	UNP P34750
C	-250	HIS	-	insertion	UNP P34750
C	-249	HIS	-	insertion	UNP P34750
C	330	GLY	-	expression tag	UNP P34750
C	331	HIS	-	expression tag	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
C	332	HIS	-	expression tag	UNP P34750
C	333	HIS	-	expression tag	UNP P34750
C	334	HIS	-	expression tag	UNP P34750
C	335	HIS	-	expression tag	UNP P34750
C	336	HIS	-	expression tag	UNP P34750
C	337	HIS	-	expression tag	UNP P34750
C	338	HIS	-	expression tag	UNP P34750
D	-256	HIS	-	insertion	UNP P34750
D	-255	HIS	-	insertion	UNP P34750
D	-254	HIS	-	insertion	UNP P34750
D	-253	HIS	-	insertion	UNP P34750
D	-252	HIS	-	insertion	UNP P34750
D	-251	HIS	-	insertion	UNP P34750
D	-250	HIS	-	insertion	UNP P34750
D	-249	HIS	-	insertion	UNP P34750
D	330	GLY	-	expression tag	UNP P34750
D	331	HIS	-	expression tag	UNP P34750
D	332	HIS	-	expression tag	UNP P34750
D	333	HIS	-	expression tag	UNP P34750
D	334	HIS	-	expression tag	UNP P34750
D	335	HIS	-	expression tag	UNP P34750
D	336	HIS	-	expression tag	UNP P34750
D	337	HIS	-	expression tag	UNP P34750
D	338	HIS	-	expression tag	UNP P34750
E	-256	HIS	-	insertion	UNP P34750
E	-255	HIS	-	insertion	UNP P34750
E	-254	HIS	-	insertion	UNP P34750
E	-253	HIS	-	insertion	UNP P34750
E	-252	HIS	-	insertion	UNP P34750
E	-251	HIS	-	insertion	UNP P34750
E	-250	HIS	-	insertion	UNP P34750
E	-249	HIS	-	insertion	UNP P34750
E	330	GLY	-	expression tag	UNP P34750
E	331	HIS	-	expression tag	UNP P34750
E	332	HIS	-	expression tag	UNP P34750
E	333	HIS	-	expression tag	UNP P34750
E	334	HIS	-	expression tag	UNP P34750
E	335	HIS	-	expression tag	UNP P34750
E	336	HIS	-	expression tag	UNP P34750
E	337	HIS	-	expression tag	UNP P34750
E	338	HIS	-	expression tag	UNP P34750
F	-256	HIS	-	insertion	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-255	HIS	-	insertion	UNP P34750
F	-254	HIS	-	insertion	UNP P34750
F	-253	HIS	-	insertion	UNP P34750
F	-252	HIS	-	insertion	UNP P34750
F	-251	HIS	-	insertion	UNP P34750
F	-250	HIS	-	insertion	UNP P34750
F	-249	HIS	-	insertion	UNP P34750
F	330	GLY	-	expression tag	UNP P34750
F	331	HIS	-	expression tag	UNP P34750
F	332	HIS	-	expression tag	UNP P34750
F	333	HIS	-	expression tag	UNP P34750
F	334	HIS	-	expression tag	UNP P34750
F	335	HIS	-	expression tag	UNP P34750
F	336	HIS	-	expression tag	UNP P34750
F	337	HIS	-	expression tag	UNP P34750
F	338	HIS	-	expression tag	UNP P34750
G	-256	HIS	-	insertion	UNP P34750
G	-255	HIS	-	insertion	UNP P34750
G	-254	HIS	-	insertion	UNP P34750
G	-253	HIS	-	insertion	UNP P34750
G	-252	HIS	-	insertion	UNP P34750
G	-251	HIS	-	insertion	UNP P34750
G	-250	HIS	-	insertion	UNP P34750
G	-249	HIS	-	insertion	UNP P34750
G	330	GLY	-	expression tag	UNP P34750
G	331	HIS	-	expression tag	UNP P34750
G	332	HIS	-	expression tag	UNP P34750
G	333	HIS	-	expression tag	UNP P34750
G	334	HIS	-	expression tag	UNP P34750
G	335	HIS	-	expression tag	UNP P34750
G	336	HIS	-	expression tag	UNP P34750
G	337	HIS	-	expression tag	UNP P34750
G	338	HIS	-	expression tag	UNP P34750
H	-256	HIS	-	insertion	UNP P34750
H	-255	HIS	-	insertion	UNP P34750
H	-254	HIS	-	insertion	UNP P34750
H	-253	HIS	-	insertion	UNP P34750
H	-252	HIS	-	insertion	UNP P34750
H	-251	HIS	-	insertion	UNP P34750
H	-250	HIS	-	insertion	UNP P34750
H	-249	HIS	-	insertion	UNP P34750
H	330	GLY	-	expression tag	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
H	331	HIS	-	expression tag	UNP P34750
H	332	HIS	-	expression tag	UNP P34750
H	333	HIS	-	expression tag	UNP P34750
H	334	HIS	-	expression tag	UNP P34750
H	335	HIS	-	expression tag	UNP P34750
H	336	HIS	-	expression tag	UNP P34750
H	337	HIS	-	expression tag	UNP P34750
H	338	HIS	-	expression tag	UNP P34750
I	-256	HIS	-	insertion	UNP P34750
I	-255	HIS	-	insertion	UNP P34750
I	-254	HIS	-	insertion	UNP P34750
I	-253	HIS	-	insertion	UNP P34750
I	-252	HIS	-	insertion	UNP P34750
I	-251	HIS	-	insertion	UNP P34750
I	-250	HIS	-	insertion	UNP P34750
I	-249	HIS	-	insertion	UNP P34750
I	330	GLY	-	expression tag	UNP P34750
I	331	HIS	-	expression tag	UNP P34750
I	332	HIS	-	expression tag	UNP P34750
I	333	HIS	-	expression tag	UNP P34750
I	334	HIS	-	expression tag	UNP P34750
I	335	HIS	-	expression tag	UNP P34750
I	336	HIS	-	expression tag	UNP P34750
I	337	HIS	-	expression tag	UNP P34750
I	338	HIS	-	expression tag	UNP P34750
J	-256	HIS	-	insertion	UNP P34750
J	-255	HIS	-	insertion	UNP P34750
J	-254	HIS	-	insertion	UNP P34750
J	-253	HIS	-	insertion	UNP P34750
J	-252	HIS	-	insertion	UNP P34750
J	-251	HIS	-	insertion	UNP P34750
J	-250	HIS	-	insertion	UNP P34750
J	-249	HIS	-	insertion	UNP P34750
J	330	GLY	-	expression tag	UNP P34750
J	331	HIS	-	expression tag	UNP P34750
J	332	HIS	-	expression tag	UNP P34750
J	333	HIS	-	expression tag	UNP P34750
J	334	HIS	-	expression tag	UNP P34750
J	335	HIS	-	expression tag	UNP P34750
J	336	HIS	-	expression tag	UNP P34750
J	337	HIS	-	expression tag	UNP P34750
J	338	HIS	-	expression tag	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-256	HIS	-	insertion	UNP P34750
K	-255	HIS	-	insertion	UNP P34750
K	-254	HIS	-	insertion	UNP P34750
K	-253	HIS	-	insertion	UNP P34750
K	-252	HIS	-	insertion	UNP P34750
K	-251	HIS	-	insertion	UNP P34750
K	-250	HIS	-	insertion	UNP P34750
K	-249	HIS	-	insertion	UNP P34750
K	330	GLY	-	expression tag	UNP P34750
K	331	HIS	-	expression tag	UNP P34750
K	332	HIS	-	expression tag	UNP P34750
K	333	HIS	-	expression tag	UNP P34750
K	334	HIS	-	expression tag	UNP P34750
K	335	HIS	-	expression tag	UNP P34750
K	336	HIS	-	expression tag	UNP P34750
K	337	HIS	-	expression tag	UNP P34750
K	338	HIS	-	expression tag	UNP P34750
L	-256	HIS	-	insertion	UNP P34750
L	-255	HIS	-	insertion	UNP P34750
L	-254	HIS	-	insertion	UNP P34750
L	-253	HIS	-	insertion	UNP P34750
L	-252	HIS	-	insertion	UNP P34750
L	-251	HIS	-	insertion	UNP P34750
L	-250	HIS	-	insertion	UNP P34750
L	-249	HIS	-	insertion	UNP P34750
L	330	GLY	-	expression tag	UNP P34750
L	331	HIS	-	expression tag	UNP P34750
L	332	HIS	-	expression tag	UNP P34750
L	333	HIS	-	expression tag	UNP P34750
L	334	HIS	-	expression tag	UNP P34750
L	335	HIS	-	expression tag	UNP P34750
L	336	HIS	-	expression tag	UNP P34750
L	337	HIS	-	expression tag	UNP P34750
L	338	HIS	-	expression tag	UNP P34750
M	-256	HIS	-	insertion	UNP P34750
M	-255	HIS	-	insertion	UNP P34750
M	-254	HIS	-	insertion	UNP P34750
M	-253	HIS	-	insertion	UNP P34750
M	-252	HIS	-	insertion	UNP P34750
M	-251	HIS	-	insertion	UNP P34750
M	-250	HIS	-	insertion	UNP P34750
M	-249	HIS	-	insertion	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
M	330	GLY	-	expression tag	UNP P34750
M	331	HIS	-	expression tag	UNP P34750
M	332	HIS	-	expression tag	UNP P34750
M	333	HIS	-	expression tag	UNP P34750
M	334	HIS	-	expression tag	UNP P34750
M	335	HIS	-	expression tag	UNP P34750
M	336	HIS	-	expression tag	UNP P34750
M	337	HIS	-	expression tag	UNP P34750
M	338	HIS	-	expression tag	UNP P34750
N	-256	HIS	-	insertion	UNP P34750
N	-255	HIS	-	insertion	UNP P34750
N	-254	HIS	-	insertion	UNP P34750
N	-253	HIS	-	insertion	UNP P34750
N	-252	HIS	-	insertion	UNP P34750
N	-251	HIS	-	insertion	UNP P34750
N	-250	HIS	-	insertion	UNP P34750
N	-249	HIS	-	insertion	UNP P34750
N	330	GLY	-	expression tag	UNP P34750
N	331	HIS	-	expression tag	UNP P34750
N	332	HIS	-	expression tag	UNP P34750
N	333	HIS	-	expression tag	UNP P34750
N	334	HIS	-	expression tag	UNP P34750
N	335	HIS	-	expression tag	UNP P34750
N	336	HIS	-	expression tag	UNP P34750
N	337	HIS	-	expression tag	UNP P34750
N	338	HIS	-	expression tag	UNP P34750

- Molecule 2 is a protein called LysM domain-containing protein.

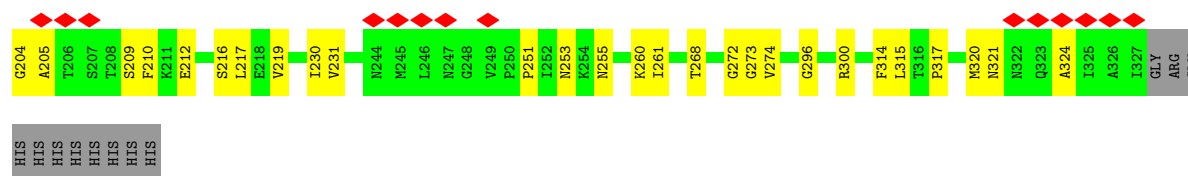
Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	225	Total	C	N	O	0	0
			1102	652	225	225		
2	P	225	Total	C	N	O	0	0
			1102	652	225	225		
2	Q	225	Total	C	N	O	0	0
			1102	652	225	225		
2	R	225	Total	C	N	O	0	0
			1102	652	225	225		
2	S	225	Total	C	N	O	0	0
			1102	652	225	225		
2	T	225	Total	C	N	O	0	0
			1102	652	225	225		

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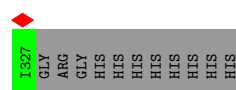
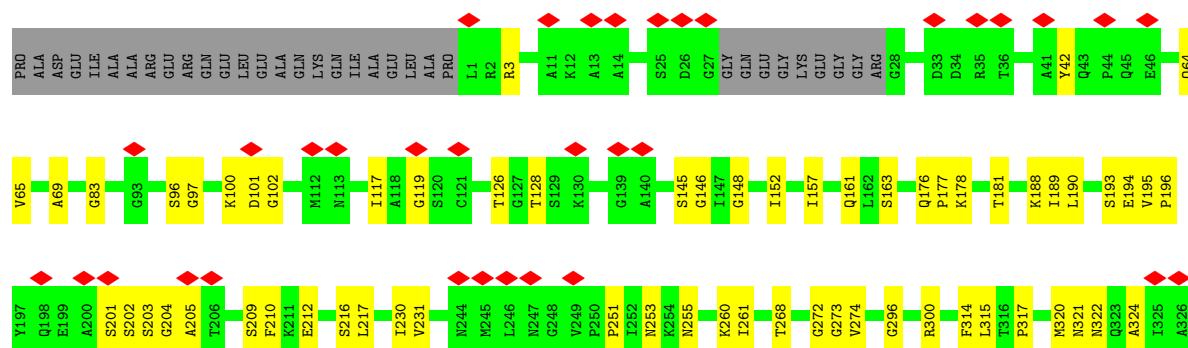
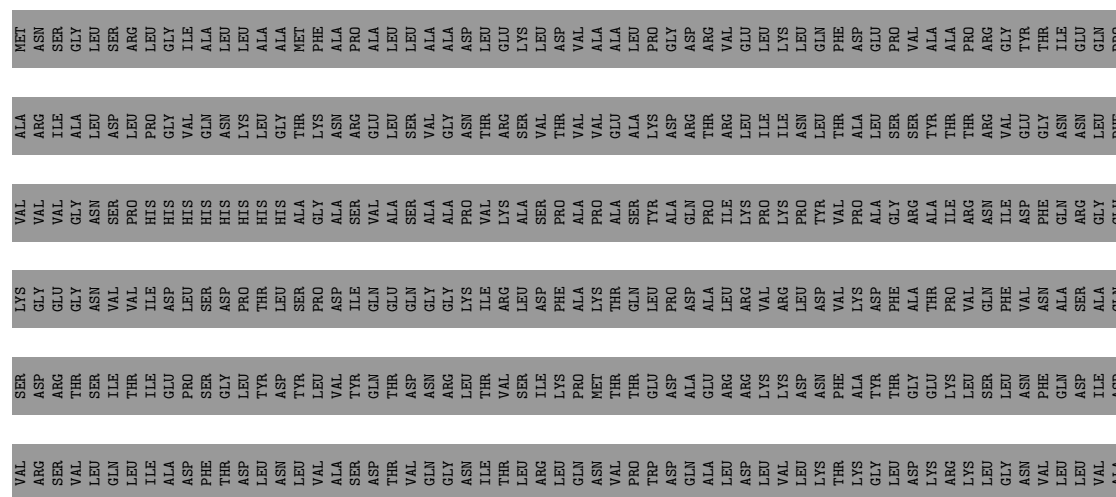
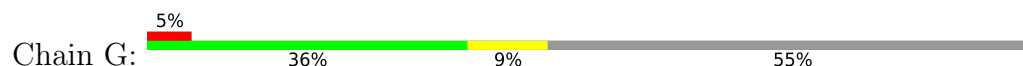
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Mol	Chain	Residues	Atoms				AltConf	Trace
2	U	225	Total	C	N	O	0	0
			1102	652	225	225		

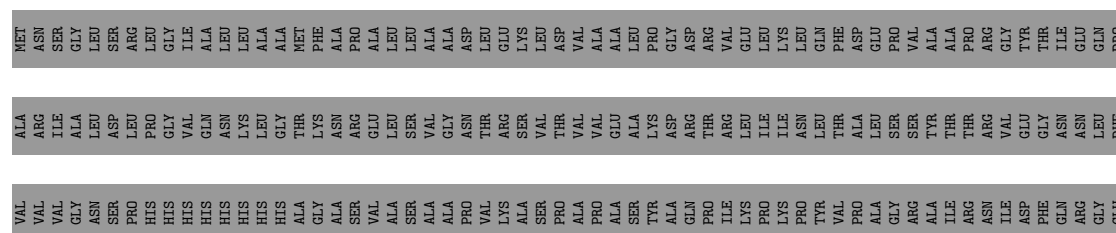
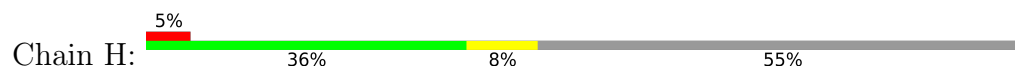


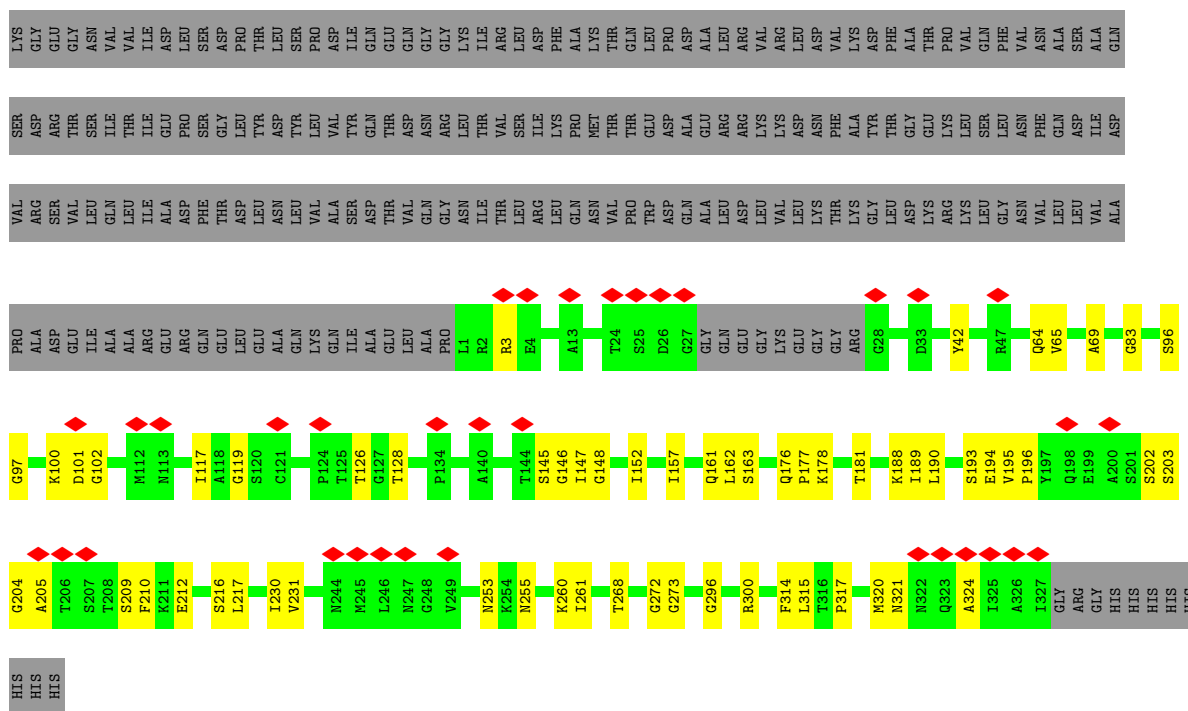


• Molecule 1: Fimbrial assembly protein PilQ

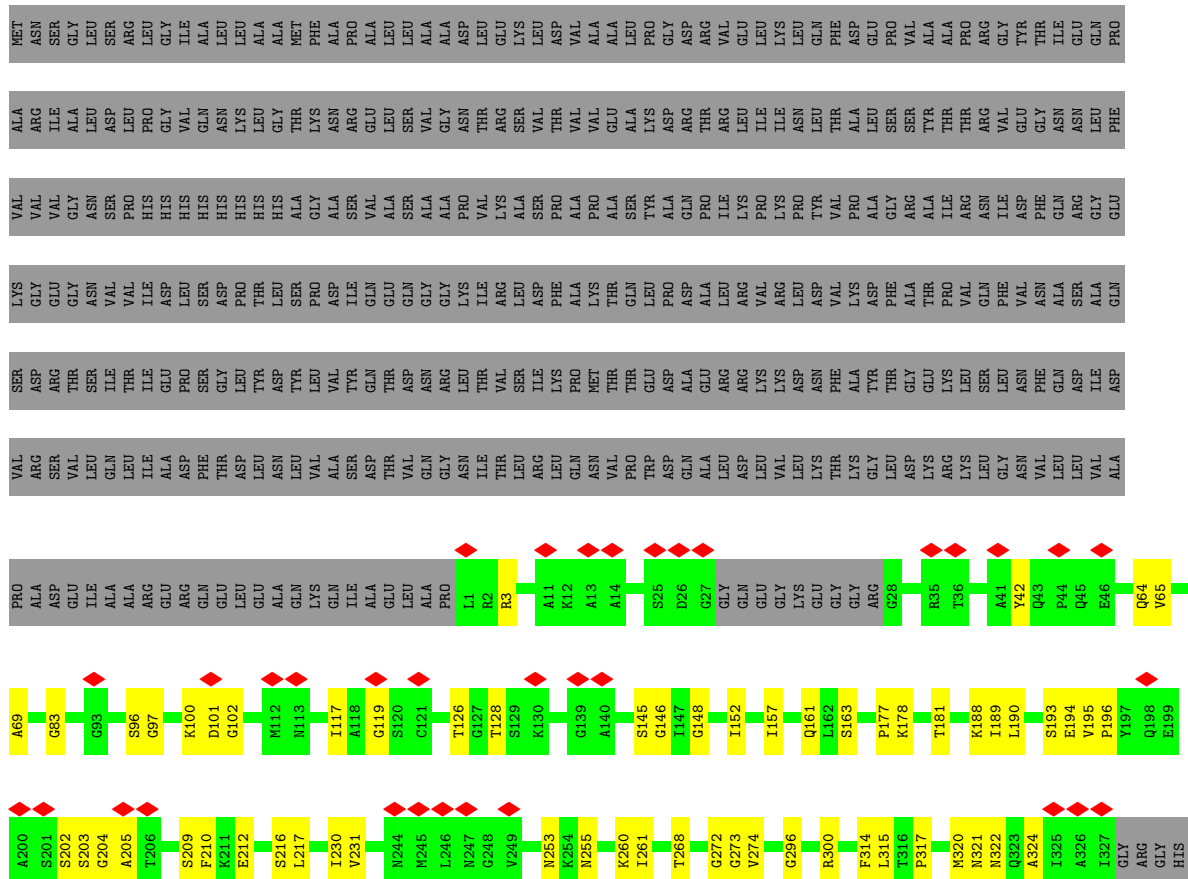
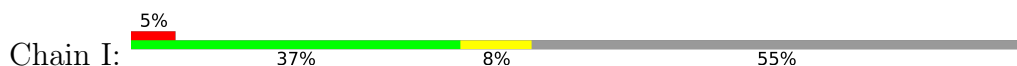


• Molecule 1: Fimbrial assembly protein PilQ



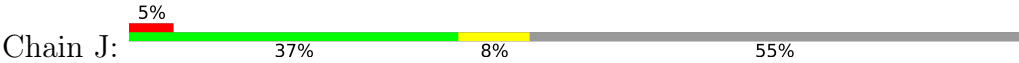


- Molecule 1: Fimbrial assembly protein PilQ



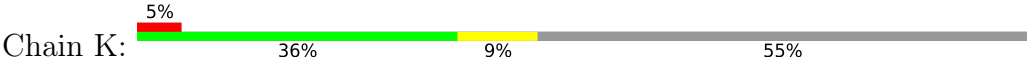
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● Molecule 1: Fimbrial assembly protein PilQ

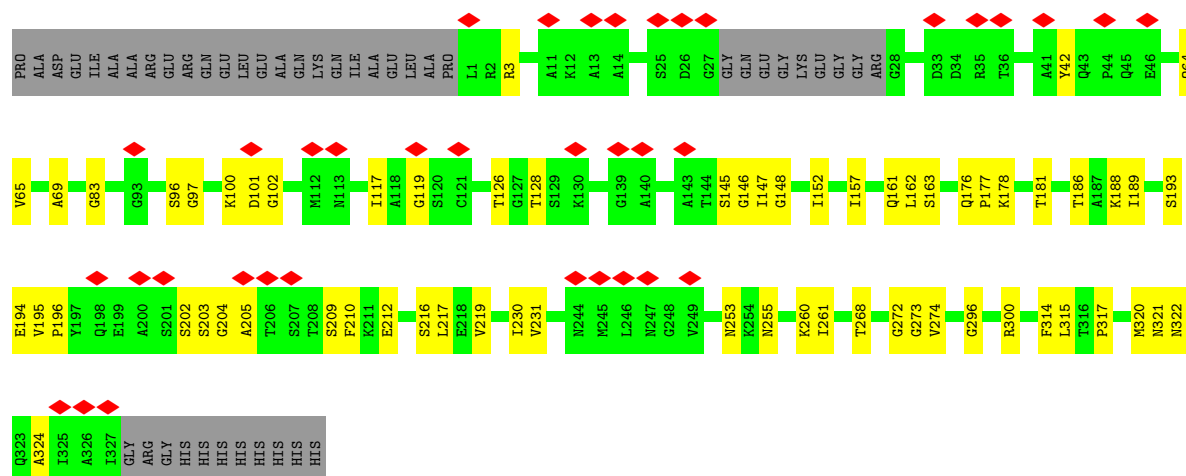


T206	S207	T208	S209	F210	K211	E212	S216	L217	T230	V231	N244	M245	L246	N247	G248	V249	N253	K260	I261	T268	G272	G273	V274	G296	R300	F314	L315	T316	F317	M320	N321	N322	Q323	A324	I325	A326	I327	GLY	ARG	GLY	HIS	HIS	HIS	HIS	HIS	HIS	HIS
K100	D101	G102	M112	M113	I117	A118	G119	S120	G121	P124	T125	T126	G127	T128	P134	A140	T144	S145	G146	T147	G148	I152	I157	Q161	L162	S163	Q176	P177	K178	T181	K188	I189	L190	S193	E194	V195	P196	Y197	Q198	E199	A200	S201	S202	G203	G204	A205	
PRO	ALA	ASP	GLU	ILE	ALA	ALA	ARG	GLU	ARG	GLN	GLN	LYS	GLN	ILE	ALA	LEU	PRO	L1	R2	R3	E4	T24	S25	D26	G27	GLY	GLN	GLU	GLY	LYS	GLY	ASP	LYS	ARG	GLY	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
VAL	ARG	SER	VAL	LEU	GLN	LEU	ILE	ALA	ASP	ASN	LEU	VAL	ALA	THR	VAL	GLN	GLY	THR	ILE	THR	LEU	ARG	ILE	LYS	GLN	ALA	GLN	ASN	VAL	PRO	TRP	ASP	GLN	GLN	GLY	GLY	LYS	THR	LYS	GLY	LEU	ASN	GLY	VAL	VAL	ALA	
SER	ASP	THR	SER	ILE	THR	ILE	GLU	PRO	THR	THR	THR	THR	THR	THR	THR	ASP	ASN	THR	GLY	THR	THR	THR	THR	THR	GLU	ALA	ALA	GLU	ARG	THR	GLU	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
LYS	GLY	GLY	ASN	VAL	VAL	ILE	ASP	LEU	THR	GLN	GLY	ASP	THR	THR	GLN	GLN	GLY	THR	ILE	THR	LEU	THR	THR	LYS	PRO	ALA	ALA	GLU	ILE	ARG	LYS	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
VAL	VAL	VAL	ASN	SER	HIS	HIS	ASP	LEU	THR	SER	PRO	GLY	ALA	THR	SER	GLN	GLN	GLY	ILE	VAL	ARG	LYS	SER	ASP	PRO	ALA	VAL	THR	ILE	ARG	LYS	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
ALA	ARG	ILE	ASN	SER	HIS	HIS	GLY	VAL	GLN	THR	MET	PHE	ALA	THR	LEU	ALA	ALA	GLY	ALA	VAL	THR	THR	VAL	THR	ALA	ASP	GLN	VAL	THR	ILE	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
MET	ASN	ILE	GLY	SER	LEU	ILE	GLY	ALA	ALA	LEU	ALA	ALA	ALA	LEU	SER	LEU	ALA	GLY	ALA	GLY	THR	VAL	VAL	THR	PRO	GLY	VAL	ALA	GLU	ILE	LYS	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	

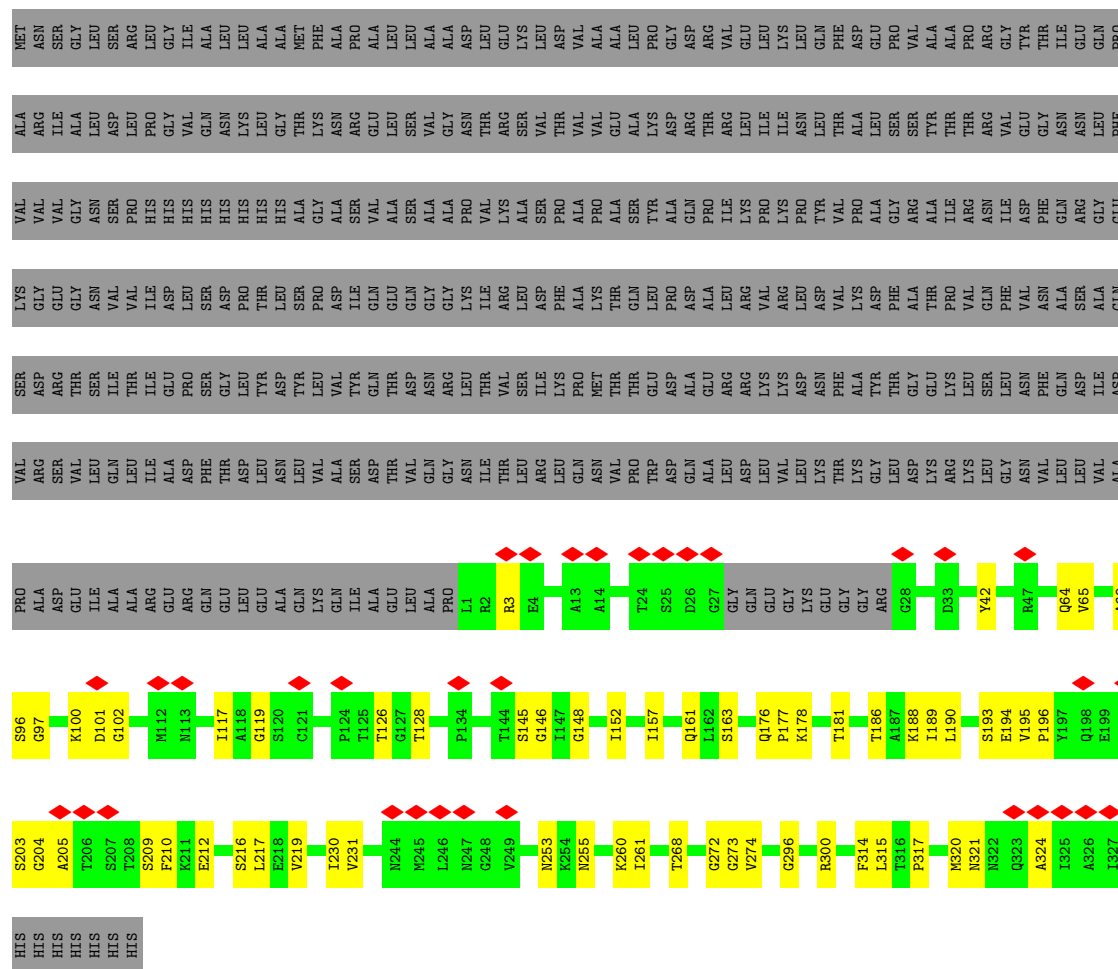
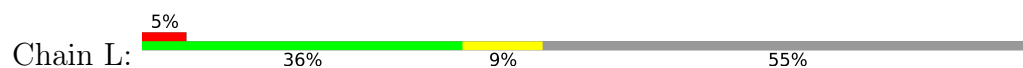
● Molecule 1: Fimbrial assembly protein PilQ



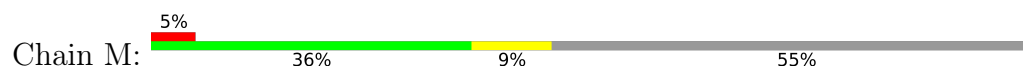
MET	ASN	GLY	LEU	SER	ARG	LEU	GLY	ILE	ALA	LEU	LEU	ALA	ALA	GLY	ASP	LEU	THR	VAL	VAL	ALA	LEU	LEU	PRO	LYS	PRO	GLY	ARG	VAL	LEU	ILE	LYS	LEU	ASN	GLN	PHE	ASP	ALA	GLU	GLY	THR	ILE	ASN	GLN	PRO	PHE		
ALA	ARG	ILE	GLY	ILE	PRO	VAL	GLY	VAL	GLN	VAL	ASN	LYS	LEU	LEU	GLY	ASP	LEU	THR	VAL	VAL	ALA	ALA	LEU	LEU	PRO	LYS	PRO	GLY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



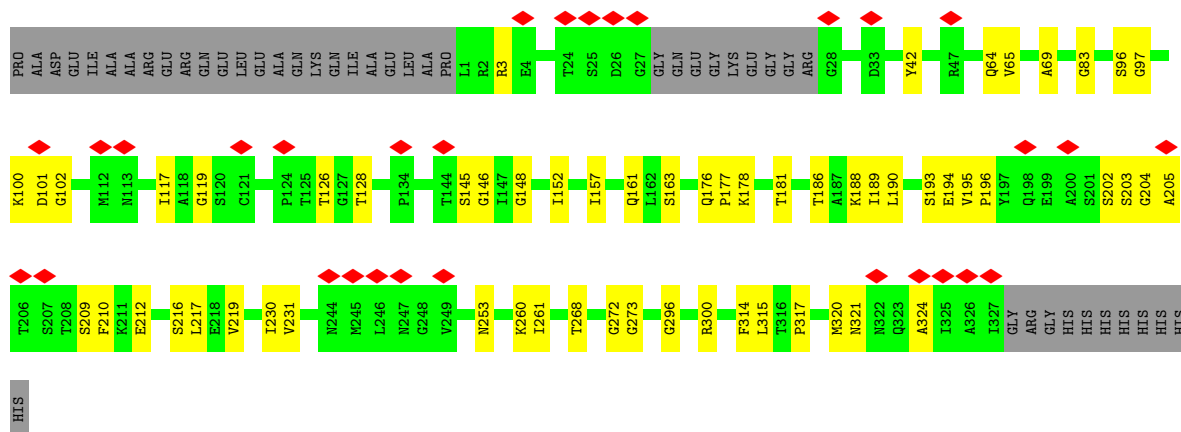
• Molecule 1: Fimbrial assembly protein PilQ



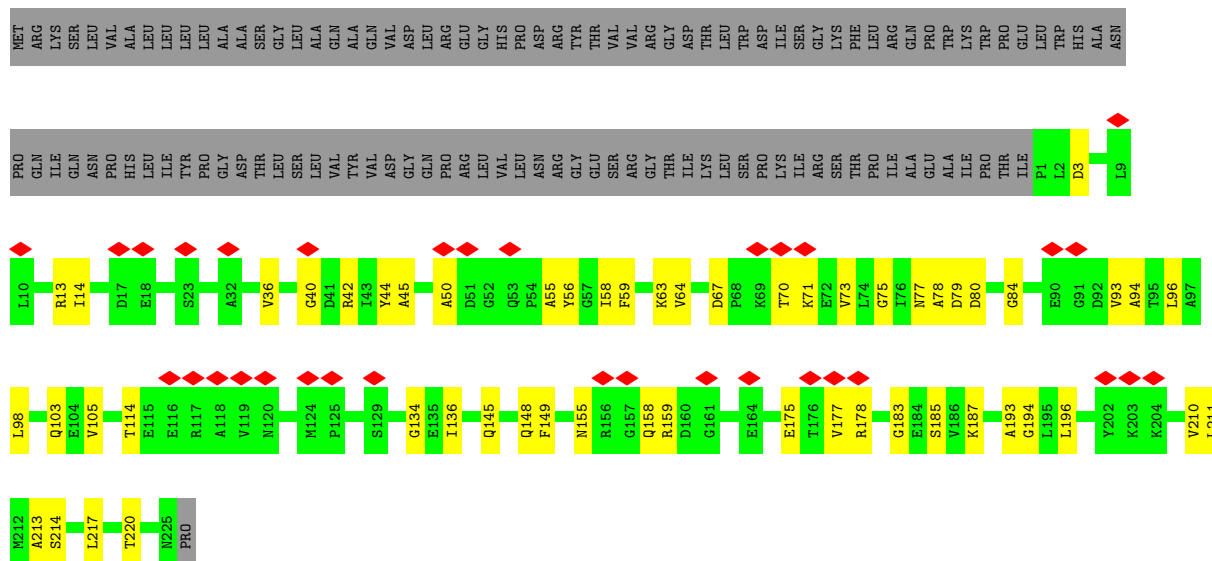
• Molecule 1: Fimbrial assembly protein PilQ



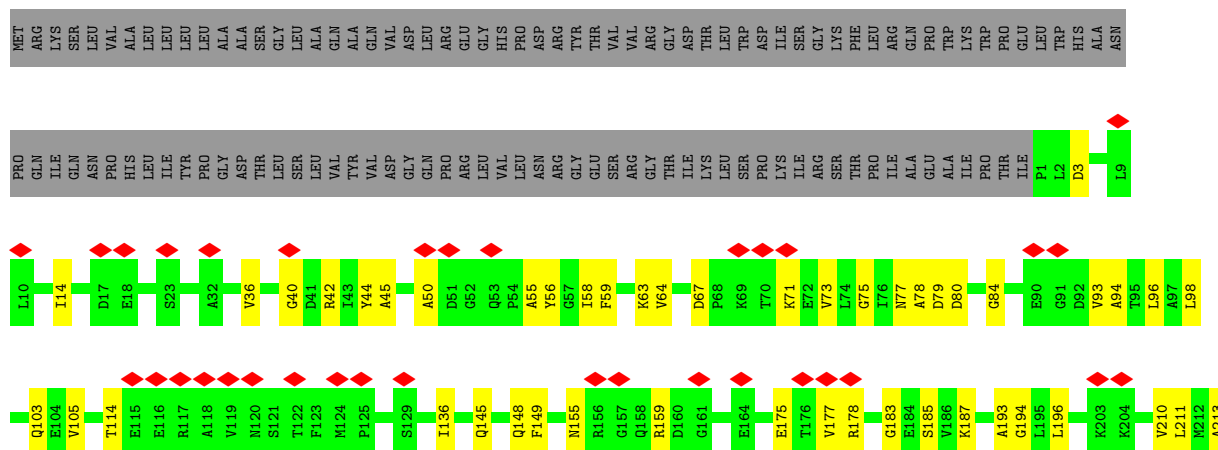




• Molecule 2: LysM domain-containing protein

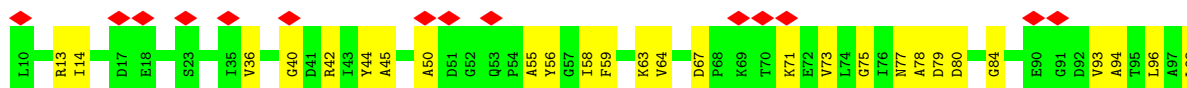
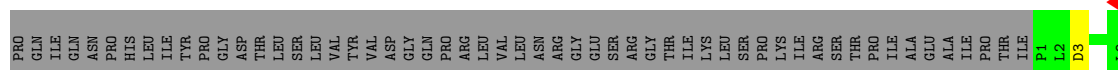


• Molecule 2: LysM domain-containing protein

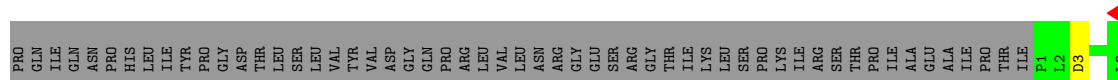




- Molecule 2: LysM domain-containing protein

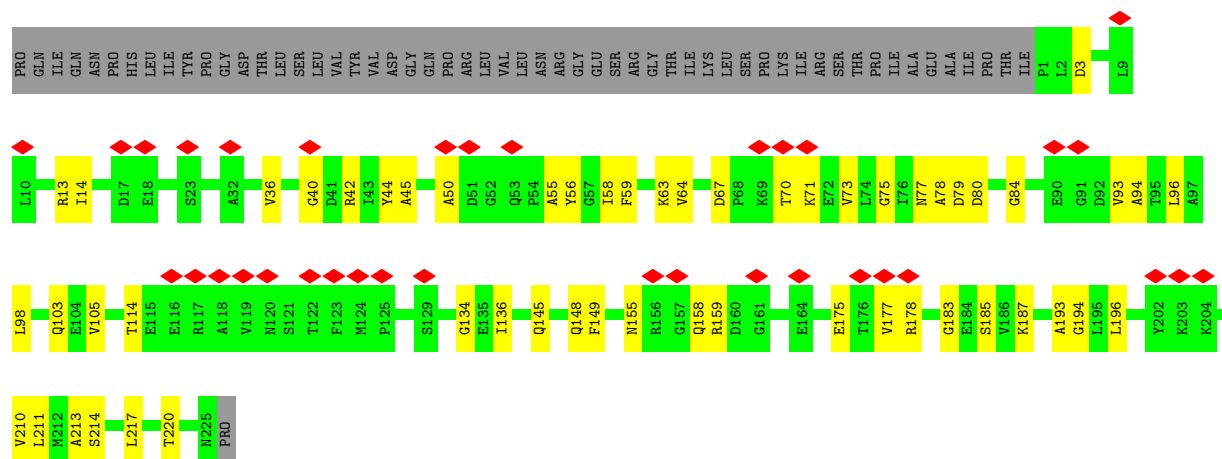


- Molecule 2: LysM domain-containing protein

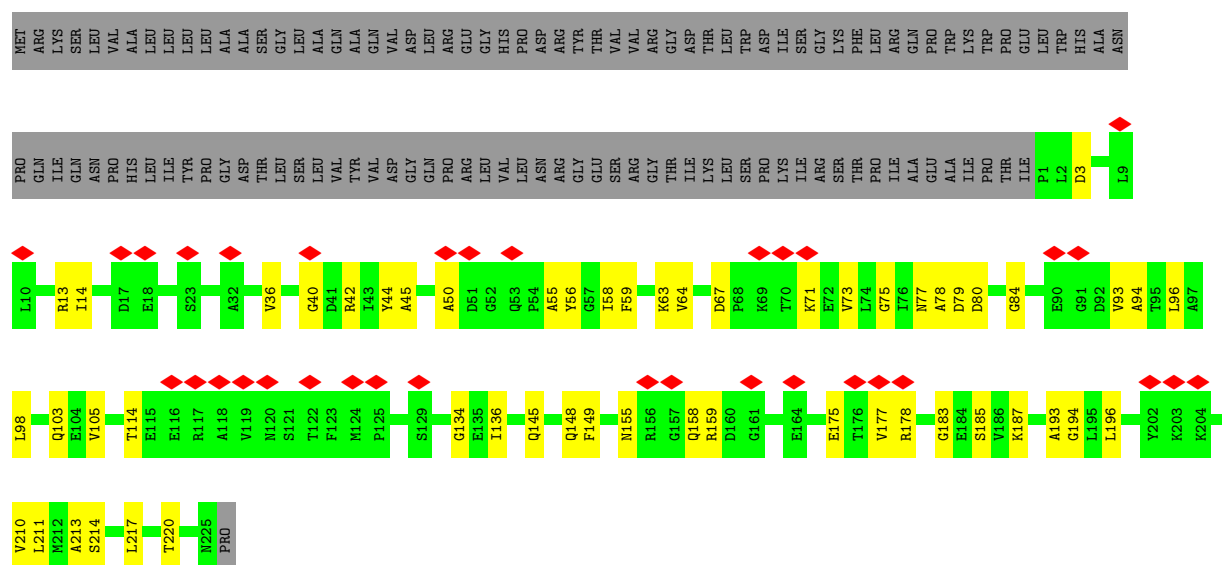


- Molecule 2: LysM domain-containing protein

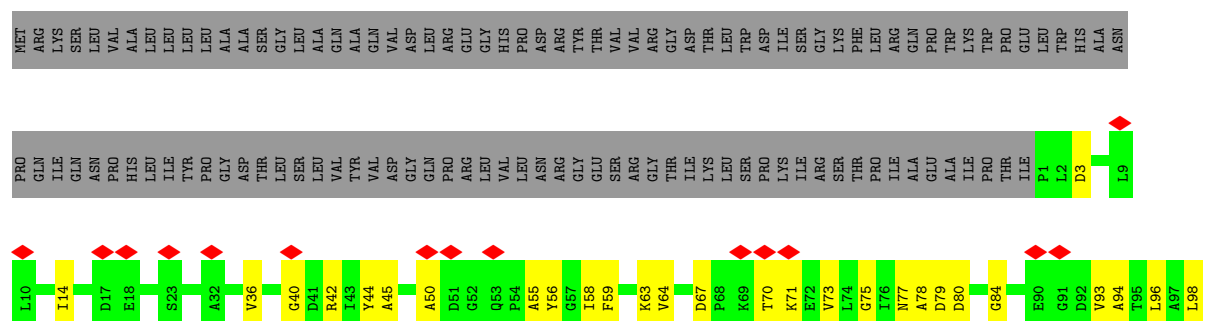


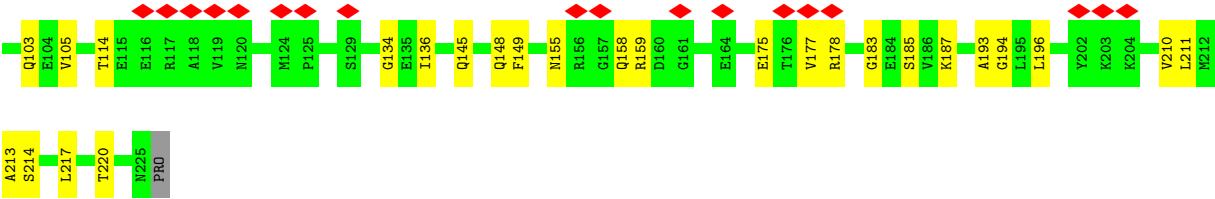


• Molecule 2: LysM domain-containing protein



• Molecule 2: LysM domain-containing protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	47468	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.116	Depositor
Minimum map value	-0.270	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.46	Depositor
Map size (Å)	371.2, 371.2, 371.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	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	0.39	0/1604	0.65	0/2225
1	B	0.39	0/1604	0.65	0/2225
1	C	0.39	0/1604	0.65	0/2225
1	D	0.39	0/1604	0.65	0/2225
1	E	0.39	0/1604	0.65	0/2225
1	F	0.39	0/1604	0.65	0/2225
1	G	0.39	0/1604	0.65	0/2225
1	H	0.39	0/1604	0.65	0/2225
1	I	0.39	0/1604	0.65	0/2225
1	J	0.39	0/1604	0.65	0/2225
1	K	0.39	0/1604	0.65	0/2225
1	L	0.39	0/1604	0.65	0/2225
1	M	0.39	0/1604	0.65	0/2225
1	N	0.39	0/1604	0.65	0/2225
2	O	0.36	0/1101	0.67	0/1526
2	P	0.36	0/1101	0.67	0/1526
2	Q	0.36	0/1101	0.67	0/1526
2	R	0.36	0/1101	0.67	0/1526
2	S	0.36	0/1101	0.67	0/1526
2	T	0.36	0/1101	0.67	0/1526
2	U	0.36	0/1101	0.67	0/1526
All	All	0.38	0/30163	0.65	0/41832

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

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	1606	0	731	46	0
1	B	1606	0	731	56	0
1	C	1606	0	731	51	0
1	D	1606	0	731	45	0
1	E	1606	0	731	47	0
1	F	1606	0	731	50	0
1	G	1606	0	731	49	0
1	H	1606	0	731	46	0
1	I	1606	0	731	44	0
1	J	1606	0	731	41	0
1	K	1606	0	731	43	0
1	L	1606	0	731	51	0
1	M	1606	0	731	51	0
1	N	1606	0	731	44	0
2	O	1102	0	514	34	0
2	P	1102	0	514	32	0
2	Q	1102	0	514	33	0
2	R	1102	0	514	34	0
2	S	1102	0	514	34	0
2	T	1102	0	514	34	0
2	U	1102	0	514	34	0
All	All	30198	0	13832	727	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 17.

The worst 5 of 727 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)
2:S:149:PHE:HA	2:S:210:VAL:O	1.60	1.02
2:P:149:PHE:HA	2:P:210:VAL:O	1.60	1.01
2:O:149:PHE:HA	2:O:210:VAL:O	1.61	1.01
2:R:149:PHE:HA	2:R:210:VAL:O	1.61	1.01
2:T:149:PHE:HA	2:T:210:VAL:O	1.61	1.01

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	B	323/731 (44%)	306 (95%)	15 (5%)	2 (1%)	25	65
1	C	323/731 (44%)	306 (95%)	15 (5%)	2 (1%)	25	65
1	D	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	E	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	F	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	G	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	H	323/731 (44%)	306 (95%)	15 (5%)	2 (1%)	25	65
1	I	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	J	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	K	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
1	L	323/731 (44%)	306 (95%)	15 (5%)	2 (1%)	25	65
1	M	323/731 (44%)	306 (95%)	15 (5%)	2 (1%)	25	65
1	N	323/731 (44%)	307 (95%)	14 (4%)	2 (1%)	25	65
2	O	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
2	P	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
2	Q	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
2	R	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
2	S	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
2	T	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
2	U	223/341 (65%)	211 (95%)	12 (5%)	0	100	100
All	All	6083/12621 (48%)	5770 (95%)	285 (5%)	28 (0%)	32	68

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	SER
1	B	145	SER
1	C	145	SER
1	D	145	SER
1	E	145	SER

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.

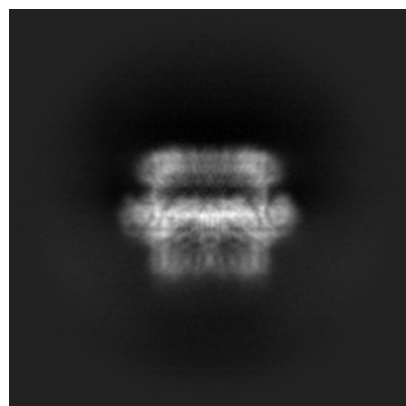
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21152. These allow visual inspection of the internal detail of the map and identification of artifacts.

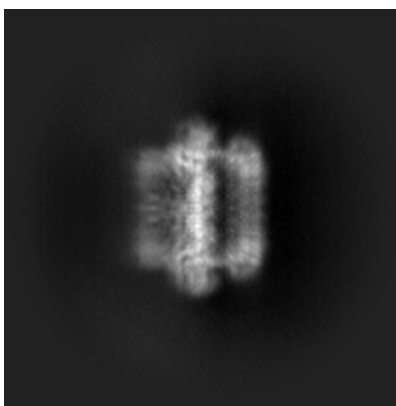
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

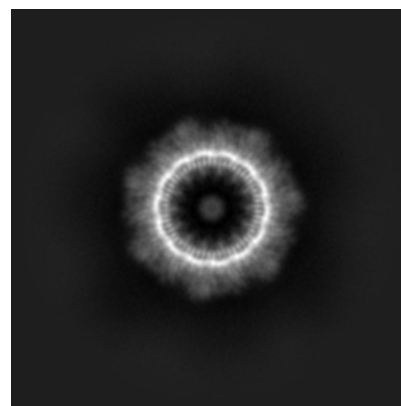
6.1.1 Primary map



X

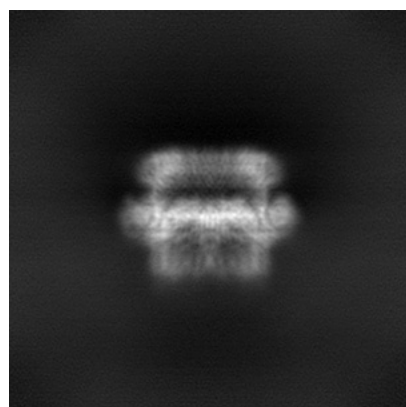


Y

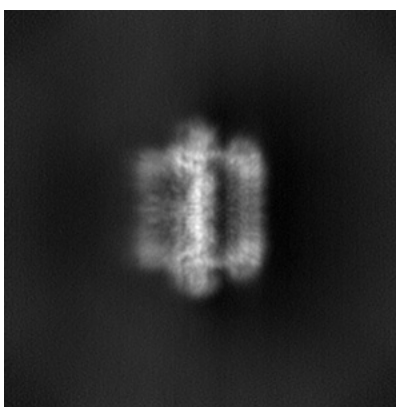


Z

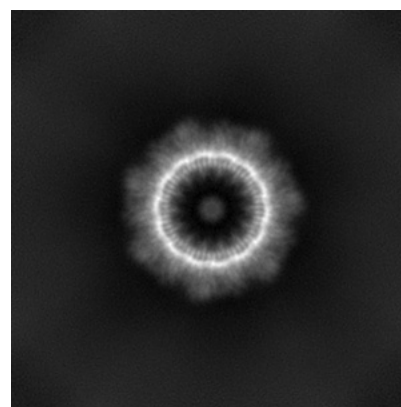
6.1.2 Raw map



X



Y

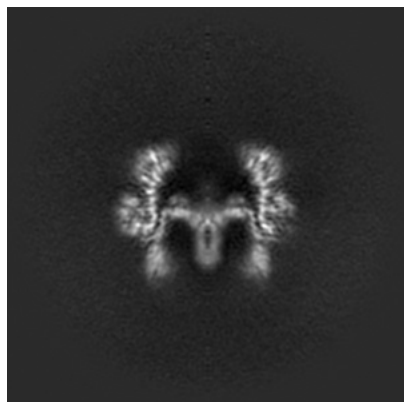


Z

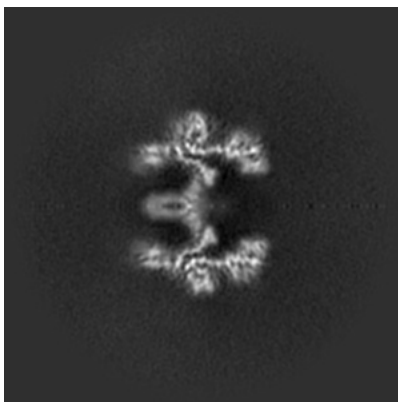
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

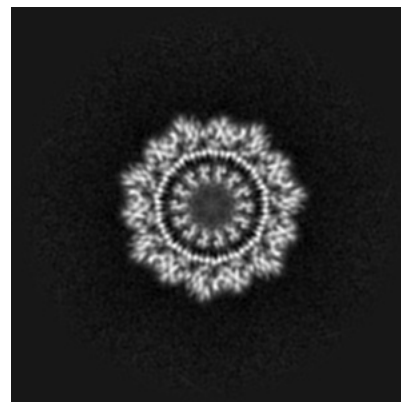
6.2.1 Primary map



X Index: 128

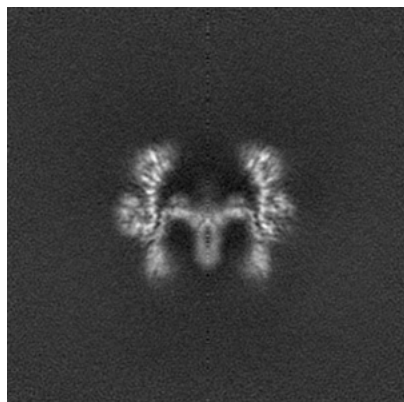


Y Index: 128

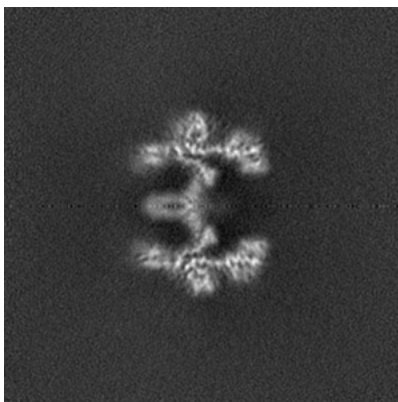


Z Index: 128

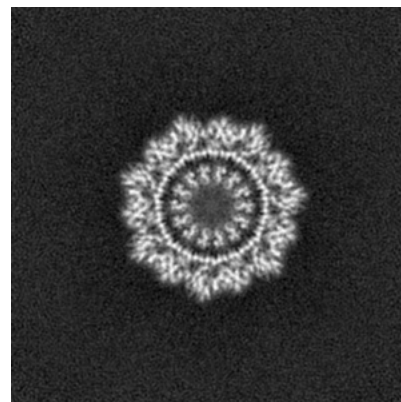
6.2.2 Raw map



X Index: 128



Y Index: 128

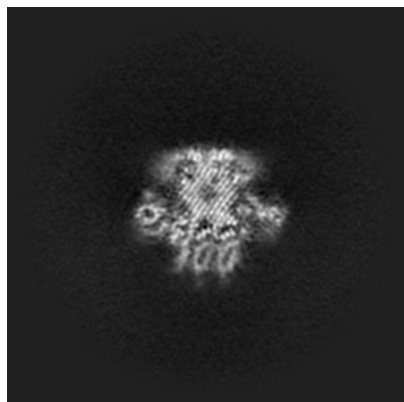


Z Index: 128

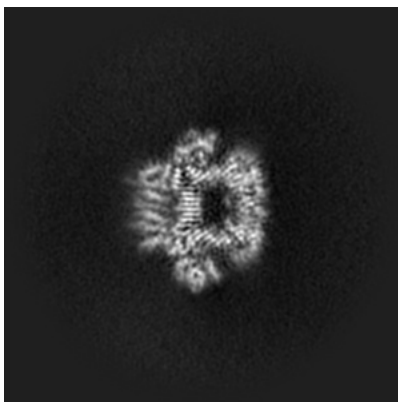
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

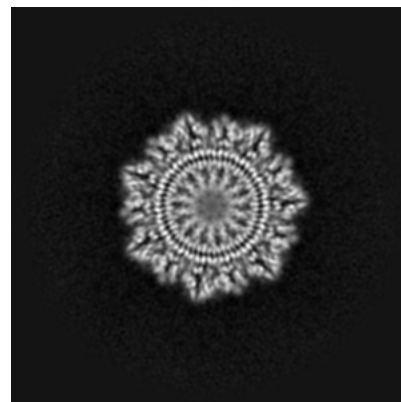
6.3.1 Primary map



X Index: 162

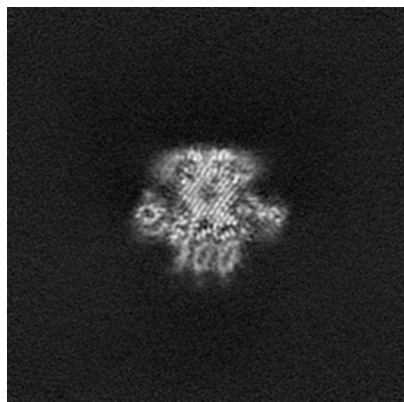


Y Index: 99

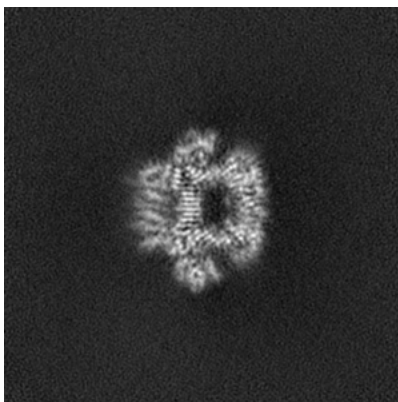


Z Index: 124

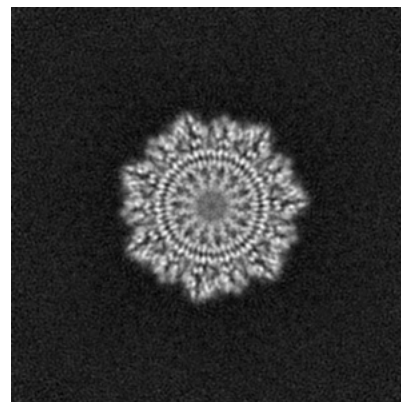
6.3.2 Raw map



X Index: 162



Y Index: 99

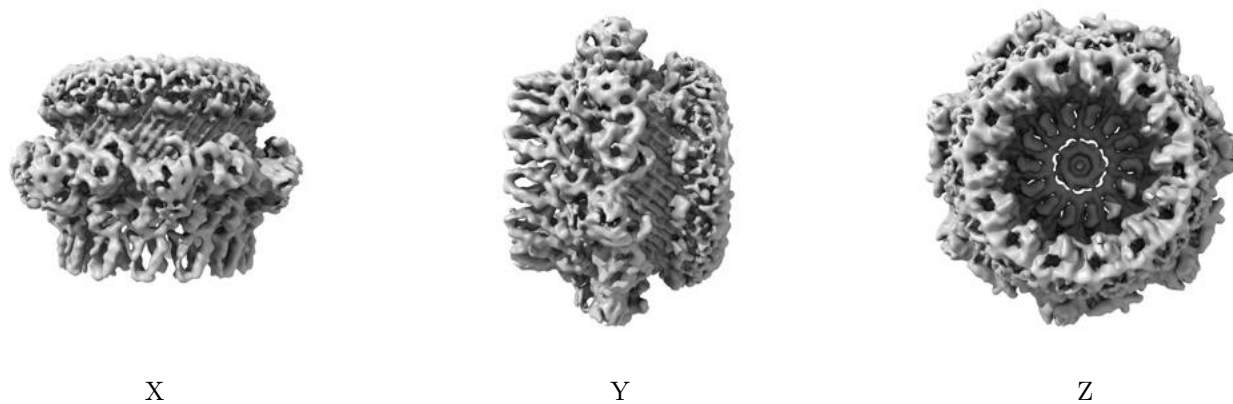


Z Index: 124

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

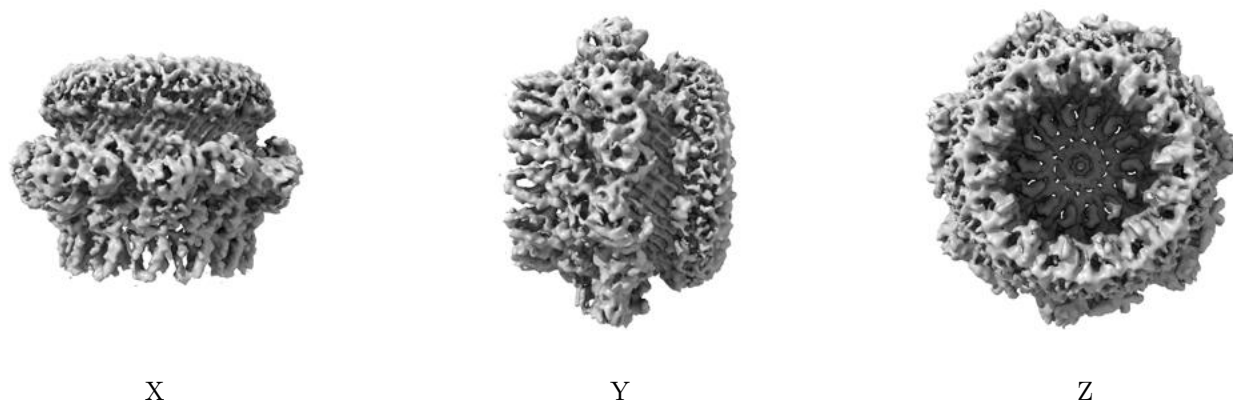
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.46. 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.

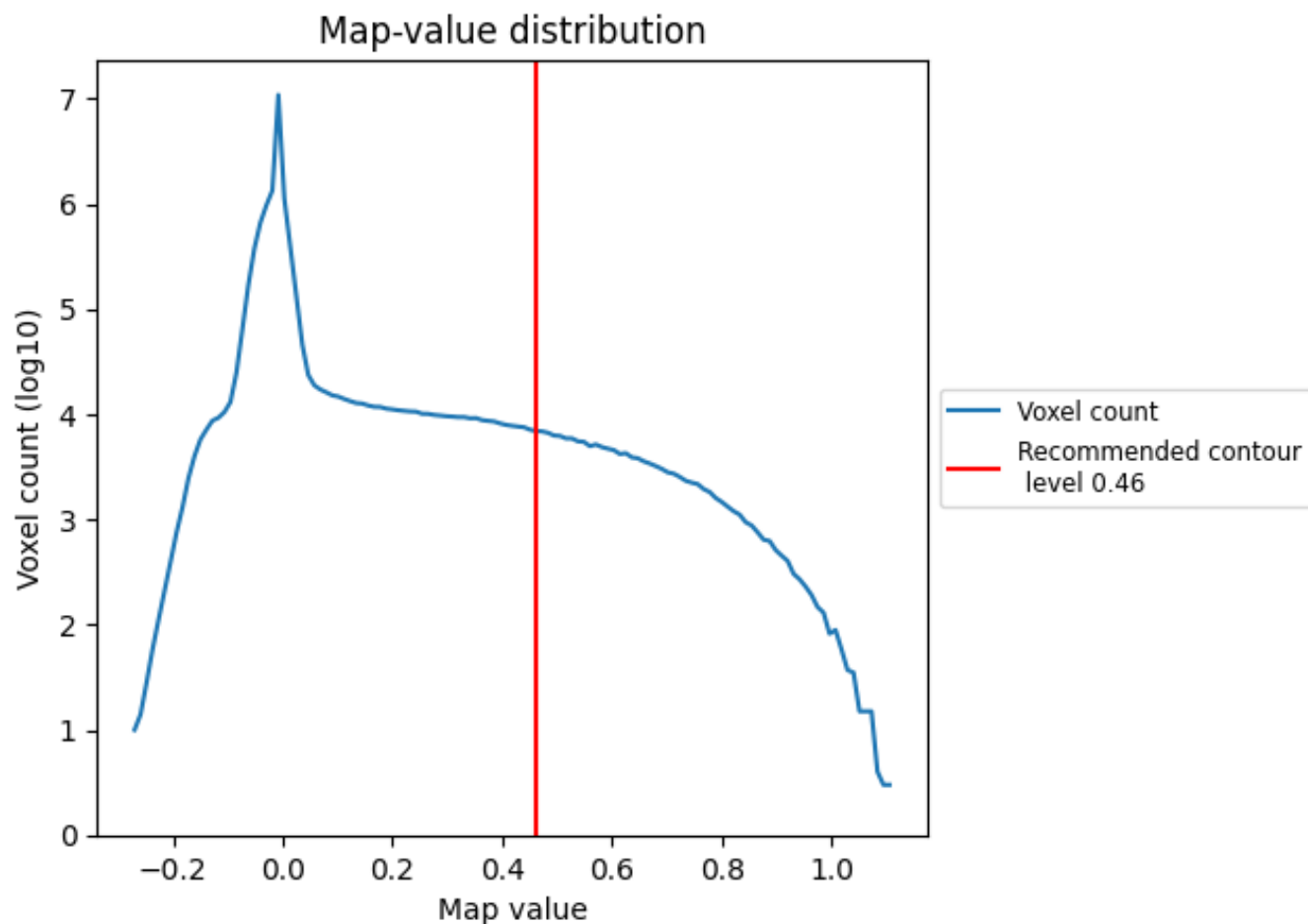
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

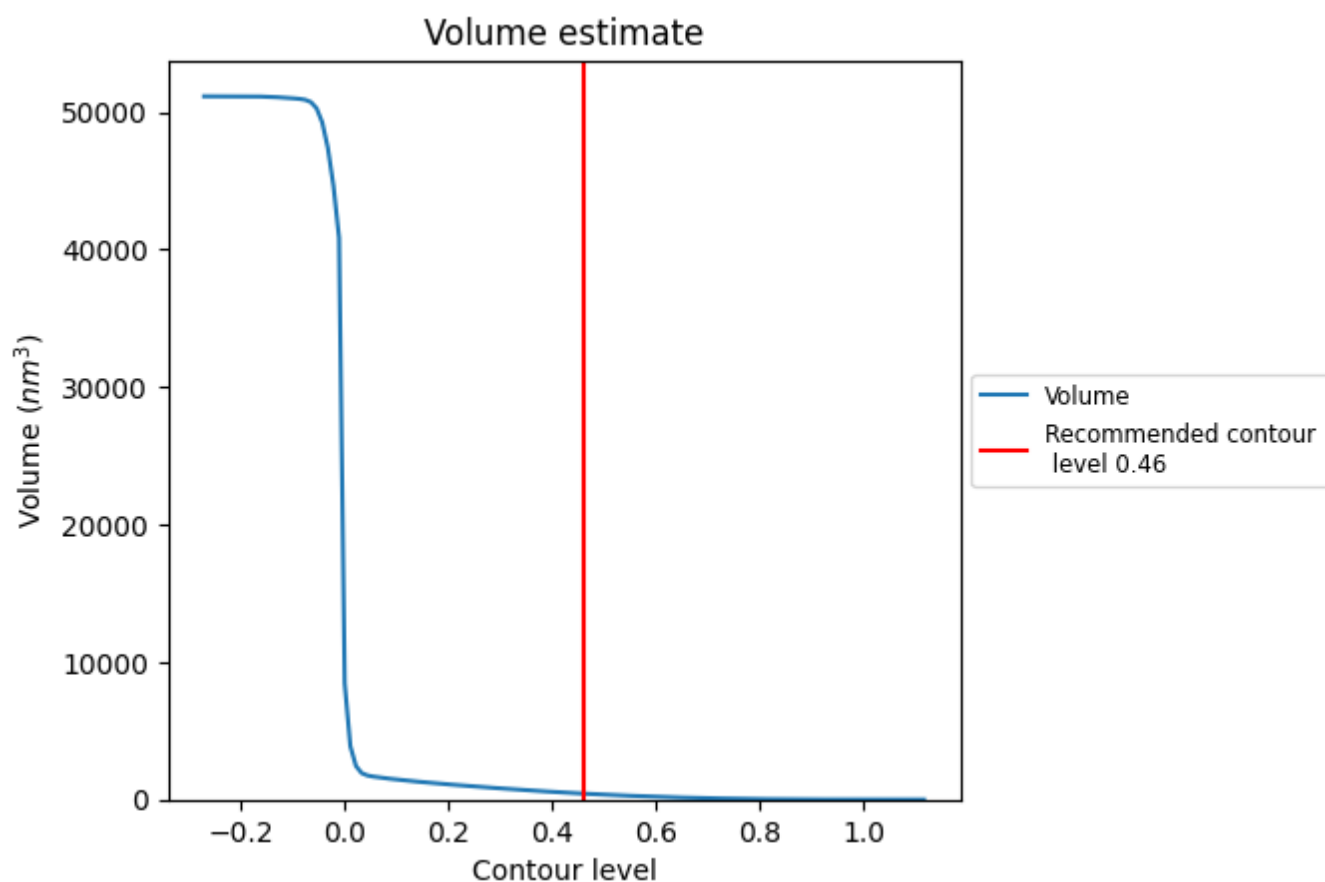
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

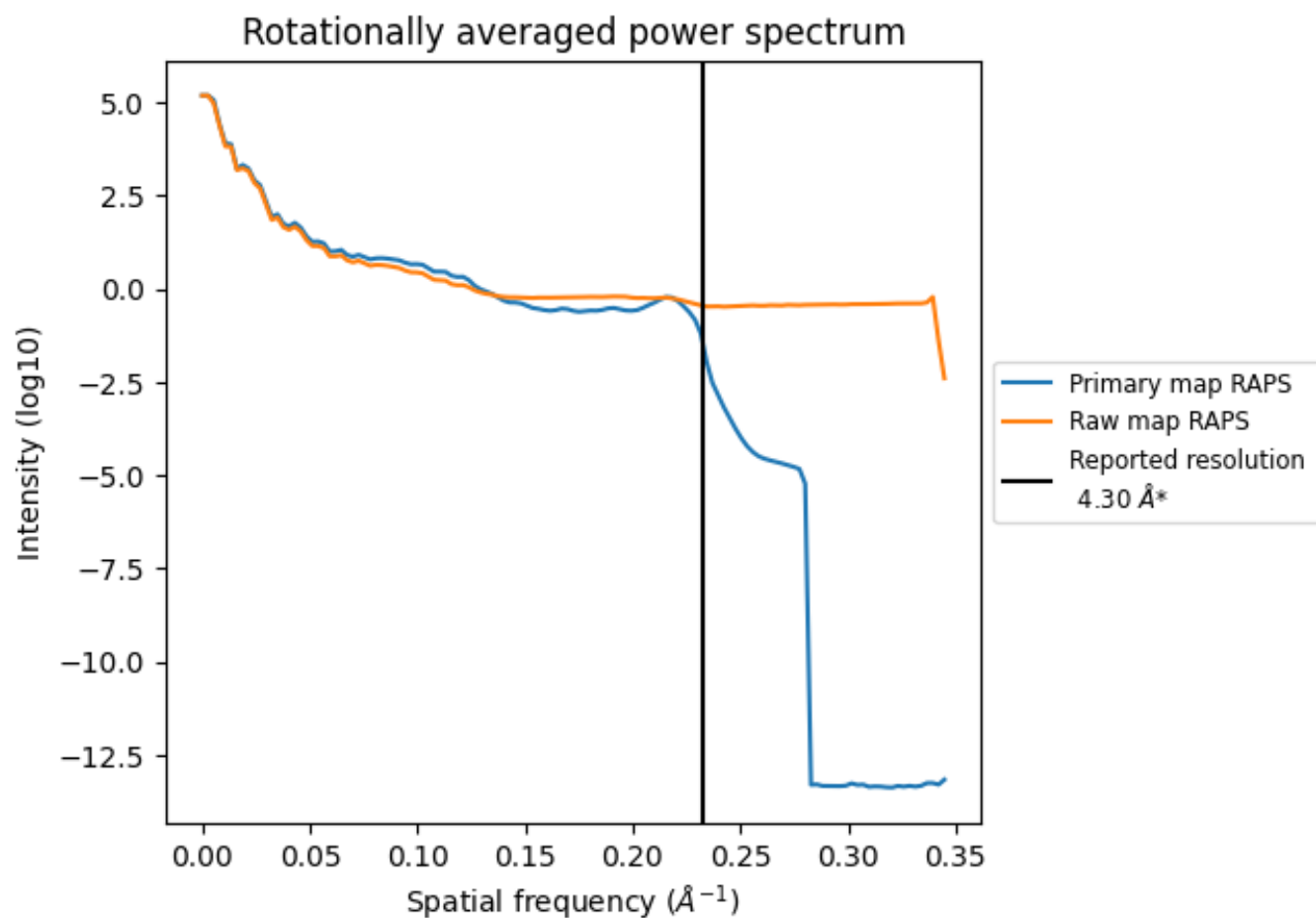
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 434 nm³; this corresponds to an approximate mass of 392 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 ⓘ

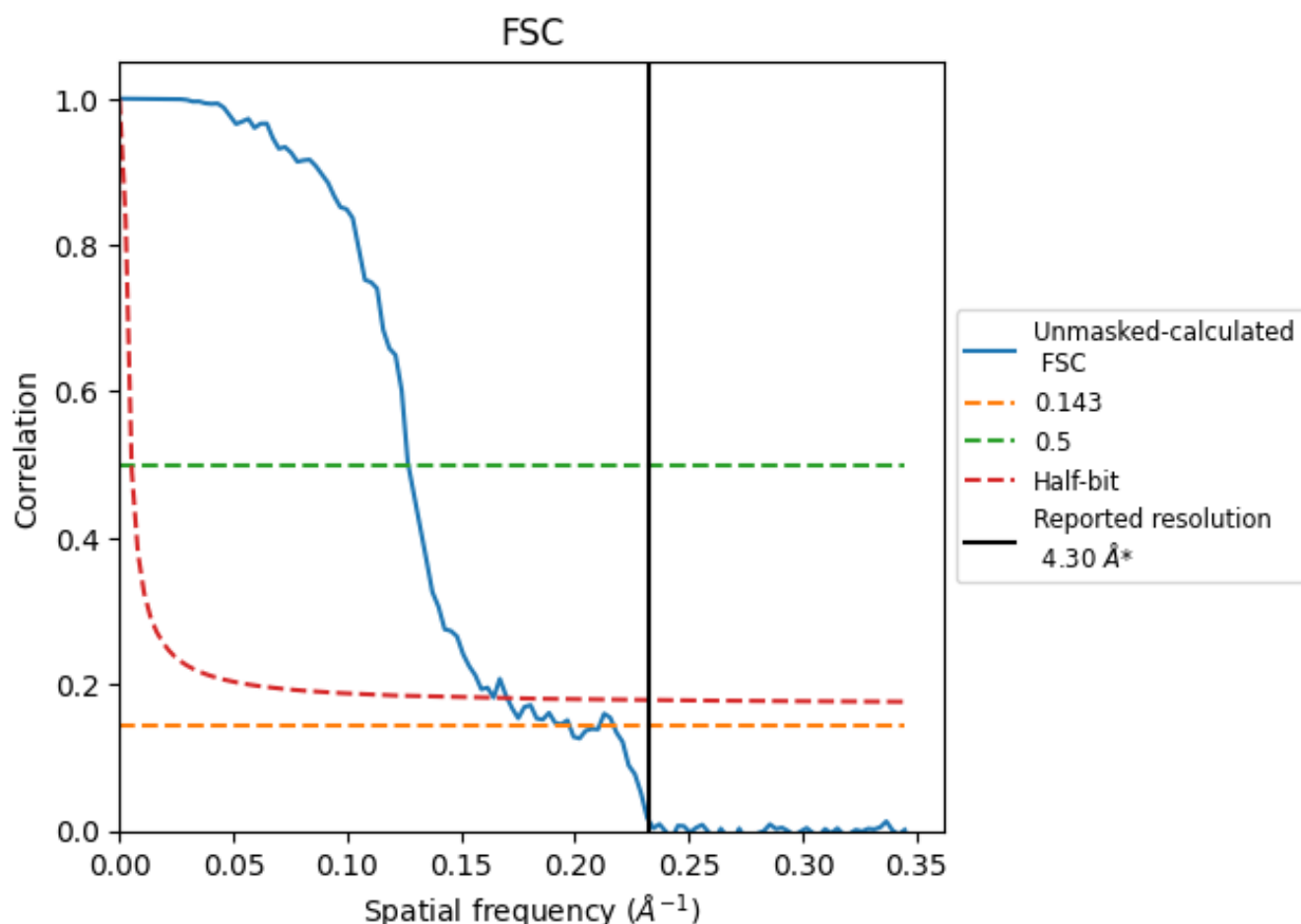


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

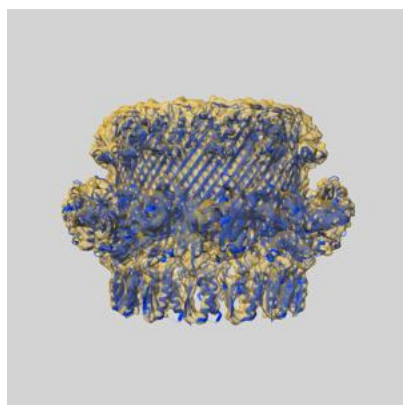
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.06	7.89	5.87

*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 5.06 differs from the reported value 4.3 by more than 10 %

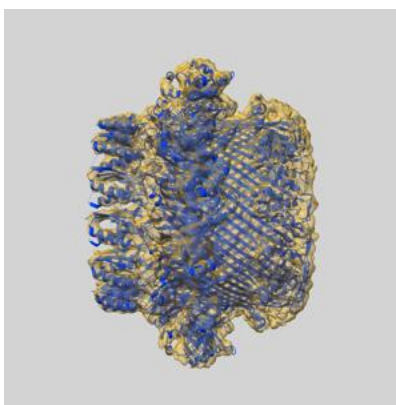
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21152 and PDB model 6VE2. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

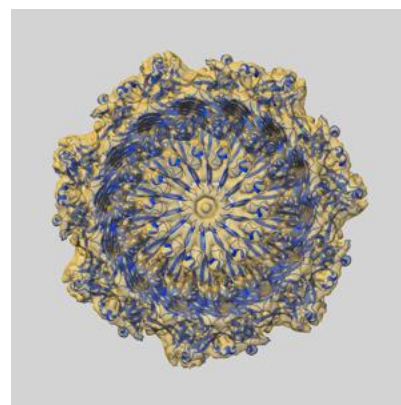
9.1 Map-model overlay [i](#)



X



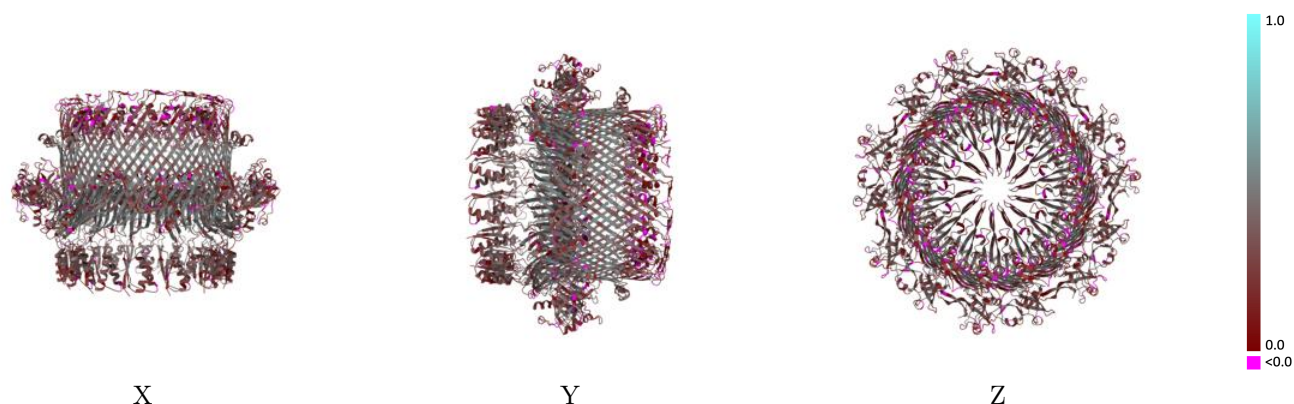
Y



Z

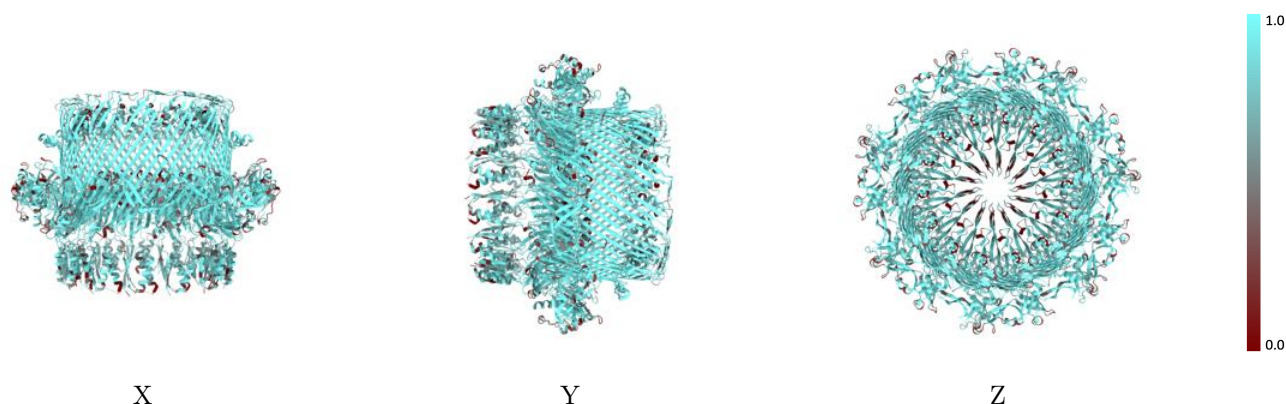
The images above show the 3D surface view of the map at the recommended contour level 0.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



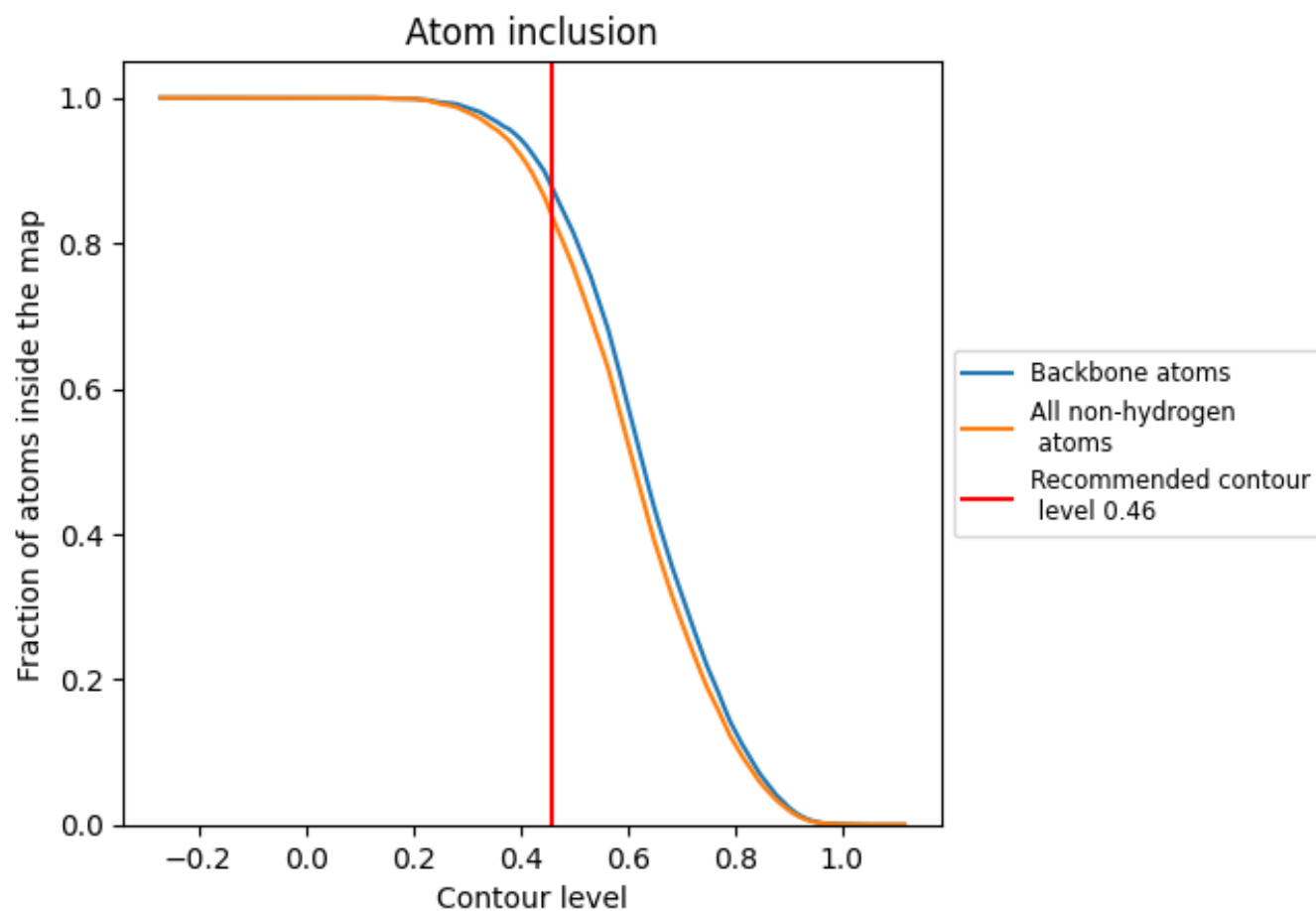
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.46).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% 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 (0.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8356	 0.3020
A	 0.8487	 0.3140
B	 0.8524	 0.3160
C	 0.8481	 0.3160
D	 0.8531	 0.3160
E	 0.8493	 0.3140
F	 0.8518	 0.3150
G	 0.8493	 0.3180
H	 0.8499	 0.3170
I	 0.8481	 0.3180
J	 0.8531	 0.3190
K	 0.8481	 0.3150
L	 0.8531	 0.3160
M	 0.8499	 0.3140
N	 0.8537	 0.3170
O	 0.7931	 0.2630
P	 0.7886	 0.2620
Q	 0.7913	 0.2630
R	 0.7958	 0.2640
S	 0.7904	 0.2620
T	 0.7940	 0.2620
U	 0.7904	 0.2600

