wwPDB EM Validation Summary Report (i)

Feb 27, 2024 – 10:19 AM EST

PDB ID	:	6VE4
EMDB ID	:	EMD-21154
Title	:	Pentadecameric PilQ from Pseudomonas aeruginosa
Authors	:	McCallum, M.; Tammam, S.; Rubinstein, J.L.; Burrows, L.L.; Howell, P.L.
Deposited on	:	2019-12-28
Resolution	:	6.90 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 (i) 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 (i)) were used in the production of this report:

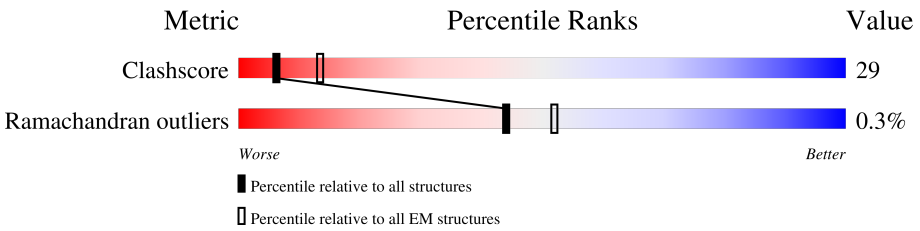
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.90 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 <=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	5% 28% 13% 58%
1	B	731	5% 28% 13% 58%
1	C	731	5% 28% 13% 58%
1	D	731	5% 27% 14% 58%
1	E	731	5% 28% 14% 58%
1	F	731	5% 28% 14% 58%
1	G	731	5% 28% 14% 58%
1	H	731	5% 28% 14% 58%
1	I	731	5% 28% 14% 58%

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Mol	Chain	Length	Quality of chain
1	J	731	5% 27% 14% 58%
1	K	731	5% 27% 14% 58%
1	L	731	5% 28% 14% 58%
1	M	731	5% 28% 13% 58%
1	N	731	5% 29% 13% 58%
1	O	731	5% 29% 13% 58%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 22425 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
			Total	C	N	O		
1	A	304	1495	887	304	304	0	0
1	B	304	1495	887	304	304	0	0
1	C	304	1495	887	304	304	0	0
1	D	304	1495	887	304	304	0	0
1	E	304	1495	887	304	304	0	0
1	F	304	1495	887	304	304	0	0
1	G	304	1495	887	304	304	0	0
1	H	304	1495	887	304	304	0	0
1	I	304	1495	887	304	304	0	0
1	J	304	1495	887	304	304	0	0
1	K	304	1495	887	304	304	0	0
1	L	304	1495	887	304	304	0	0
1	M	304	1495	887	304	304	0	0
1	N	304	1495	887	304	304	0	0
1	O	304	1495	887	304	304	0	0

There are 255 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
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	307	GLY	-	expression tag	UNP P34750
A	308	HIS	-	expression tag	UNP P34750
A	309	HIS	-	expression tag	UNP P34750
A	310	HIS	-	expression tag	UNP P34750
A	311	HIS	-	expression tag	UNP P34750
A	312	HIS	-	expression tag	UNP P34750
A	313	HIS	-	expression tag	UNP P34750
A	314	HIS	-	expression tag	UNP P34750
A	315	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	307	GLY	-	expression tag	UNP P34750
B	308	HIS	-	expression tag	UNP P34750
B	309	HIS	-	expression tag	UNP P34750
B	310	HIS	-	expression tag	UNP P34750
B	311	HIS	-	expression tag	UNP P34750
B	312	HIS	-	expression tag	UNP P34750
B	313	HIS	-	expression tag	UNP P34750
B	314	HIS	-	expression tag	UNP P34750
B	315	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	307	GLY	-	expression tag	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
C	308	HIS	-	expression tag	UNP P34750
C	309	HIS	-	expression tag	UNP P34750
C	310	HIS	-	expression tag	UNP P34750
C	311	HIS	-	expression tag	UNP P34750
C	312	HIS	-	expression tag	UNP P34750
C	313	HIS	-	expression tag	UNP P34750
C	314	HIS	-	expression tag	UNP P34750
C	315	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	307	GLY	-	expression tag	UNP P34750
D	308	HIS	-	expression tag	UNP P34750
D	309	HIS	-	expression tag	UNP P34750
D	310	HIS	-	expression tag	UNP P34750
D	311	HIS	-	expression tag	UNP P34750
D	312	HIS	-	expression tag	UNP P34750
D	313	HIS	-	expression tag	UNP P34750
D	314	HIS	-	expression tag	UNP P34750
D	315	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	307	GLY	-	expression tag	UNP P34750
E	308	HIS	-	expression tag	UNP P34750
E	309	HIS	-	expression tag	UNP P34750
E	310	HIS	-	expression tag	UNP P34750
E	311	HIS	-	expression tag	UNP P34750
E	312	HIS	-	expression tag	UNP P34750
E	313	HIS	-	expression tag	UNP P34750
E	314	HIS	-	expression tag	UNP P34750
E	315	HIS	-	expression tag	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-256	HIS	-	insertion	UNP P34750
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	307	GLY	-	expression tag	UNP P34750
F	308	HIS	-	expression tag	UNP P34750
F	309	HIS	-	expression tag	UNP P34750
F	310	HIS	-	expression tag	UNP P34750
F	311	HIS	-	expression tag	UNP P34750
F	312	HIS	-	expression tag	UNP P34750
F	313	HIS	-	expression tag	UNP P34750
F	314	HIS	-	expression tag	UNP P34750
F	315	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	307	GLY	-	expression tag	UNP P34750
G	308	HIS	-	expression tag	UNP P34750
G	309	HIS	-	expression tag	UNP P34750
G	310	HIS	-	expression tag	UNP P34750
G	311	HIS	-	expression tag	UNP P34750
G	312	HIS	-	expression tag	UNP P34750
G	313	HIS	-	expression tag	UNP P34750
G	314	HIS	-	expression tag	UNP P34750
G	315	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

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Chain	Residue	Modelled	Actual	Comment	Reference
H	307	GLY	-	expression tag	UNP P34750
H	308	HIS	-	expression tag	UNP P34750
H	309	HIS	-	expression tag	UNP P34750
H	310	HIS	-	expression tag	UNP P34750
H	311	HIS	-	expression tag	UNP P34750
H	312	HIS	-	expression tag	UNP P34750
H	313	HIS	-	expression tag	UNP P34750
H	314	HIS	-	expression tag	UNP P34750
H	315	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	307	GLY	-	expression tag	UNP P34750
I	308	HIS	-	expression tag	UNP P34750
I	309	HIS	-	expression tag	UNP P34750
I	310	HIS	-	expression tag	UNP P34750
I	311	HIS	-	expression tag	UNP P34750
I	312	HIS	-	expression tag	UNP P34750
I	313	HIS	-	expression tag	UNP P34750
I	314	HIS	-	expression tag	UNP P34750
I	315	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	307	GLY	-	expression tag	UNP P34750
J	308	HIS	-	expression tag	UNP P34750
J	309	HIS	-	expression tag	UNP P34750
J	310	HIS	-	expression tag	UNP P34750
J	311	HIS	-	expression tag	UNP P34750
J	312	HIS	-	expression tag	UNP P34750
J	313	HIS	-	expression tag	UNP P34750
J	314	HIS	-	expression tag	UNP P34750

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Chain	Residue	Modelled	Actual	Comment	Reference
J	315	HIS	-	expression tag	UNP P34750
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	307	GLY	-	expression tag	UNP P34750
K	308	HIS	-	expression tag	UNP P34750
K	309	HIS	-	expression tag	UNP P34750
K	310	HIS	-	expression tag	UNP P34750
K	311	HIS	-	expression tag	UNP P34750
K	312	HIS	-	expression tag	UNP P34750
K	313	HIS	-	expression tag	UNP P34750
K	314	HIS	-	expression tag	UNP P34750
K	315	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	307	GLY	-	expression tag	UNP P34750
L	308	HIS	-	expression tag	UNP P34750
L	309	HIS	-	expression tag	UNP P34750
L	310	HIS	-	expression tag	UNP P34750
L	311	HIS	-	expression tag	UNP P34750
L	312	HIS	-	expression tag	UNP P34750
L	313	HIS	-	expression tag	UNP P34750
L	314	HIS	-	expression tag	UNP P34750
L	315	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

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-249	HIS	-	insertion	UNP P34750
M	307	GLY	-	expression tag	UNP P34750
M	308	HIS	-	expression tag	UNP P34750
M	309	HIS	-	expression tag	UNP P34750
M	310	HIS	-	expression tag	UNP P34750
M	311	HIS	-	expression tag	UNP P34750
M	312	HIS	-	expression tag	UNP P34750
M	313	HIS	-	expression tag	UNP P34750
M	314	HIS	-	expression tag	UNP P34750
M	315	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	307	GLY	-	expression tag	UNP P34750
N	308	HIS	-	expression tag	UNP P34750
N	309	HIS	-	expression tag	UNP P34750
N	310	HIS	-	expression tag	UNP P34750
N	311	HIS	-	expression tag	UNP P34750
N	312	HIS	-	expression tag	UNP P34750
N	313	HIS	-	expression tag	UNP P34750
N	314	HIS	-	expression tag	UNP P34750
N	315	HIS	-	expression tag	UNP P34750
O	-256	HIS	-	insertion	UNP P34750
O	-255	HIS	-	insertion	UNP P34750
O	-254	HIS	-	insertion	UNP P34750
O	-253	HIS	-	insertion	UNP P34750
O	-252	HIS	-	insertion	UNP P34750
O	-251	HIS	-	insertion	UNP P34750
O	-250	HIS	-	insertion	UNP P34750
O	-249	HIS	-	insertion	UNP P34750
O	307	GLY	-	expression tag	UNP P34750
O	308	HIS	-	expression tag	UNP P34750
O	309	HIS	-	expression tag	UNP P34750
O	310	HIS	-	expression tag	UNP P34750
O	311	HIS	-	expression tag	UNP P34750
O	312	HIS	-	expression tag	UNP P34750
O	313	HIS	-	expression tag	UNP P34750

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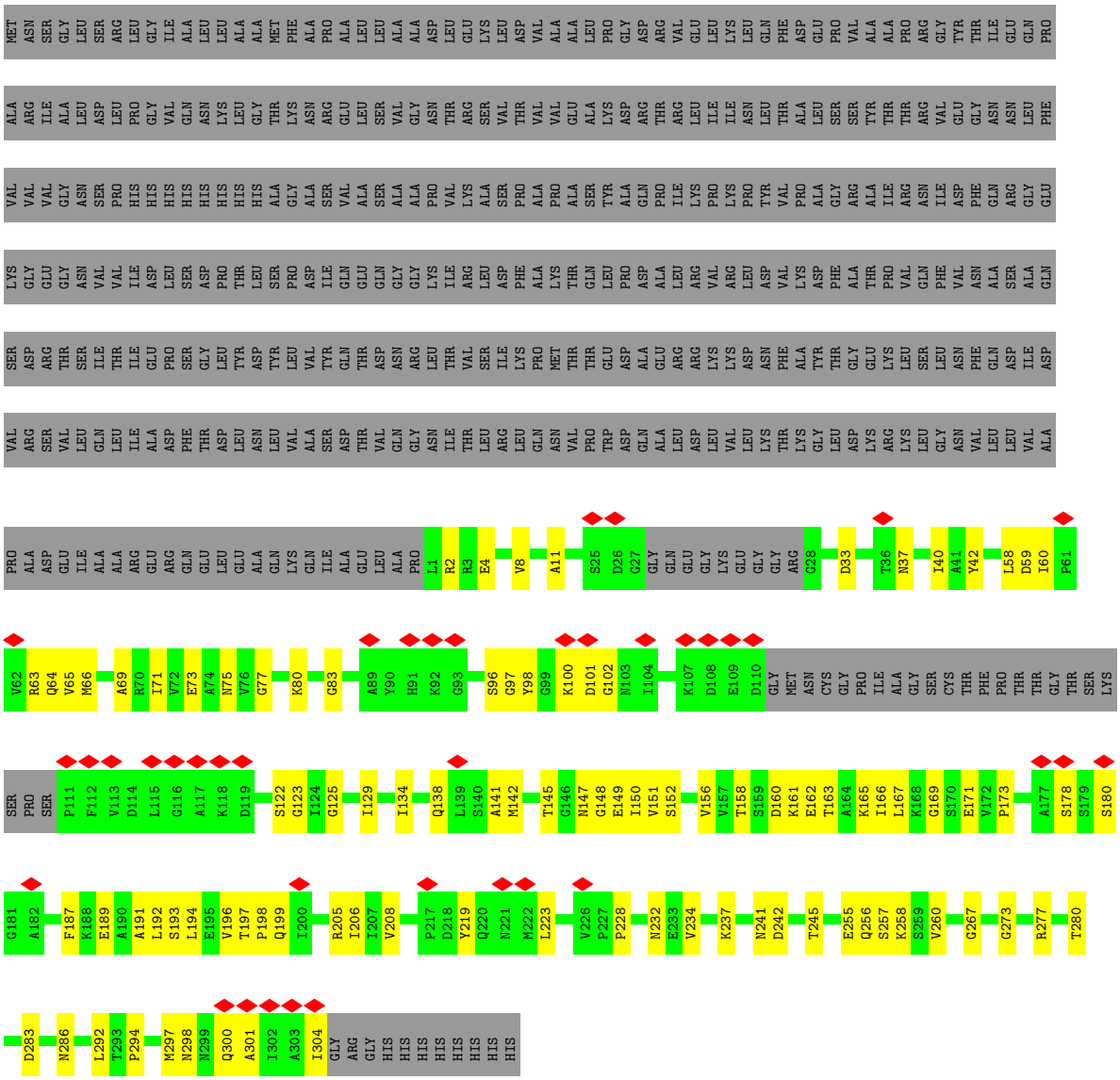
Chain	Residue	Modelled	Actual	Comment	Reference
O	314	HIS	-	expression tag	UNP P34750
O	315	HIS	-	expression tag	UNP P34750

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

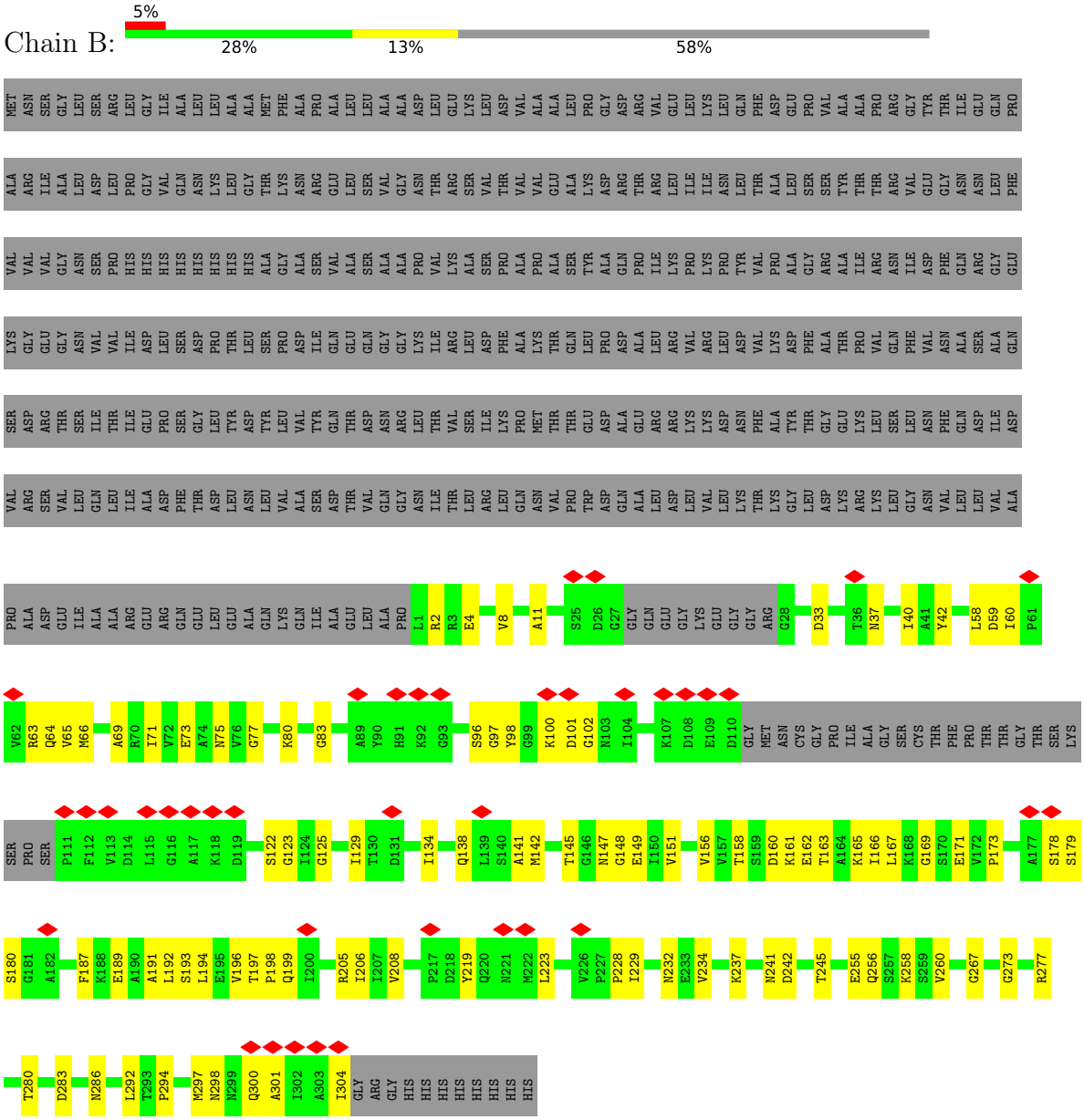
- Molecule 1: Fimbrial assembly protein PilQ

Chain A: 5% 28% 13% 58%



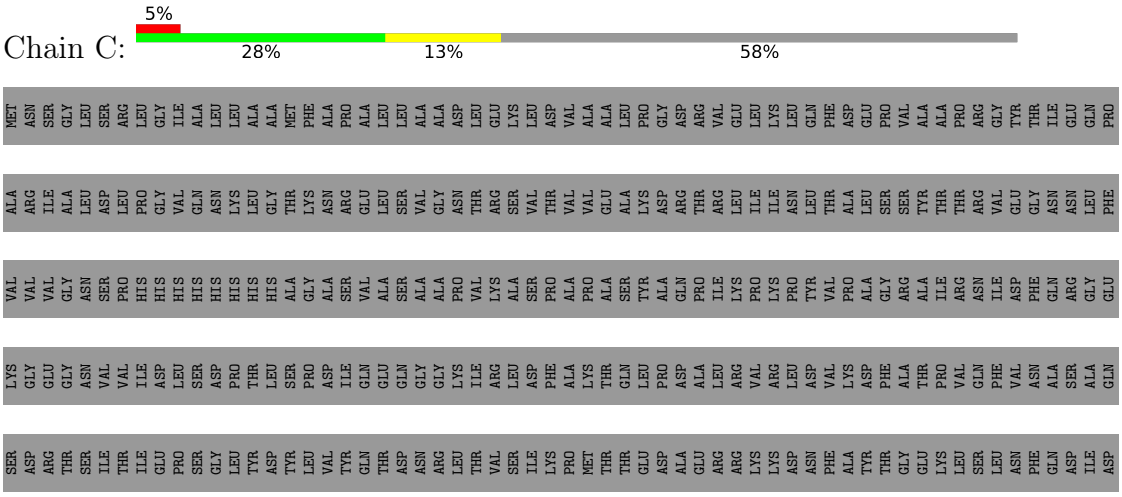
- Molecule 1: Fimbrial assembly protein PilQ

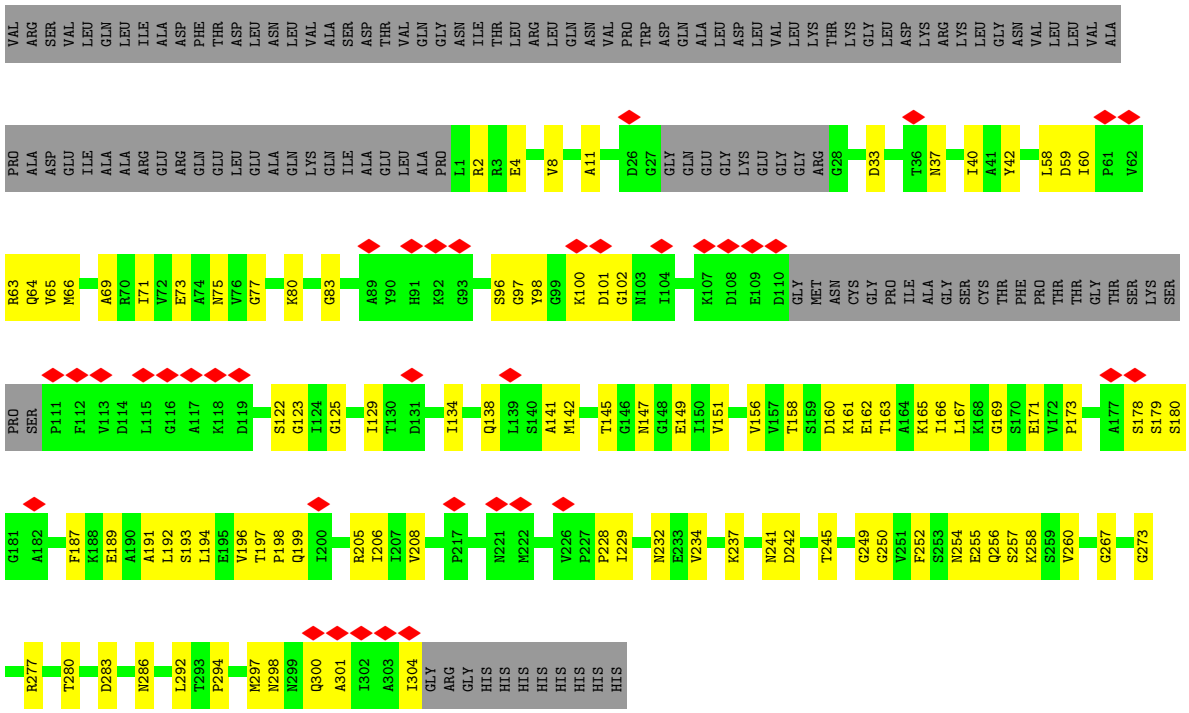
Chain B:



• Molecule 1: Fimbrial assembly protein PilQ

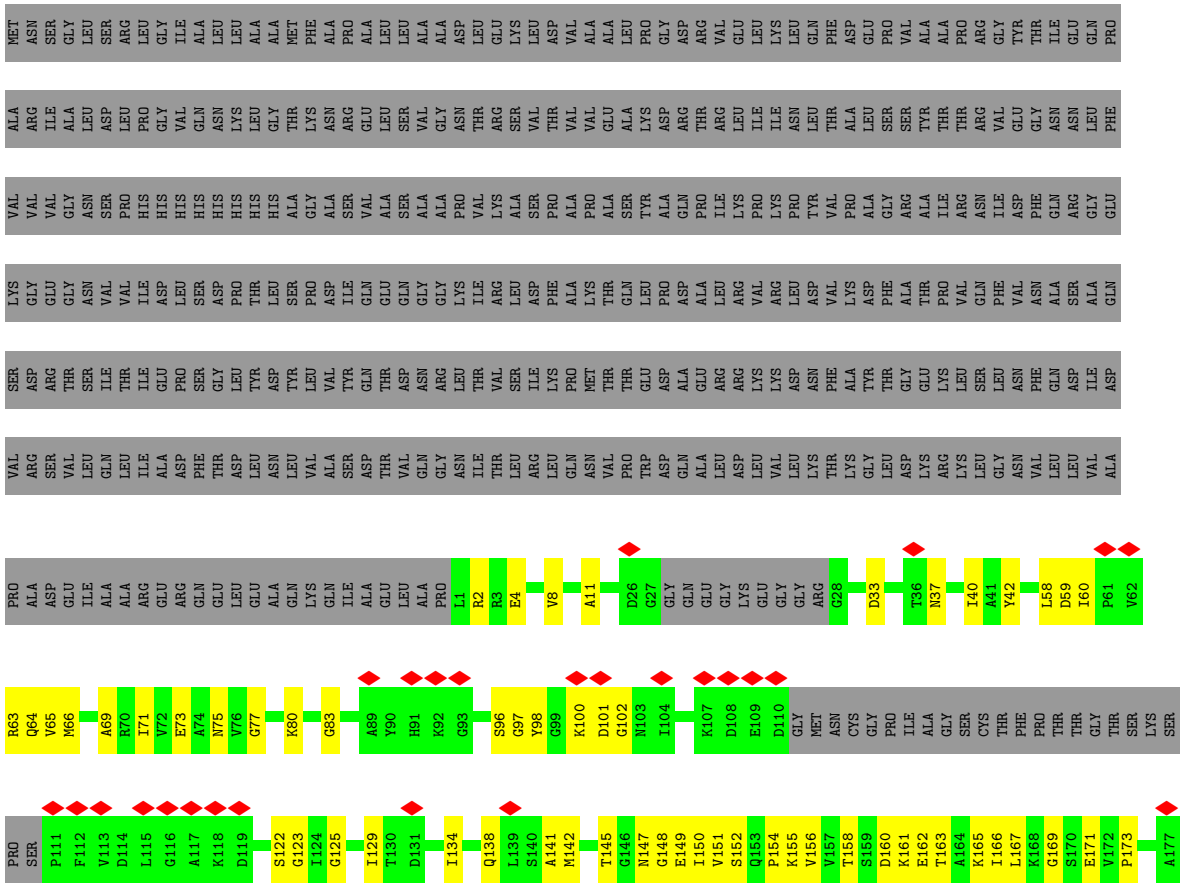
Chain C:

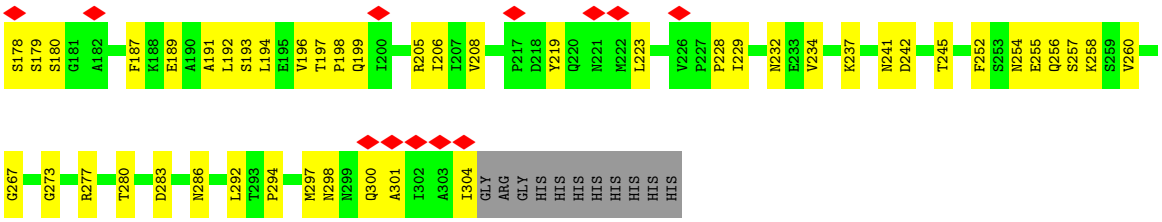




- Molecule 1: Fimbrial assembly protein PilQ

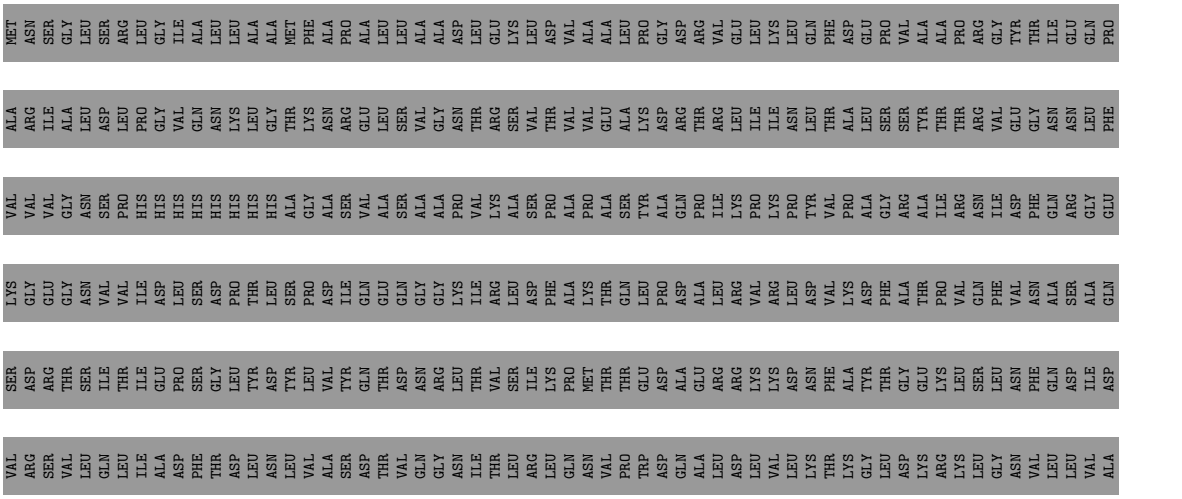
Chain D:





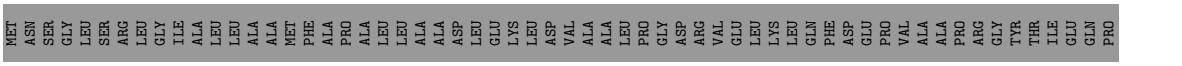
• Molecule 1: Fimbrial assembly protein PilQ

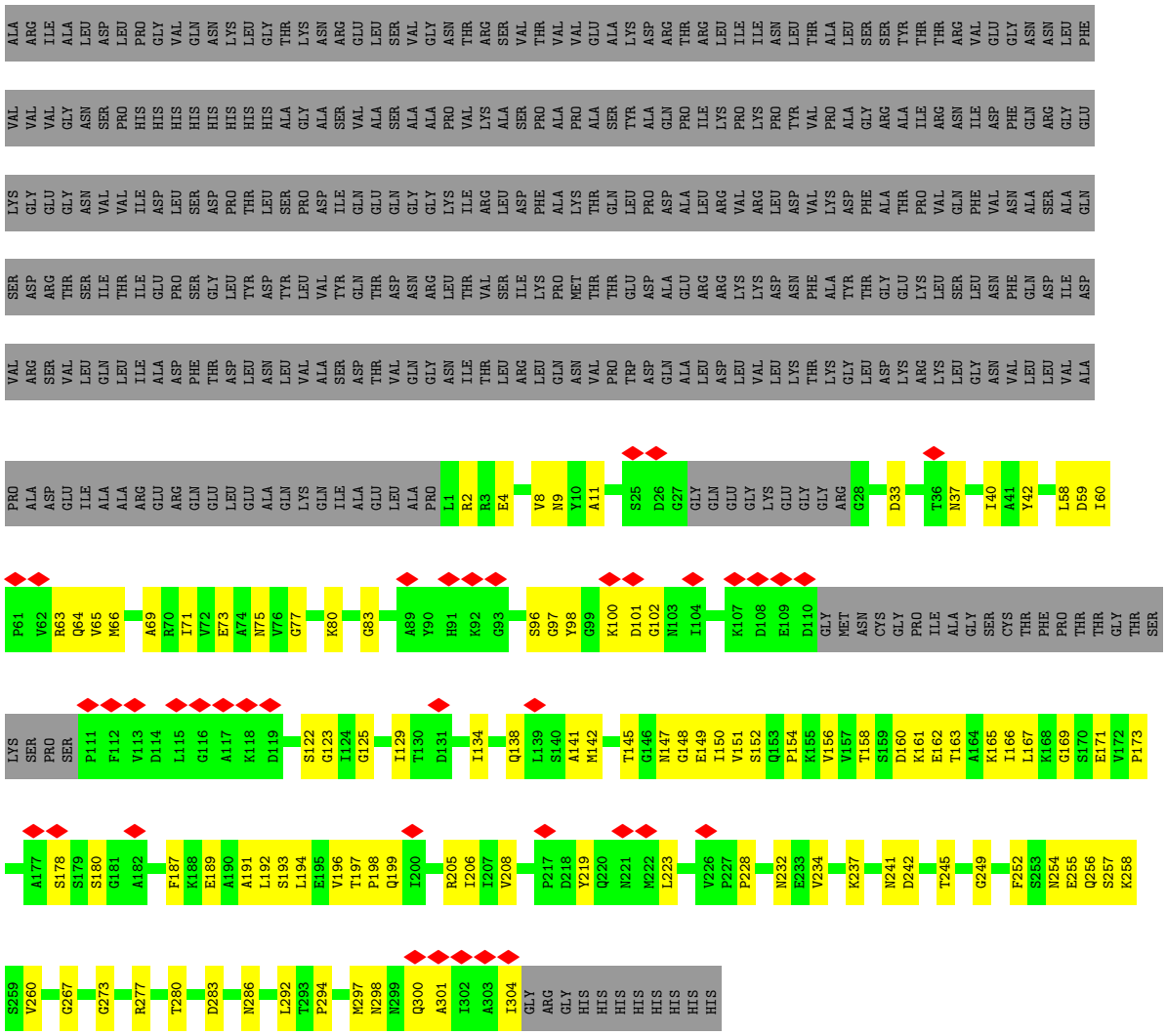
Chain E:



• Molecule 1: Fimbrial assembly protein PilQ

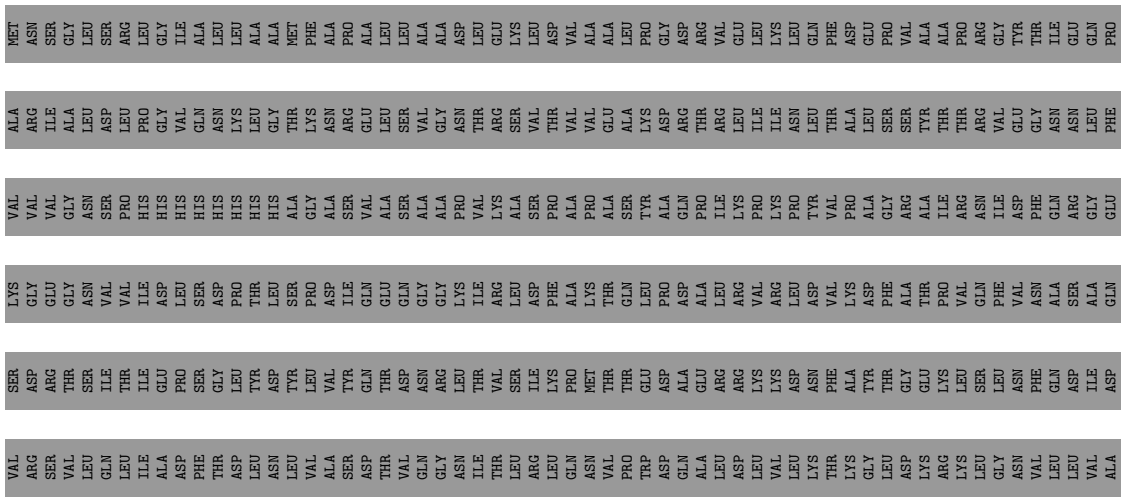
Chain F:

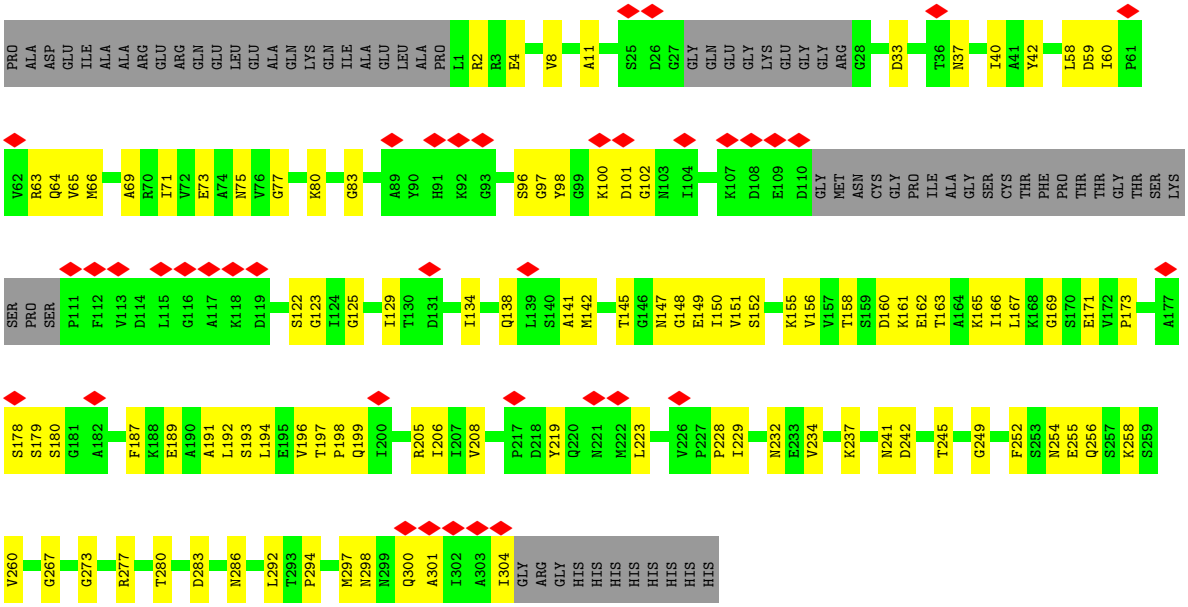




- Molecule 1: Fimbrial assembly protein PilQ

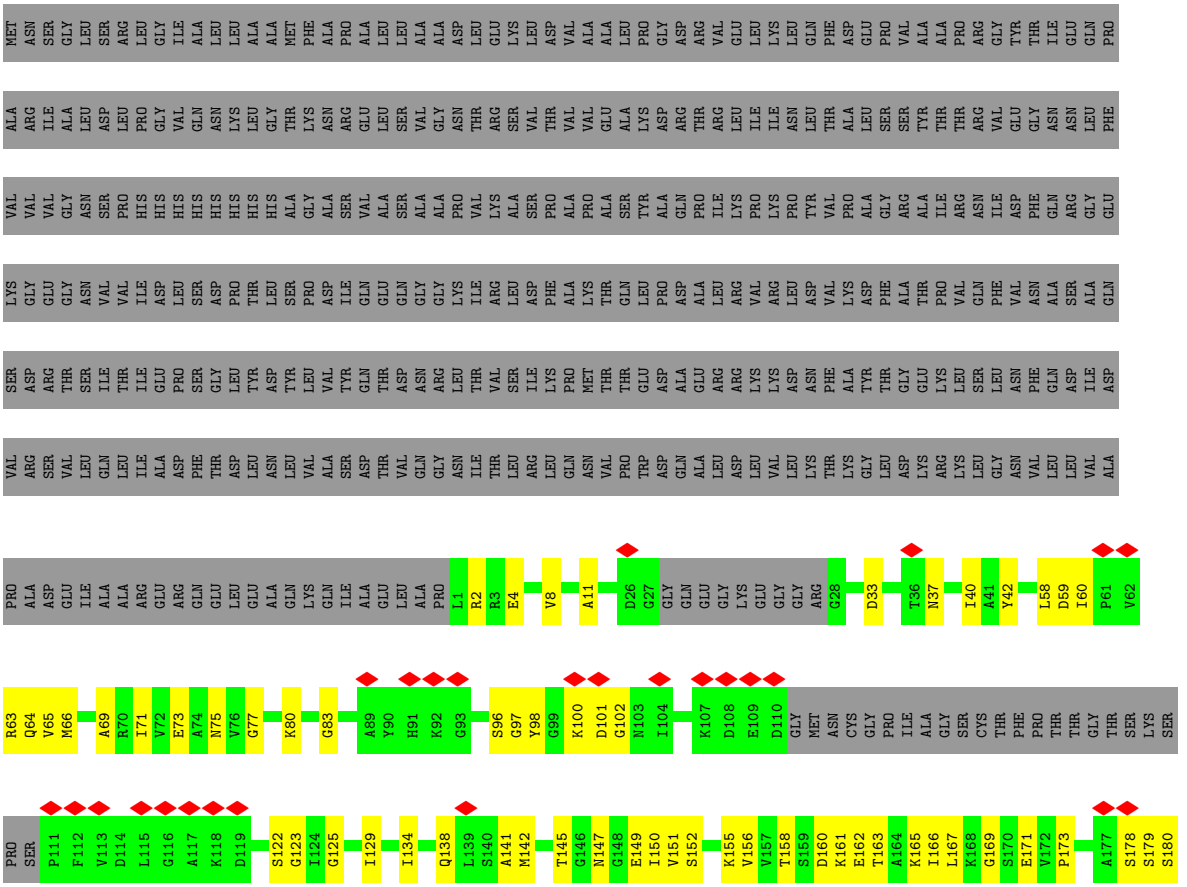
Chain G: 5% 28% 14% 58%

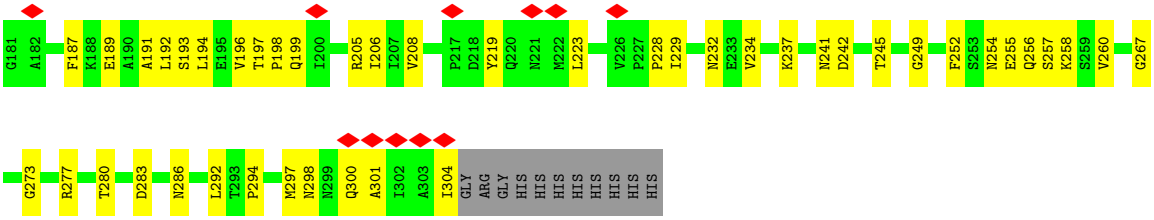




- Molecule 1: Fimbrial assembly protein PilQ

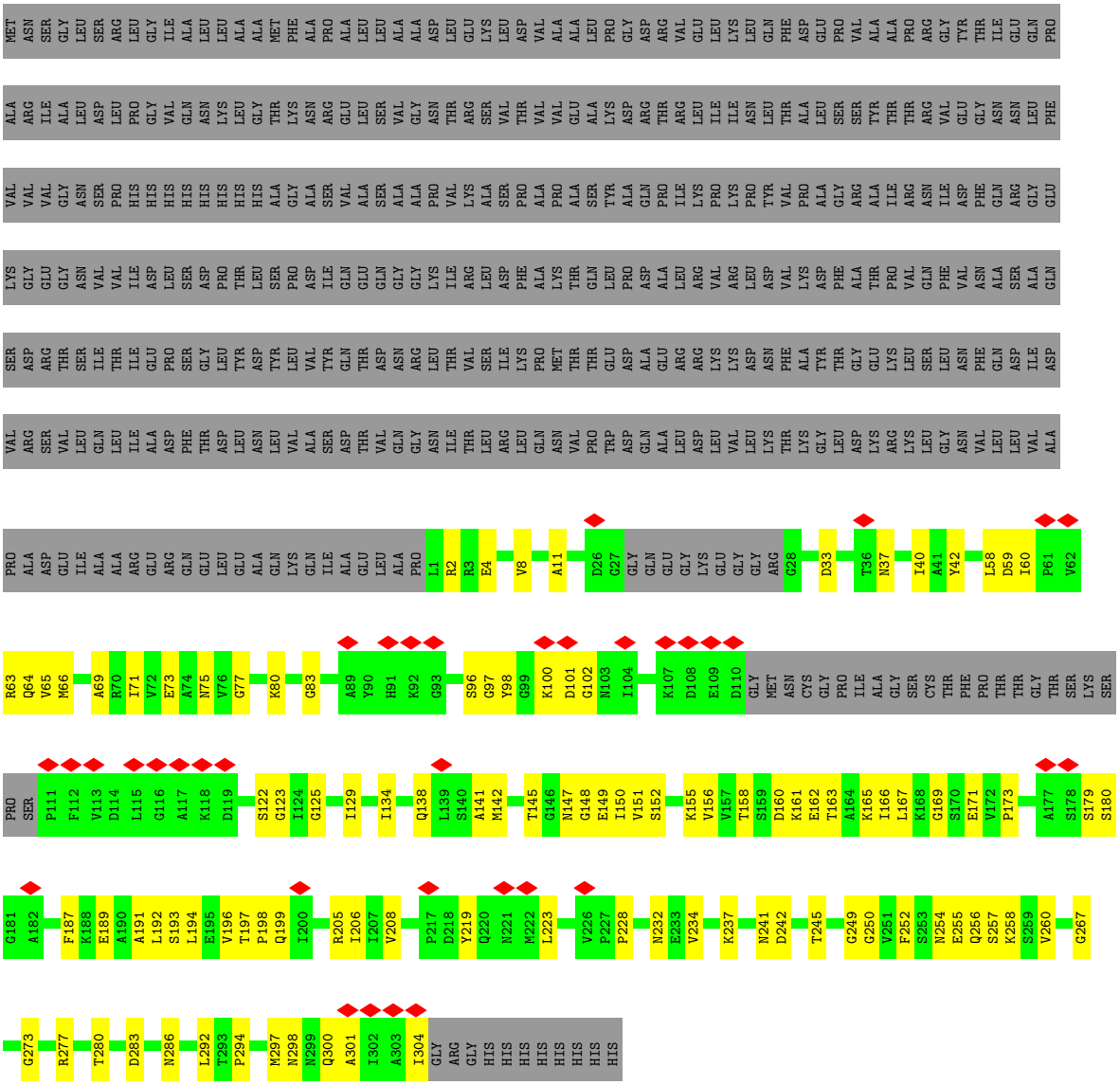
Chain H:





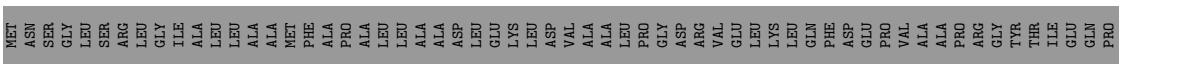
• Molecule 1: Fimbrial assembly protein PilQ

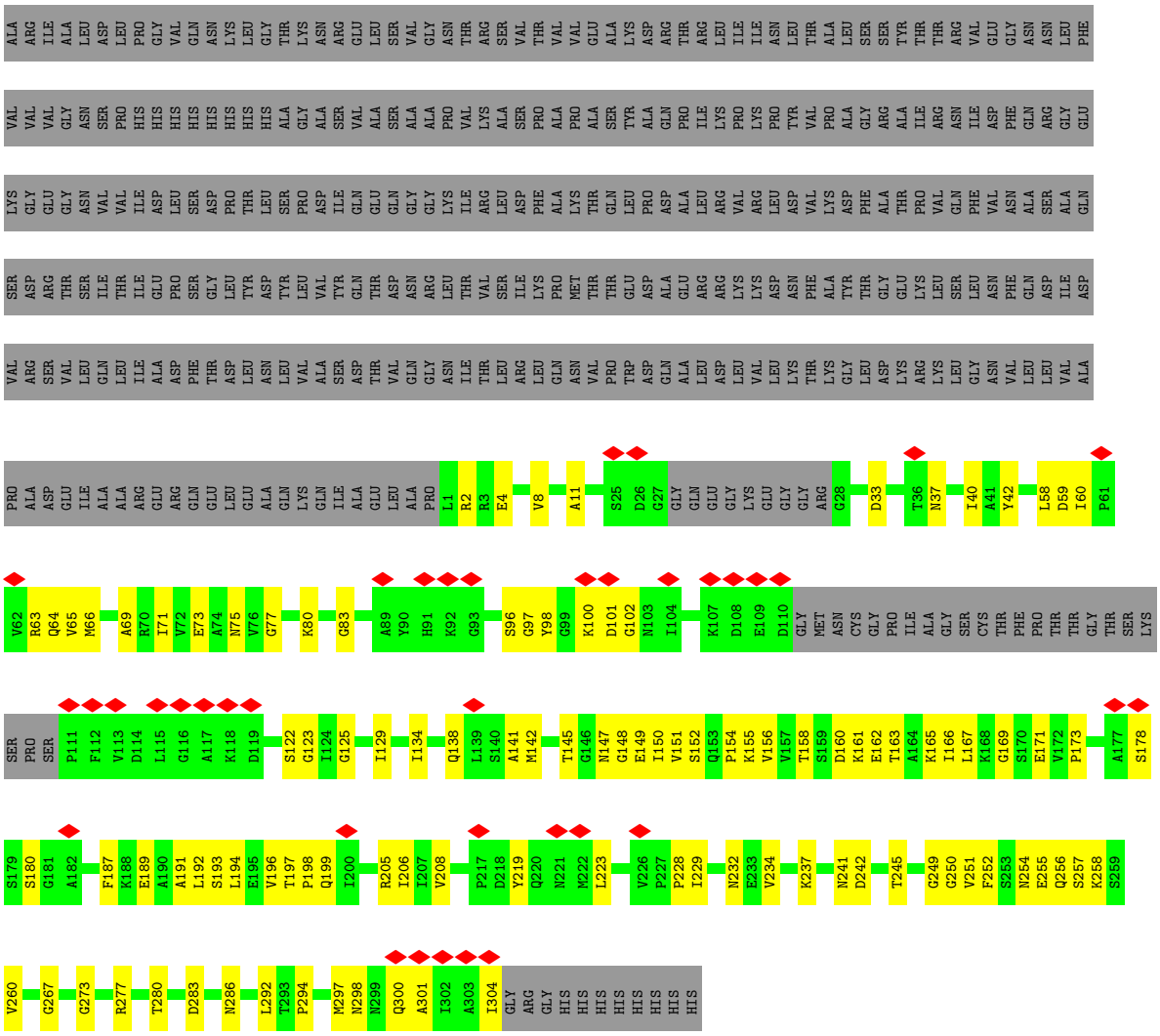
Chain I:



• Molecule 1: Fimbrial assembly protein PilQ

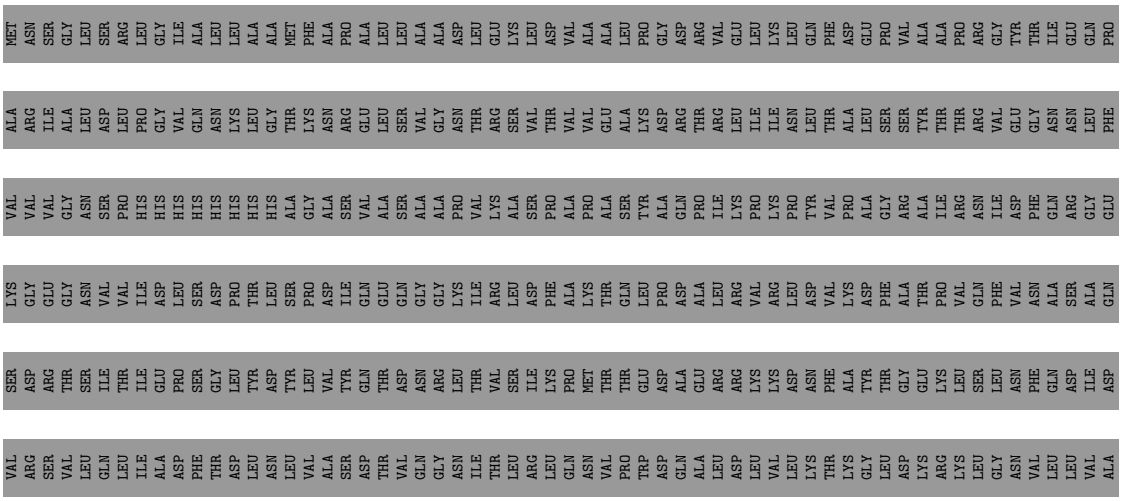
Chain J:

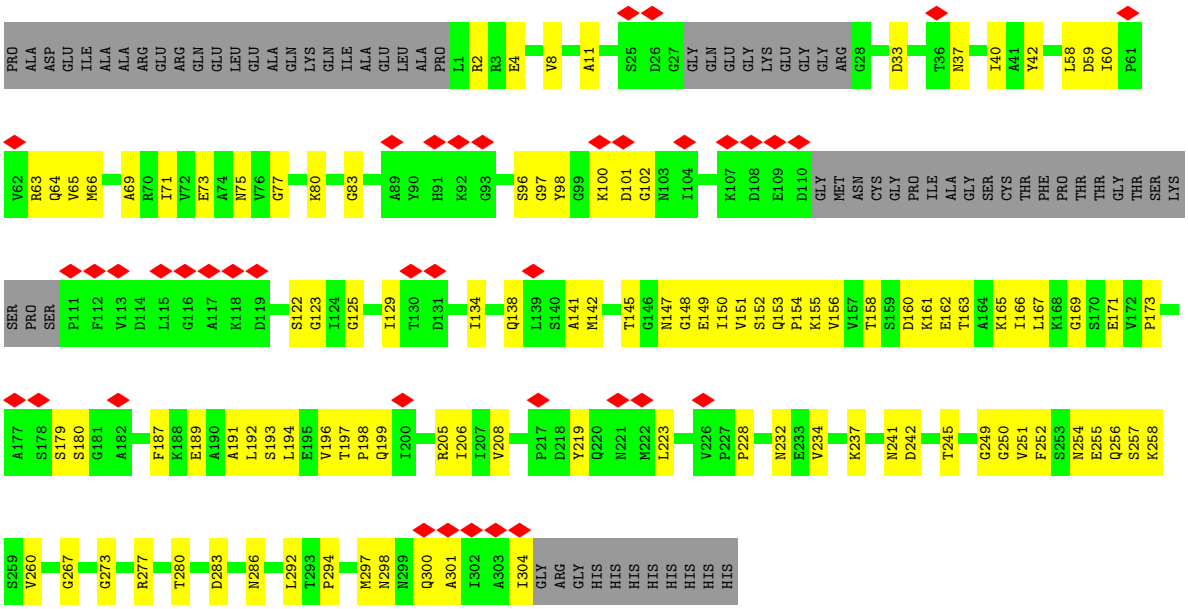




- Molecule 1: Fimbrial assembly protein PilQ

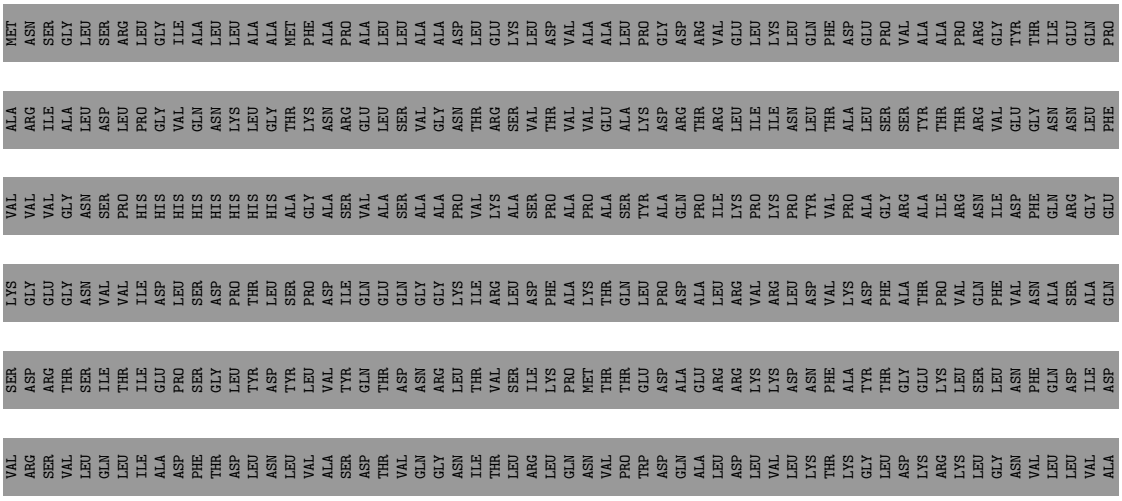
Chain K:

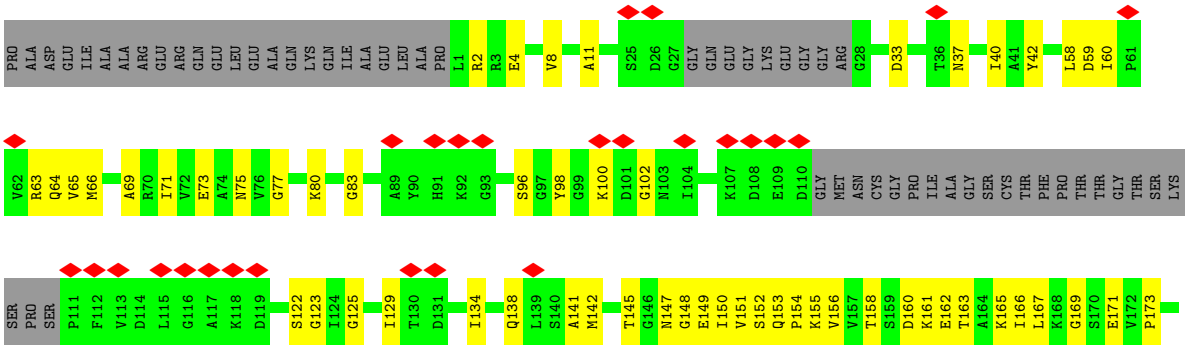


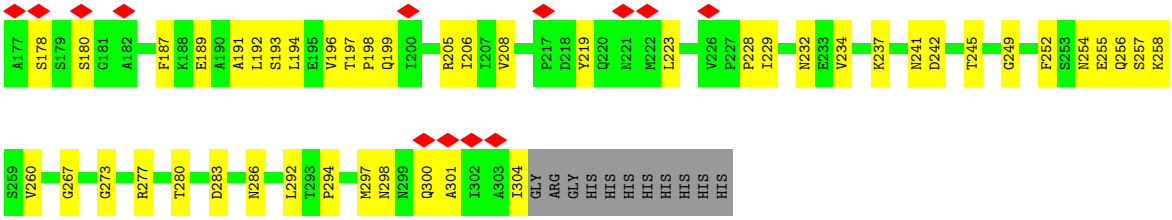


- Molecule 1: Fimbrial assembly protein PilQ

Chain L:

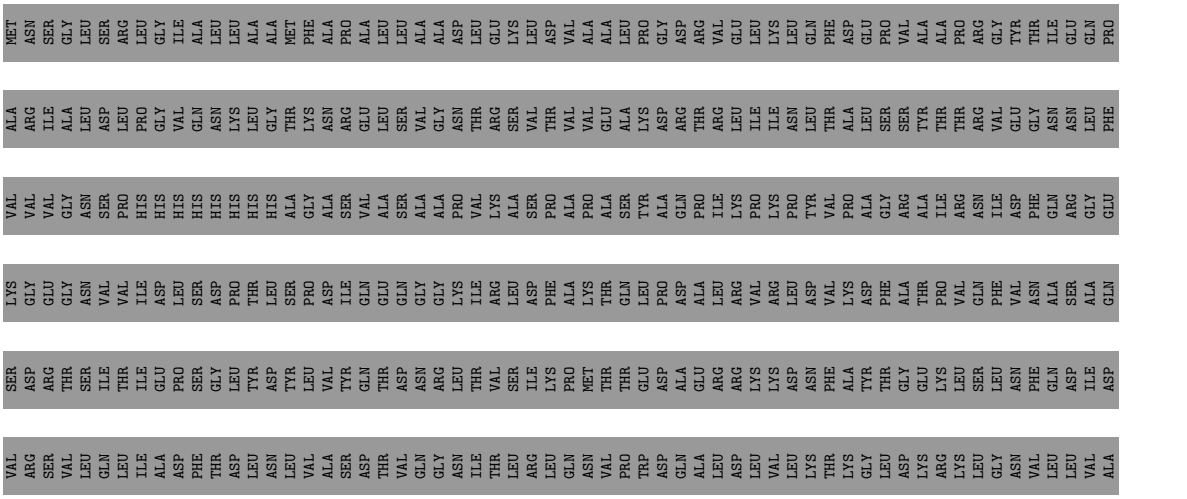






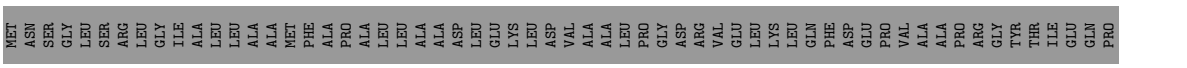
• Molecule 1: Fimbrial assembly protein PilQ

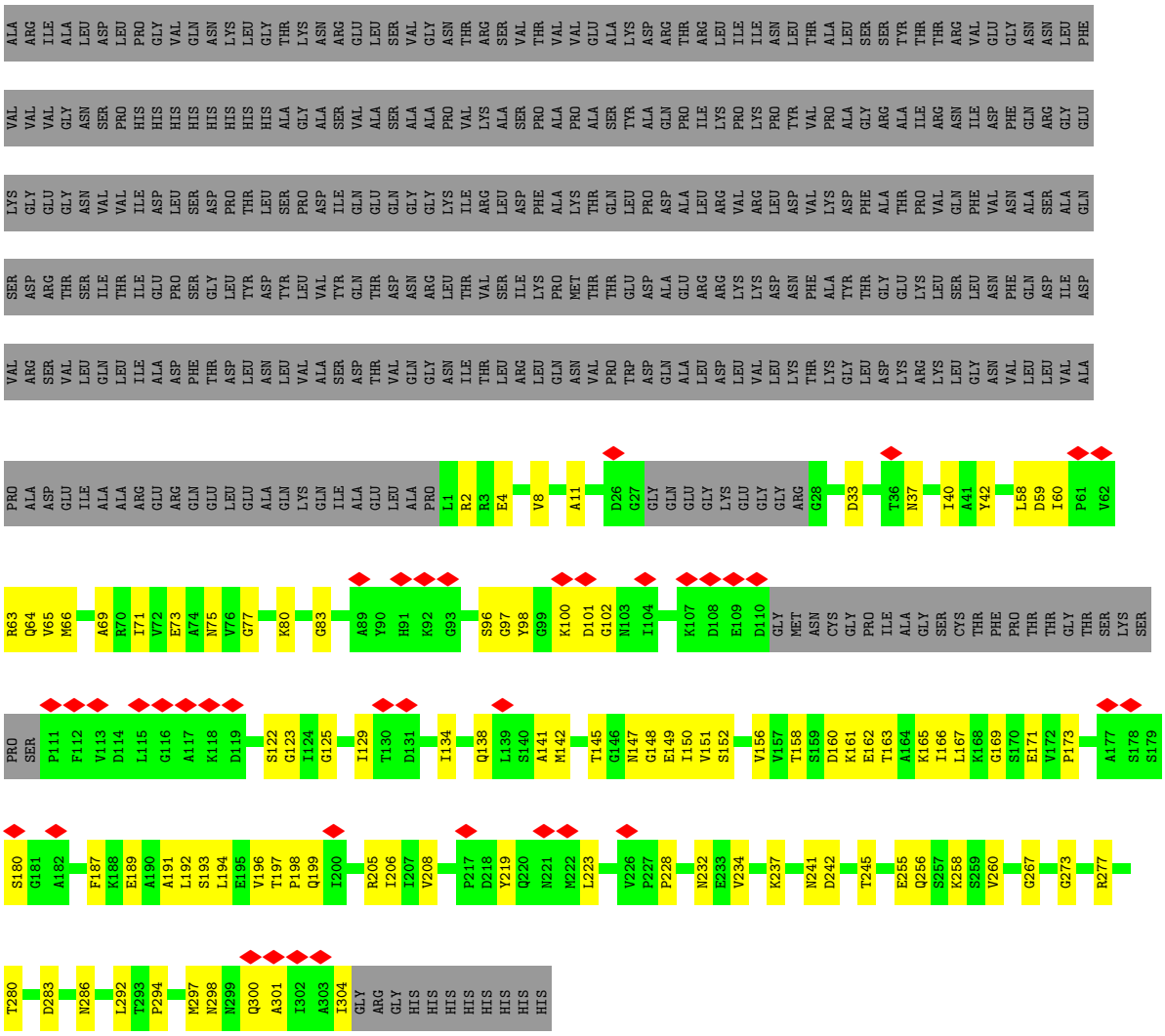
Chain M:



• Molecule 1: Fimbrial assembly protein PilQ

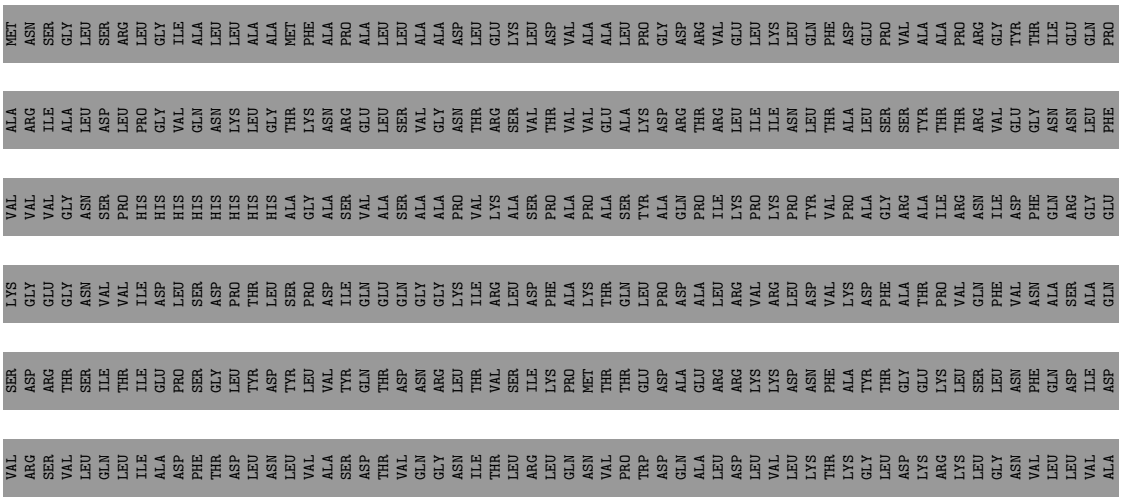
Chain N:

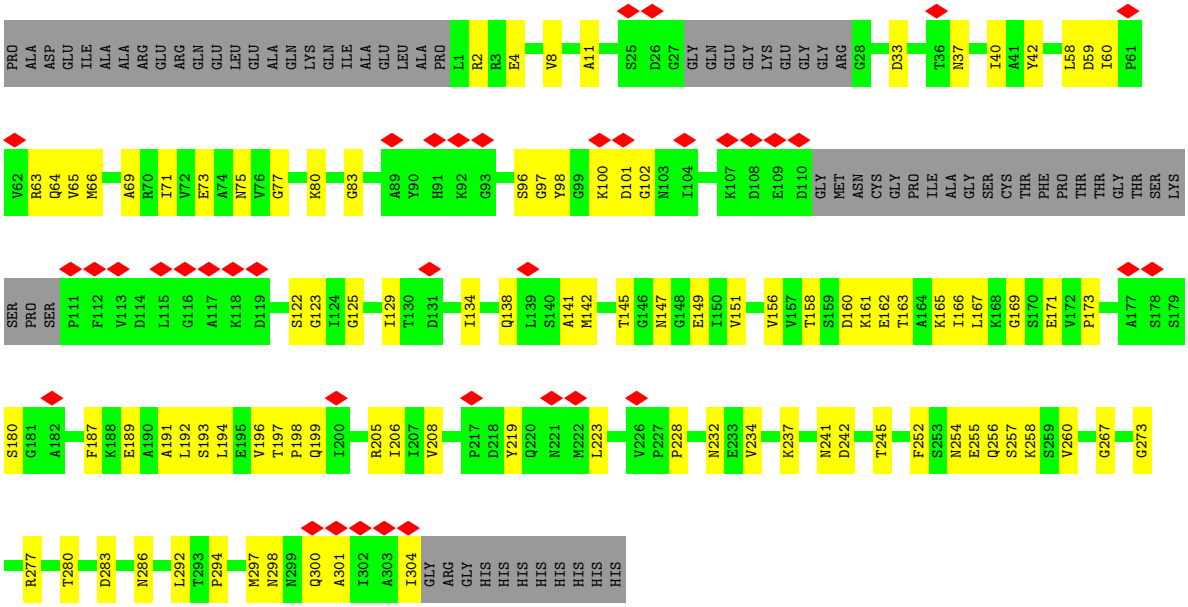




- Molecule 1: Fimbrial assembly protein PilQ

Chain O:




PRO ALA ASP GLU ILE ALA ALA ARG GLU ARG GLN GLU LEU GLU ALA GLN LYS GLN ILE ALA GLU LEU ALA PRO L1 R2 R3 E4 V8 A11 S25 D26 G27 GLY GLN GLU GLY LYS GLU GLY GLY ARG G28 D33 T36 N37 I40 A41 Y42 L58 D59 I60 P61
V62 R63 Q64 V65 M66 A69 R70 I71 V72 E73 A74 N75 V76 G77 K80 G83 A89 Y90 H91 K92 G93 S96 G97 Y98 G99 K100 D101 G102 N103 I104 K107 D108 E109 D110 GLY MET ASN CYS GLY PRO ILE ALA GLY SER CYS THR PHE PRO THR THR GLY THR SER LYS
SER PRO SER P111 F112 V113 D114 L115 G116 A117 K118 D119 S122 G123 I124 G125 I129 T130 D131 I134 Q138 L139 S140 A141 M142 T145 G146 N147 G148 E149 I150 V151 V156 V157 T158 S159 D160 K161 E162 T163 A164 K165 I166 L167 K168 G169 S170 E171 V172 P173 A177 S178 S179
S180 G181 A182 F187 K188 E189 A190 A191 L192 S193 L194 E195 V196 T197 P198 Q199 I200 R205 I206 I207 V208 P217 D218 Y219 Q220 N221 M222 L223 V226 P227 P228 N232 E233 V234 K237 N241 D242 T245 F252 S253 N254 E255 Q256 S257 K258 S259 V260 G267 G273
R277 T280 D283 N286 L292 T293 P294 M297 N298 N299 Q300 A301 I302 A303 I304 GLY ARG GLY HIS HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C15	Depositor
Number of particles used	8725	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 ($e^-/Å^2$)	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	1.744	Depositor
Minimum map value	-0.711	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.48	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 (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	0.37	0/1492	0.73	0/2069
1	B	0.37	0/1492	0.73	0/2069
1	C	0.37	0/1492	0.73	0/2069
1	D	0.37	0/1492	0.73	0/2069
1	E	0.37	0/1492	0.73	0/2069
1	F	0.37	0/1492	0.73	0/2069
1	G	0.37	0/1492	0.73	0/2069
1	H	0.37	0/1492	0.73	0/2069
1	I	0.37	0/1492	0.73	0/2069
1	J	0.37	0/1492	0.73	0/2069
1	K	0.37	0/1492	0.73	0/2069
1	L	0.37	0/1492	0.73	0/2069
1	M	0.37	0/1492	0.73	0/2069
1	N	0.37	0/1492	0.73	0/2069
1	O	0.37	0/1492	0.73	0/2069
All	All	0.37	0/22380	0.73	0/31035

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)

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	1495	0	681	74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1495	0	681	70	0
1	C	1495	0	681	75	0
1	D	1495	0	681	81	0
1	E	1495	0	681	79	0
1	F	1495	0	681	79	0
1	G	1495	0	681	76	0
1	H	1495	0	681	78	0
1	I	1495	0	681	81	0
1	J	1495	0	681	84	0
1	K	1495	0	681	85	0
1	L	1495	0	681	80	0
1	M	1495	0	681	76	0
1	N	1495	0	681	69	0
1	O	1495	0	681	70	0
All	All	22425	0	10215	944	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 29.

The worst 5 of 944 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:O:171:GLU:HA	1:O:189:GLU:HA	1.59	0.85
1:L:171:GLU:HA	1:L:189:GLU:HA	1.59	0.85
1:B:171:GLU:HA	1:B:189:GLU:HA	1.59	0.84
1:M:171:GLU:HA	1:M:189:GLU:HA	1.59	0.84
1:N:171:GLU:HA	1:N:189:GLU:HA	1.59	0.84

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	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	B	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	C	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	D	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	E	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	F	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	G	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	H	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	I	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	J	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	K	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	L	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	M	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	N	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
1	O	298/731 (41%)	286 (96%)	11 (4%)	1 (0%)	41	77
All	All	4470/10965 (41%)	4290 (96%)	165 (4%)	15 (0%)	44	77

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	SER
1	D	122	SER
1	F	122	SER
1	G	122	SER
1	I	122	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)

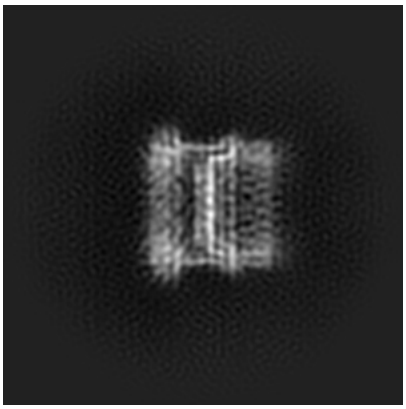
This section contains visualisations of the EMDB entry EMD-21154. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

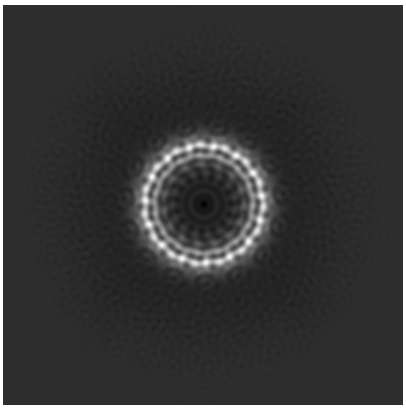
6.1 Orthogonal projections (i)

6.1.1 Primary map

X

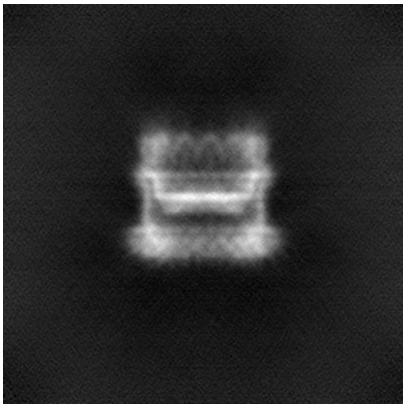


Y

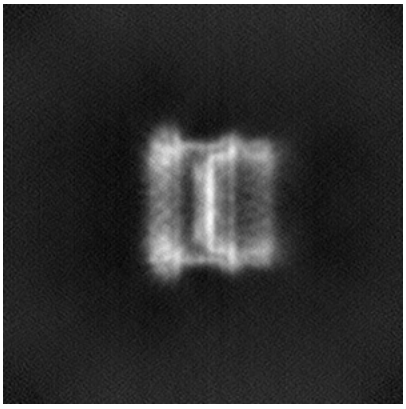


Z

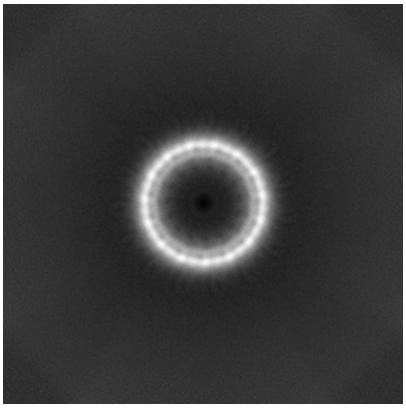
6.1.2 Raw map



X



Y

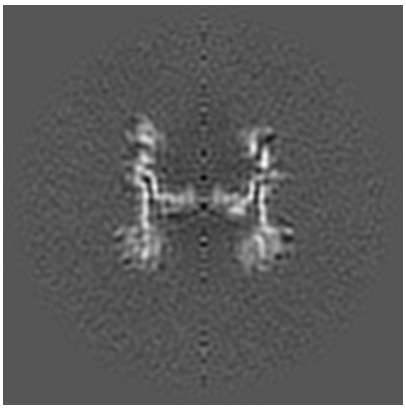


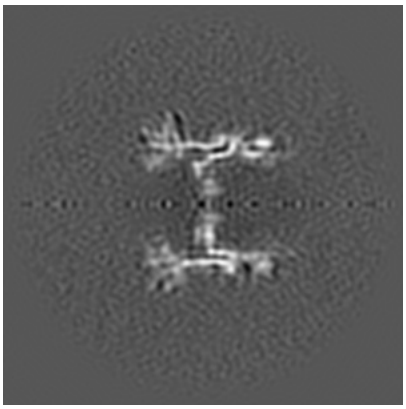
Z

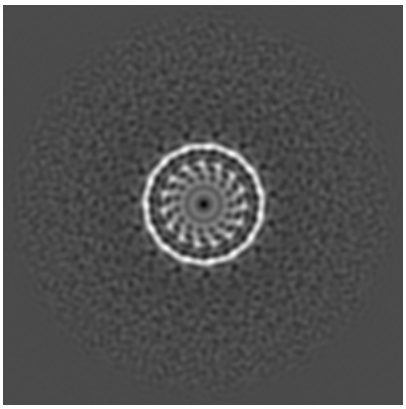
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

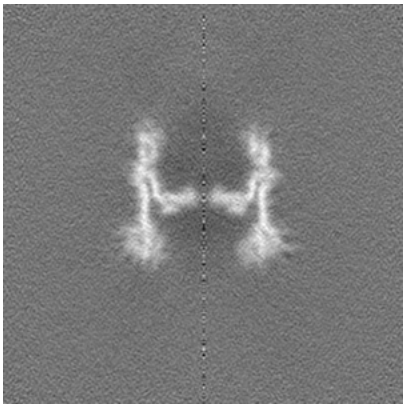
6.2.1 Primary map

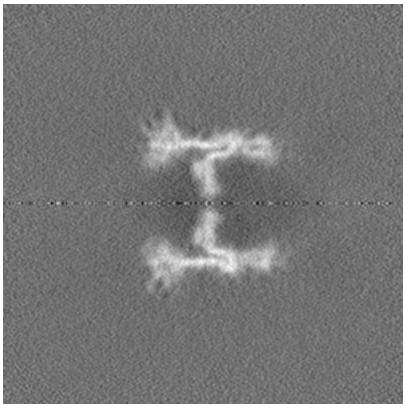

X Index: 128

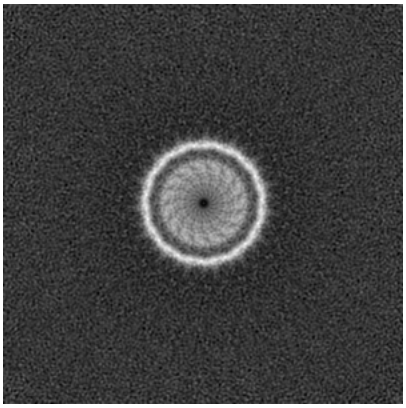

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

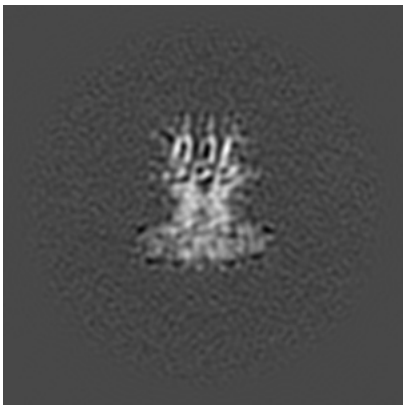

Y Index: 128


Z Index: 128

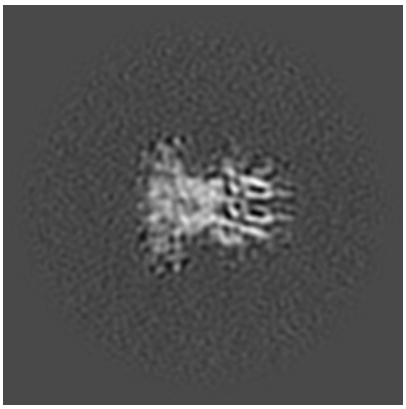
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

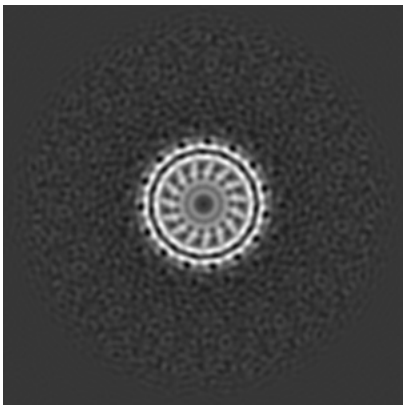
6.3.1 Primary map



X Index: 164

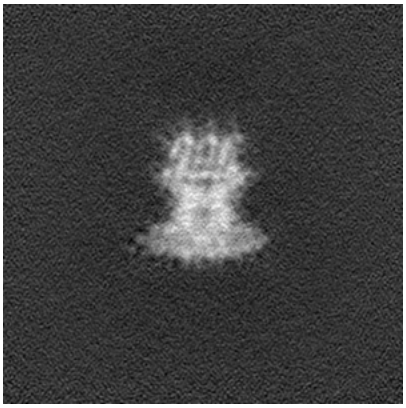


Y Index: 164

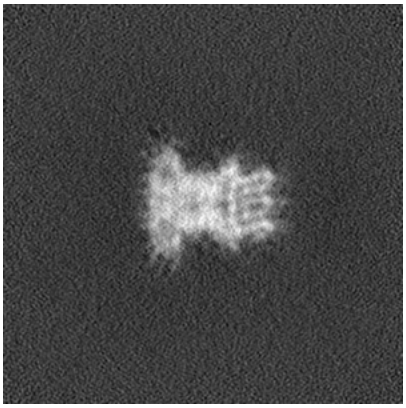


Z Index: 133

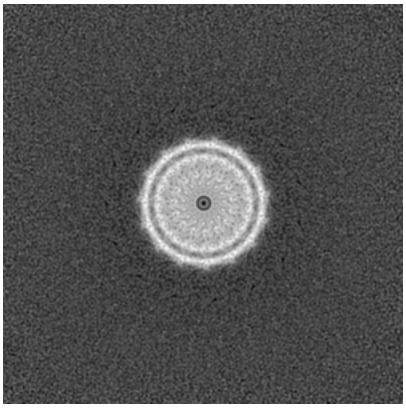
6.3.2 Raw map



X Index: 164



Y Index: 92

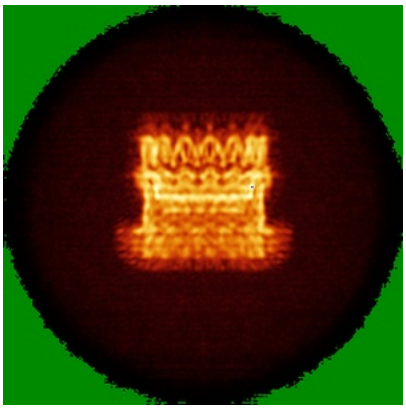


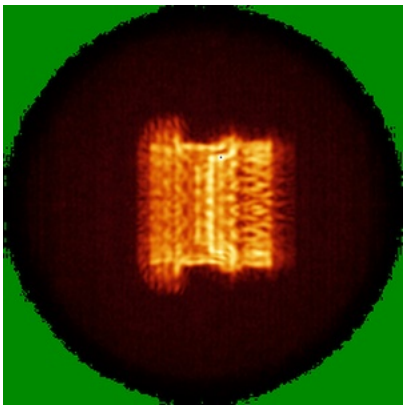
Z Index: 132

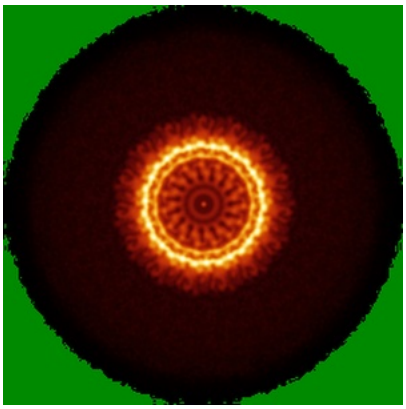
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

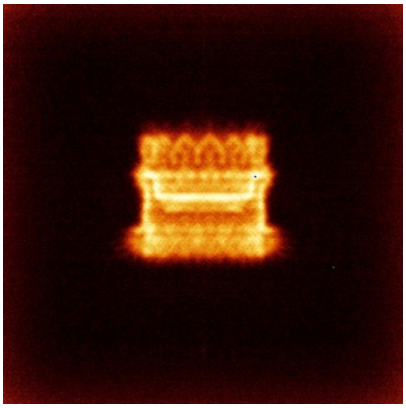
6.4.1 Primary map

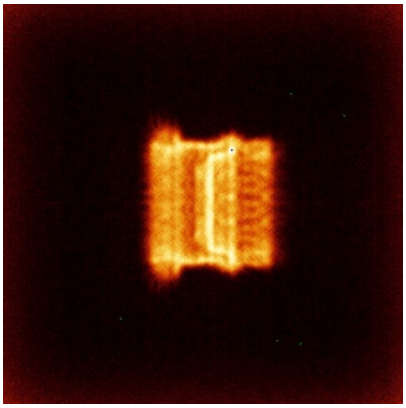

X

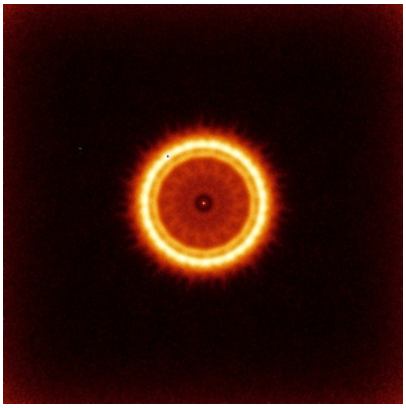

Y


Z

6.4.2 Raw map


X

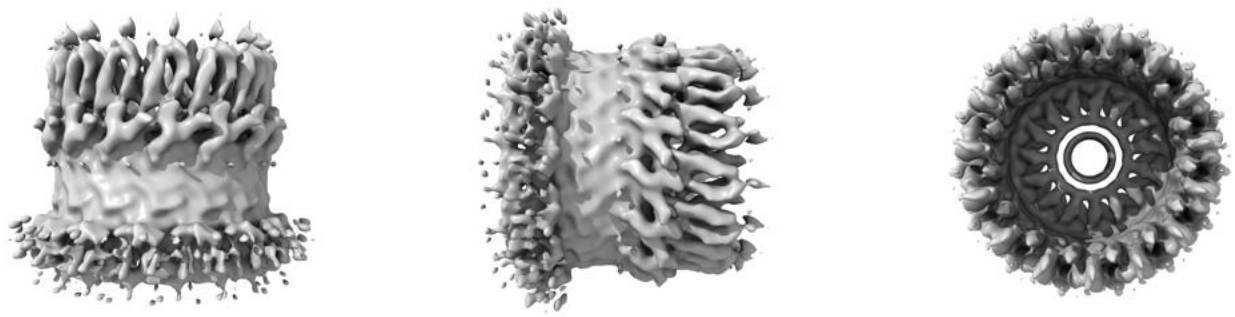

Y


Z

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

6.5 Orthogonal surface views (i)

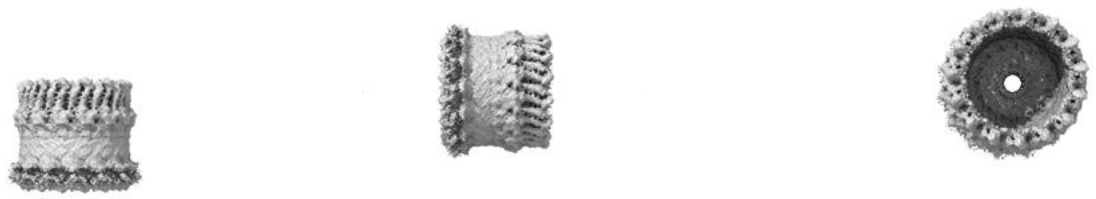
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.48. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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.

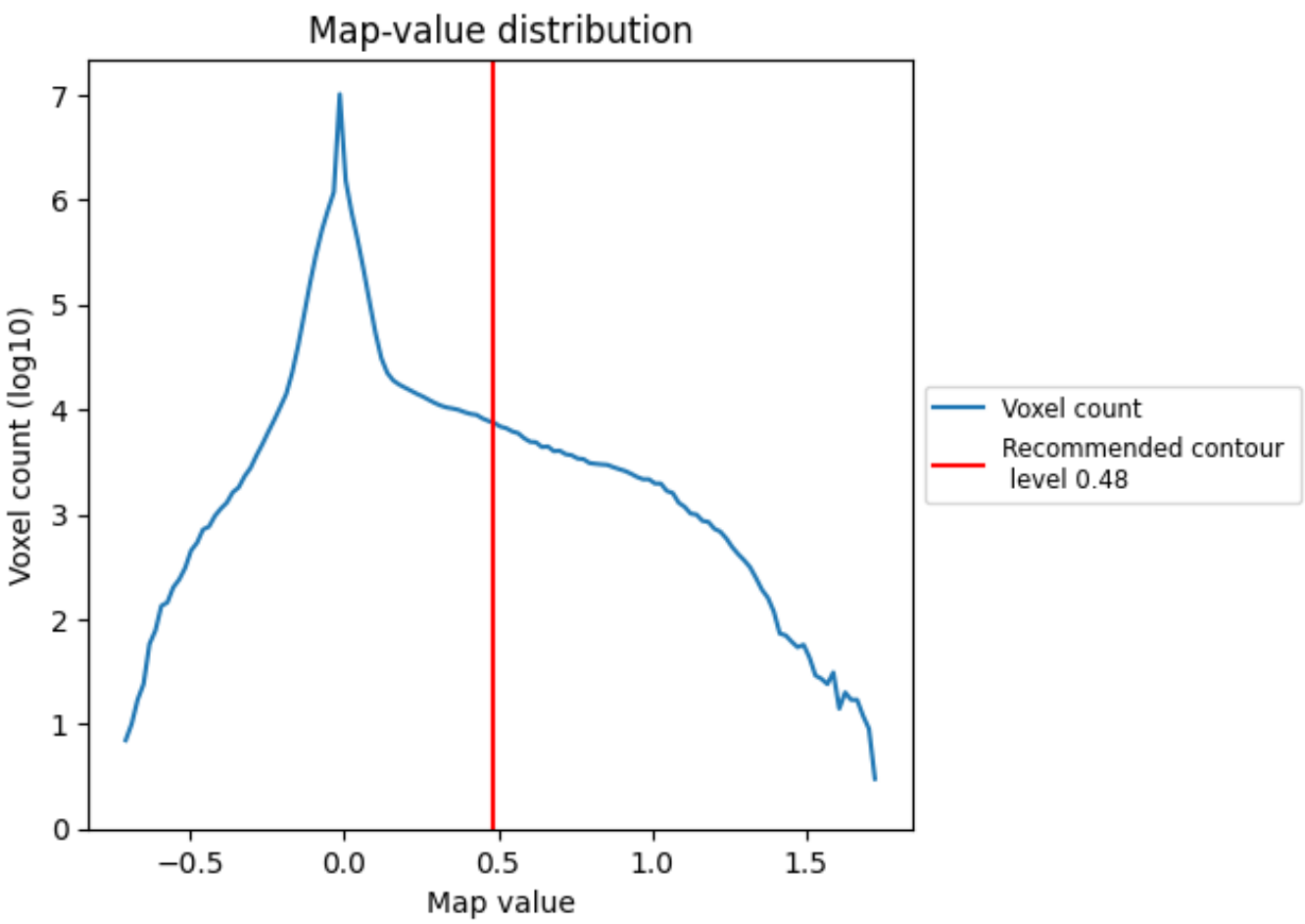
6.6 Mask visualisation (i)

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

7 Map analysis (i)

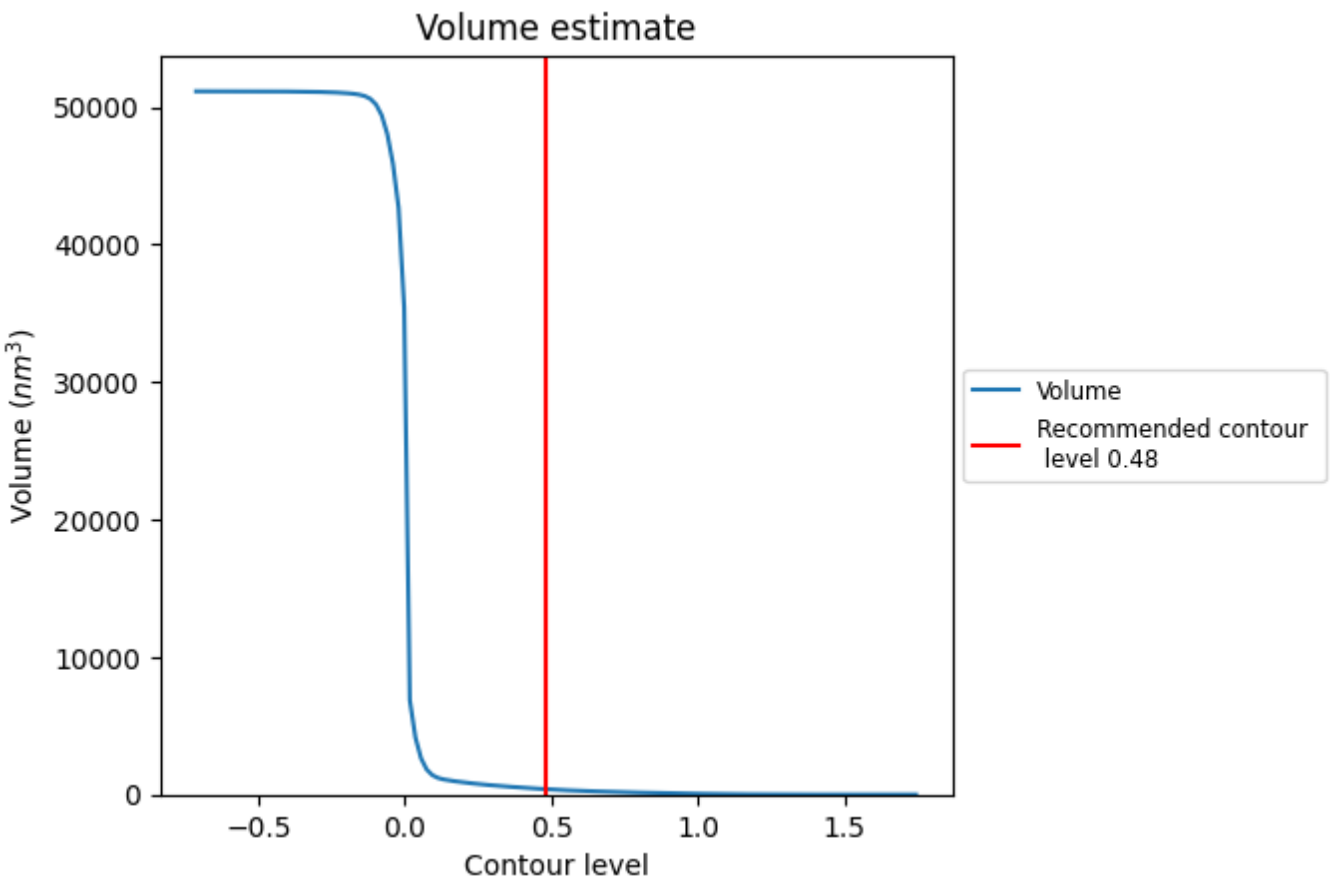
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

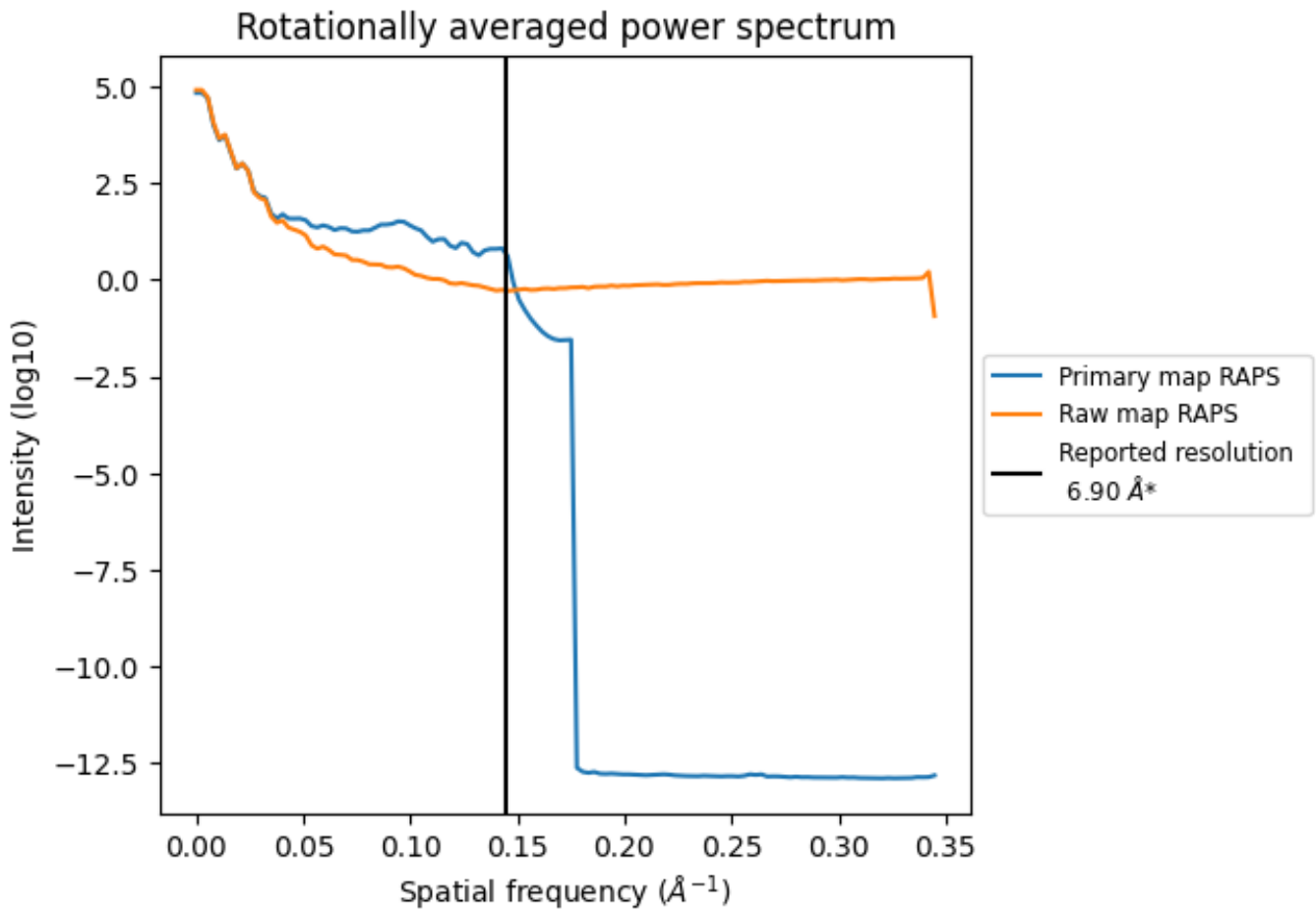
7.2 Volume estimate (i)



The volume at the recommended contour level is 395 nm^3; this corresponds to an approximate mass of 357 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)

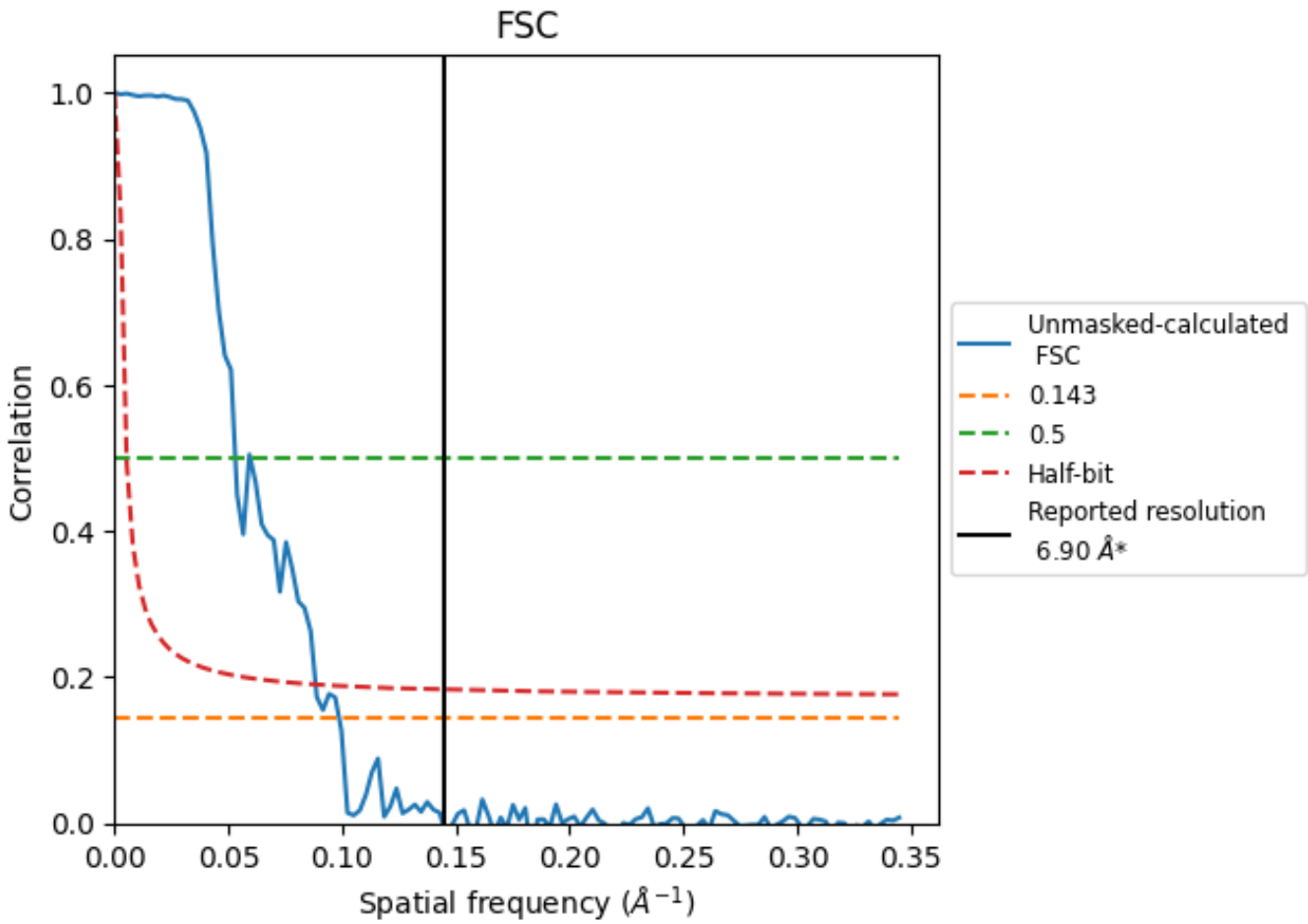


*Reported resolution corresponds to spatial frequency of 0.145 Å^{-1}

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 0.145 Å^{-1}

8.2 Resolution estimates (i)

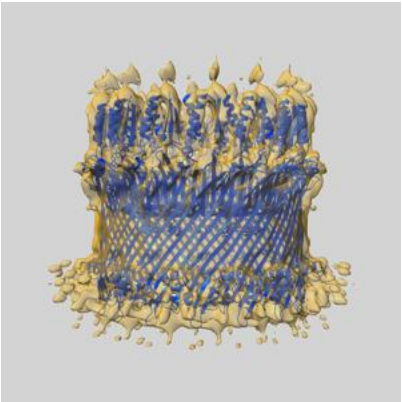
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.13	18.83	11.31

*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 10.13 differs from the reported value 6.9 by more than 10 %

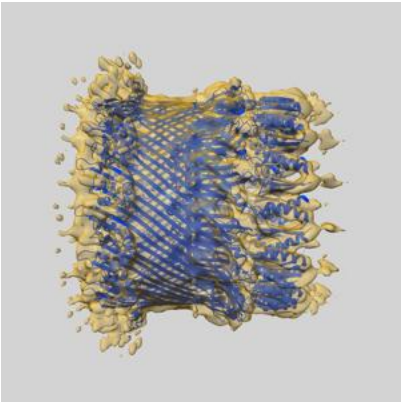
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21154 and PDB model 6VE4. Per-residue inclusion information can be found in section 3 on page 12.

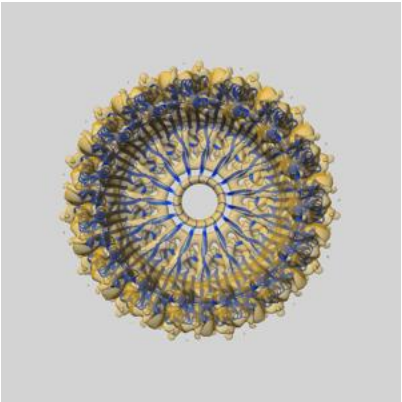
9.1 Map-model overlay (i)



X



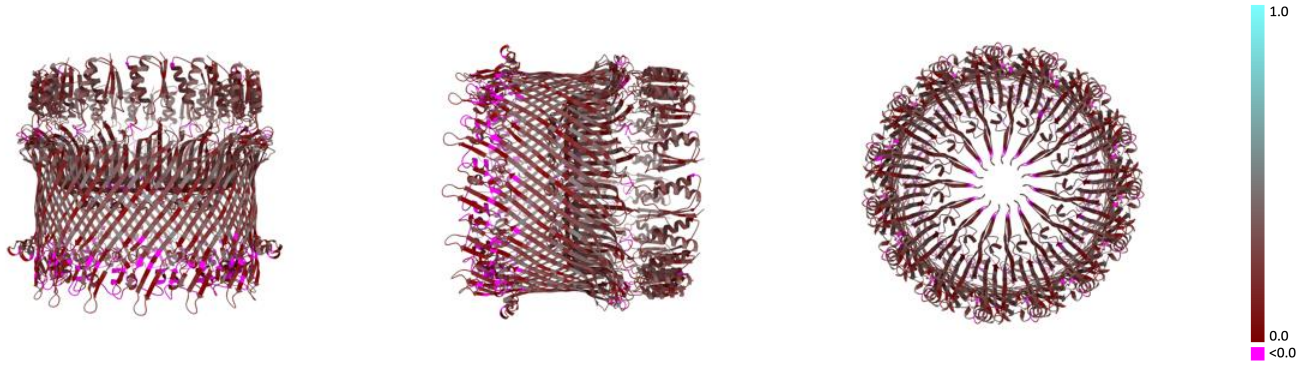
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.48 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.

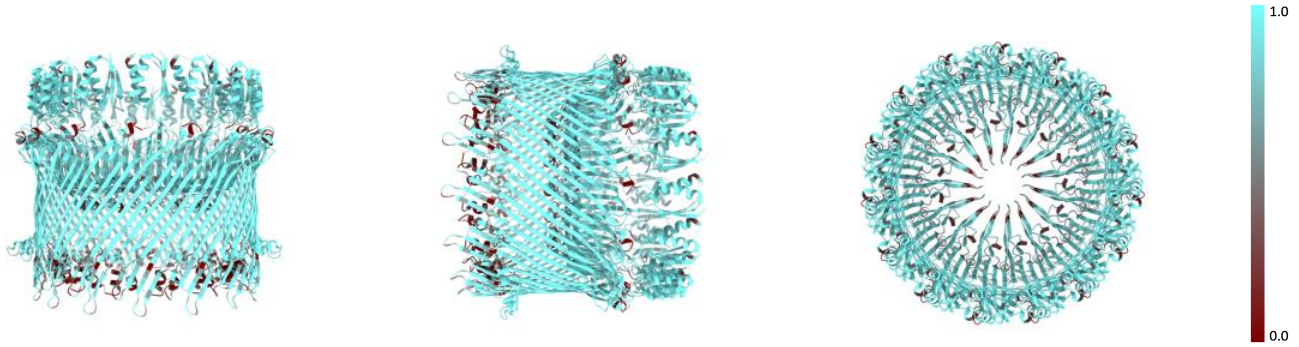
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

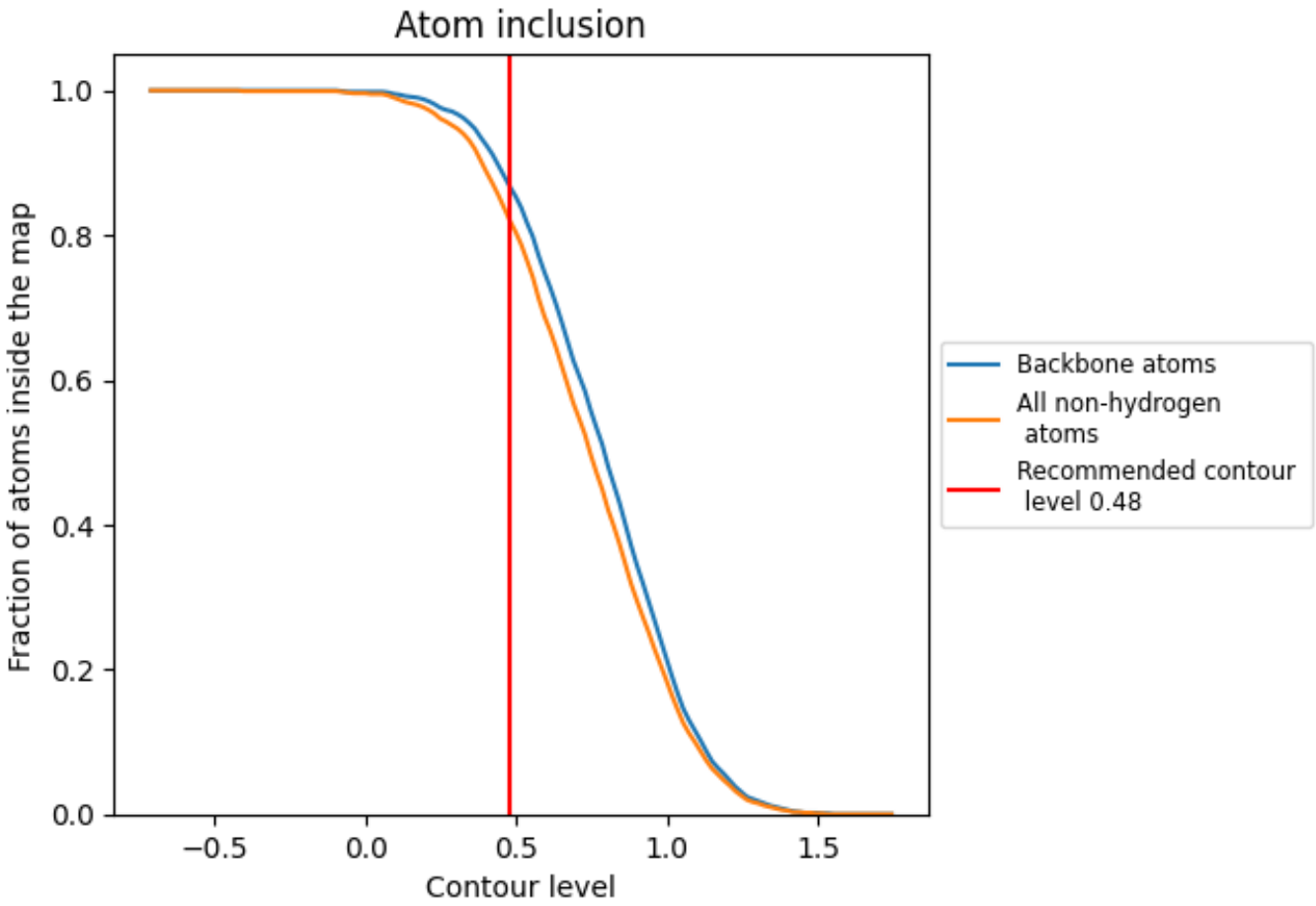
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.48).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.48) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8190	0.2010
A	0.8190	0.2010
B	0.8200	0.2010
C	0.8200	0.2010
D	0.8190	0.2020
E	0.8190	0.2000
F	0.8190	0.2000
G	0.8170	0.2010
H	0.8180	0.2000
I	0.8210	0.2020
J	0.8210	0.2020
K	0.8170	0.2020
L	0.8190	0.2030
M	0.8190	0.2010
N	0.8170	0.2020
O	0.8190	0.2000