



## wwPDB EM Validation Summary Report ⓘ

Nov 9, 2024 – 11:11 am GMT

PDB ID : 6F8L  
EMDB ID : EMD-4194  
Title : Thermus thermophilus PilF ATPase (AMPPNP-bound form)  
Authors : Derrick, J.P.; Collins, R.F.  
Deposited on : 2017-12-13  
Resolution : 8.00 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.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

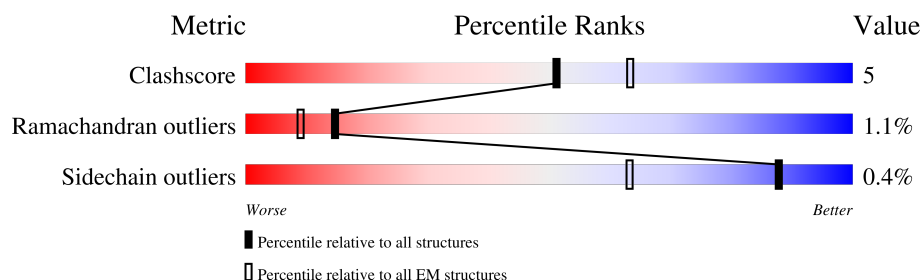
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.00 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.



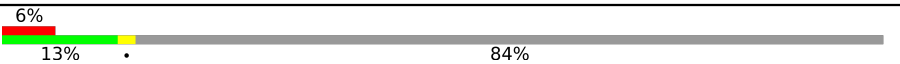

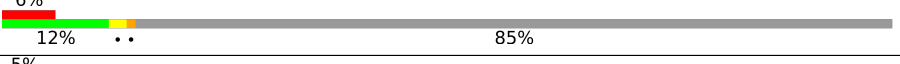




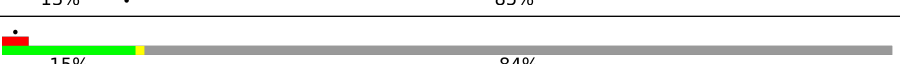
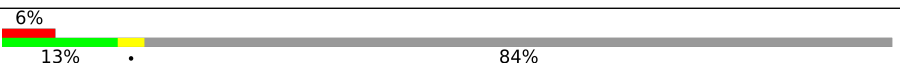

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	913	<div> <div>10%</div> <div>37%</div> <div>58%</div> </div>
1	B	913	<div> <div>11%</div> <div>36%</div> <div>5%</div> <div>58%</div> </div>
1	C	913	<div> <div>11%</div> <div>35%</div> <div>7%</div> <div>58%</div> </div>
1	D	913	<div> <div>11%</div> <div>35%</div> <div>5%</div> <div>58%</div> </div>
1	E	913	<div> <div>13%</div> <div>37%</div> <div>5%</div> <div>58%</div> </div>
1	F	913	<div> <div>12%</div> <div>36%</div> <div>5%</div> <div>58%</div> </div>
1	G	913	<div> <div>5%</div> <div>13%</div> <div>84%</div> </div>
1	H	913	<div> <div>14%</div> <div>84%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	913	
1	J	913	
1	K	913	
1	L	913	
1	M	913	
1	N	913	
1	O	913	
1	P	913	
1	Q	913	
1	R	913	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31239 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 assembly protein PilF.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	146	Total	C	N	O	S	0	0
			1143	726	205	210	2		
1	J	137	Total	C	N	O		0	0
			1090	699	190	201			
1	K	137	Total	C	N	O		0	0
			1090	699	190	201			
1	L	137	Total	C	N	O		0	0
			1090	699	190	201			
1	H	146	Total	C	N	O	S	0	0
			1143	726	205	210	2		
1	I	146	Total	C	N	O	S	0	0
			1143	726	205	210	2		
1	M	146	Total	C	N	O	S	0	0
			1143	726	205	210	2		
1	N	137	Total	C	N	O		0	0
			1090	699	190	201			
1	O	137	Total	C	N	O		0	0
			1090	699	190	201			
1	P	137	Total	C	N	O		0	0
			1090	699	190	201			
1	Q	146	Total	C	N	O	S	0	0
			1143	726	205	210	2		
1	R	146	Total	C	N	O	S	0	0
			1143	726	205	210	2		
1	A	384	Total	C	N	O	S	0	0
			2975	1874	535	556	10		
1	B	383	Total	C	N	O	S	0	0
			2966	1868	534	554	10		
1	C	384	Total	C	N	O	S	0	0
			2975	1874	535	556	10		
1	D	384	Total	C	N	O	S	0	0
			2975	1874	535	556	10		
1	E	384	Total	C	N	O	S	0	0
			2975	1874	535	556	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	384	Total	C	N	O	S	0	0
			2975	1874	535	556	10		

There are 432 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	890	ALA	-	expression tag	UNP Q5SLC9
G	891	ALA	-	expression tag	UNP Q5SLC9
G	892	ALA	-	expression tag	UNP Q5SLC9
G	893	GLU	-	expression tag	UNP Q5SLC9
G	894	LEU	-	expression tag	UNP Q5SLC9
G	895	ALA	-	expression tag	UNP Q5SLC9
G	896	LEU	-	expression tag	UNP Q5SLC9
G	897	VAL	-	expression tag	UNP Q5SLC9
G	898	PRO	-	expression tag	UNP Q5SLC9
G	899	ARG	-	expression tag	UNP Q5SLC9
G	900	GLY	-	expression tag	UNP Q5SLC9
G	901	SER	-	expression tag	UNP Q5SLC9
G	902	SER	-	expression tag	UNP Q5SLC9
G	903	ALA	-	expression tag	UNP Q5SLC9
G	904	HIS	-	expression tag	UNP Q5SLC9
G	905	HIS	-	expression tag	UNP Q5SLC9
G	906	HIS	-	expression tag	UNP Q5SLC9
G	907	HIS	-	expression tag	UNP Q5SLC9
G	908	HIS	-	expression tag	UNP Q5SLC9
G	909	HIS	-	expression tag	UNP Q5SLC9
G	910	HIS	-	expression tag	UNP Q5SLC9
G	911	HIS	-	expression tag	UNP Q5SLC9
G	912	HIS	-	expression tag	UNP Q5SLC9
G	913	HIS	-	expression tag	UNP Q5SLC9
J	890	ALA	-	expression tag	UNP Q5SLC9
J	891	ALA	-	expression tag	UNP Q5SLC9
J	892	ALA	-	expression tag	UNP Q5SLC9
J	893	GLU	-	expression tag	UNP Q5SLC9
J	894	LEU	-	expression tag	UNP Q5SLC9
J	895	ALA	-	expression tag	UNP Q5SLC9
J	896	LEU	-	expression tag	UNP Q5SLC9
J	897	VAL	-	expression tag	UNP Q5SLC9
J	898	PRO	-	expression tag	UNP Q5SLC9
J	899	ARG	-	expression tag	UNP Q5SLC9
J	900	GLY	-	expression tag	UNP Q5SLC9
J	901	SER	-	expression tag	UNP Q5SLC9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	902	SER	-	expression tag	UNP Q5SLC9
J	903	ALA	-	expression tag	UNP Q5SLC9
J	904	HIS	-	expression tag	UNP Q5SLC9
J	905	HIS	-	expression tag	UNP Q5SLC9
J	906	HIS	-	expression tag	UNP Q5SLC9
J	907	HIS	-	expression tag	UNP Q5SLC9
J	908	HIS	-	expression tag	UNP Q5SLC9
J	909	HIS	-	expression tag	UNP Q5SLC9
J	910	HIS	-	expression tag	UNP Q5SLC9
J	911	HIS	-	expression tag	UNP Q5SLC9
J	912	HIS	-	expression tag	UNP Q5SLC9
J	913	HIS	-	expression tag	UNP Q5SLC9
K	890	ALA	-	expression tag	UNP Q5SLC9
K	891	ALA	-	expression tag	UNP Q5SLC9
K	892	ALA	-	expression tag	UNP Q5SLC9
K	893	GLU	-	expression tag	UNP Q5SLC9
K	894	LEU	-	expression tag	UNP Q5SLC9
K	895	ALA	-	expression tag	UNP Q5SLC9
K	896	LEU	-	expression tag	UNP Q5SLC9
K	897	VAL	-	expression tag	UNP Q5SLC9
K	898	PRO	-	expression tag	UNP Q5SLC9
K	899	ARG	-	expression tag	UNP Q5SLC9
K	900	GLY	-	expression tag	UNP Q5SLC9
K	901	SER	-	expression tag	UNP Q5SLC9
K	902	SER	-	expression tag	UNP Q5SLC9
K	903	ALA	-	expression tag	UNP Q5SLC9
K	904	HIS	-	expression tag	UNP Q5SLC9
K	905	HIS	-	expression tag	UNP Q5SLC9
K	906	HIS	-	expression tag	UNP Q5SLC9
K	907	HIS	-	expression tag	UNP Q5SLC9
K	908	HIS	-	expression tag	UNP Q5SLC9
K	909	HIS	-	expression tag	UNP Q5SLC9
K	910	HIS	-	expression tag	UNP Q5SLC9
K	911	HIS	-	expression tag	UNP Q5SLC9
K	912	HIS	-	expression tag	UNP Q5SLC9
K	913	HIS	-	expression tag	UNP Q5SLC9
L	890	ALA	-	expression tag	UNP Q5SLC9
L	891	ALA	-	expression tag	UNP Q5SLC9
L	892	ALA	-	expression tag	UNP Q5SLC9
L	893	GLU	-	expression tag	UNP Q5SLC9
L	894	LEU	-	expression tag	UNP Q5SLC9
L	895	ALA	-	expression tag	UNP Q5SLC9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	896	LEU	-	expression tag	UNP Q5SLC9
L	897	VAL	-	expression tag	UNP Q5SLC9
L	898	PRO	-	expression tag	UNP Q5SLC9
L	899	ARG	-	expression tag	UNP Q5SLC9
L	900	GLY	-	expression tag	UNP Q5SLC9
L	901	SER	-	expression tag	UNP Q5SLC9
L	902	SER	-	expression tag	UNP Q5SLC9
L	903	ALA	-	expression tag	UNP Q5SLC9
L	904	HIS	-	expression tag	UNP Q5SLC9
L	905	HIS	-	expression tag	UNP Q5SLC9
L	906	HIS	-	expression tag	UNP Q5SLC9
L	907	HIS	-	expression tag	UNP Q5SLC9
L	908	HIS	-	expression tag	UNP Q5SLC9
L	909	HIS	-	expression tag	UNP Q5SLC9
L	910	HIS	-	expression tag	UNP Q5SLC9
L	911	HIS	-	expression tag	UNP Q5SLC9
L	912	HIS	-	expression tag	UNP Q5SLC9
L	913	HIS	-	expression tag	UNP Q5SLC9
H	890	ALA	-	expression tag	UNP Q5SLC9
H	891	ALA	-	expression tag	UNP Q5SLC9
H	892	ALA	-	expression tag	UNP Q5SLC9
H	893	GLU	-	expression tag	UNP Q5SLC9
H	894	LEU	-	expression tag	UNP Q5SLC9
H	895	ALA	-	expression tag	UNP Q5SLC9
H	896	LEU	-	expression tag	UNP Q5SLC9
H	897	VAL	-	expression tag	UNP Q5SLC9
H	898	PRO	-	expression tag	UNP Q5SLC9
H	899	ARG	-	expression tag	UNP Q5SLC9
H	900	GLY	-	expression tag	UNP Q5SLC9
H	901	SER	-	expression tag	UNP Q5SLC9
H	902	SER	-	expression tag	UNP Q5SLC9
H	903	ALA	-	expression tag	UNP Q5SLC9
H	904	HIS	-	expression tag	UNP Q5SLC9
H	905	HIS	-	expression tag	UNP Q5SLC9
H	906	HIS	-	expression tag	UNP Q5SLC9
H	907	HIS	-	expression tag	UNP Q5SLC9
H	908	HIS	-	expression tag	UNP Q5SLC9
H	909	HIS	-	expression tag	UNP Q5SLC9
H	910	HIS	-	expression tag	UNP Q5SLC9
H	911	HIS	-	expression tag	UNP Q5SLC9
H	912	HIS	-	expression tag	UNP Q5SLC9
H	913	HIS	-	expression tag	UNP Q5SLC9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	890	ALA	-	expression tag	UNP Q5SLC9
I	891	ALA	-	expression tag	UNP Q5SLC9
I	892	ALA	-	expression tag	UNP Q5SLC9
I	893	GLU	-	expression tag	UNP Q5SLC9
I	894	LEU	-	expression tag	UNP Q5SLC9
I	895	ALA	-	expression tag	UNP Q5SLC9
I	896	LEU	-	expression tag	UNP Q5SLC9
I	897	VAL	-	expression tag	UNP Q5SLC9
I	898	PRO	-	expression tag	UNP Q5SLC9
I	899	ARG	-	expression tag	UNP Q5SLC9
I	900	GLY	-	expression tag	UNP Q5SLC9
I	901	SER	-	expression tag	UNP Q5SLC9
I	902	SER	-	expression tag	UNP Q5SLC9
I	903	ALA	-	expression tag	UNP Q5SLC9
I	904	HIS	-	expression tag	UNP Q5SLC9
I	905	HIS	-	expression tag	UNP Q5SLC9
I	906	HIS	-	expression tag	UNP Q5SLC9
I	907	HIS	-	expression tag	UNP Q5SLC9
I	908	HIS	-	expression tag	UNP Q5SLC9
I	909	HIS	-	expression tag	UNP Q5SLC9
I	910	HIS	-	expression tag	UNP Q5SLC9
I	911	HIS	-	expression tag	UNP Q5SLC9
I	912	HIS	-	expression tag	UNP Q5SLC9
I	913	HIS	-	expression tag	UNP Q5SLC9
M	890	ALA	-	expression tag	UNP Q5SLC9
M	891	ALA	-	expression tag	UNP Q5SLC9
M	892	ALA	-	expression tag	UNP Q5SLC9
M	893	GLU	-	expression tag	UNP Q5SLC9
M	894	LEU	-	expression tag	UNP Q5SLC9
M	895	ALA	-	expression tag	UNP Q5SLC9
M	896	LEU	-	expression tag	UNP Q5SLC9
M	897	VAL	-	expression tag	UNP Q5SLC9
M	898	PRO	-	expression tag	UNP Q5SLC9
M	899	ARG	-	expression tag	UNP Q5SLC9
M	900	GLY	-	expression tag	UNP Q5SLC9
M	901	SER	-	expression tag	UNP Q5SLC9
M	902	SER	-	expression tag	UNP Q5SLC9
M	903	ALA	-	expression tag	UNP Q5SLC9
M	904	HIS	-	expression tag	UNP Q5SLC9
M	905	HIS	-	expression tag	UNP Q5SLC9
M	906	HIS	-	expression tag	UNP Q5SLC9
M	907	HIS	-	expression tag	UNP Q5SLC9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	908	HIS	-	expression tag	UNP Q5SLC9
M	909	HIS	-	expression tag	UNP Q5SLC9
M	910	HIS	-	expression tag	UNP Q5SLC9
M	911	HIS	-	expression tag	UNP Q5SLC9
M	912	HIS	-	expression tag	UNP Q5SLC9
M	913	HIS	-	expression tag	UNP Q5SLC9
N	890	ALA	-	expression tag	UNP Q5SLC9
N	891	ALA	-	expression tag	UNP Q5SLC9
N	892	ALA	-	expression tag	UNP Q5SLC9
N	893	GLU	-	expression tag	UNP Q5SLC9
N	894	LEU	-	expression tag	UNP Q5SLC9
N	895	ALA	-	expression tag	UNP Q5SLC9
N	896	LEU	-	expression tag	UNP Q5SLC9
N	897	VAL	-	expression tag	UNP Q5SLC9
N	898	PRO	-	expression tag	UNP Q5SLC9
N	899	ARG	-	expression tag	UNP Q5SLC9
N	900	GLY	-	expression tag	UNP Q5SLC9
N	901	SER	-	expression tag	UNP Q5SLC9
N	902	SER	-	expression tag	UNP Q5SLC9
N	903	ALA	-	expression tag	UNP Q5SLC9
N	904	HIS	-	expression tag	UNP Q5SLC9
N	905	HIS	-	expression tag	UNP Q5SLC9
N	906	HIS	-	expression tag	UNP Q5SLC9
N	907	HIS	-	expression tag	UNP Q5SLC9
N	908	HIS	-	expression tag	UNP Q5SLC9
N	909	HIS	-	expression tag	UNP Q5SLC9
N	910	HIS	-	expression tag	UNP Q5SLC9
N	911	HIS	-	expression tag	UNP Q5SLC9
N	912	HIS	-	expression tag	UNP Q5SLC9
N	913	HIS	-	expression tag	UNP Q5SLC9
O	890	ALA	-	expression tag	UNP Q5SLC9
O	891	ALA	-	expression tag	UNP Q5SLC9
O	892	ALA	-	expression tag	UNP Q5SLC9
O	893	GLU	-	expression tag	UNP Q5SLC9
O	894	LEU	-	expression tag	UNP Q5SLC9
O	895	ALA	-	expression tag	UNP Q5SLC9
O	896	LEU	-	expression tag	UNP Q5SLC9
O	897	VAL	-	expression tag	UNP Q5SLC9
O	898	PRO	-	expression tag	UNP Q5SLC9
O	899	ARG	-	expression tag	UNP Q5SLC9
O	900	GLY	-	expression tag	UNP Q5SLC9
O	901	SER	-	expression tag	UNP Q5SLC9

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Chain	Residue	Modelled	Actual	Comment	Reference
O	902	SER	-	expression tag	UNP Q5SLC9
O	903	ALA	-	expression tag	UNP Q5SLC9
O	904	HIS	-	expression tag	UNP Q5SLC9
O	905	HIS	-	expression tag	UNP Q5SLC9
O	906	HIS	-	expression tag	UNP Q5SLC9
O	907	HIS	-	expression tag	UNP Q5SLC9
O	908	HIS	-	expression tag	UNP Q5SLC9
O	909	HIS	-	expression tag	UNP Q5SLC9
O	910	HIS	-	expression tag	UNP Q5SLC9
O	911	HIS	-	expression tag	UNP Q5SLC9
O	912	HIS	-	expression tag	UNP Q5SLC9
O	913	HIS	-	expression tag	UNP Q5SLC9
P	890	ALA	-	expression tag	UNP Q5SLC9
P	891	ALA	-	expression tag	UNP Q5SLC9
P	892	ALA	-	expression tag	UNP Q5SLC9
P	893	GLU	-	expression tag	UNP Q5SLC9
P	894	LEU	-	expression tag	UNP Q5SLC9
P	895	ALA	-	expression tag	UNP Q5SLC9
P	896	LEU	-	expression tag	UNP Q5SLC9
P	897	VAL	-	expression tag	UNP Q5SLC9
P	898	PRO	-	expression tag	UNP Q5SLC9
P	899	ARG	-	expression tag	UNP Q5SLC9
P	900	GLY	-	expression tag	UNP Q5SLC9
P	901	SER	-	expression tag	UNP Q5SLC9
P	902	SER	-	expression tag	UNP Q5SLC9
P	903	ALA	-	expression tag	UNP Q5SLC9
P	904	HIS	-	expression tag	UNP Q5SLC9
P	905	HIS	-	expression tag	UNP Q5SLC9
P	906	HIS	-	expression tag	UNP Q5SLC9
P	907	HIS	-	expression tag	UNP Q5SLC9
P	908	HIS	-	expression tag	UNP Q5SLC9
P	909	HIS	-	expression tag	UNP Q5SLC9
P	910	HIS	-	expression tag	UNP Q5SLC9
P	911	HIS	-	expression tag	UNP Q5SLC9
P	912	HIS	-	expression tag	UNP Q5SLC9
P	913	HIS	-	expression tag	UNP Q5SLC9
Q	890	ALA	-	expression tag	UNP Q5SLC9
Q	891	ALA	-	expression tag	UNP Q5SLC9
Q	892	ALA	-	expression tag	UNP Q5SLC9
Q	893	GLU	-	expression tag	UNP Q5SLC9
Q	894	LEU	-	expression tag	UNP Q5SLC9
Q	895	ALA	-	expression tag	UNP Q5SLC9

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	896	LEU	-	expression tag	UNP Q5SLC9
Q	897	VAL	-	expression tag	UNP Q5SLC9
Q	898	PRO	-	expression tag	UNP Q5SLC9
Q	899	ARG	-	expression tag	UNP Q5SLC9
Q	900	GLY	-	expression tag	UNP Q5SLC9
Q	901	SER	-	expression tag	UNP Q5SLC9
Q	902	SER	-	expression tag	UNP Q5SLC9
Q	903	ALA	-	expression tag	UNP Q5SLC9
Q	904	HIS	-	expression tag	UNP Q5SLC9
Q	905	HIS	-	expression tag	UNP Q5SLC9
Q	906	HIS	-	expression tag	UNP Q5SLC9
Q	907	HIS	-	expression tag	UNP Q5SLC9
Q	908	HIS	-	expression tag	UNP Q5SLC9
Q	909	HIS	-	expression tag	UNP Q5SLC9
Q	910	HIS	-	expression tag	UNP Q5SLC9
Q	911	HIS	-	expression tag	UNP Q5SLC9
Q	912	HIS	-	expression tag	UNP Q5SLC9
Q	913	HIS	-	expression tag	UNP Q5SLC9
R	890	ALA	-	expression tag	UNP Q5SLC9
R	891	ALA	-	expression tag	UNP Q5SLC9
R	892	ALA	-	expression tag	UNP Q5SLC9
R	893	GLU	-	expression tag	UNP Q5SLC9
R	894	LEU	-	expression tag	UNP Q5SLC9
R	895	ALA	-	expression tag	UNP Q5SLC9
R	896	LEU	-	expression tag	UNP Q5SLC9
R	897	VAL	-	expression tag	UNP Q5SLC9
R	898	PRO	-	expression tag	UNP Q5SLC9
R	899	ARG	-	expression tag	UNP Q5SLC9
R	900	GLY	-	expression tag	UNP Q5SLC9
R	901	SER	-	expression tag	UNP Q5SLC9
R	902	SER	-	expression tag	UNP Q5SLC9
R	903	ALA	-	expression tag	UNP Q5SLC9
R	904	HIS	-	expression tag	UNP Q5SLC9
R	905	HIS	-	expression tag	UNP Q5SLC9
R	906	HIS	-	expression tag	UNP Q5SLC9
R	907	HIS	-	expression tag	UNP Q5SLC9
R	908	HIS	-	expression tag	UNP Q5SLC9
R	909	HIS	-	expression tag	UNP Q5SLC9
R	910	HIS	-	expression tag	UNP Q5SLC9
R	911	HIS	-	expression tag	UNP Q5SLC9
R	912	HIS	-	expression tag	UNP Q5SLC9
R	913	HIS	-	expression tag	UNP Q5SLC9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	890	ALA	-	expression tag	UNP Q5SLC9
A	891	ALA	-	expression tag	UNP Q5SLC9
A	892	ALA	-	expression tag	UNP Q5SLC9
A	893	GLU	-	expression tag	UNP Q5SLC9
A	894	LEU	-	expression tag	UNP Q5SLC9
A	895	ALA	-	expression tag	UNP Q5SLC9
A	896	LEU	-	expression tag	UNP Q5SLC9
A	897	VAL	-	expression tag	UNP Q5SLC9
A	898	PRO	-	expression tag	UNP Q5SLC9
A	899	ARG	-	expression tag	UNP Q5SLC9
A	900	GLY	-	expression tag	UNP Q5SLC9
A	901	SER	-	expression tag	UNP Q5SLC9
A	902	SER	-	expression tag	UNP Q5SLC9
A	903	ALA	-	expression tag	UNP Q5SLC9
A	904	HIS	-	expression tag	UNP Q5SLC9
A	905	HIS	-	expression tag	UNP Q5SLC9
A	906	HIS	-	expression tag	UNP Q5SLC9
A	907	HIS	-	expression tag	UNP Q5SLC9
A	908	HIS	-	expression tag	UNP Q5SLC9
A	909	HIS	-	expression tag	UNP Q5SLC9
A	910	HIS	-	expression tag	UNP Q5SLC9
A	911	HIS	-	expression tag	UNP Q5SLC9
A	912	HIS	-	expression tag	UNP Q5SLC9
A	913	HIS	-	expression tag	UNP Q5SLC9
B	890	ALA	-	expression tag	UNP Q5SLC9
B	891	ALA	-	expression tag	UNP Q5SLC9
B	892	ALA	-	expression tag	UNP Q5SLC9
B	893	GLU	-	expression tag	UNP Q5SLC9
B	894	LEU	-	expression tag	UNP Q5SLC9
B	895	ALA	-	expression tag	UNP Q5SLC9
B	896	LEU	-	expression tag	UNP Q5SLC9
B	897	VAL	-	expression tag	UNP Q5SLC9
B	898	PRO	-	expression tag	UNP Q5SLC9
B	899	ARG	-	expression tag	UNP Q5SLC9
B	900	GLY	-	expression tag	UNP Q5SLC9
B	901	SER	-	expression tag	UNP Q5SLC9
B	902	SER	-	expression tag	UNP Q5SLC9
B	903	ALA	-	expression tag	UNP Q5SLC9
B	904	HIS	-	expression tag	UNP Q5SLC9
B	905	HIS	-	expression tag	UNP Q5SLC9
B	906	HIS	-	expression tag	UNP Q5SLC9
B	907	HIS	-	expression tag	UNP Q5SLC9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	908	HIS	-	expression tag	UNP Q5SLC9
B	909	HIS	-	expression tag	UNP Q5SLC9
B	910	HIS	-	expression tag	UNP Q5SLC9
B	911	HIS	-	expression tag	UNP Q5SLC9
B	912	HIS	-	expression tag	UNP Q5SLC9
B	913	HIS	-	expression tag	UNP Q5SLC9
C	890	ALA	-	expression tag	UNP Q5SLC9
C	891	ALA	-	expression tag	UNP Q5SLC9
C	892	ALA	-	expression tag	UNP Q5SLC9
C	893	GLU	-	expression tag	UNP Q5SLC9
C	894	LEU	-	expression tag	UNP Q5SLC9
C	895	ALA	-	expression tag	UNP Q5SLC9
C	896	LEU	-	expression tag	UNP Q5SLC9
C	897	VAL	-	expression tag	UNP Q5SLC9
C	898	PRO	-	expression tag	UNP Q5SLC9
C	899	ARG	-	expression tag	UNP Q5SLC9
C	900	GLY	-	expression tag	UNP Q5SLC9
C	901	SER	-	expression tag	UNP Q5SLC9
C	902	SER	-	expression tag	UNP Q5SLC9
C	903	ALA	-	expression tag	UNP Q5SLC9
C	904	HIS	-	expression tag	UNP Q5SLC9
C	905	HIS	-	expression tag	UNP Q5SLC9
C	906	HIS	-	expression tag	UNP Q5SLC9
C	907	HIS	-	expression tag	UNP Q5SLC9
C	908	HIS	-	expression tag	UNP Q5SLC9
C	909	HIS	-	expression tag	UNP Q5SLC9
C	910	HIS	-	expression tag	UNP Q5SLC9
C	911	HIS	-	expression tag	UNP Q5SLC9
C	912	HIS	-	expression tag	UNP Q5SLC9
C	913	HIS	-	expression tag	UNP Q5SLC9
D	890	ALA	-	expression tag	UNP Q5SLC9
D	891	ALA	-	expression tag	UNP Q5SLC9
D	892	ALA	-	expression tag	UNP Q5SLC9
D	893	GLU	-	expression tag	UNP Q5SLC9
D	894	LEU	-	expression tag	UNP Q5SLC9
D	895	ALA	-	expression tag	UNP Q5SLC9
D	896	LEU	-	expression tag	UNP Q5SLC9
D	897	VAL	-	expression tag	UNP Q5SLC9
D	898	PRO	-	expression tag	UNP Q5SLC9
D	899	ARG	-	expression tag	UNP Q5SLC9
D	900	GLY	-	expression tag	UNP Q5SLC9
D	901	SER	-	expression tag	UNP Q5SLC9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	902	SER	-	expression tag	UNP Q5SLC9
D	903	ALA	-	expression tag	UNP Q5SLC9
D	904	HIS	-	expression tag	UNP Q5SLC9
D	905	HIS	-	expression tag	UNP Q5SLC9
D	906	HIS	-	expression tag	UNP Q5SLC9
D	907	HIS	-	expression tag	UNP Q5SLC9
D	908	HIS	-	expression tag	UNP Q5SLC9
D	909	HIS	-	expression tag	UNP Q5SLC9
D	910	HIS	-	expression tag	UNP Q5SLC9
D	911	HIS	-	expression tag	UNP Q5SLC9
D	912	HIS	-	expression tag	UNP Q5SLC9
D	913	HIS	-	expression tag	UNP Q5SLC9
E	890	ALA	-	expression tag	UNP Q5SLC9
E	891	ALA	-	expression tag	UNP Q5SLC9
E	892	ALA	-	expression tag	UNP Q5SLC9
E	893	GLU	-	expression tag	UNP Q5SLC9
E	894	LEU	-	expression tag	UNP Q5SLC9
E	895	ALA	-	expression tag	UNP Q5SLC9
E	896	LEU	-	expression tag	UNP Q5SLC9
E	897	VAL	-	expression tag	UNP Q5SLC9
E	898	PRO	-	expression tag	UNP Q5SLC9
E	899	ARG	-	expression tag	UNP Q5SLC9
E	900	GLY	-	expression tag	UNP Q5SLC9
E	901	SER	-	expression tag	UNP Q5SLC9
E	902	SER	-	expression tag	UNP Q5SLC9
E	903	ALA	-	expression tag	UNP Q5SLC9
E	904	HIS	-	expression tag	UNP Q5SLC9
E	905	HIS	-	expression tag	UNP Q5SLC9
E	906	HIS	-	expression tag	UNP Q5SLC9
E	907	HIS	-	expression tag	UNP Q5SLC9
E	908	HIS	-	expression tag	UNP Q5SLC9
E	909	HIS	-	expression tag	UNP Q5SLC9
E	910	HIS	-	expression tag	UNP Q5SLC9
E	911	HIS	-	expression tag	UNP Q5SLC9
E	912	HIS	-	expression tag	UNP Q5SLC9
E	913	HIS	-	expression tag	UNP Q5SLC9
F	890	ALA	-	expression tag	UNP Q5SLC9
F	891	ALA	-	expression tag	UNP Q5SLC9
F	892	ALA	-	expression tag	UNP Q5SLC9
F	893	GLU	-	expression tag	UNP Q5SLC9
F	894	LEU	-	expression tag	UNP Q5SLC9
F	895	ALA	-	expression tag	UNP Q5SLC9

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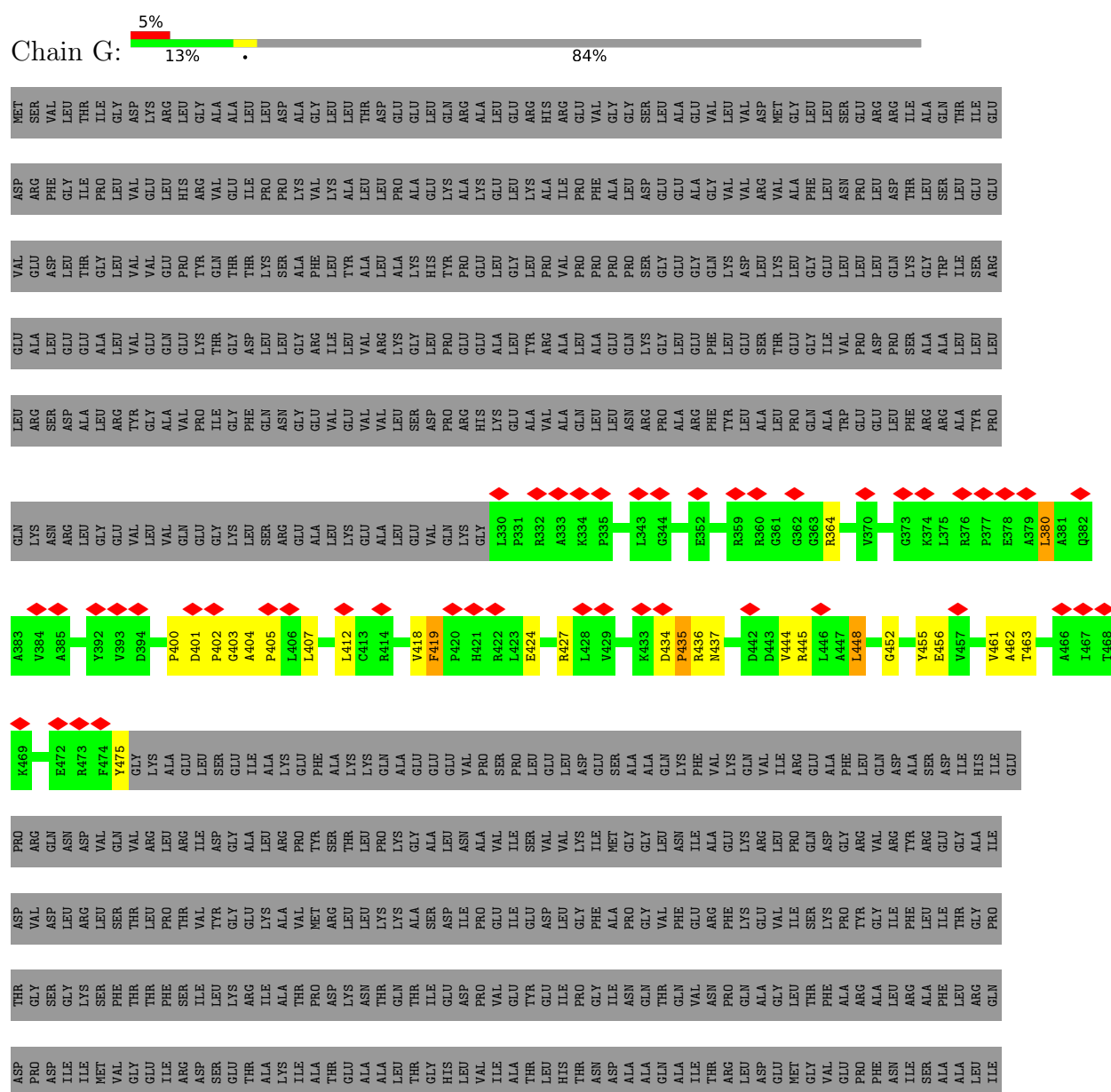
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Chain	Residue	Modelled	Actual	Comment	Reference
F	896	LEU	-	expression tag	UNP Q5SLC9
F	897	VAL	-	expression tag	UNP Q5SLC9
F	898	PRO	-	expression tag	UNP Q5SLC9
F	899	ARG	-	expression tag	UNP Q5SLC9
F	900	GLY	-	expression tag	UNP Q5SLC9
F	901	SER	-	expression tag	UNP Q5SLC9
F	902	SER	-	expression tag	UNP Q5SLC9
F	903	ALA	-	expression tag	UNP Q5SLC9
F	904	HIS	-	expression tag	UNP Q5SLC9
F	905	HIS	-	expression tag	UNP Q5SLC9
F	906	HIS	-	expression tag	UNP Q5SLC9
F	907	HIS	-	expression tag	UNP Q5SLC9
F	908	HIS	-	expression tag	UNP Q5SLC9
F	909	HIS	-	expression tag	UNP Q5SLC9
F	910	HIS	-	expression tag	UNP Q5SLC9
F	911	HIS	-	expression tag	UNP Q5SLC9
F	912	HIS	-	expression tag	UNP Q5SLC9
F	913	HIS	-	expression tag	UNP Q5SLC9

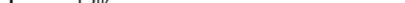
### 3 Residue-property plots

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: Type IV pilus assembly protein PilF

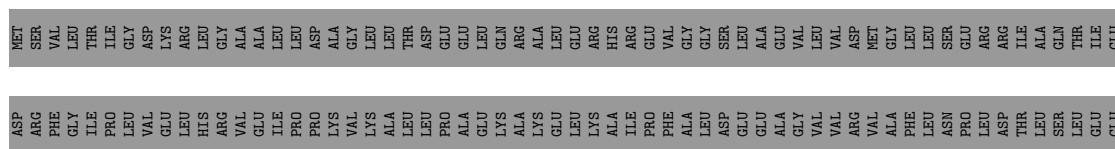


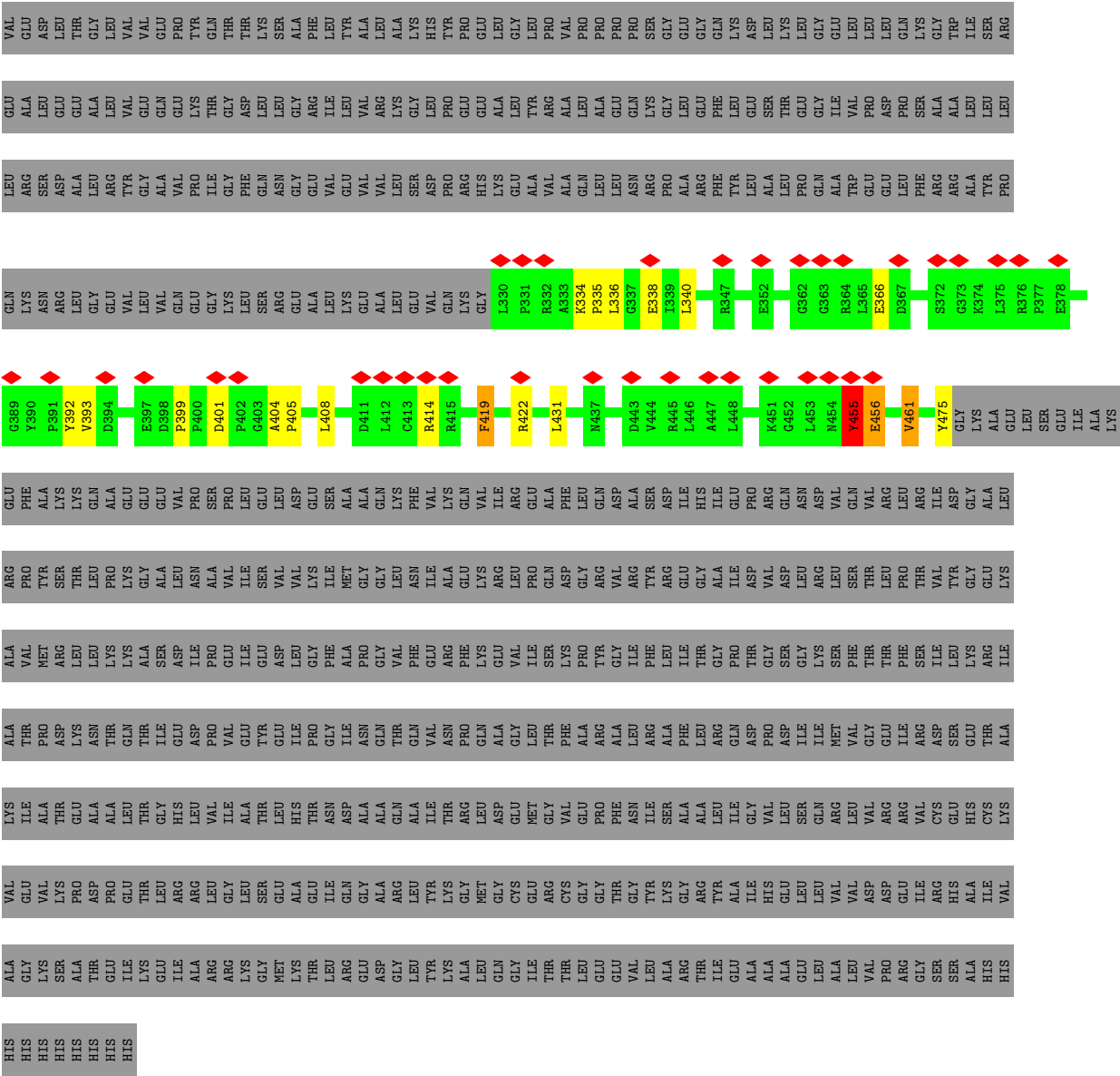
ALA  
ALA  
ALA  
GLU  
LEU  
ALA  
LEU  
VAL  
PRO  
ARG  
GLY  
SER  
SER  
ALA  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

Chain J:  5% 13% 85%

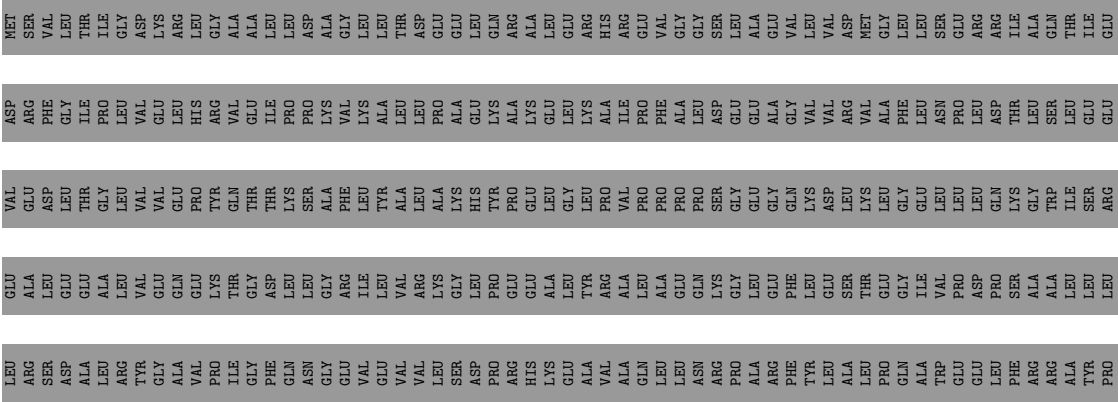








● Molecule 1: Type IV pilus assembly protein PilF







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

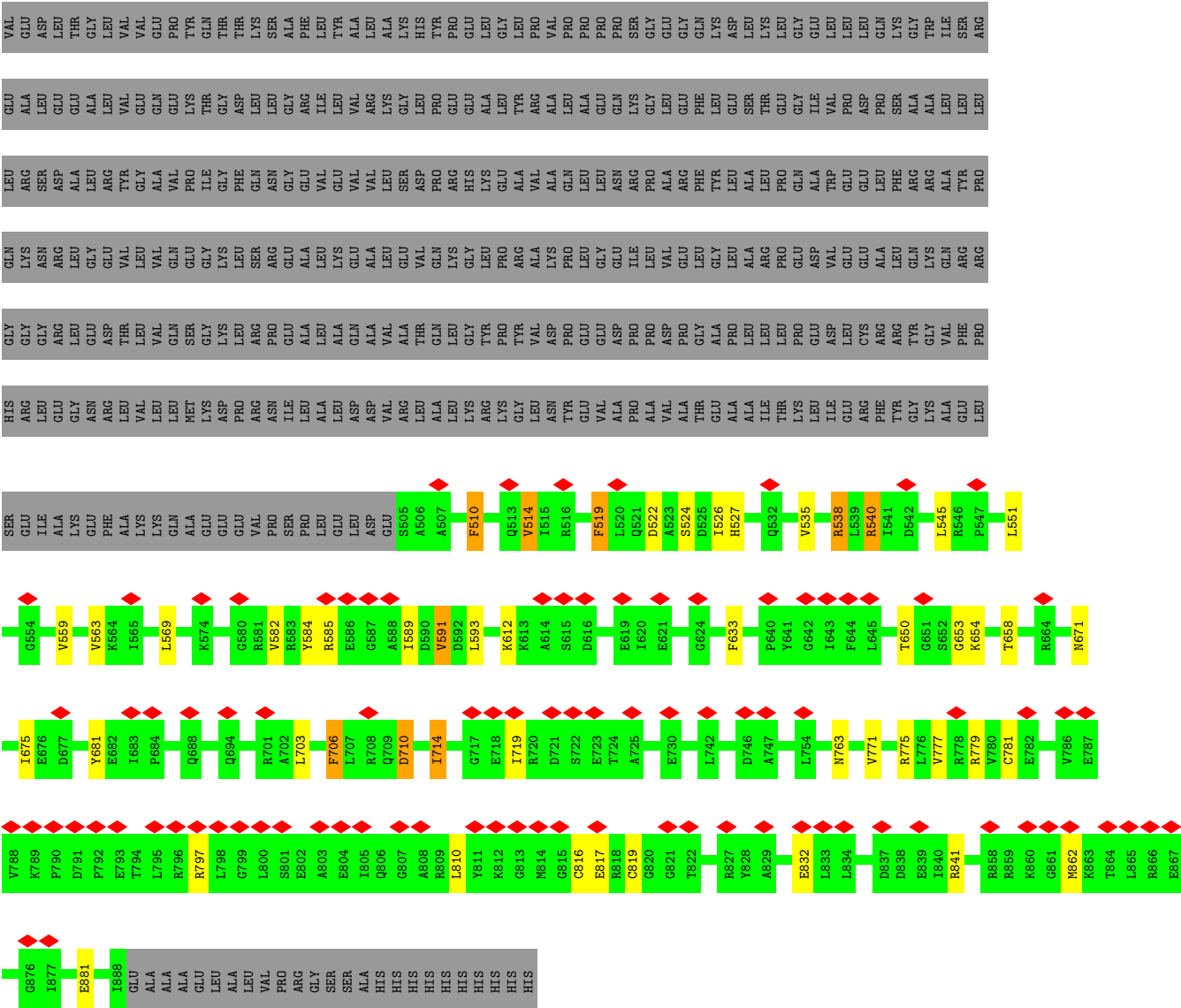
- Molecule 1: Type IV pilus assembly protein PilF

[illegible]

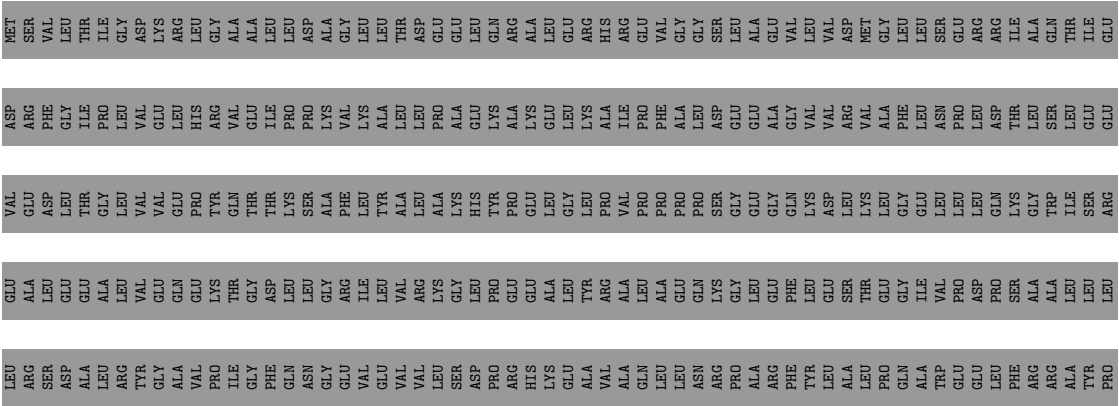
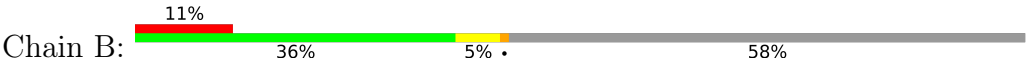


Chain R:  6% 13% 84%

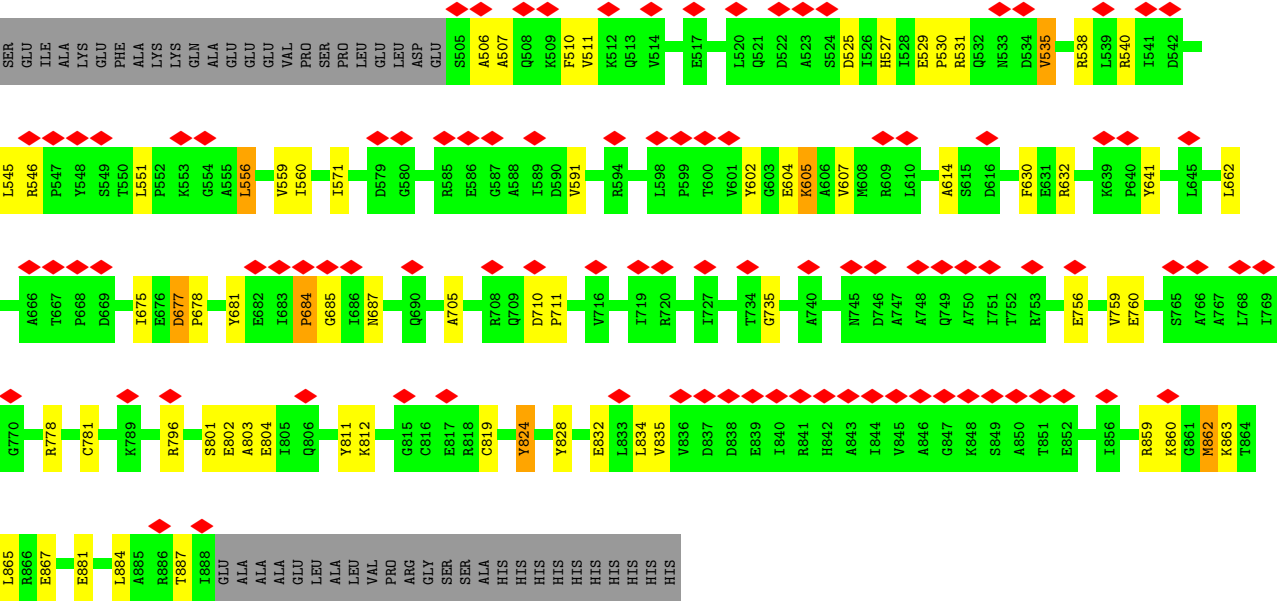




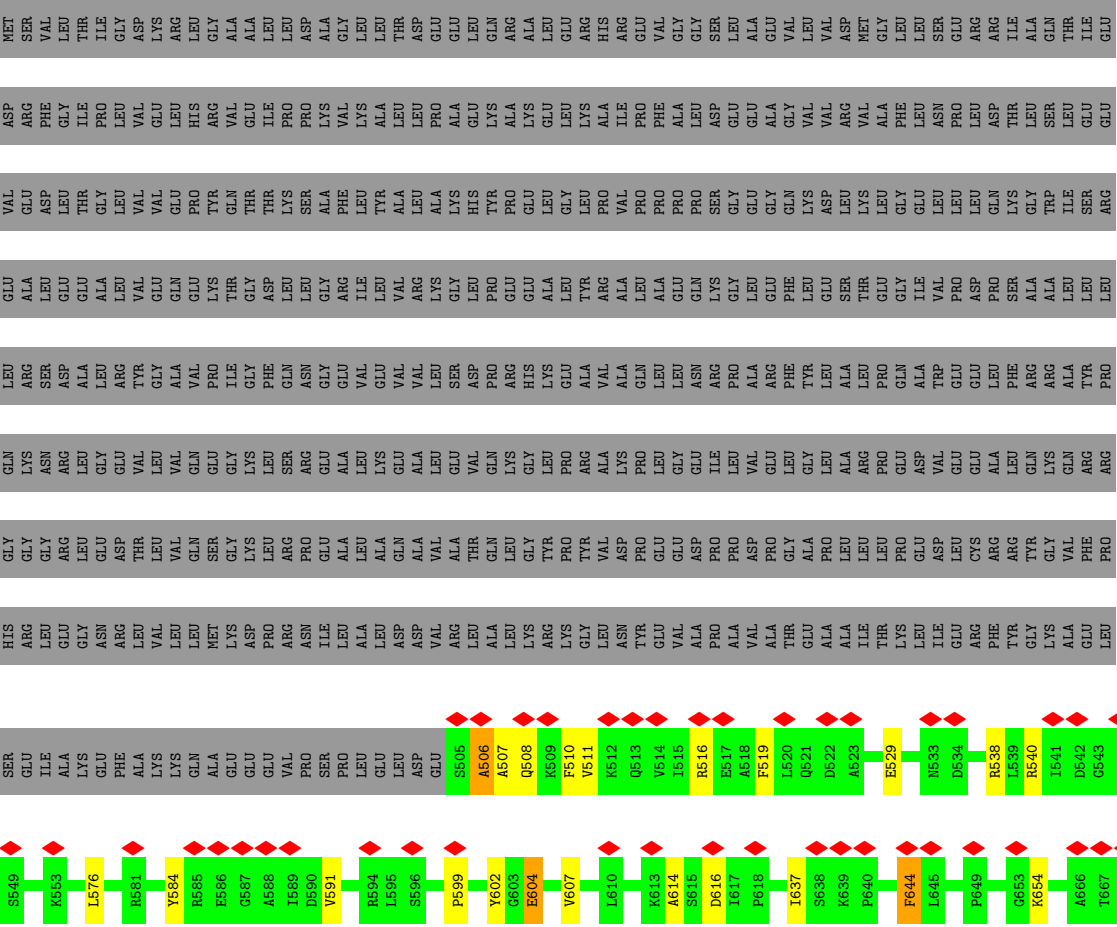
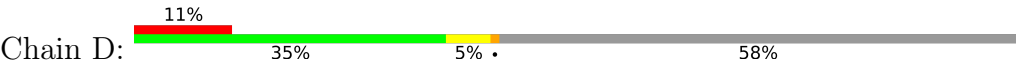
● Molecule 1: Type IV pilus assembly protein PilF

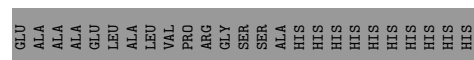
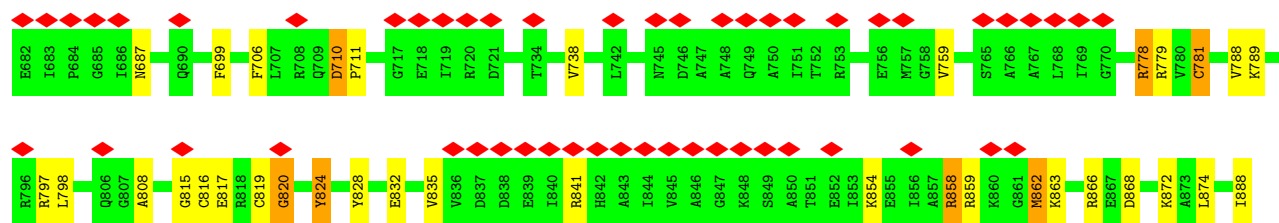




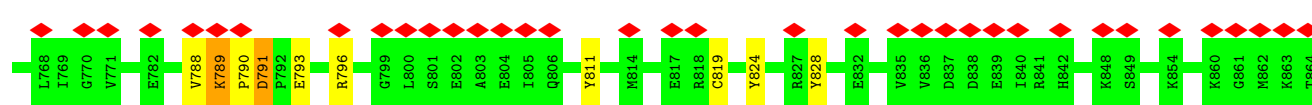
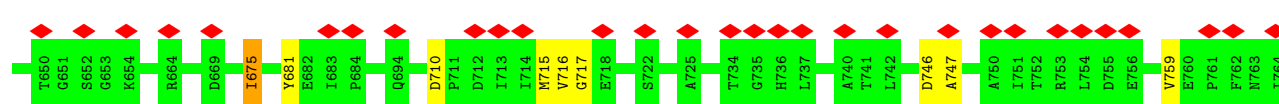
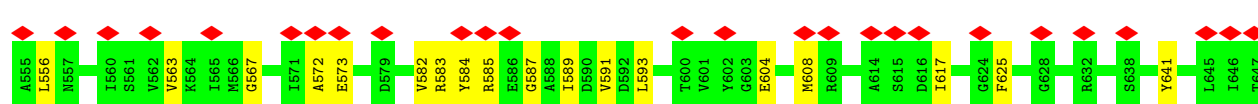
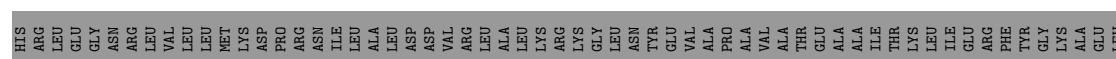
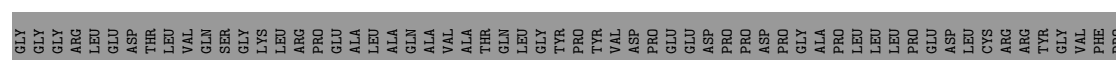
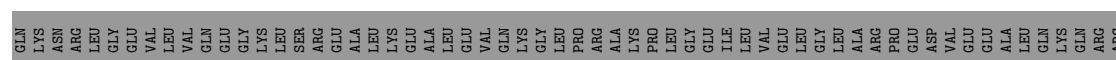
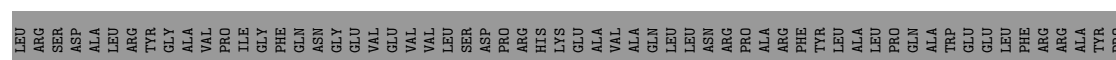
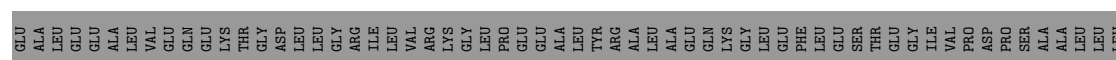
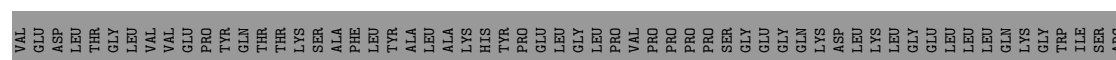
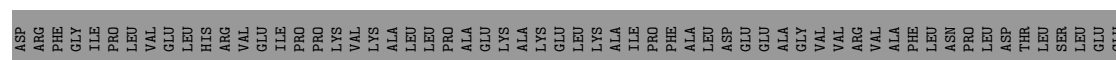
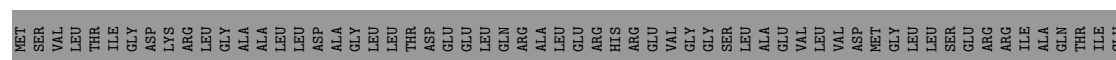
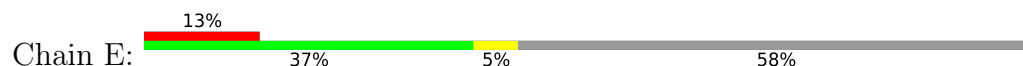


● Molecule 1: Type IV pilus assembly protein PilF





# • Molecule 1: Type IV pilus assembly protein PilF





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	450000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	5.398	Depositor
Minimum map value	-4.813	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.290	Depositor
Recommended contour level	1.45	Depositor
Map size ( $\text{\AA}$ )	341.76, 341.76, 341.76	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.7800001, 1.7800001, 1.7800001	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	1.29	21/3017 (0.7%)	1.10	12/4073 (0.3%)
1	B	1.25	17/3008 (0.6%)	1.03	6/4061 (0.1%)
1	C	1.27	19/3017 (0.6%)	1.11	10/4073 (0.2%)
1	D	1.28	18/3017 (0.6%)	1.13	14/4073 (0.3%)
1	E	1.22	13/3017 (0.4%)	1.07	13/4073 (0.3%)
1	F	1.23	20/3017 (0.7%)	1.07	9/4073 (0.2%)
1	G	1.21	4/1164 (0.3%)	1.03	4/1580 (0.3%)
1	H	1.16	6/1164 (0.5%)	1.12	7/1580 (0.4%)
1	I	1.09	2/1164 (0.2%)	1.09	6/1580 (0.4%)
1	J	1.21	7/1109 (0.6%)	1.08	6/1499 (0.4%)
1	K	1.23	6/1109 (0.5%)	1.06	5/1499 (0.3%)
1	L	1.27	7/1109 (0.6%)	1.07	4/1499 (0.3%)
1	M	1.17	5/1164 (0.4%)	1.00	2/1580 (0.1%)
1	N	1.29	11/1109 (1.0%)	1.17	9/1499 (0.6%)
1	O	1.24	7/1109 (0.6%)	1.08	6/1499 (0.4%)
1	P	1.22	5/1109 (0.5%)	1.11	4/1499 (0.3%)
1	Q	1.28	11/1164 (0.9%)	1.07	1/1580 (0.1%)
1	R	1.19	6/1164 (0.5%)	1.05	4/1580 (0.3%)
All	All	1.24	185/31731 (0.6%)	1.08	122/42900 (0.3%)

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	C	0	4
1	D	0	8
1	E	0	2
1	F	0	4
All	All	0	18

The worst 5 of 185 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	784	CYS	CB-SG	-11.09	1.63	1.82
1	D	529	GLU	CG-CD	-10.54	1.36	1.51
1	N	212	TYR	CB-CG	-9.85	1.36	1.51
1	C	529	GLU	CG-CD	-9.80	1.37	1.51
1	B	527	HIS	CB-CG	-9.76	1.32	1.50

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	248	TYR	CB-CG-CD2	-11.44	114.13	121.00
1	H	414	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	A	585	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	O	284	TYR	CB-CG-CD2	-9.33	115.40	121.00
1	M	445	ARG	NE-CZ-NH2	-9.01	115.80	120.30

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	506	ALA	Mainchain,Peptide
1	C	684	PRO	Mainchain,Peptide
1	D	506	ALA	Mainchain,Peptide
1	D	815	GLY	Mainchain,Peptide
1	D	819	CYS	Mainchain

## 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	2975	0	3080	26	0
1	B	2966	0	3066	28	0
1	C	2975	0	3080	37	0
1	D	2975	0	3080	32	0
1	E	2975	0	3080	19	0
1	F	2975	0	3078	27	0
1	G	1143	0	1182	16	0
1	H	1143	0	1182	13	0
1	I	1143	0	1182	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1090	0	1117	13	0
1	K	1090	0	1117	21	0
1	L	1090	0	1117	16	0
1	M	1143	0	1182	12	0
1	N	1090	0	1117	16	0
1	O	1090	0	1117	21	0
1	P	1090	0	1117	13	0
1	Q	1143	0	1182	15	0
1	R	1143	0	1182	11	0
All	All	31239	0	32258	339	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 5.

The worst 5 of 339 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:Q:336:LEU:HD13	1:Q:336:LEU:O	1.43	1.17
1:F:683:ILE:HG22	1:F:683:ILE:O	1.50	1.06
1:Q:336:LEU:HD13	1:Q:336:LEU:C	1.78	1.02
1:B:679:VAL:HG12	1:B:679:VAL:O	1.58	1.01
1:K:263:VAL:HG23	1:K:263:VAL:O	1.63	0.96

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	382/913 (42%)	374 (98%)	7 (2%)	1 (0%)	37 73
1	B	381/913 (42%)	369 (97%)	10 (3%)	2 (0%)	25 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	382/913 (42%)	368 (96%)	8 (2%)	6 (2%)	8	38
1	D	382/913 (42%)	366 (96%)	13 (3%)	3 (1%)	16	55
1	E	382/913 (42%)	367 (96%)	13 (3%)	2 (0%)	25	64
1	F	382/913 (42%)	367 (96%)	13 (3%)	2 (0%)	25	64
1	G	144/913 (16%)	133 (92%)	6 (4%)	5 (4%)	3	20
1	H	144/913 (16%)	132 (92%)	9 (6%)	3 (2%)	5	30
1	I	144/913 (16%)	137 (95%)	6 (4%)	1 (1%)	19	57
1	J	135/913 (15%)	123 (91%)	10 (7%)	2 (2%)	8	40
1	K	135/913 (15%)	126 (93%)	7 (5%)	2 (2%)	8	40
1	L	135/913 (15%)	123 (91%)	9 (7%)	3 (2%)	5	29
1	M	144/913 (16%)	133 (92%)	8 (6%)	3 (2%)	5	30
1	N	135/913 (15%)	128 (95%)	6 (4%)	1 (1%)	19	57
1	O	135/913 (15%)	124 (92%)	10 (7%)	1 (1%)	19	57
1	P	135/913 (15%)	130 (96%)	3 (2%)	2 (2%)	8	40
1	Q	144/913 (16%)	135 (94%)	8 (6%)	1 (1%)	19	57
1	R	144/913 (16%)	135 (94%)	7 (5%)	2 (1%)	9	41
All	All	3965/16434 (24%)	3770 (95%)	153 (4%)	42 (1%)	15	47

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	435	PRO
1	J	259	GLU
1	H	399	PRO
1	H	456	GLU
1	I	456	GLU

### 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	317/751 (42%)	316 (100%)	1 (0%)	91	92
1	B	315/751 (42%)	313 (99%)	2 (1%)	84	88
1	C	317/751 (42%)	317 (100%)	0	100	100
1	D	317/751 (42%)	315 (99%)	2 (1%)	84	88
1	E	317/751 (42%)	317 (100%)	0	100	100
1	F	317/751 (42%)	316 (100%)	1 (0%)	91	92
1	G	120/751 (16%)	119 (99%)	1 (1%)	79	85
1	H	120/751 (16%)	120 (100%)	0	100	100
1	I	120/751 (16%)	120 (100%)	0	100	100
1	J	112/751 (15%)	112 (100%)	0	100	100
1	K	112/751 (15%)	111 (99%)	1 (1%)	75	83
1	L	112/751 (15%)	110 (98%)	2 (2%)	54	71
1	M	120/751 (16%)	120 (100%)	0	100	100
1	N	112/751 (15%)	111 (99%)	1 (1%)	75	83
1	O	112/751 (15%)	110 (98%)	2 (2%)	54	71
1	P	112/751 (15%)	111 (99%)	1 (1%)	75	83
1	Q	120/751 (16%)	120 (100%)	0	100	100
1	R	120/751 (16%)	120 (100%)	0	100	100
All	All	3292/13518 (24%)	3278 (100%)	14 (0%)	88	91

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	291	TRP
1	A	519	PHE
1	F	656	PHE
1	D	644	PHE
1	D	858	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	218	GLN
1	A	745	ASN
1	B	736	HIS
1	E	743	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

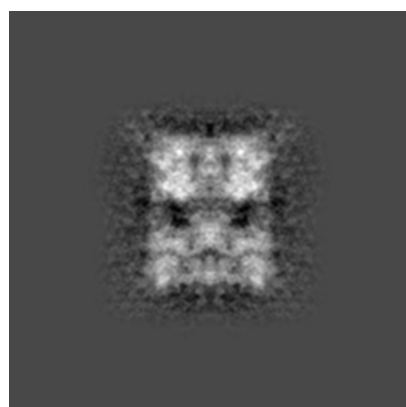
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4194. These allow visual inspection of the internal detail of the map and identification of artifacts.

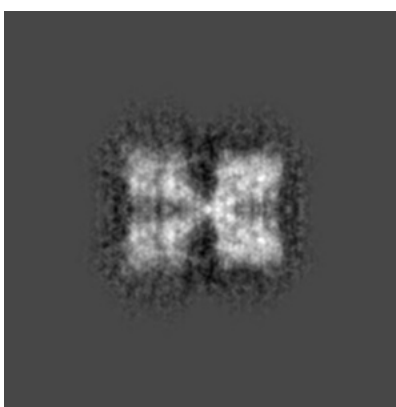
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

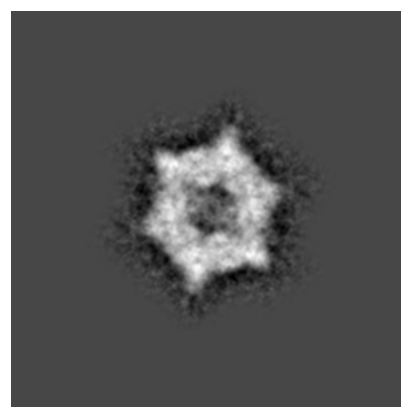
#### 6.1.1 Primary map



X



Y

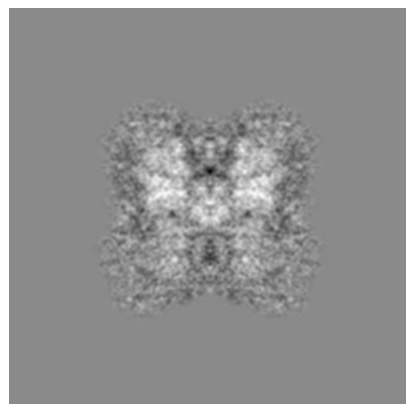


Z

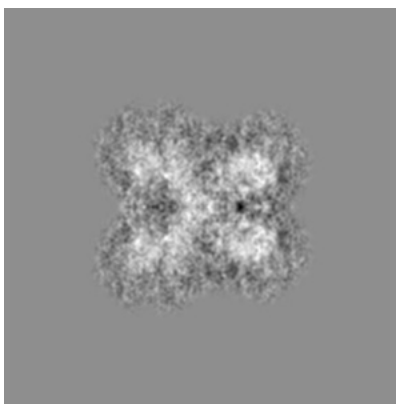
The images above show the map projected in three orthogonal directions.

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

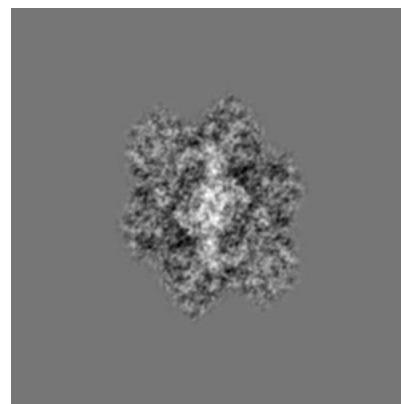
#### 6.2.1 Primary map



X Index: 96



Y Index: 96

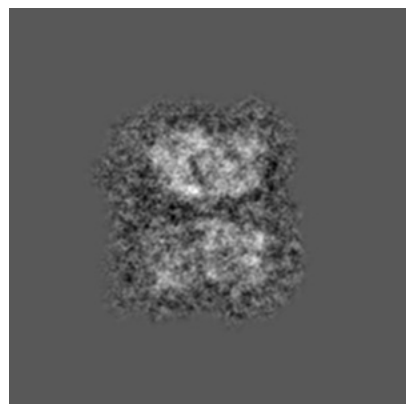


Z Index: 96

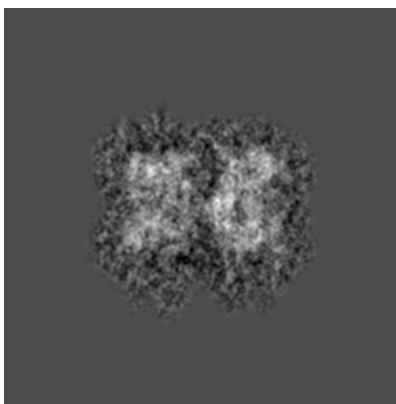
The images above show central slices of the map in three orthogonal directions.

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

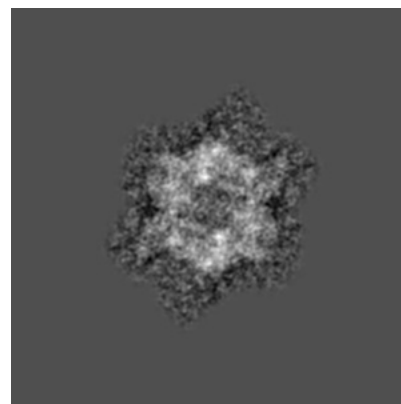
### 6.3.1 Primary map



X Index: 80



Y Index: 75

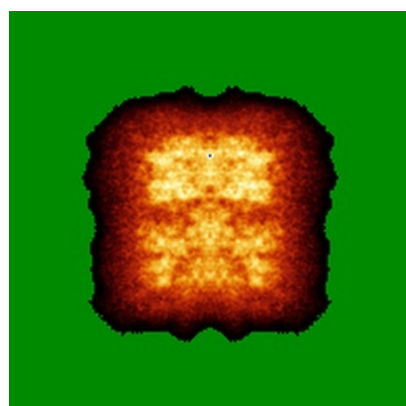


Z Index: 108

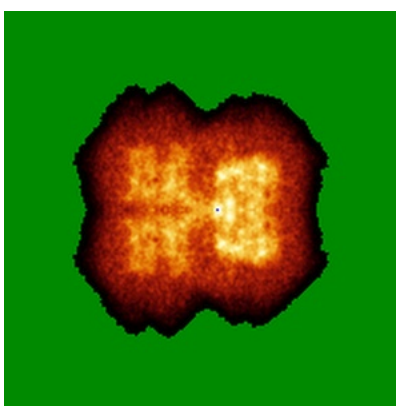
The images above show the largest variance slices of the map in three orthogonal directions.

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

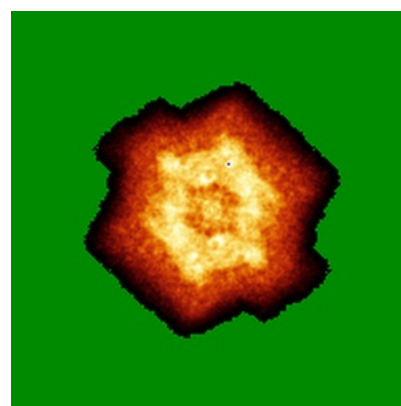
### 6.4.1 Primary map



X



Y

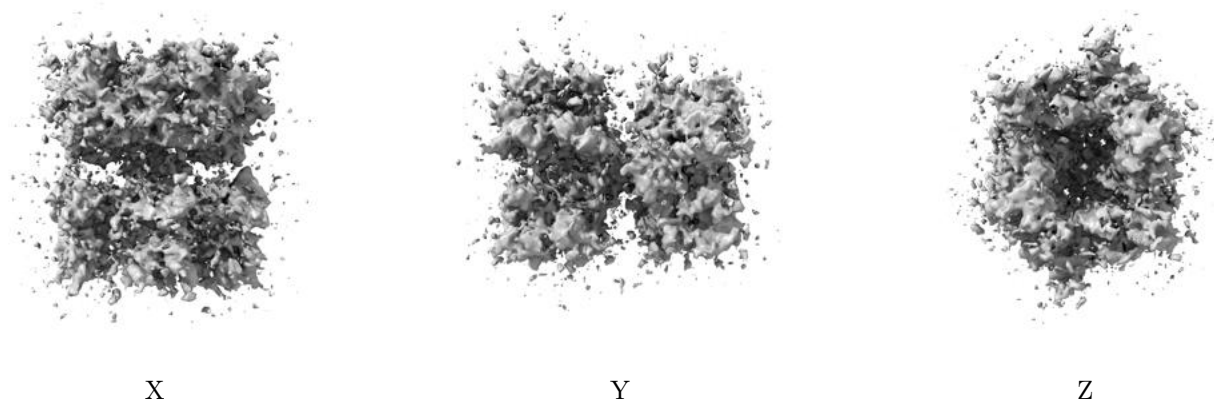


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

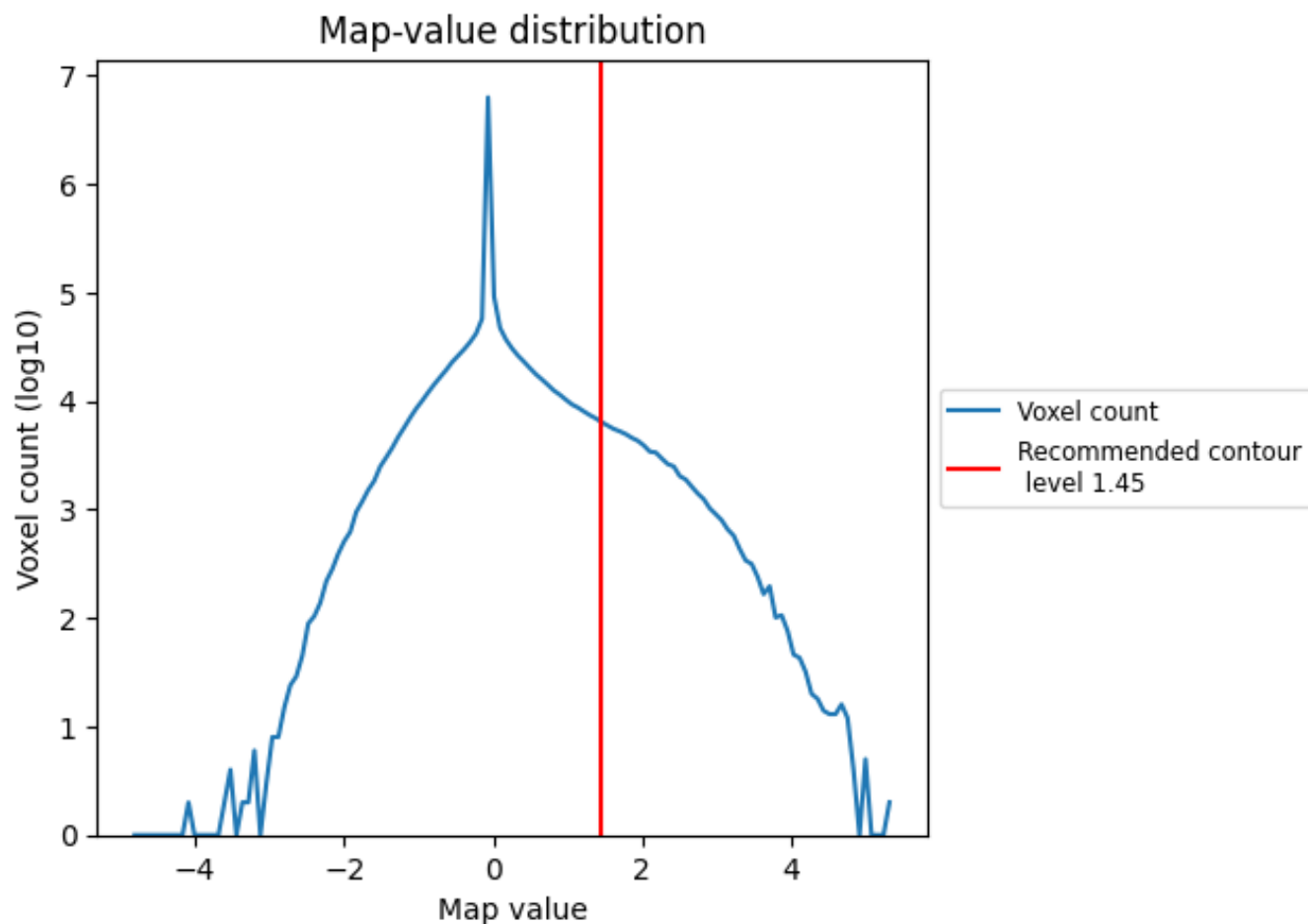
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

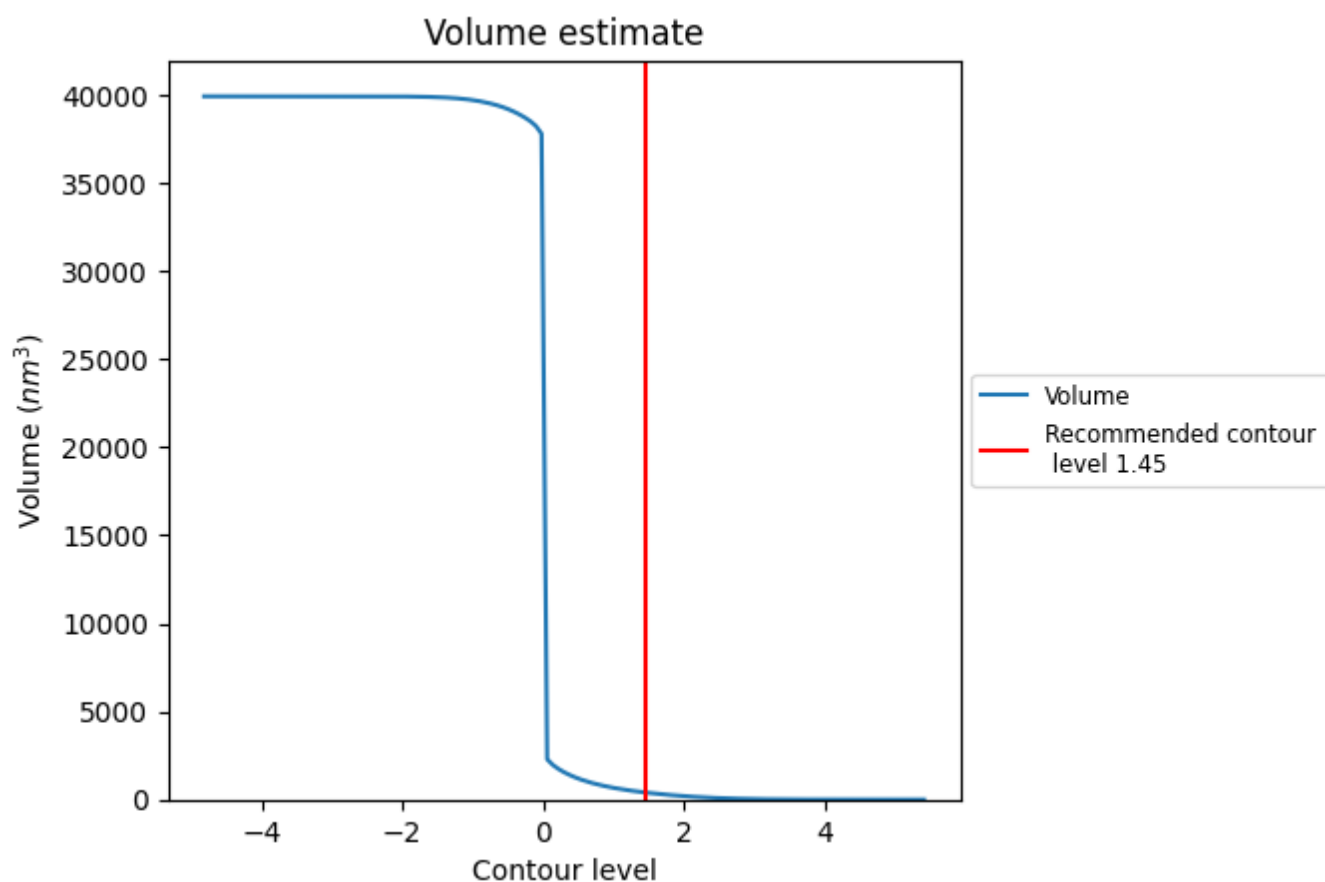
This section contains the results of statistical analysis of the map.

### 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.

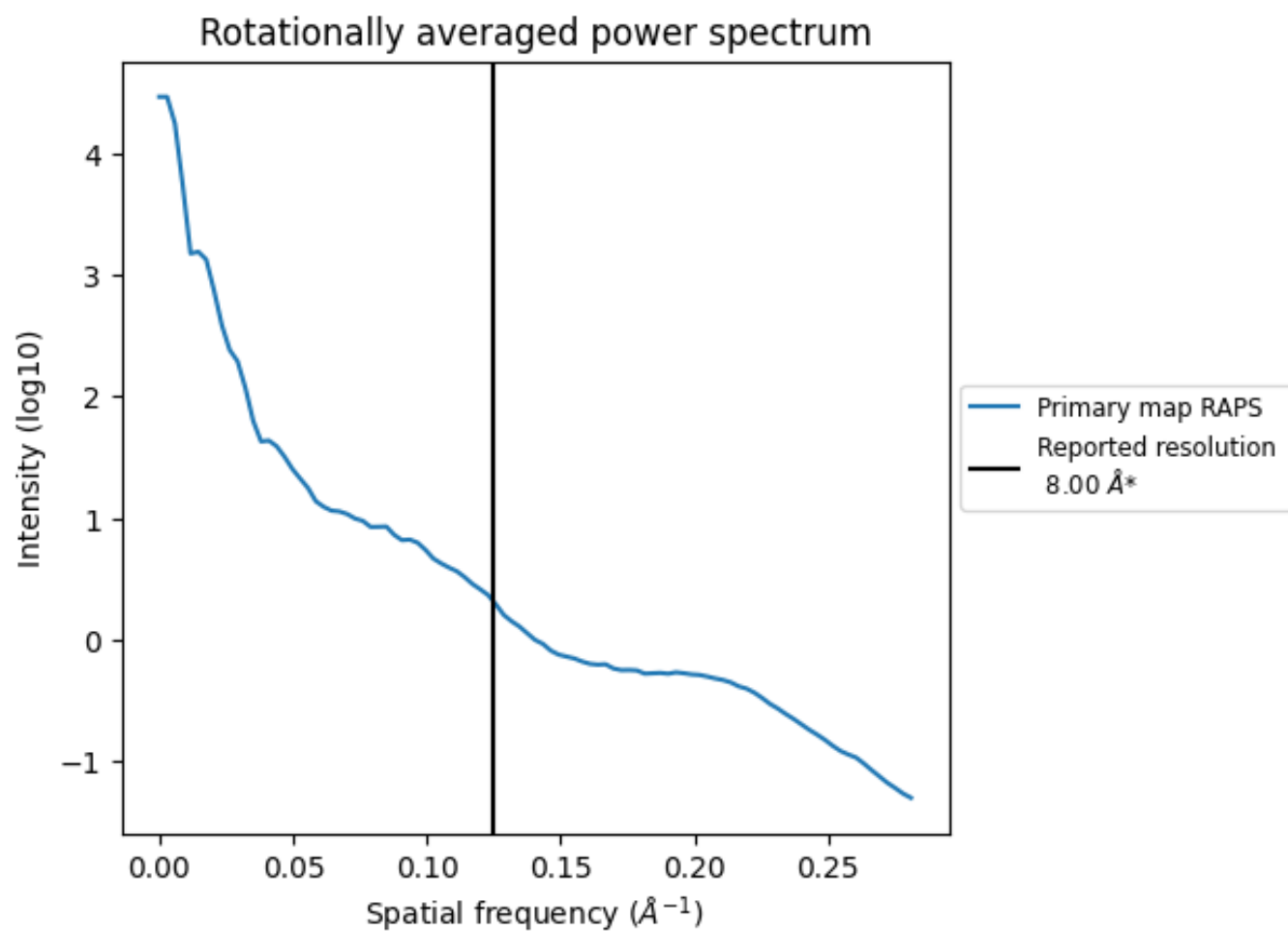
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 398 nm<sup>3</sup>; this corresponds to an approximate mass of 360 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 0.125 Å<sup>-1</sup>

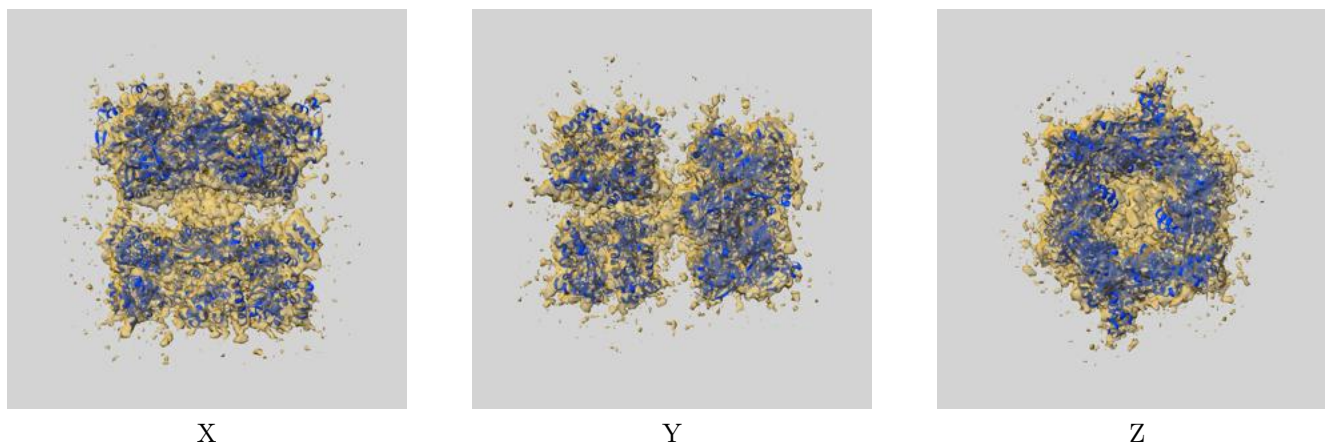
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

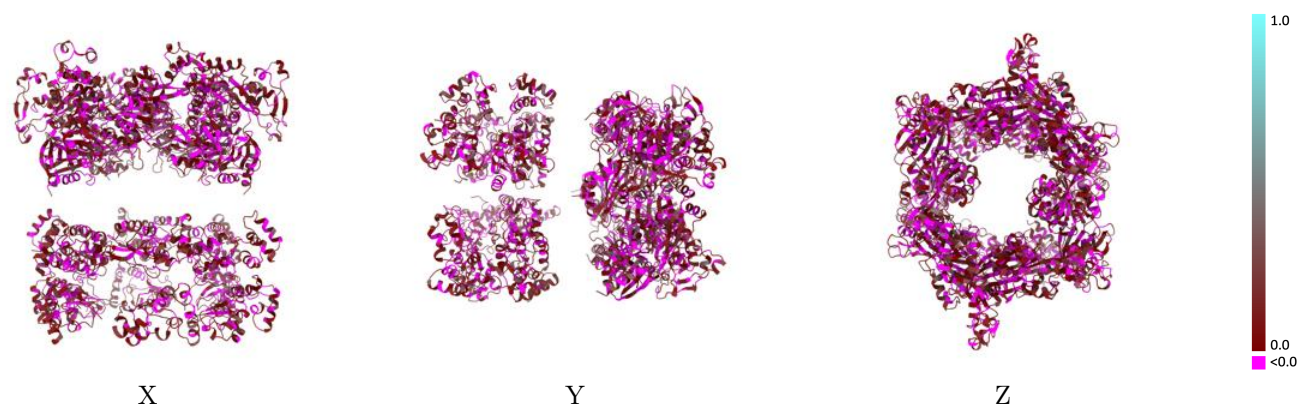
This section contains information regarding the fit between EMDB map EMD-4194 and PDB model 6F8L. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

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



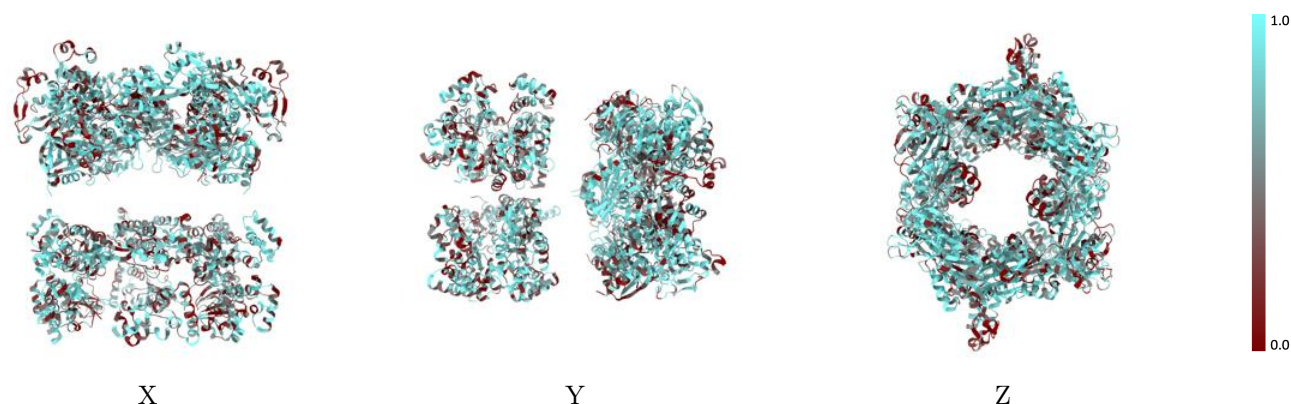
The images above show the 3D surface view of the map at the recommended contour level 1.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



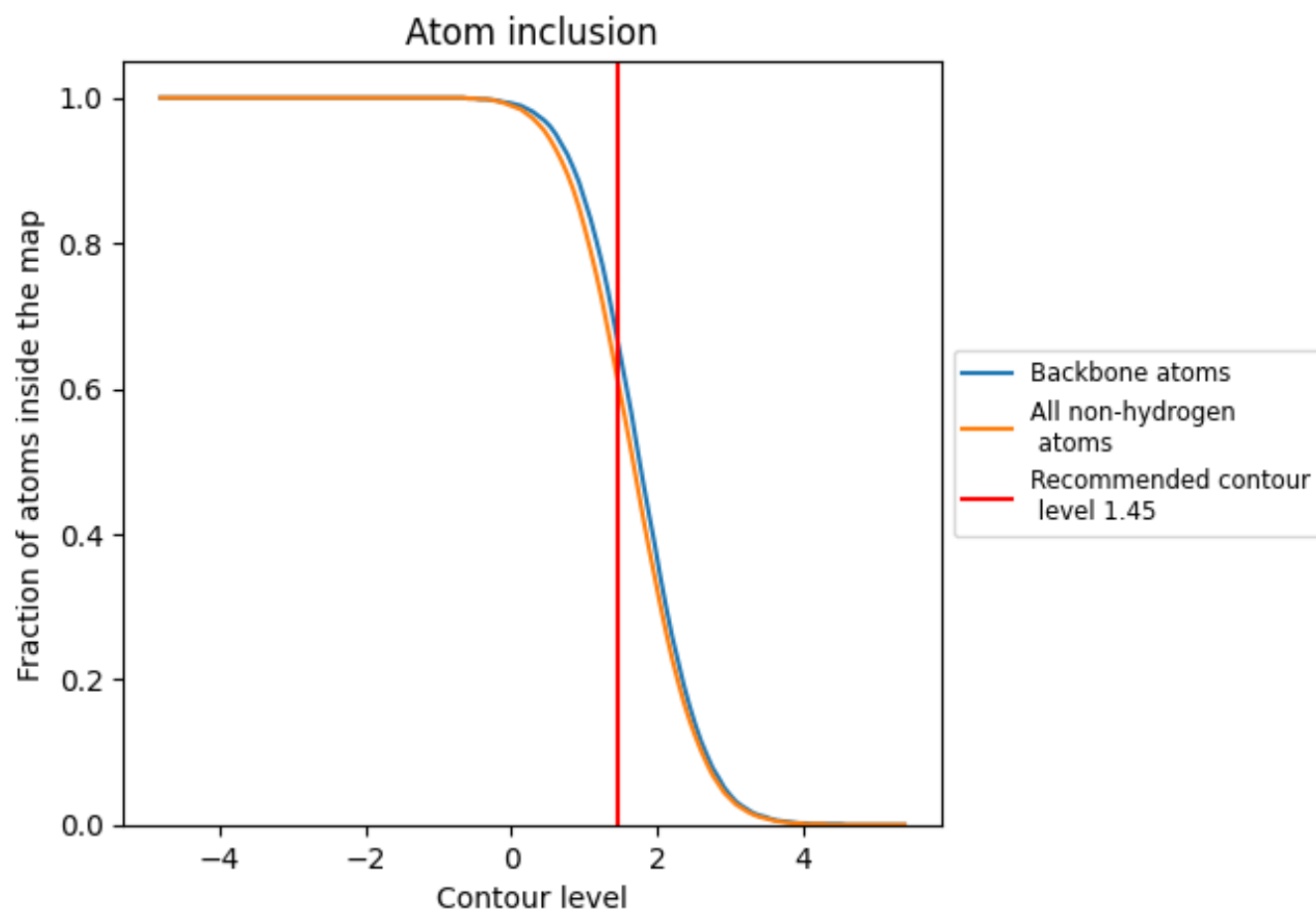
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.45).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 62% 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 (1.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6160	 0.0750
A	 0.6660	 0.0610
B	 0.6840	 0.0670
C	 0.6760	 0.0700
D	 0.6720	 0.0730
E	 0.6140	 0.0730
F	 0.6200	 0.0780
G	 0.5290	 0.0720
H	 0.6480	 0.0860
I	 0.5550	 0.0720
J	 0.5560	 0.1040
K	 0.5330	 0.0710
L	 0.5770	 0.0800
M	 0.5570	 0.0840
N	 0.5270	 0.0900
O	 0.5380	 0.0810
P	 0.5550	 0.0850
Q	 0.6510	 0.0890
R	 0.5430	 0.0570

