



## Full wwPDB EM Validation 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 Full wwPDB EM Validation 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

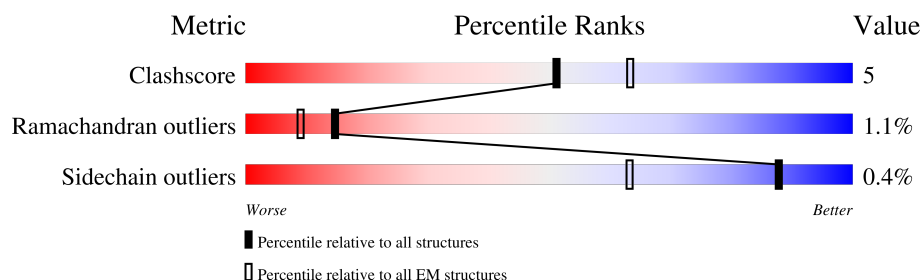
# 1 Overall quality at a glance

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.



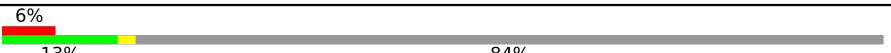







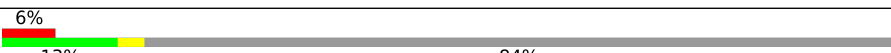

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
1	B	913	
1	C	913	
1	D	913	
1	E	913	
1	F	913	
1	G	913	
1	H	913	

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Mol	Chain	Length	Quality of chain
1	I	913	 6% 13% 84%
1	J	913	 5% 13% 85%
1	K	913	 6% 12% 85%
1	L	913	 5% 13% 85%
1	M	913	 5% 14% 84%
1	N	913	 6% 13% 85%
1	O	913	 6% 12% 85%
1	P	913	 6% 13% 85%
1	Q	913	 15% 84%
1	R	913	 6% 13% 84%

## 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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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





ALA  
ALA  
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- Molecule 1: Type IV pilus assembly protein PilF



ASP	ARG	PHE	GLY	ILE	PRO	LEU	VAL	GLU	LEU	HIS	ARG	VAL	GLU	ILE	PRO	PRO	LYS	VAL	LYS	ALA	ALA	LEU	LEU	PRO	ALA	LYS	LYS	GLU	GLY	LEU	LYS	ALA	ILE	PRO	PHE	ALA	ALA	ASP	GLY	GLU	GLY	ALA	ALA	GLY	VAL	VAL	VAL	ARG	VAL	ALA	ALA	PHE	ASN	LEU	PRO	LEU	ASP	THR	LEU	LEU	SER	LEU	LEU	GLY	THR
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[illegible]

L183	E184	E185	L196	R199	V202	R203	G204	G205	L206	P207	E208	E209	A210	L211	Y212	R213	A214	L215	A216	G220	L221	E225	G229	P232	D233	P234	S235	A236	A237	L240	L241	R242	S243	D244	A245	L246	R247	Y248	G249	A250	V251	P252	I253	G254	F255	Q256	N257	G258	E259	V260	F261
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Category	Value	Color
L264	1	Green
S265	1	Green
D266	1	Red
K270	1	Yellow
V273	1	Orange
L276	1	Yellow
L277	1	Green
N278	1	Red
R282	1	Red
L287	1	Yellow
P288	1	Yellow
R296	1	Yellow
K297	1	Green
Y299	1	Green
PRO	1	Grey
GLN	1	Grey
LYS	1	Grey
ASN	1	Grey
ARG	1	Grey
LEU	1	Grey
GLY	1	Grey
GLU	1	Grey
VAL	1	Grey
LEU	1	Grey
VAL	1	Grey
GLN	1	Grey
GLU	1	Grey
GLY	1	Grey
LYS	1	Grey
LYS	1	Grey
SER	1	Grey
ARG	1	Grey
GLU	1	Grey
ALA	1	Grey
LEU	1	Grey
LYS	1	Grey
GLU	1	Grey
LEU	1	Grey
ALA	1	Grey
GLU	1	Grey
VAL	1	Grey
GLN	1	Grey
LYS	1	Grey
GLY	1	Grey
LEU	1	Grey
PRO	1	Grey
ARG	1	Grey
ALA	1	Grey
LYS	1	Grey
PRO	1	Grey
LEU	1	Grey
GLY	1	Grey
TYR	1	Grey

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

ASP  
GLY  
VAL  
ARG  
THR  
ARG  
GLY  
GLY  
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ASP  
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LEU  
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THR  
PRO  
VAL  
VAL  
GLY  
LEU  
LYS  
ALA  
ALA  
MET  
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LEU  
LEU  
LYS  
LYS  
ALA  
SER  
ASP  
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PRO  
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LEU  
VAL  
ILE

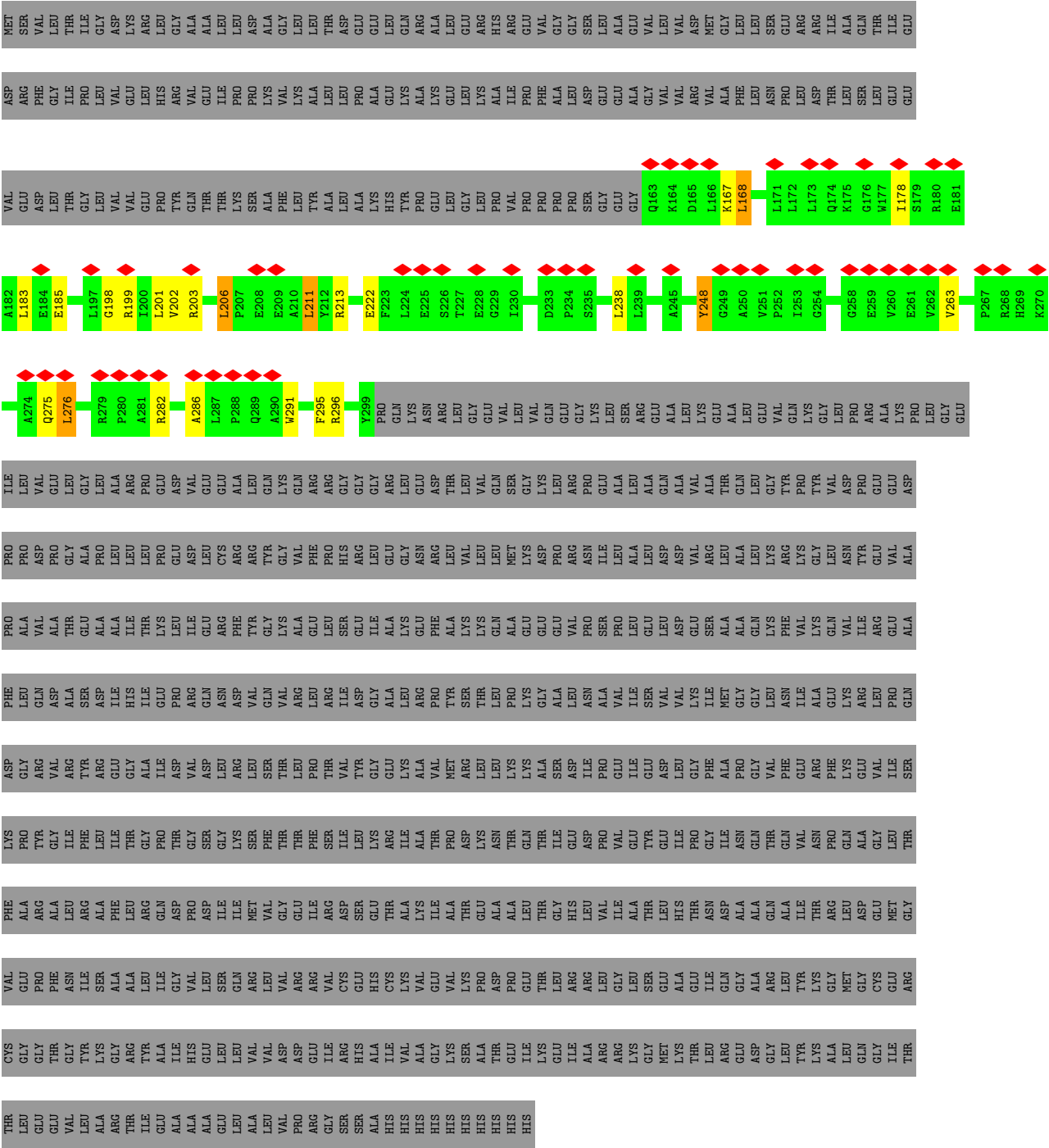
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HE	RG	LA	EU	EU	RG	LA	EU	RG	LN	SP	RD	SP	LE	LE	ET	AL	LY	LU	LE	RG	SP	ER	LU	HR	LA	YS	LE	LE	HR	LU	LA	LA	EU	HR	LY	IS	IS	AL	IE	LA	HR	IS	IS	SN	SP	LA	LN	LN	IE	HR	RG	SP	ET
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[illegible][illegible]

THR  
LEU  
GLU  
GLU  
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GLY  
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ARG  
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ALA  
ALA  
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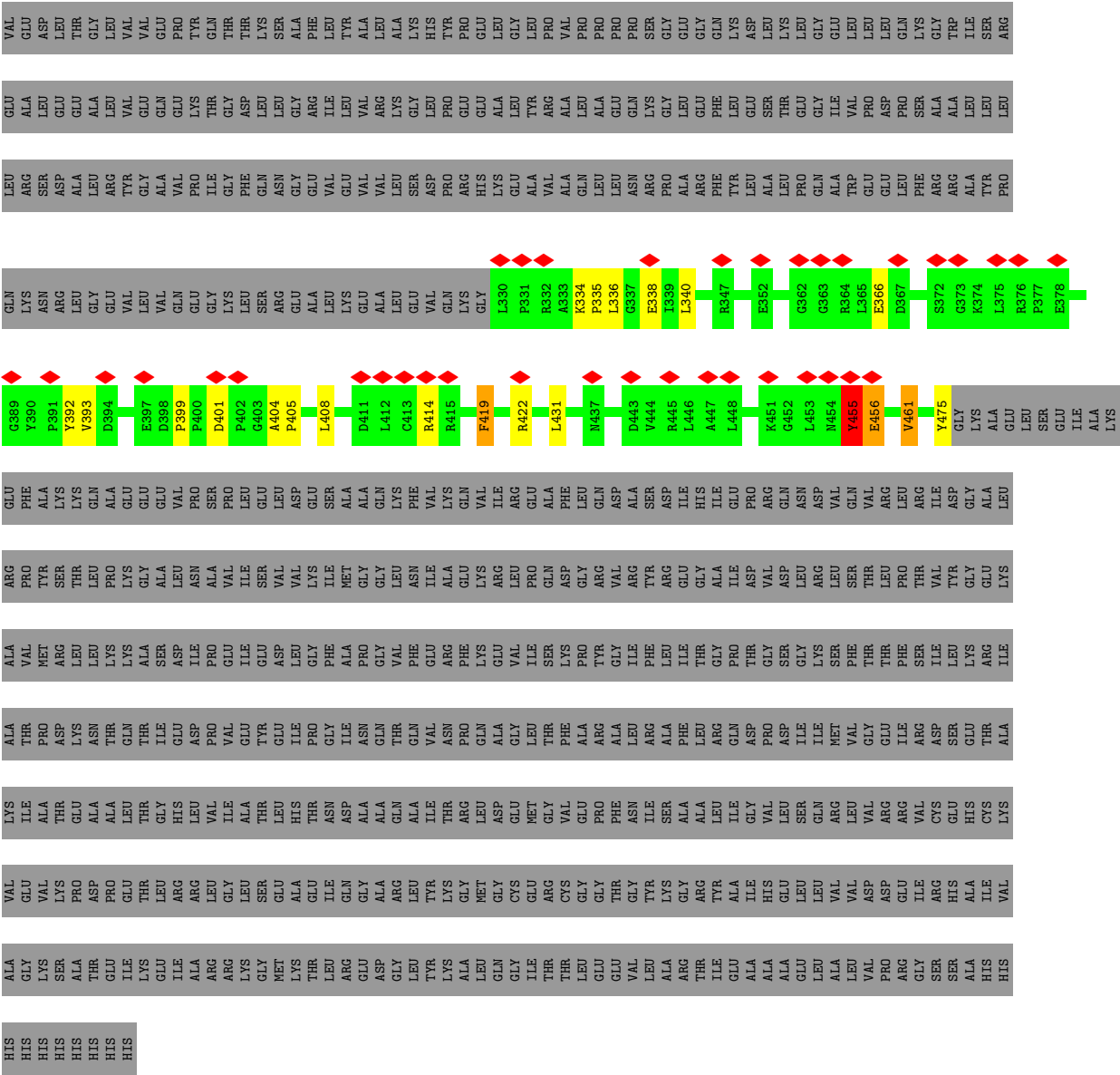
● Molecule 1: Type IV pilus assembly protein PilF



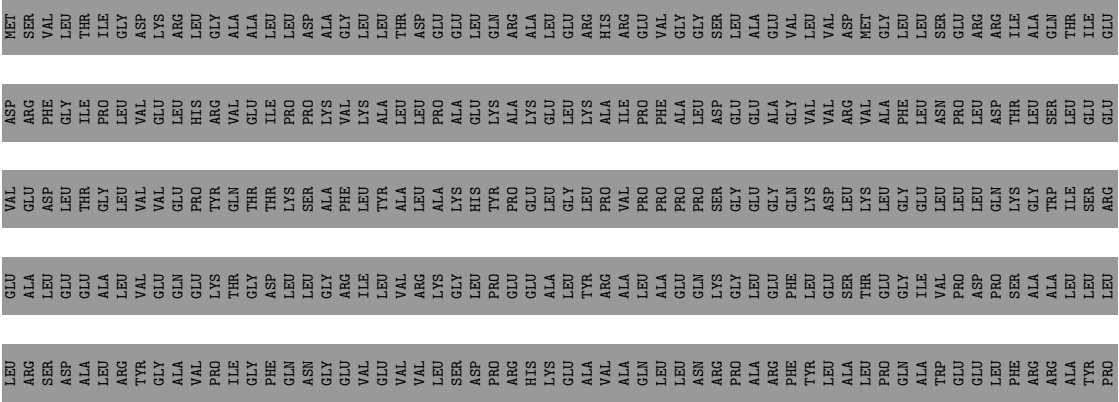
● Molecule 1: Type IV pilus assembly protein PilF

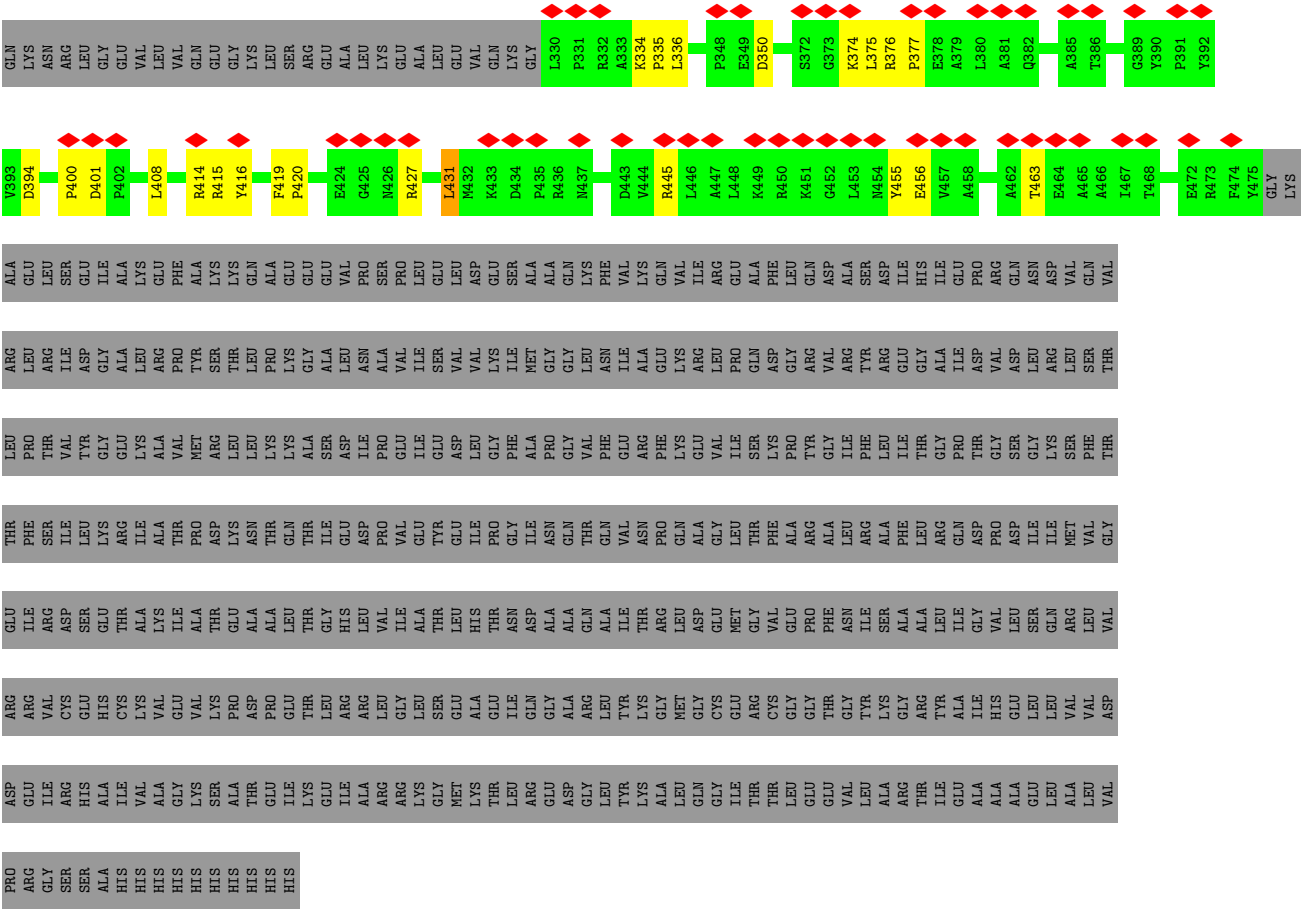




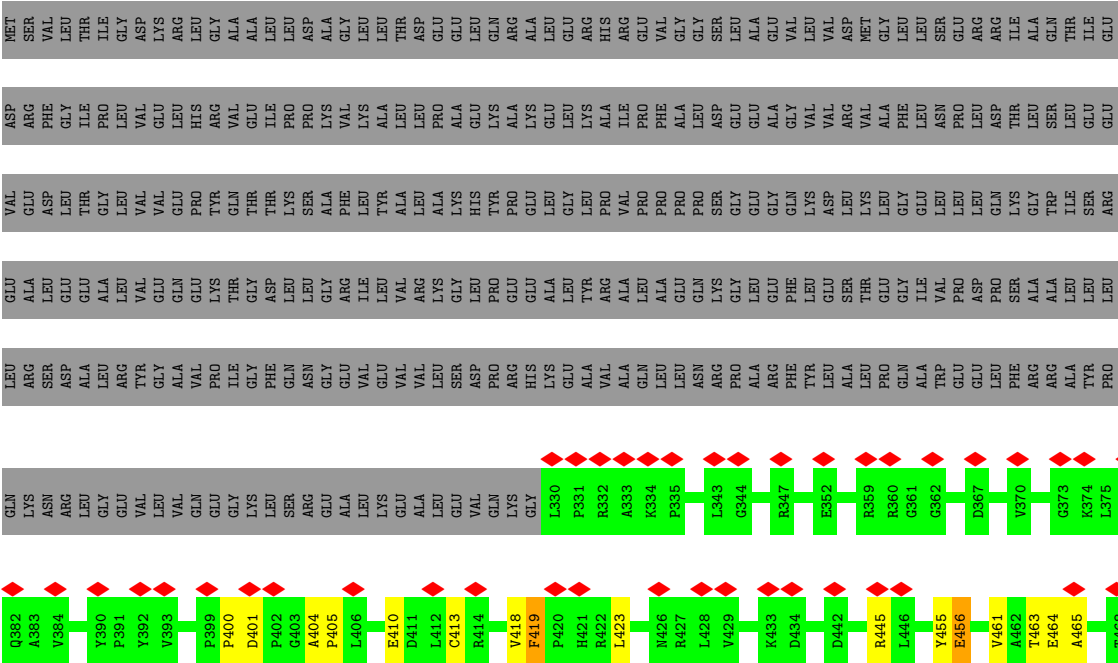


● Molecule 1: Type IV pilus assembly protein PilF





● Molecule 1: Type IV pilus assembly protein PilF







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- Molecule 1: Type IV pilus assembly protein PilF

[illegible]



ARG	THR	ILE	GLU	ALA	ALA	GLU	LEU	ALA	LEU	VAL	ASP	ASP	GLU	ILE	ARG	HIS	ILE	VAL	ALA	GLY	LYS	SER	THR	GLU	ILE	LYS	GLU	ILE	ALA	ARG	ARG	LYS	GLY	MET	THR	THR	LEU	ARG	GLU	ASP	GLY	LEU	THR	TYR	THR	LYS	ALA	LEU	GLN	GLY	THR	THR	ILE	HIS	GLU	VAL	VAL	ALA	LEU	ALA	
THR	ILE	GLU	ALA	ALA	GLU	LEU	ALA	LEU	VAL	ASP	ASP	GLU	ILE	ARG	SER	SER	ALA	HIS	HIS	HIS	HIS	HIS	HIS	THR	GLU	ILE	LYS	GLU	ILE	ALA	ARG	ARG	LYS	GLY	MET	THR	THR	LEU	ARG	GLU	ASP	GLY	LEU	THR	TYR	THR	LYS	ALA	LEU	GLN	GLY	THR	THR	ILE	HIS	GLU	VAL	VAL	ALA	LEU	ALA

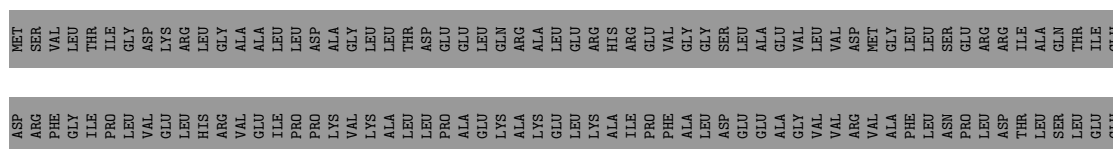
- Molecule 1: Type IV pilus assembly protein PilF

Chain Q:  15% 84%

LEU	ARG	GLU	GLY	ASP	ASN	GLY	PHE	ILE	SER	L412	GLN	LEU	GLU	VAL	ASP	MET
GLU	GLY	ASN	PRO	ALA	ASN	ILE	ALA	MET	ALA	C413	LYS	ARG	ALA	ARG	ARG	SER
ALA	ASP	ALA	GLY	GLN	GLN	GLY	GLN	GLY	GLN	R414	ASN	ASP	GLY	VAL	PHE	GLY
GLY	GLY	GLN	VAL	PHE	ASN	PHE	VAL	ASN	PHE	R415	LEU	ALA	GLY	THR	ILE	THR
LEU	LEU	ALA	GLY	ILE	ILE	VAL	GLY	ILE	VAL	Y416	GLY	LEU	ALA	LEU	PRO	ILE
TYR	LYS	ASN	ARG	ILE	LYS	VAL	GLY	ALA	LYS	F419	GLU	ARG	VAL	ASP	GLY	GLY
LYS	GLY	PRO	GLY	GLY	GLN	GLY	GLY	GLY	GLY	R422	VAL	TYR	VAL	VAL	VAL	ASP
ALA	LEU	PRO	PHE	GLY	LYS	VAL	VAL	GLY	VAL	R422	LEU	GLY	GLN	GLY	GLY	ARG
LEU	LEU	GLY	VAL	GLY	LYS	VAL	VAL	ARG	ILE	R437	GLN	VAL	GLY	PRO	TYR	GLY
GLN	GLY	ASP	GLY	VAL	ILE	ARG	ARG	PRO	ARG	R437	GLY	PRO	LYS	LYS	ARG	GLY
CYS	GLY	GLY	VAL	ILE	GLY	ILE	VAL	ILE	GLY	I438	GLY	ILE	THR	THR	ALA	ALA
GLY	THR	GLY	SER	SER	GLN	ALA	ALA	GLN	ALA	I438	LYS	PHE	ASP	THR	GLY	ALA
THR	ARG	LYS	LYS	LYS	ASP	PHE	PHE	GLN	PHE		LEU	PHE	GLY	ILE	GLY	ALA
LEU	LEU	GLY	PRO	GLY	GLY	LEU	LEU	GLY	LEU	D443	ARG	ASN	LEU	GLY	PRO	ASP
GLY	GLY	VAL	TYR	VAL	VAL	GLN	GLY	VAL	ASP	V444	GLY	GLY	GLY	ALA	LYS	GLY
GLY	THR	THR	ILE	ILE	ARG	ALA	ILE	ILE	ALA	R445	ALA	GLY	ARG	VAL	VAL	GLY
VAL	VAL	THR	ILE	ILE	ARG	ALA	ILE	ILE	ALA	I446	ALA	GLY	ILE	VAL	VAL	GLY
LEU	LEU	ILE	GLY	GLY	ASP	ASP	ASP	GLY	ASP	A447	LYS	VAL	GLY	ALA	LYS	LEU
ALA	ALA	LYS	ILE	ILE	ILE	ILE	ILE	GLY	ILE	I448	GLY	VAL	VAL	ALA	ALA	LEU
ARG	THR	ARG	GLY	GLY	GLY	GLY	GLY	GLY	HIS		ALA	VAL	ARG	LEU	THR	THR
THR	ARG	GLY	THR	GLY	GLY	GLY	GLY	GLY	ILE		LEU	VAL	ARG	LEU	ASP	ASP
ILE	ILE	TYR	GLY	GLY	ILE	GLY	GLY	GLY	ILE	R451	LEU	LEU	LYS	LEU	GLY	GLY
GLY	GLY	ALA	ALA	ILE	GLY	GLY	PRO	ILE	GLY	C452	GLY	LEU	GLY	ALA	ALA	GLY
ALA	ALA	ILE	THR	GLY	ASP	ASP	GLY	ILE	PRO	I453	VAL	SER	GLY	THR	GLY	GLY
ALA	ALA	HIS	THR	GLY	VAL	ARG	GLY	ASP	ARG	V457	GLN	THR	GLY	ARG	ARG	ARG
VAL	VAL	VAL	GLY	VAL	GLY	VAL	VAL	THR	VAL		LYS	ARG	GLY	ILE	ALA	HIS
ASP	ASP	ASP	GLY	ASP	GLY	ASP	THR	THR	GLY	L470	GLY	ALA	ALA	VAL	ILE	GLY
PRO	PRO	GLY	THR	THR	GLY	GLY	THR	THR	GLY		ALA	GLN	ALA	VAL	ALA	GLY
ARG	ARG	GLY	PHE	PHE	ILE	LYS	PHE	PRO	LEU	V475	GLY	GLN	LEU	PRO	PHE	GLY
GLY	SER	ILE	SER	ILE	ARG	ILE	ILE	THR	ILE	GLY	L336	LEU	ALA	ALA	ALA	VAL
SER	SER	ARG	LEU	VAL	ASP	VAL	VAL	VAL	ASP	LYS	L340	ASN	GLN	GLY	GLY	GLY
ALA	ALA	HIS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L340	ASN	GLN	GLY	LEU	GLY
HIS	HIS	ILE	GLY	GLY	GLY	GLY	GLY	GLY	ALA	LEU	F352	PRO	GLY	GLY	GLY	GLY
HIS	HIS	VAL	ARG	GLY	GLY	GLY	GLY	GLY	ALA	SER		ALA	LEU	GLY	GLY	ALA
HIS	HIS	ALA	ILE	ILE	LYS	ILE	ALA	ALA	ARG	GLY	G362	ARG	GLY	GLY	ALA	GLY
HIS	HIS	GLY	THR	THR	VAL	VAL	THR	VAL	PRO	ILE	G363	PHE	PHE	GLY</		

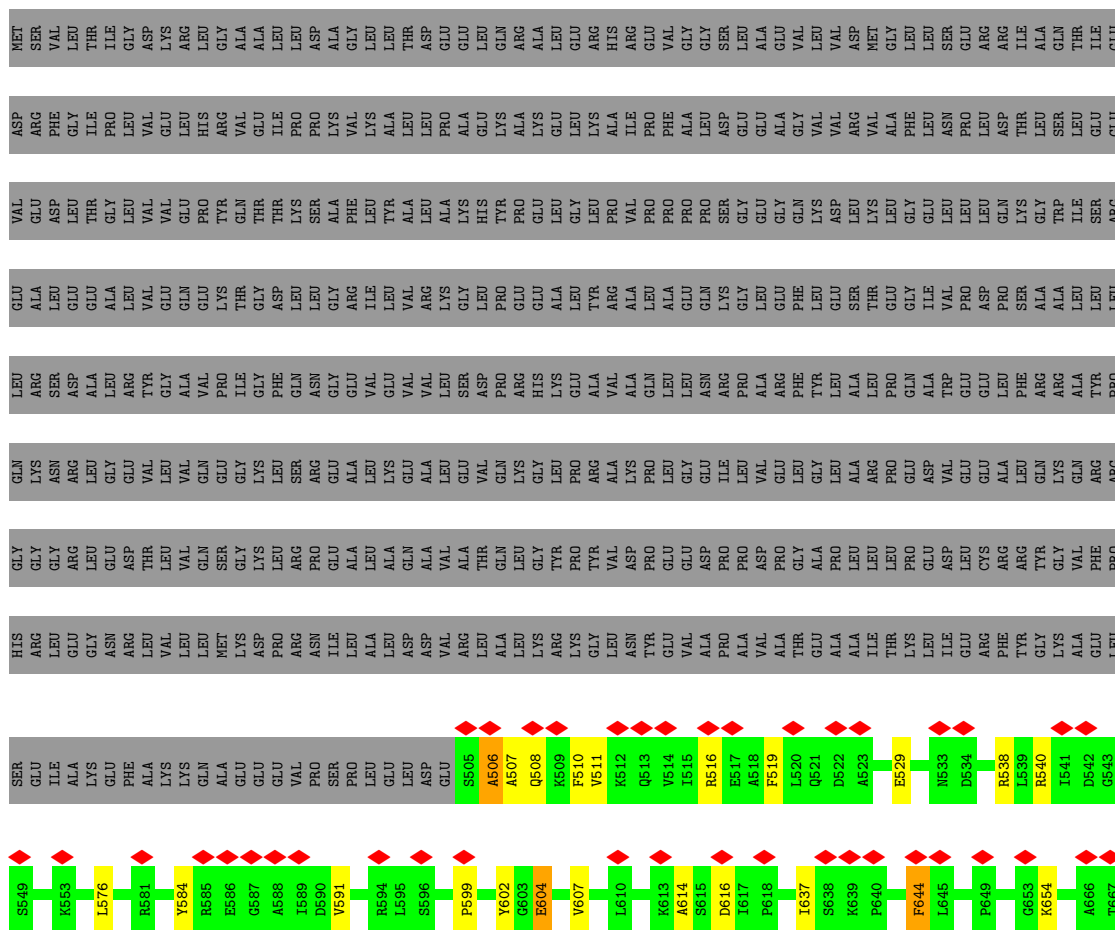
- Molecule 1: Type IV pilus assembly protein PilF

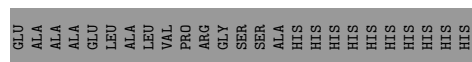
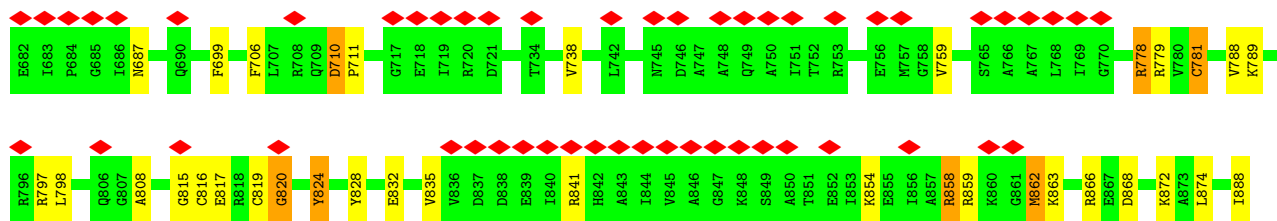
Chain R:  6% 13% 84%



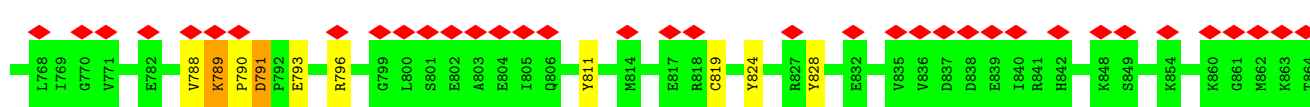
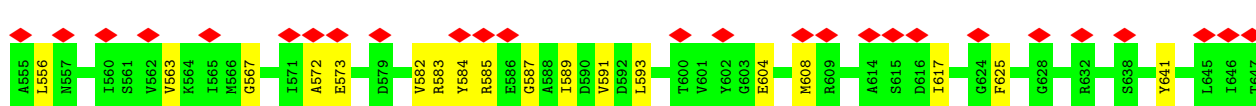
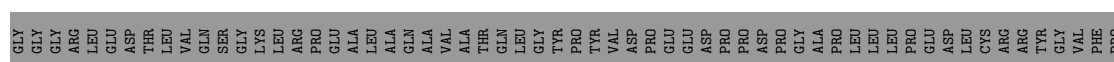
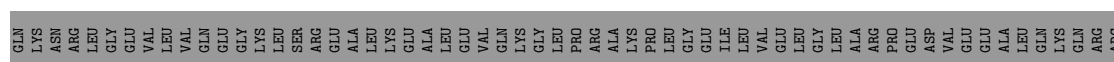
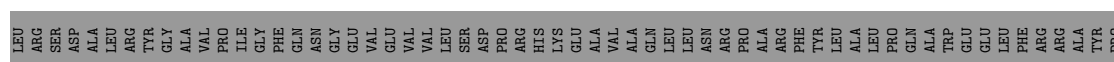
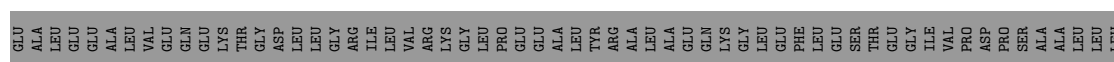
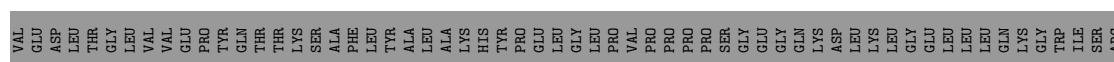
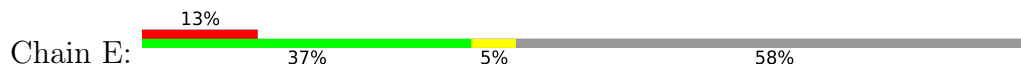


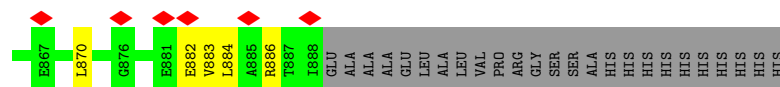






### • Molecule 1: Type IV pilus assembly protein PilF





## 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 (Å)	341.76, 341.76, 341.76	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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

All (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
1	E	591	VAL	CB-CG1	-9.48	1.32	1.52
1	F	582	VAL	CB-CG2	-9.31	1.33	1.52
1	B	510	PHE	CB-CG	-9.10	1.35	1.51
1	A	514	VAL	CB-CG2	-8.68	1.34	1.52
1	C	607	VAL	CB-CG2	-8.62	1.34	1.52
1	B	511	VAL	CB-CG2	-8.27	1.35	1.52
1	A	819	CYS	CB-SG	-8.25	1.68	1.82
1	Q	475	TYR	CB-CG	-7.95	1.39	1.51
1	C	605	LYS	CE-NZ	-7.92	1.29	1.49
1	R	413	CYS	CB-SG	-7.83	1.69	1.82
1	D	602	TYR	CB-CG	-7.81	1.40	1.51
1	F	733	LEU	CB-CG	-7.72	1.30	1.52
1	D	654	LYS	CE-NZ	-7.63	1.29	1.49
1	D	824	TYR	CB-CG	-7.60	1.40	1.51
1	A	591	VAL	CB-CG1	-7.56	1.36	1.52
1	N	178	ILE	CB-CG2	-7.52	1.29	1.52
1	A	510	PHE	CB-CG	-7.50	1.38	1.51
1	N	284	TYR	CB-CG	-7.45	1.40	1.51
1	Q	336	LEU	CB-CG	-7.44	1.30	1.52
1	F	673	GLN	CG-CD	-7.43	1.33	1.51
1	B	777	VAL	CB-CG1	-7.41	1.37	1.52
1	O	284	TYR	CB-CG	-7.38	1.40	1.51
1	E	811	TYR	CG-CD2	-7.25	1.29	1.39
1	I	431	LEU	CB-CG	-7.22	1.31	1.52
1	A	563	VAL	CB-CG2	-7.19	1.37	1.52
1	D	529	GLU	CB-CG	-7.18	1.38	1.52
1	F	675	ILE	CB-CG1	-7.11	1.34	1.54
1	K	211	LEU	CB-CG	-7.07	1.32	1.52
1	E	811	TYR	CG-CD1	-7.01	1.30	1.39
1	C	828	TYR	CB-CG	-6.99	1.41	1.51
1	A	681	TYR	CB-CG	-6.97	1.41	1.51
1	D	710	ASP	CB-CG	6.93	1.66	1.51
1	D	681	TYR	CG-CD1	-6.89	1.30	1.39
1	C	867	GLU	CG-CD	-6.85	1.41	1.51
1	N	212	TYR	CG-CD2	-6.82	1.30	1.39
1	E	675	ILE	CB-CG1	-6.81	1.34	1.54
1	G	419	PHE	CB-CG	-6.80	1.39	1.51
1	L	223	PHE	CB-CG	-6.76	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	475	TYR	CG-CD1	-6.76	1.30	1.39
1	Q	475	TYR	CD1-CE1	-6.71	1.29	1.39
1	J	178	ILE	CB-CG2	-6.71	1.32	1.52
1	E	828	TYR	CE2-CZ	-6.68	1.29	1.38
1	D	607	VAL	CB-CG2	-6.67	1.38	1.52
1	H	340	LEU	CG-CD1	-6.67	1.27	1.51
1	R	431	LEU	CB-CG	-6.67	1.33	1.52
1	C	591	VAL	CB-CG1	-6.66	1.38	1.52
1	Q	413	CYS	CB-SG	-6.65	1.71	1.82
1	Q	366	GLU	CD-OE1	-6.62	1.18	1.25
1	B	675	ILE	CB-CG1	-6.61	1.35	1.54
1	L	291	TRP	CB-CG	-6.60	1.38	1.50
1	M	413	CYS	CB-SG	-6.59	1.71	1.82
1	J	273	VAL	CB-CG2	-6.52	1.39	1.52
1	L	217	GLU	CD-OE1	-6.48	1.18	1.25
1	A	816	CYS	CB-SG	-6.42	1.71	1.82
1	C	535	VAL	CB-CG1	-6.35	1.39	1.52
1	F	688	GLN	CG-CD	-6.34	1.36	1.51
1	D	738	VAL	CB-CG2	-6.30	1.39	1.52
1	N	248	TYR	CG-CD2	-6.29	1.30	1.39
1	P	178	ILE	CB-CG2	-6.27	1.33	1.52
1	F	681	TYR	CB-CG	-6.26	1.42	1.51
1	R	393	VAL	CB-CG2	-6.25	1.39	1.52
1	A	763	ASN	CB-CG	-6.24	1.36	1.51
1	R	366	GLU	CG-CD	-6.24	1.42	1.51
1	C	881	GLU	CD-OE1	-6.23	1.18	1.25
1	A	777	VAL	CB-CG1	-6.23	1.39	1.52
1	F	680	GLU	CG-CD	6.22	1.61	1.51
1	E	819	CYS	CB-SG	-6.20	1.71	1.82
1	A	771	VAL	CB-CG1	-6.19	1.39	1.52
1	E	759	VAL	CB-CG1	-6.17	1.39	1.52
1	F	710	ASP	CB-CG	-6.13	1.38	1.51
1	F	733	LEU	CG-CD2	-6.11	1.29	1.51
1	D	604	GLU	CD-OE1	-6.11	1.19	1.25
1	A	559	VAL	CB-CG1	-6.08	1.40	1.52
1	C	781	CYS	CB-SG	-6.08	1.72	1.82
1	L	263	VAL	CB-CG2	-6.02	1.40	1.52
1	P	212	TYR	CE1-CZ	-6.01	1.30	1.38
1	R	419	PHE	CB-CG	6.00	1.61	1.51
1	J	248	TYR	CG-CD1	-6.00	1.31	1.39
1	M	419	PHE	CB-CG	-5.98	1.41	1.51
1	N	199	ARG	CD-NE	-5.97	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	819	CYS	CB-SG	-5.94	1.72	1.81
1	D	781	CYS	CB-SG	-5.93	1.72	1.81
1	E	625	PHE	CB-CG	-5.93	1.41	1.51
1	A	710	ASP	CB-CG	-5.92	1.39	1.51
1	D	687	ASN	CB-CG	-5.92	1.37	1.51
1	D	759	VAL	CB-CG2	-5.90	1.40	1.52
1	E	715	MET	CG-SD	-5.90	1.65	1.81
1	K	201	LEU	CB-CG	-5.89	1.35	1.52
1	Q	419	PHE	CB-CG	-5.88	1.41	1.51
1	K	222	GLU	CD-OE2	-5.87	1.19	1.25
1	Q	419	PHE	CG-CD2	-5.85	1.29	1.38
1	J	178	ILE	CB-CG1	-5.83	1.37	1.54
1	K	222	GLU	CD-OE1	-5.80	1.19	1.25
1	G	461	VAL	CB-CG1	-5.80	1.40	1.52
1	B	762	PHE	CB-CG	-5.75	1.41	1.51
1	L	223	PHE	CG-CD1	-5.74	1.30	1.38
1	O	291	TRP	CB-CG	-5.70	1.40	1.50
1	F	673	GLN	CB-CG	-5.67	1.37	1.52
1	J	202	VAL	CB-CG1	-5.66	1.41	1.52
1	F	882	GLU	CG-CD	-5.66	1.43	1.51
1	C	559	VAL	CB-CG1	-5.62	1.41	1.52
1	E	529	GLU	CG-CD	-5.60	1.43	1.51
1	E	604	GLU	CG-CD	-5.58	1.43	1.51
1	H	419	PHE	CB-CG	-5.56	1.41	1.51
1	F	529	GLU	CD-OE2	-5.56	1.19	1.25
1	C	630	PHE	CB-CG	-5.55	1.42	1.51
1	G	448	LEU	CG-CD2	-5.54	1.31	1.51
1	A	810	LEU	CB-CG	-5.54	1.36	1.52
1	F	819	CYS	CB-SG	-5.51	1.72	1.81
1	I	420	PRO	N-CD	-5.51	1.40	1.47
1	B	816	CYS	CB-SG	-5.50	1.72	1.81
1	D	584	TYR	CG-CD2	-5.48	1.32	1.39
1	B	510	PHE	CD2-CE2	-5.47	1.28	1.39
1	P	178	ILE	CB-CG1	-5.46	1.38	1.54
1	C	604	GLU	CD-OE2	-5.46	1.19	1.25
1	B	582	VAL	CB-CG2	-5.45	1.41	1.52
1	D	680	GLU	CG-CD	5.45	1.60	1.51
1	O	284	TYR	CD2-CE2	-5.43	1.31	1.39
1	J	211	LEU	CB-CG	-5.42	1.36	1.52
1	O	291	TRP	CZ3-CH2	-5.42	1.31	1.40
1	F	630	PHE	CB-CG	-5.42	1.42	1.51
1	A	781	CYS	CB-SG	-5.41	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	266	ASP	CB-CG	5.41	1.63	1.51
1	M	419	PHE	CG-CD2	-5.41	1.30	1.38
1	N	248	TYR	CE2-CZ	-5.40	1.31	1.38
1	D	854	LYS	CB-CG	-5.39	1.38	1.52
1	E	514	VAL	CB-CG1	-5.39	1.41	1.52
1	N	263	VAL	CB-CG2	-5.36	1.41	1.52
1	J	288	PRO	N-CD	-5.36	1.40	1.47
1	L	295	PHE	CB-CG	-5.36	1.42	1.51
1	G	444	VAL	CB-CG1	-5.35	1.41	1.52
1	Q	340	LEU	CG-CD1	-5.35	1.32	1.51
1	P	177	TRP	CZ3-CH2	-5.35	1.31	1.40
1	C	687	ASN	CB-CG	-5.34	1.38	1.51
1	M	418	VAL	CB-CG1	-5.32	1.41	1.52
1	Q	475	TYR	CE1-CZ	-5.31	1.31	1.38
1	H	393	VAL	CB-CG2	-5.30	1.41	1.52
1	O	222	GLU	CD-OE2	-5.29	1.19	1.25
1	C	529	GLU	CD-OE2	-5.26	1.19	1.25
1	A	527	HIS	CB-CG	-5.26	1.40	1.50
1	F	721	ASP	CB-CG	5.26	1.62	1.51
1	A	775	ARG	CG-CD	-5.25	1.38	1.51
1	C	759	VAL	CB-CG2	-5.25	1.41	1.52
1	N	212	TYR	CD2-CE2	-5.23	1.31	1.39
1	C	641	TYR	CB-CG	-5.21	1.43	1.51
1	B	529	GLU	CD-OE2	-5.19	1.20	1.25
1	N	248	TYR	CD2-CE2	-5.19	1.31	1.39
1	A	526	ILE	CB-CG1	-5.17	1.39	1.54
1	F	683	ILE	CB-CG2	-5.17	1.36	1.52
1	H	431	LEU	CB-CG	-5.17	1.37	1.52
1	O	201	LEU	CB-CG	-5.17	1.37	1.52
1	A	658	THR	CB-CG2	-5.16	1.35	1.52
1	C	756	GLU	CG-CD	5.15	1.59	1.51
1	H	461	VAL	CB-CG1	-5.15	1.42	1.52
1	M	461	VAL	CB-CG1	-5.14	1.42	1.52
1	A	832	GLU	CD-OE2	-5.14	1.20	1.25
1	D	591	VAL	CB-CG1	-5.14	1.42	1.52
1	D	699	PHE	CB-CG	-5.13	1.42	1.51
1	A	589	ILE	CB-CG2	-5.12	1.36	1.52
1	Q	475	TYR	CG-CD2	-5.12	1.32	1.39
1	F	529	GLU	CG-CD	-5.12	1.44	1.51
1	B	760	GLU	CG-CD	5.11	1.59	1.51
1	F	775	ARG	CG-CD	-5.11	1.39	1.51
1	B	529	GLU	CG-CD	-5.10	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	556	LEU	CB-CG	-5.10	1.37	1.52
1	B	560	ILE	CB-CG1	-5.10	1.39	1.54
1	F	681	TYR	CG-CD2	-5.10	1.32	1.39
1	B	591	VAL	CB-CG1	-5.09	1.42	1.52
1	N	199	ARG	CZ-NH2	-5.09	1.26	1.33
1	R	418	VAL	CB-CG2	-5.08	1.42	1.52
1	C	681	TYR	CG-CD1	-5.07	1.32	1.39
1	O	248	TYR	CE1-CZ	-5.07	1.31	1.38
1	F	542	ASP	CB-CG	-5.07	1.41	1.51
1	B	828	TYR	CE2-CZ	-5.05	1.31	1.38
1	E	828	TYR	CD2-CE2	-5.04	1.31	1.39
1	K	185	GLU	CD-OE1	-5.03	1.20	1.25
1	K	206	LEU	CG-CD2	-5.01	1.33	1.51
1	H	393	VAL	CB-CG1	-5.01	1.42	1.52
1	P	264	LEU	CB-CG	-5.01	1.38	1.52
1	A	633	PHE	CB-CG	-5.00	1.42	1.51

All (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
1	C	546	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	N	248	TYR	CB-CG-CD1	8.95	126.37	121.00
1	J	213	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	C	796	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	G	445	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	O	213	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	K	213	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	D	841	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	A	797	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	H	475	TYR	CB-CG-CD1	-7.69	116.39	121.00
1	C	546	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	P	213	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	I	445	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	C	632	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	R	414	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	Q	414	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	E	546	ARG	NE-CZ-NH1	7.22	123.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	584	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	B	720	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	F	704	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	H	414	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	A	540	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	797	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	D	516	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	R	427	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	N	213	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	E	828	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	L	223	PHE	CB-CG-CD1	-6.64	116.15	120.80
1	G	475	TYR	CB-CG-CD2	-6.64	117.02	121.00
1	F	778	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	E	791	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	779	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	J	211	LEU	CB-CA-C	-6.50	97.86	110.20
1	A	540	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	E	585	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	M	445	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	G	445	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	824	TYR	CB-CG-CD1	-6.43	117.14	121.00
1	E	540	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	827	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	E	681	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	J	297	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	C	630	PHE	CB-CG-CD1	-6.35	116.36	120.80
1	E	641	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	B	510	PHE	CB-CG-CD2	-6.25	116.42	120.80
1	I	414	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	D	859	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	B	644	PHE	CB-CG-CD1	-6.17	116.48	120.80
1	D	824	TYR	CB-CG-CD1	-6.15	117.31	121.00
1	A	681	TYR	CB-CG-CD1	-6.13	117.32	121.00
1	N	297	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	N	282	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	F	733	LEU	CB-CA-C	-5.99	98.81	110.20
1	P	177	TRP	CB-CG-CD2	5.94	134.32	126.60
1	L	282	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	D	779	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	O	279	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	H	404	ALA	CB-CA-C	5.83	118.84	110.10
1	I	416	TYR	CB-CG-CD2	-5.83	117.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	811	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	H	455	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	J	213	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	714	ILE	CG1-CB-CG2	-5.80	98.64	111.40
1	N	284	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	D	778	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	L	212	TYR	CB-CG-CD2	-5.73	117.56	121.00
1	E	789	LYS	C-N-CD	-5.72	108.01	120.60
1	E	538	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	D	858	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	I	427	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	G	364	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	K	282	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	R	392	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	J	248	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	R	436	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	632	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	C	531	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	862	MET	CG-SD-CE	-5.58	91.28	100.20
1	N	227	THR	CA-CB-CG2	-5.52	104.67	112.40
1	A	633	PHE	CB-CG-CD2	-5.52	116.94	120.80
1	F	720	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	P	199	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	F	585	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	N	212	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	F	609	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	F	886	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	E	583	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	H	422	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	584	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	H	392	TYR	CB-CG-CD1	-5.34	117.79	121.00
1	P	264	LEU	CB-CA-C	-5.28	100.17	110.20
1	K	168	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	D	797	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	J	178	ILE	CB-CA-C	-5.24	101.13	111.60
1	A	841	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	E	796	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	O	212	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	D	828	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	O	296	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	K	199	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	D	820	GLY	CA-C-O	-5.15	111.33	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	538	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	I	455	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	A	706	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	C	540	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	I	415	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	E	791	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	862	MET	CB-CA-C	-5.09	100.22	110.40
1	D	706	PHE	CB-CG-CD2	5.08	124.36	120.80
1	E	811	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	F	841	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	D	538	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	K	296	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	N	264	LEU	CB-CA-C	-5.04	100.63	110.20
1	F	710	ASP	CB-CA-C	-5.02	100.37	110.40
1	L	264	LEU	CB-CA-C	-5.00	100.69	110.20
1	O	255	PHE	CB-CG-CD1	-5.00	117.30	120.80

There are no chirality outliers.

All (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,Peptide
1	D	820	GLY	Mainchain,Peptide
1	E	587	GLY	Mainchain,Peptide
1	F	533	ASN	Mainchain,Peptide
1	F	682	GLU	Mainchain,Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2975	0	3080	26	0
1	B	2966	0	3066	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:O:291:TRP:HE3	1:O:291:TRP:HA	1.32	0.94
1:O:291:TRP:HA	1:O:291:TRP:CE3	2.01	0.91
1:D:832:GLU:O	1:D:832:GLU:HG3	1.72	0.89
1:L:248:TYR:HD1	1:L:248:TYR:O	1.63	0.82
1:L:291:TRP:HA	1:L:291:TRP:CE3	2.18	0.79
1:Q:336:LEU:C	1:Q:336:LEU:CD1	2.50	0.78
1:O:291:TRP:CE3	1:O:291:TRP:CA	2.68	0.76
1:G:401:ASP:OD1	1:G:401:ASP:O	2.04	0.76
1:L:291:TRP:HA	1:L:291:TRP:HE3	1.50	0.76
1:C:862:MET:O	1:C:862:MET:HG2	1.86	0.74
1:B:679:VAL:O	1:B:679:VAL:CG1	2.33	0.74
1:C:525:ASP:OD1	1:C:525:ASP:O	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:ASP:OD1	1:C:525:ASP:C	2.26	0.73
1:P:291:TRP:CE3	1:P:291:TRP:HA	2.25	0.71
1:J:276:LEU:C	1:J:276:LEU:HD23	2.11	0.71
1:D:862:MET:O	1:D:862:MET:HG2	1.91	0.71
1:K:291:TRP:HE3	1:K:291:TRP:HA	1.56	0.71
1:F:710:ASP:O	1:F:710:ASP:OD2	2.08	0.71
1:A:519:PHE:HD1	1:A:519:PHE:N	1.89	0.70
1:B:650:THR:HG23	1:B:650:THR:O	1.90	0.70
1:K:291:TRP:HA	1:K:291:TRP:CE3	2.27	0.70
1:L:248:TYR:CD1	1:L:248:TYR:C	2.65	0.69
1:P:291:TRP:HA	1:P:291:TRP:HE3	1.58	0.68
1:P:263:VAL:HG23	1:P:263:VAL:O	1.94	0.68
1:O:263:VAL:HG23	1:O:263:VAL:O	1.94	0.66
1:O:212:TYR:C	1:O:212:TYR:CD1	2.67	0.66
1:G:412:LEU:C	1:G:412:LEU:HD23	2.16	0.66
1:D:888:ILE:HG22	1:D:888:ILE:O	1.96	0.66
1:H:419:PHE:O	1:H:419:PHE:CD2	2.49	0.65
1:L:291:TRP:CE3	1:L:291:TRP:CA	2.79	0.65
1:L:248:TYR:O	1:L:248:TYR:CD1	2.48	0.65
1:Q:419:PHE:CD1	1:Q:419:PHE:C	2.70	0.65
1:G:412:LEU:HD23	1:G:412:LEU:O	1.97	0.65
1:N:276:LEU:C	1:N:276:LEU:HD23	2.17	0.64
1:A:519:PHE:N	1:A:519:PHE:CD1	2.65	0.64
1:O:295:PHE:CD1	1:O:295:PHE:N	2.61	0.63
1:D:832:GLU:O	1:D:832:GLU:CG	2.40	0.63
1:K:178:ILE:HG23	1:K:178:ILE:O	1.99	0.63
1:R:407:LEU:O	1:R:407:LEU:HD12	2.00	0.62
1:R:401:ASP:OD1	1:R:401:ASP:O	2.16	0.62
1:M:410:GLU:CD	1:M:410:GLU:H	2.03	0.61
1:F:595:LEU:N	1:F:595:LEU:HD12	2.16	0.61
1:K:248:TYR:HD1	1:K:248:TYR:C	2.04	0.61
1:F:683:ILE:O	1:F:683:ILE:CG2	2.32	0.61
1:H:419:PHE:CD2	1:H:419:PHE:C	2.74	0.60
1:O:178:ILE:HG23	1:O:178:ILE:O	2.01	0.60
1:F:710:ASP:O	1:F:710:ASP:CG	2.30	0.60
1:K:248:TYR:HD1	1:K:248:TYR:O	1.84	0.60
1:K:248:TYR:C	1:K:248:TYR:CD1	2.73	0.60
1:J:276:LEU:HD23	1:J:276:LEU:O	2.01	0.60
1:E:582:VAL:HG13	1:E:582:VAL:O	2.03	0.59
1:M:419:PHE:CD1	1:M:419:PHE:C	2.76	0.58
1:L:248:TYR:HD1	1:L:248:TYR:C	2.05	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:862:MET:O	1:D:862:MET:HE3	2.04	0.58
1:B:686:ILE:O	1:B:686:ILE:HG23	2.03	0.57
1:B:677:ASP:C	1:B:677:ASP:OD1	2.42	0.57
1:K:263:VAL:O	1:K:263:VAL:CG2	2.42	0.57
1:J:287:LEU:HD12	1:J:287:LEU:N	2.19	0.57
1:L:263:VAL:O	1:L:263:VAL:HG23	2.03	0.56
1:A:714:ILE:CG2	1:A:714:ILE:O	2.52	0.56
1:M:410:GLU:OE1	1:M:410:GLU:N	2.25	0.56
1:R:366:GLU:OE1	1:R:366:GLU:N	2.36	0.56
1:H:336:LEU:HD22	1:H:336:LEU:O	2.05	0.56
1:B:671:ASN:HB2	1:C:545:LEU:HG	1.86	0.56
1:N:276:LEU:HD23	1:N:276:LEU:O	2.06	0.56
1:B:691:VAL:O	1:B:692:ASN:C	2.45	0.56
1:C:862:MET:O	1:C:862:MET:HE3	2.06	0.55
1:F:837:ASP:OD2	1:F:860:LYS:NZ	2.40	0.55
1:I:336:LEU:HD13	1:I:336:LEU:C	2.26	0.55
1:Q:408:LEU:C	1:Q:408:LEU:HD23	2.27	0.55
1:A:862:MET:HG2	1:A:862:MET:O	2.06	0.55
1:C:862:MET:O	1:C:862:MET:CG	2.44	0.55
1:B:650:THR:O	1:B:650:THR:CG2	2.54	0.54
1:C:527:HIS:ND1	1:C:605:LYS:NZ	2.54	0.54
1:R:404:ALA:O	1:R:475:TYR:OH	2.24	0.54
1:F:884:LEU:C	1:F:884:LEU:HD23	2.28	0.54
1:R:422:ARG:O	1:R:422:ARG:HG3	2.07	0.54
1:E:582:VAL:O	1:E:582:VAL:CG1	2.56	0.54
1:O:277:LEU:O	1:O:277:LEU:HG	2.07	0.54
1:R:401:ASP:O	1:R:403:GLY:N	2.40	0.54
1:D:644:PHE:C	1:D:644:PHE:HD1	2.12	0.54
1:P:202:VAL:O	1:P:203:ARG:CB	2.55	0.53
1:D:781:CYS:O	1:D:781:CYS:SG	2.63	0.53
1:C:859:ARG:O	1:C:860:LYS:HB2	2.09	0.53
1:G:435:PRO:O	1:G:436:ARG:C	2.47	0.53
1:N:178:ILE:HG22	1:N:206:LEU:HB2	1.90	0.53
1:R:451:LYS:HG3	1:R:451:LYS:O	2.08	0.53
1:D:519:PHE:HD1	1:D:519:PHE:N	2.05	0.53
1:D:519:PHE:N	1:D:519:PHE:CD1	2.76	0.53
1:D:778:ARG:HB3	1:D:824:TYR:HB3	1.90	0.52
1:C:801:SER:O	1:C:803:ALA:N	2.42	0.52
1:L:255:PHE:C	1:L:255:PHE:CD2	2.80	0.52
1:B:641:TYR:OH	1:C:812:LYS:NZ	2.31	0.52
1:J:259:GLU:O	1:J:259:GLU:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:212:TYR:CD1	1:L:212:TYR:C	2.82	0.52
1:E:584:TYR:CD1	1:E:584:TYR:C	2.83	0.52
1:E:791:ASP:HB2	1:E:793:GLU:H	1.74	0.52
1:B:777:VAL:HG13	1:B:882:GLU:HB3	1.92	0.52
1:J:276:LEU:C	1:J:276:LEU:CD2	2.78	0.52
1:I:375:LEU:C	1:I:375:LEU:HD12	2.30	0.52
1:D:576:LEU:C	1:D:576:LEU:HD12	2.31	0.52
1:D:862:MET:O	1:D:863:LYS:C	2.48	0.51
1:F:765:SER:OG	1:F:766:ALA:N	2.44	0.51
1:L:255:PHE:CD2	1:L:255:PHE:O	2.64	0.51
1:B:677:ASP:HB2	1:B:678:PRO:HD2	1.93	0.51
1:E:710:ASP:CG	1:E:710:ASP:O	2.49	0.51
1:O:212:TYR:C	1:O:212:TYR:HD1	2.13	0.50
1:C:710:ASP:CG	1:C:710:ASP:O	2.48	0.50
1:K:291:TRP:CE3	1:K:291:TRP:CA	2.94	0.50
1:A:650:THR:O	1:A:650:THR:HG23	2.10	0.50
1:A:551:LEU:N	1:A:551:LEU:HD12	2.27	0.50
1:B:595:LEU:HD12	1:B:595:LEU:N	2.26	0.50
1:A:522:ASP:OD1	1:A:612:LYS:NZ	2.43	0.50
1:L:202:VAL:O	1:L:203:ARG:HB3	2.12	0.50
1:I:463:THR:HG23	1:I:463:THR:O	2.10	0.50
1:D:644:PHE:C	1:D:644:PHE:CD1	2.85	0.50
1:N:183:LEU:C	1:N:183:LEU:HD23	2.32	0.50
1:J:287:LEU:N	1:J:287:LEU:CD1	2.75	0.49
1:K:202:VAL:O	1:K:203:ARG:HB2	2.12	0.49
1:C:677:ASP:HB3	1:C:678:PRO:CD	2.41	0.49
1:G:401:ASP:O	1:G:403:GLY:N	2.45	0.49
1:D:614:ALA:HA	1:D:681:TYR:CD2	2.47	0.49
1:K:168:LEU:HD21	1:K:198:GLY:H	1.77	0.49
1:B:862:MET:O	1:B:862:MET:HG2	2.12	0.49
1:C:538:ARG:HB3	1:C:545:LEU:HB3	1.94	0.49
1:G:401:ASP:OD1	1:G:401:ASP:C	2.50	0.49
1:B:659:PHE:CD1	1:B:659:PHE:N	2.80	0.49
1:C:862:MET:O	1:C:863:LYS:C	2.48	0.49
1:O:266:ASP:OD1	1:O:266:ASP:O	2.31	0.49
1:A:510:PHE:CZ	1:A:551:LEU:HD11	2.48	0.48
1:A:519:PHE:CE2	1:A:591:VAL:HB	2.47	0.48
1:A:524:SER:N	1:A:540:ARG:O	2.46	0.48
1:A:817:GLU:H	1:A:817:GLU:CD	2.15	0.48
1:Q:393:VAL:O	1:Q:393:VAL:HG23	2.13	0.48
1:K:238:LEU:HD12	1:K:238:LEU:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:LEU:HD23	1:L:183:LEU:C	2.34	0.48
1:P:202:VAL:O	1:P:203:ARG:HB3	2.14	0.48
1:E:746:ASP:OD1	1:E:747:ALA:N	2.46	0.48
1:H:336:LEU:HD13	1:H:336:LEU:C	2.33	0.47
1:H:335:PRO:O	1:H:338:GLU:N	2.47	0.47
1:N:168:LEU:HD23	1:N:168:LEU:H	1.79	0.47
1:F:590:ASP:OD1	1:F:613:LYS:NZ	2.47	0.47
1:F:600:THR:HG22	1:F:602:TYR:H	1.79	0.47
1:G:434:ASP:O	1:G:435:PRO:C	2.53	0.47
1:O:175:LYS:NZ	1:Q:378:GLU:OE1	2.46	0.47
1:G:418:VAL:O	1:G:418:VAL:HG23	2.15	0.47
1:K:286:ALA:HB3	1:K:291:TRP:CZ2	2.50	0.47
1:B:510:PHE:CD2	1:B:510:PHE:C	2.85	0.47
1:H:408:LEU:C	1:H:408:LEU:HD23	2.35	0.47
1:I:350:ASP:HB3	1:I:374:LYS:HB3	1.96	0.47
1:A:706:PHE:CE1	1:A:714:ILE:HA	2.50	0.47
1:C:530:PRO:HB2	1:C:602:TYR:HB2	1.97	0.47
1:G:404:ALA:N	1:G:405:PRO:CD	2.77	0.46
1:G:424:GLU:HB3	1:G:427:ARG:HB3	1.97	0.46
1:O:212:TYR:HD1	1:O:212:TYR:O	1.98	0.46
1:B:677:ASP:HB2	1:B:678:PRO:CD	2.45	0.46
1:B:790:PRO:HG2	1:B:795:LEU:HD11	1.97	0.46
1:M:463:THR:O	1:M:465:ALA:N	2.48	0.46
1:D:835:VAL:HG13	1:D:835:VAL:O	2.14	0.46
1:B:535:VAL:HB	1:B:551:LEU:HB2	1.97	0.46
1:D:868:ASP:OD1	1:D:872:LYS:NZ	2.49	0.46
1:F:675:ILE:HG21	1:F:675:ILE:HD13	1.63	0.46
1:H:461:VAL:O	1:H:461:VAL:HG13	2.15	0.46
1:C:859:ARG:O	1:C:860:LYS:CB	2.64	0.46
1:D:671:ASN:OD1	1:D:671:ASN:C	2.54	0.46
1:H:336:LEU:HD22	1:H:336:LEU:C	2.35	0.46
1:N:199:ARG:NH2	1:N:265:SER:O	2.49	0.46
1:K:178:ILE:O	1:K:178:ILE:CG2	2.62	0.46
1:P:276:LEU:HD23	1:P:276:LEU:C	2.37	0.46
1:I:400:PRO:O	1:I:401:ASP:C	2.54	0.45
1:C:551:LEU:N	1:C:551:LEU:HD12	2.31	0.45
1:B:686:ILE:O	1:B:686:ILE:CG2	2.61	0.45
1:C:760:GLU:CD	1:C:760:GLU:H	2.19	0.45
1:Q:419:PHE:CE2	1:Q:470:LEU:HB3	2.50	0.45
1:A:569:LEU:HD12	1:A:569:LEU:N	2.32	0.45
1:K:202:VAL:O	1:K:202:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:778:ARG:HB3	1:C:824:TYR:CB	2.46	0.45
1:N:202:VAL:HG23	1:N:202:VAL:O	2.15	0.45
1:O:287:LEU:HA	1:O:287:LEU:HD23	1.70	0.45
1:D:798:LEU:O	1:D:866:ARG:NE	2.50	0.45
1:D:824:TYR:CD1	1:D:824:TYR:N	2.85	0.45
1:O:291:TRP:CE3	1:O:291:TRP:N	2.84	0.45
1:C:834:LEU:N	1:C:834:LEU:CD1	2.80	0.45
1:M:419:PHE:CD1	1:M:419:PHE:O	2.70	0.44
1:G:407:LEU:HD12	1:G:407:LEU:HA	1.77	0.44
1:I:408:LEU:HD23	1:I:408:LEU:C	2.37	0.44
1:P:211:LEU:O	1:P:211:LEU:HG	2.16	0.44
1:D:808:ALA:HB1	1:D:874:LEU:HD22	1.99	0.44
1:G:400:PRO:O	1:G:401:ASP:C	2.55	0.44
1:A:653:GLY:O	1:A:654:LYS:C	2.55	0.44
1:F:523:ALA:HA	1:F:541:ILE:HA	2.00	0.44
1:F:564:LYS:NZ	1:F:573:GLU:O	2.51	0.44
1:H:334:LYS:O	1:H:335:PRO:C	2.56	0.44
1:O:291:TRP:HB3	1:O:295:PHE:CZ	2.53	0.44
1:B:524:SER:N	1:B:540:ARG:O	2.48	0.44
1:F:673:GLN:HG3	1:F:706:PHE:CE2	2.52	0.44
1:J:250:ALA:HB2	1:J:264:LEU:HA	2.00	0.44
1:Q:336:LEU:HD22	1:Q:336:LEU:HA	1.57	0.44
1:C:862:MET:O	1:C:862:MET:CE	2.65	0.44
1:H:455:TYR:O	1:H:456:GLU:CB	2.66	0.44
1:B:595:LEU:HG	1:B:608:MET:HE3	1.99	0.44
1:E:589:ILE:HG23	1:E:589:ILE:O	2.17	0.44
1:K:275:GLN:O	1:K:276:LEU:CB	2.64	0.44
1:D:506:ALA:HA	1:D:508:GLN:N	2.33	0.44
1:B:662:LEU:O	1:B:666:ALA:N	2.48	0.44
1:H:401:ASP:O	1:H:405:PRO:HD2	2.18	0.44
1:Q:419:PHE:HD1	1:Q:419:PHE:O	2.00	0.44
1:D:817:GLU:H	1:D:817:GLU:CD	2.14	0.44
1:J:202:VAL:O	1:J:203:ARG:HB2	2.19	0.43
1:P:206:LEU:HA	1:P:207:PRO:HD2	1.96	0.43
1:I:394:ASP:OD1	1:I:394:ASP:C	2.56	0.43
1:D:710:ASP:N	1:D:711:PRO:HD3	2.34	0.43
1:F:682:GLU:HA	1:F:683:ILE:HB	2.00	0.43
1:A:535:VAL:HB	1:A:551:LEU:HB2	1.98	0.43
1:C:535:VAL:HB	1:C:551:LEU:HB2	2.00	0.43
1:M:419:PHE:O	1:M:419:PHE:HD1	2.02	0.43
1:N:248:TYR:HD1	1:N:248:TYR:O	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:788:VAL:O	1:E:789:LYS:C	2.57	0.43
1:E:791:ASP:HB2	1:E:793:GLU:N	2.33	0.43
1:M:419:PHE:CE2	1:M:470:LEU:HG	2.54	0.43
1:B:560:ILE:HD13	1:B:560:ILE:HA	1.78	0.43
1:C:884:LEU:HD23	1:C:884:LEU:HA	1.70	0.43
1:J:178:ILE:HG22	1:J:206:LEU:HB2	2.01	0.43
1:F:743:HIS:ND1	1:F:743:HIS:C	2.71	0.43
1:H:336:LEU:HB2	1:H:366:GLU:HG3	2.01	0.43
1:A:671:ASN:C	1:A:671:ASN:OD1	2.54	0.43
1:C:530:PRO:HB3	1:C:556:LEU:HD21	2.00	0.43
1:C:705:ALA:HB2	1:F:577:PRO:HB3	1.99	0.43
1:F:542:ASP:HB3	1:F:778:ARG:HG2	2.01	0.43
1:J:178:ILE:HG21	1:J:178:ILE:HD13	1.61	0.43
1:H:335:PRO:O	1:H:336:LEU:C	2.56	0.43
1:P:268:ARG:O	1:P:268:ARG:HG2	2.18	0.43
1:E:563:VAL:O	1:E:567:GLY:N	2.52	0.43
1:Q:457:VAL:O	1:Q:457:VAL:HG13	2.19	0.43
1:B:530:PRO:HB3	1:B:556:LEU:HD21	2.01	0.43
1:B:654:LYS:NZ	1:B:743:HIS:ND1	2.65	0.43
1:A:710:ASP:OD2	1:D:540:ARG:NE	2.51	0.42
1:G:419:PHE:C	1:G:419:PHE:CD1	2.92	0.42
1:C:778:ARG:HB3	1:C:824:TYR:HB3	2.01	0.42
1:E:593:LEU:HB3	1:E:608:MET:SD	2.60	0.42
1:E:824:TYR:CD1	1:E:824:TYR:N	2.86	0.42
1:E:535:VAL:HB	1:E:551:LEU:HB2	2.01	0.42
1:F:634:LYS:HE3	1:F:634:LYS:HB3	1.88	0.42
1:K:291:TRP:HB3	1:K:295:PHE:CZ	2.54	0.42
1:N:249:GLY:O	1:N:265:SER:N	2.53	0.42
1:N:199:ARG:HA	1:N:199:ARG:HD3	1.47	0.42
1:P:201:LEU:O	1:P:202:VAL:C	2.54	0.42
1:A:545:LEU:HB2	1:F:712:ASP:OD2	2.20	0.42
1:C:865:LEU:HB3	1:C:887:THR:HG22	2.00	0.42
1:N:177:TRP:CE3	1:N:214:ALA:HB2	2.54	0.42
1:Q:336:LEU:O	1:Q:336:LEU:CD1	2.37	0.42
1:A:675:ILE:HG21	1:A:675:ILE:HD13	1.74	0.42
1:G:448:LEU:O	1:G:452:GLY:N	2.48	0.42
1:O:178:ILE:HD13	1:O:178:ILE:HG21	1.83	0.42
1:E:878:THR:OG1	1:E:879:THR:N	2.52	0.42
1:L:291:TRP:CE3	1:L:291:TRP:N	2.87	0.42
1:O:178:ILE:O	1:O:178:ILE:CG2	2.68	0.42
1:R:357:LYS:O	1:R:361:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:617:ILE:HD13	1:E:617:ILE:HG21	1.73	0.42
1:I:334:LYS:O	1:I:335:PRO:C	2.58	0.42
1:P:202:VAL:O	1:P:202:VAL:HG13	2.20	0.42
1:A:719:ILE:HD13	1:A:719:ILE:HG21	1.91	0.42
1:C:560:ILE:HD12	1:C:560:ILE:HA	1.52	0.42
1:C:662:LEU:HD23	1:C:662:LEU:HA	1.86	0.42
1:E:675:ILE:HD13	1:E:675:ILE:HG21	1.64	0.42
1:K:183:LEU:C	1:K:183:LEU:HD23	2.40	0.42
1:L:201:LEU:C	1:L:202:VAL:O	2.55	0.42
1:C:804:GLU:OE2	1:C:863:LYS:NZ	2.44	0.42
1:M:423:LEU:HD23	1:M:423:LEU:HA	1.88	0.41
1:N:202:VAL:O	1:N:203:ARG:HB2	2.20	0.41
1:N:212:TYR:N	1:N:212:TYR:CD1	2.79	0.41
1:R:336:LEU:O	1:R:340:LEU:HG	2.20	0.41
1:B:659:PHE:N	1:B:659:PHE:HD1	2.18	0.41
1:C:510:PHE:O	1:C:511:VAL:C	2.57	0.41
1:F:870:LEU:HD23	1:F:870:LEU:HA	1.84	0.41
1:C:832:GLU:HB2	1:C:865:LEU:HG	2.02	0.41
1:D:862:MET:O	1:D:862:MET:CG	2.54	0.41
1:E:716:VAL:O	1:E:717:GLY:C	2.56	0.41
1:J:168:LEU:H	1:J:168:LEU:HD23	1.86	0.41
1:K:178:ILE:HB	1:K:206:LEU:HD13	2.02	0.41
1:N:263:VAL:HG23	1:N:263:VAL:O	2.19	0.41
1:N:276:LEU:C	1:N:276:LEU:CD2	2.85	0.41
1:Q:408:LEU:HD23	1:Q:408:LEU:O	2.20	0.41
1:M:404:ALA:N	1:M:405:PRO:HD2	2.35	0.41
1:O:252:PRO:HB3	1:O:260:VAL:HG21	2.03	0.41
1:R:401:ASP:OD1	1:R:401:ASP:C	2.59	0.41
1:K:276:LEU:HD23	1:K:276:LEU:C	2.40	0.41
1:M:456:GLU:OE1	1:M:456:GLU:HA	2.21	0.41
1:O:172:LEU:HD22	1:O:210:ALA:HB1	2.03	0.41
1:A:538:ARG:NH1	1:F:670:LYS:O	2.54	0.41
1:B:674:THR:OG1	1:B:686:ILE:HD11	2.21	0.41
1:F:697:LEU:O	1:F:697:LEU:HG	2.20	0.41
1:C:675:ILE:O	1:C:675:ILE:HG23	2.20	0.41
1:D:798:LEU:HA	1:D:798:LEU:HD23	1.89	0.41
1:M:400:PRO:O	1:M:401:ASP:C	2.59	0.41
1:O:215:LEU:HD23	1:O:215:LEU:HA	1.95	0.41
1:R:333:ALA:O	1:R:334:LYS:C	2.59	0.41
1:A:650:THR:O	1:A:650:THR:CG2	2.69	0.41
1:K:211:LEU:HA	1:K:211:LEU:HD23	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:404:ALA:N	1:M:405:PRO:CD	2.84	0.41
1:B:576:LEU:HA	1:B:576:LEU:HD23	1.88	0.41
1:C:571:ILE:HA	1:C:571:ILE:HD13	1.80	0.41
1:C:710:ASP:N	1:C:711:PRO:CD	2.83	0.41
1:C:835:VAL:O	1:C:835:VAL:CG2	2.68	0.41
1:D:788:VAL:O	1:D:789:LYS:C	2.59	0.41
1:D:874:LEU:HA	1:D:874:LEU:HD23	1.89	0.41
1:F:681:TYR:O	1:F:688:GLN:NE2	2.45	0.41
1:G:380:LEU:HA	1:G:380:LEU:HD13	1.73	0.41
1:O:206:LEU:HA	1:O:206:LEU:HD12	1.92	0.41
1:P:291:TRP:HB3	1:P:295:PHE:CZ	2.56	0.41
1:A:714:ILE:O	1:A:714:ILE:HG22	2.20	0.41
1:G:462:ALA:O	1:G:463:THR:C	2.59	0.40
1:L:216:ALA:HB3	1:L:223:PHE:CE1	2.56	0.40
1:I:419:PHE:O	1:I:431:LEU:HB3	2.21	0.40
1:P:264:LEU:N	1:P:284:TYR:O	2.53	0.40
1:D:599:PRO:HA	1:D:604:GLU:HA	2.04	0.40
1:E:530:PRO:HB3	1:E:556:LEU:CD2	2.51	0.40
1:Q:475:TYR:CD1	1:Q:475:TYR:N	2.90	0.40
1:C:684:PRO:HA	1:C:685:GLY:HA2	1.93	0.40
1:F:775:ARG:NH1	1:F:883:VAL:O	2.54	0.40
1:J:169:GLY:H	1:J:172:LEU:HD12	1.86	0.40
1:N:206:LEU:HD21	1:N:211:LEU:HB2	2.03	0.40
1:Q:419:PHE:CD1	1:Q:419:PHE:O	2.75	0.40
1:A:510:PHE:CZ	1:A:514:VAL:HG21	2.55	0.40
1:D:637:ILE:HD13	1:D:637:ILE:HG21	1.89	0.40
1:E:573:GLU:O	1:E:573:GLU:HG2	2.21	0.40
1:A:703:LEU:HD23	1:A:703:LEU:HA	1.80	0.40
1:F:583:ARG:HD2	1:F:583:ARG:N	2.36	0.40
1:F:598:LEU:HA	1:F:599:PRO:HD2	1.89	0.40
1:J:270:LYS:HA	1:J:273:VAL:HG22	2.04	0.40
1:I:376:ARG:HA	1:I:377:PRO:HD3	1.93	0.40
1:A:582:VAL:HB	1:A:593:LEU:HB2	2.04	0.40
1:D:510:PHE:O	1:D:511:VAL:C	2.59	0.40
1:D:710:ASP:N	1:D:711:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	382/913 (42%)	374 (98%)	7 (2%)	1 (0%)	37	73
1	B	381/913 (42%)	369 (97%)	10 (3%)	2 (0%)	25	64
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

All (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

*Continued on next page...*

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Mol	Chain	Res	Type
1	I	456	GLU
1	M	464	GLU
1	P	203	ARG
1	Q	456	GLU
1	B	679	VAL
1	C	614	ALA
1	C	802	GLU
1	E	790	PRO
1	G	437	ASN
1	K	276	LEU
1	R	455	TYR
1	D	507	ALA
1	E	572	ALA
1	G	402	PRO
1	K	167	LYS
1	L	255	PHE
1	L	257	ASN
1	O	167	LYS
1	A	881	GLU
1	C	507	ALA
1	D	816	CYS
1	F	807	GLY
1	G	455	TYR
1	L	167	LYS
1	R	402	PRO
1	B	678	PRO
1	C	677	ASP
1	F	735	GLY
1	G	456	GLU
1	J	167	LYS
1	H	455	TYR
1	M	455	TYR
1	M	456	GLU
1	P	167	LYS
1	C	819	CYS
1	D	616	ASP
1	N	206	LEU
1	C	735	GLY

### 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

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	380	LEU
1	K	248	TYR
1	L	212	TYR
1	L	248	TYR
1	N	248	TYR
1	O	212	TYR

*Continued on next page...*

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Mol	Chain	Res	Type
1	O	291	TRP
1	P	291	TRP
1	A	519	PHE
1	B	656	PHE
1	B	833	LEU
1	D	644	PHE
1	D	858	ARG
1	F	656	PHE

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 ⓘ

There are no chain breaks in this entry.

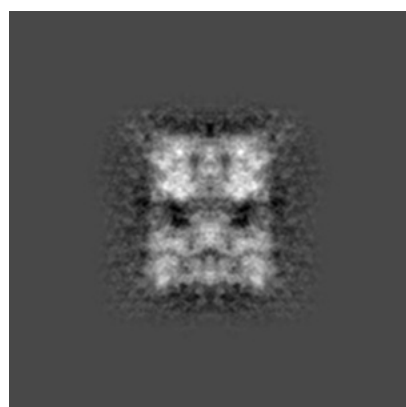
## 6 Map visualisation [i](#)

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.

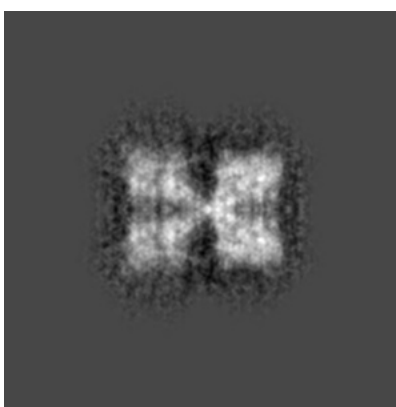
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

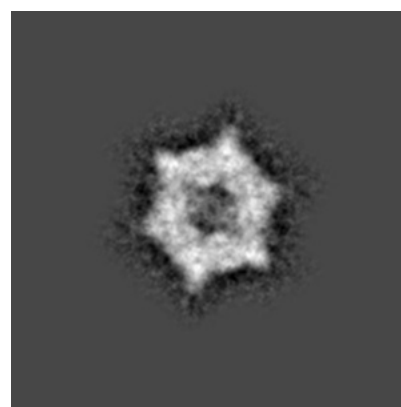
#### 6.1.1 Primary map



X



Y

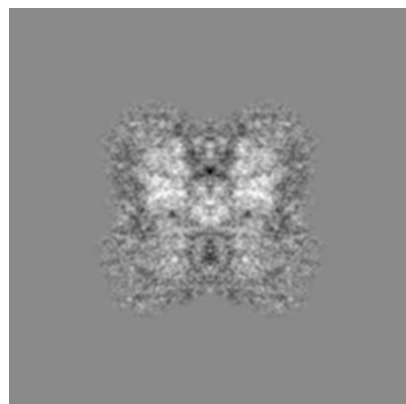


Z

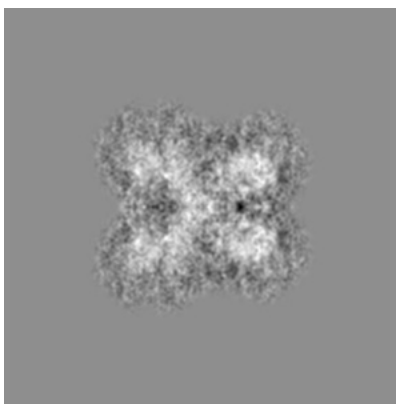
The images above show the map projected in three orthogonal directions.

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

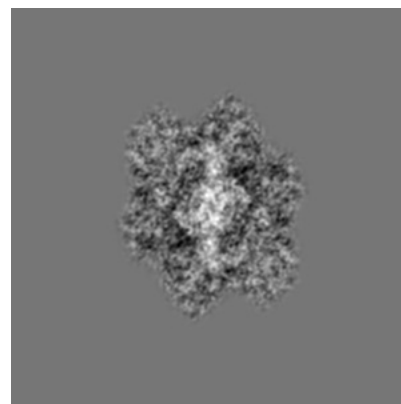
#### 6.2.1 Primary map



X Index: 96



Y Index: 96



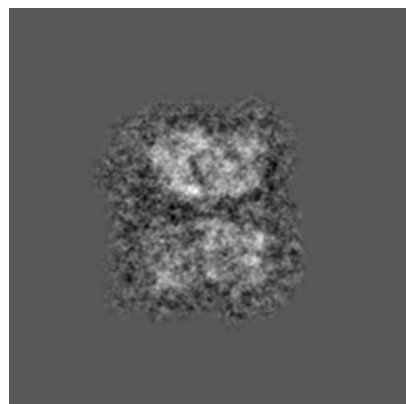
Z Index: 96



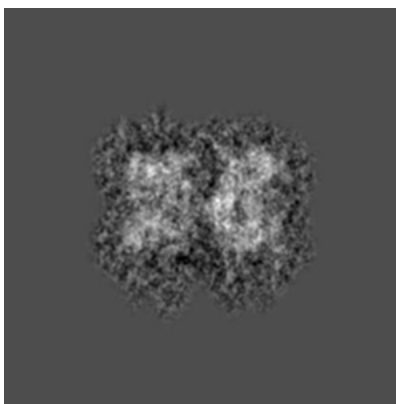
The images above show central slices of the map in three orthogonal directions.

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

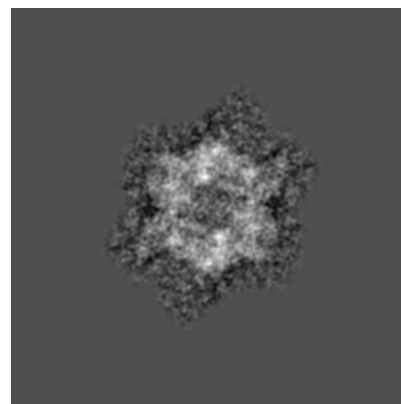
### 6.3.1 Primary map



X Index: 80



Y Index: 75

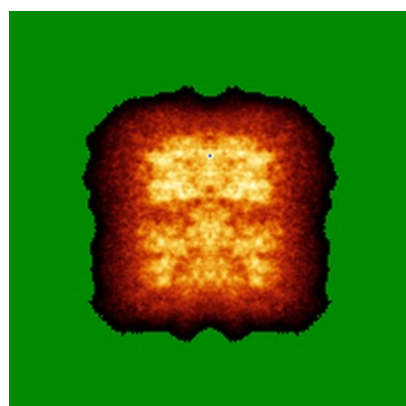


Z Index: 108

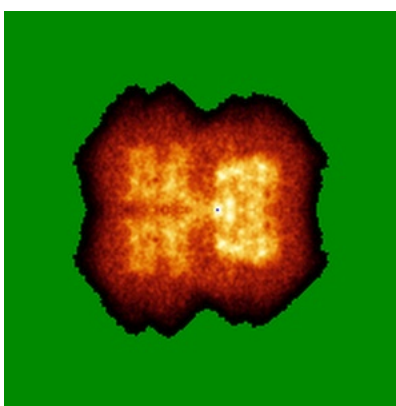
The images above show the largest variance slices of the map in three orthogonal directions.

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

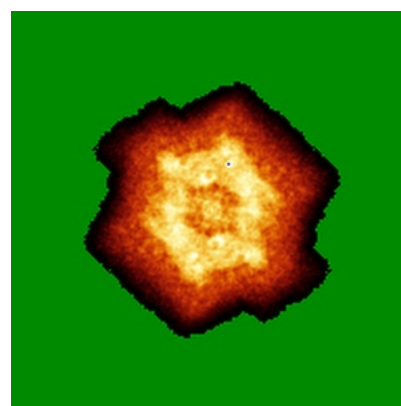
### 6.4.1 Primary map



X



Y

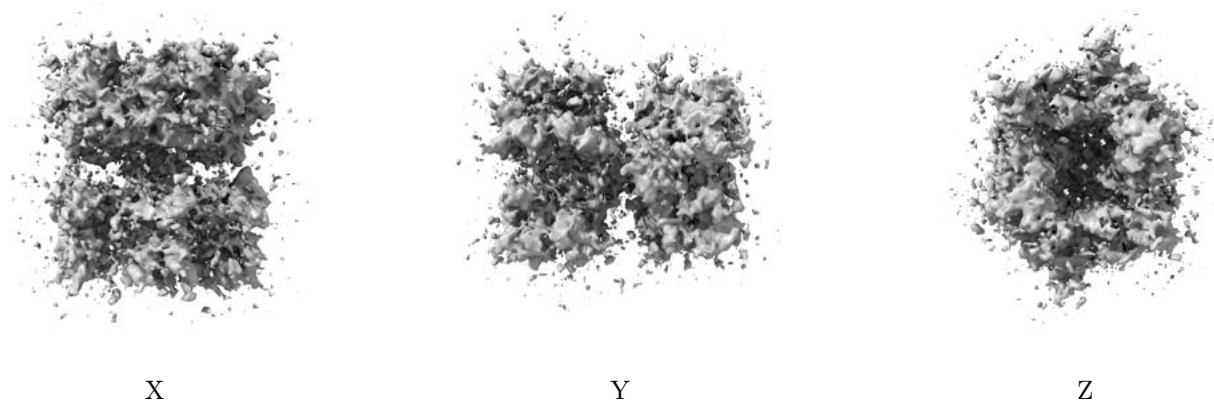


Z

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.

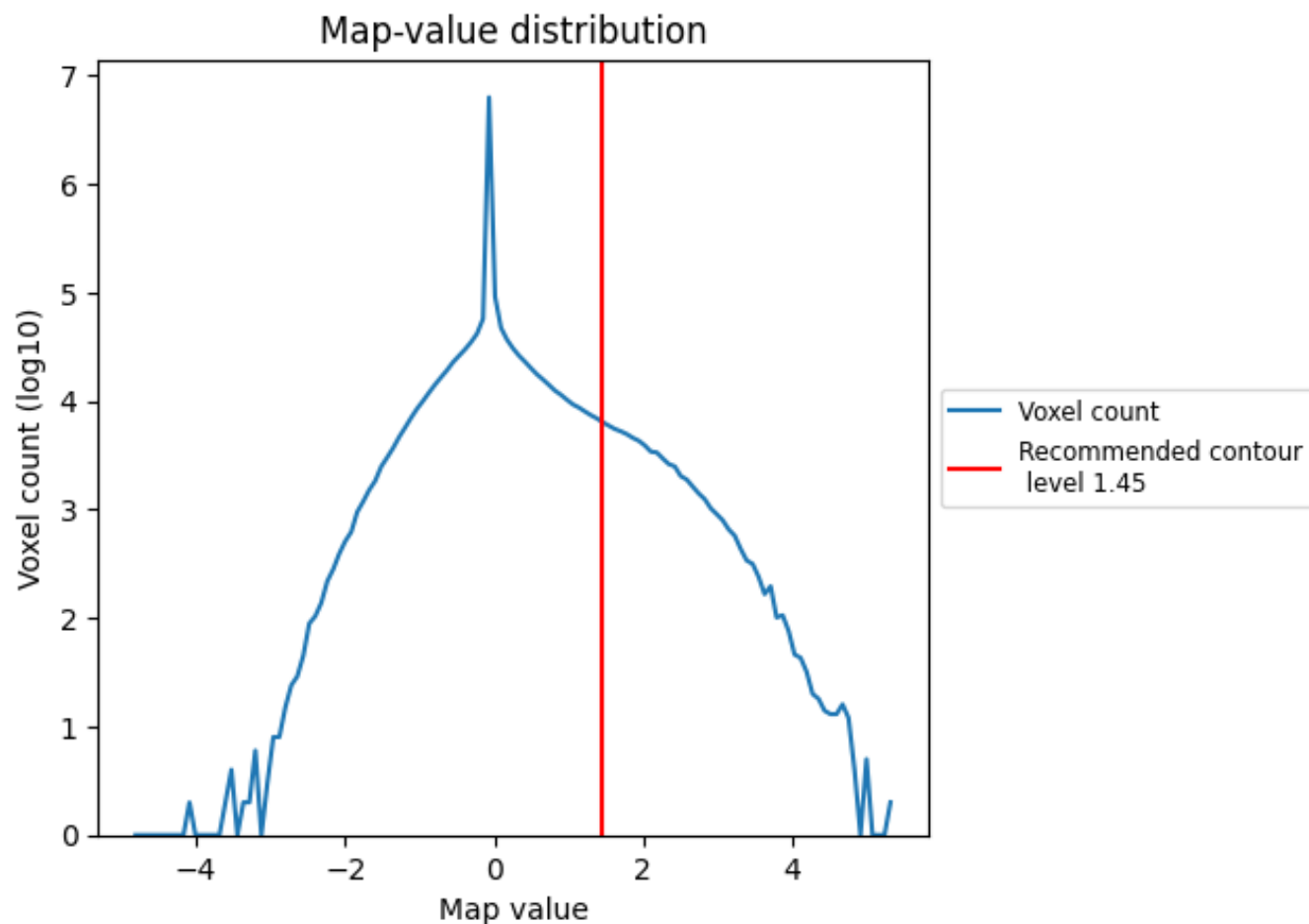
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

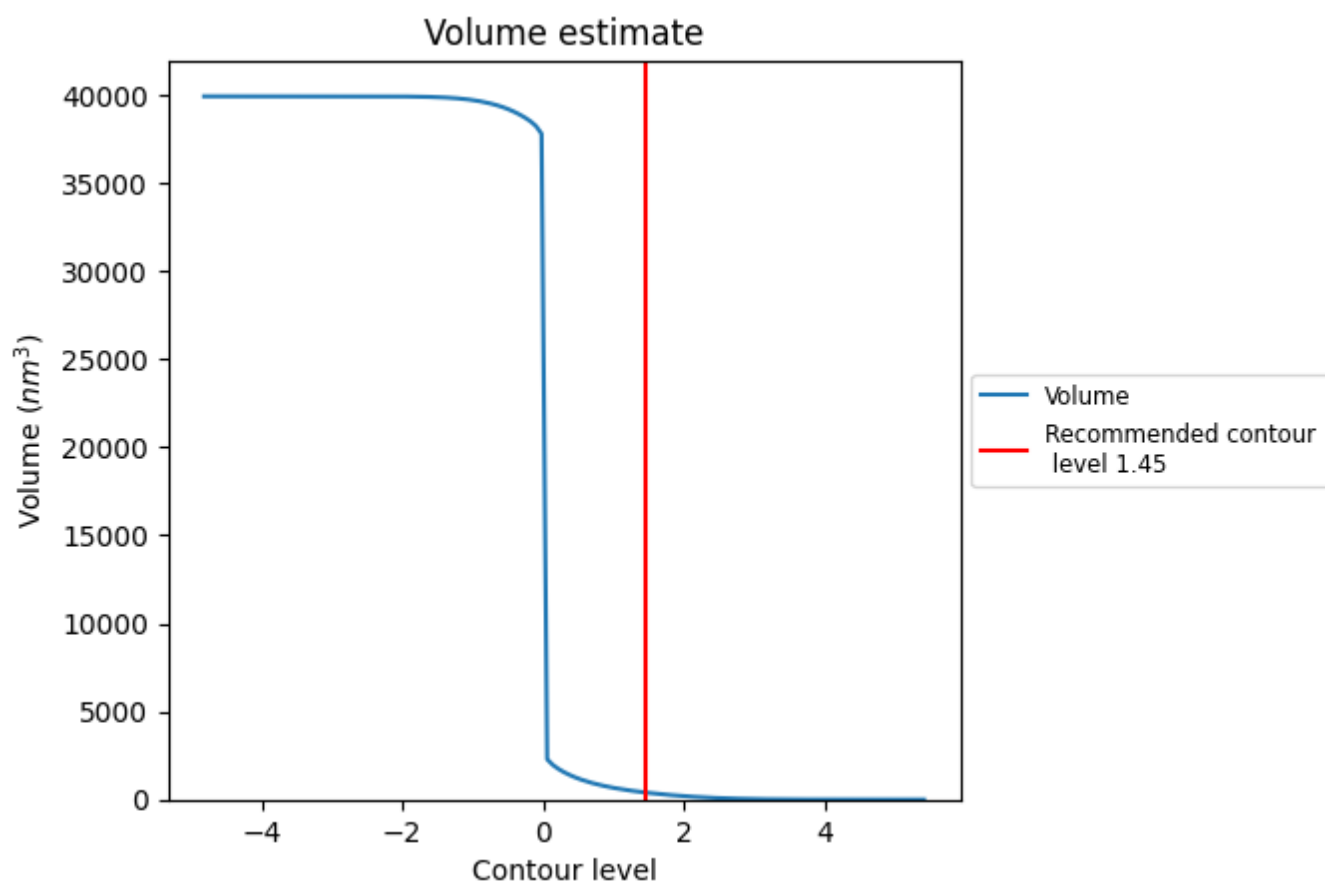
This section contains the results of statistical analysis of the map.

### 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.

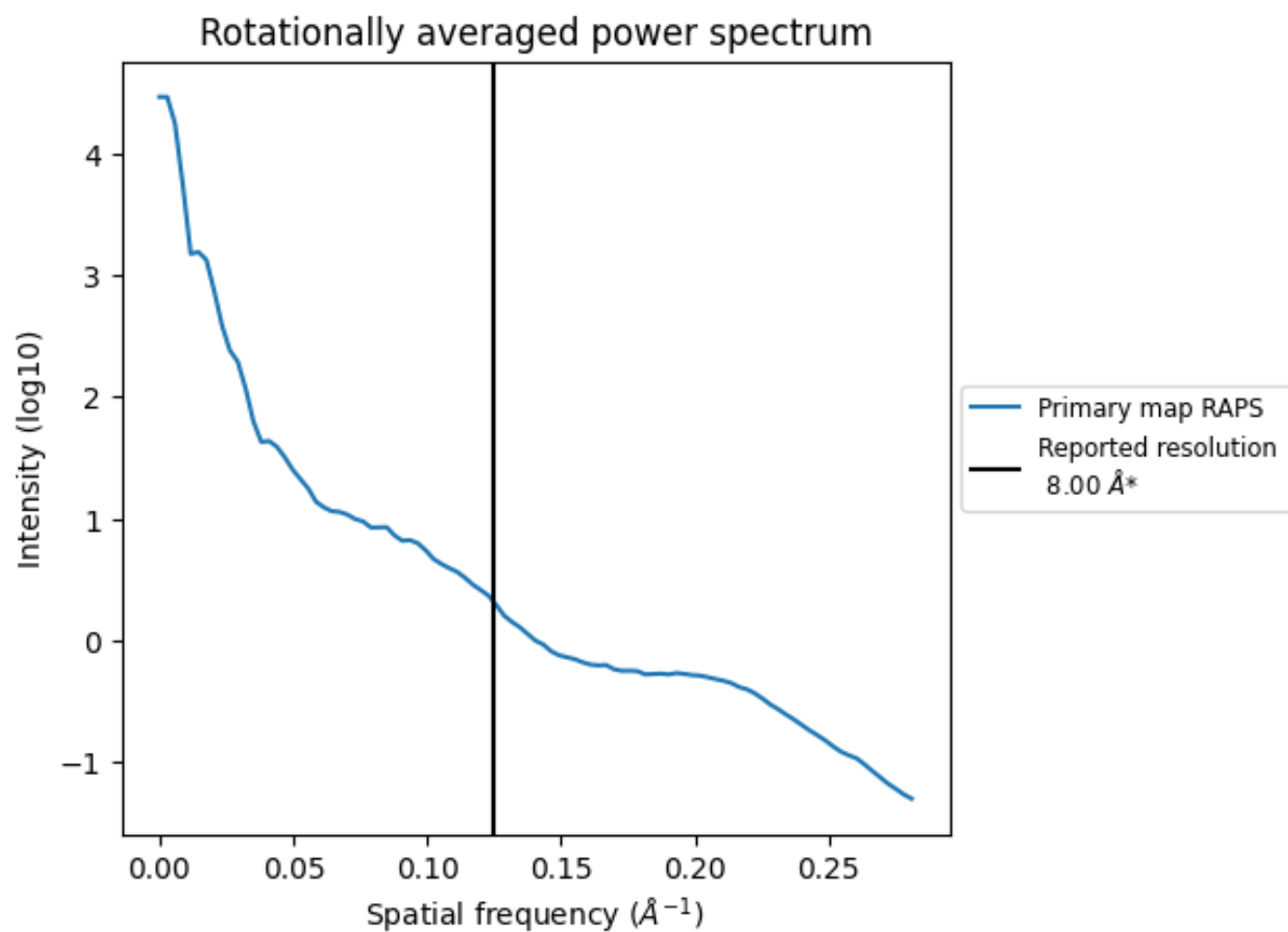
## 7.2 Volume estimate [i](#)



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>

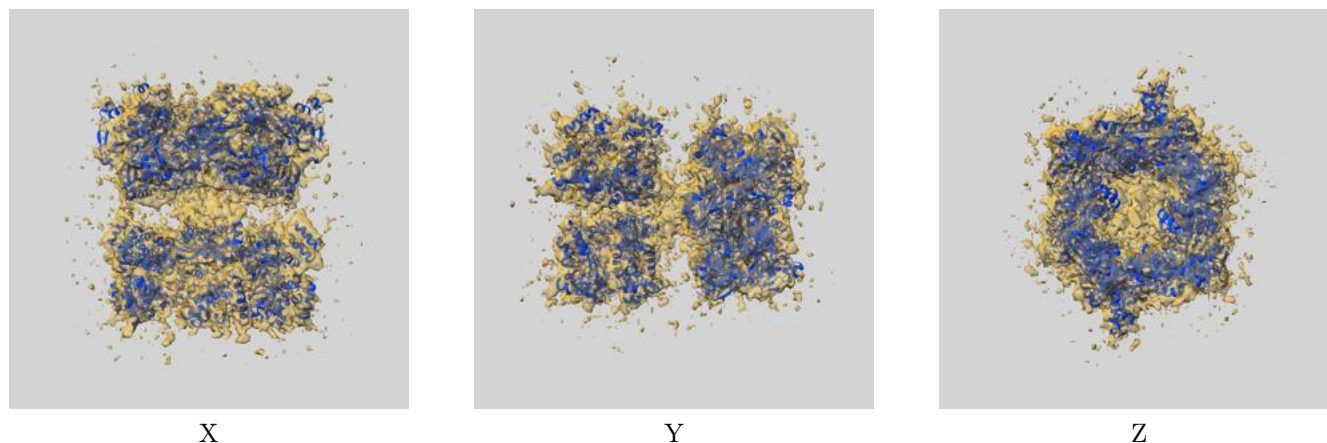
## 8 Fourier-Shell correlation

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

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

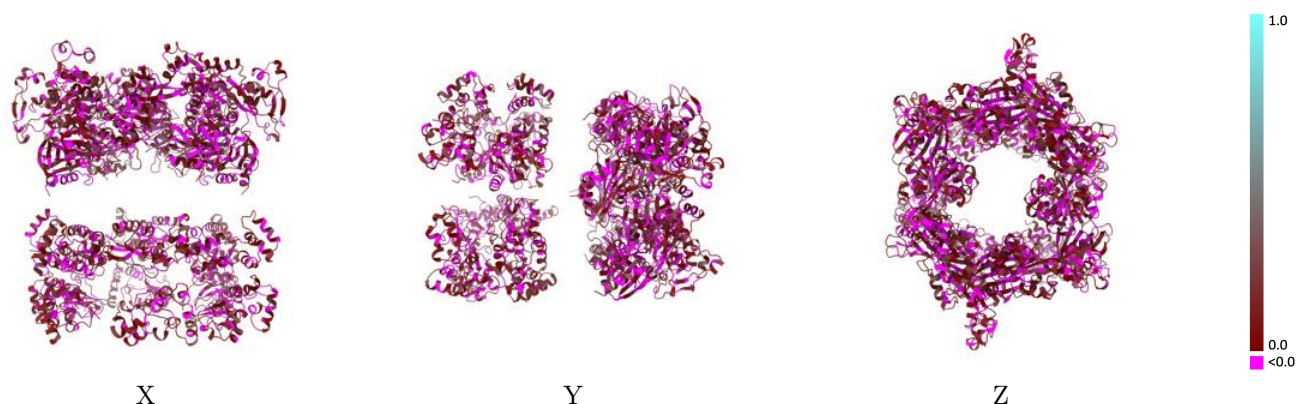
This section contains information regarding the fit between EMDB map EMD-4194 and PDB model 6F8L. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

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



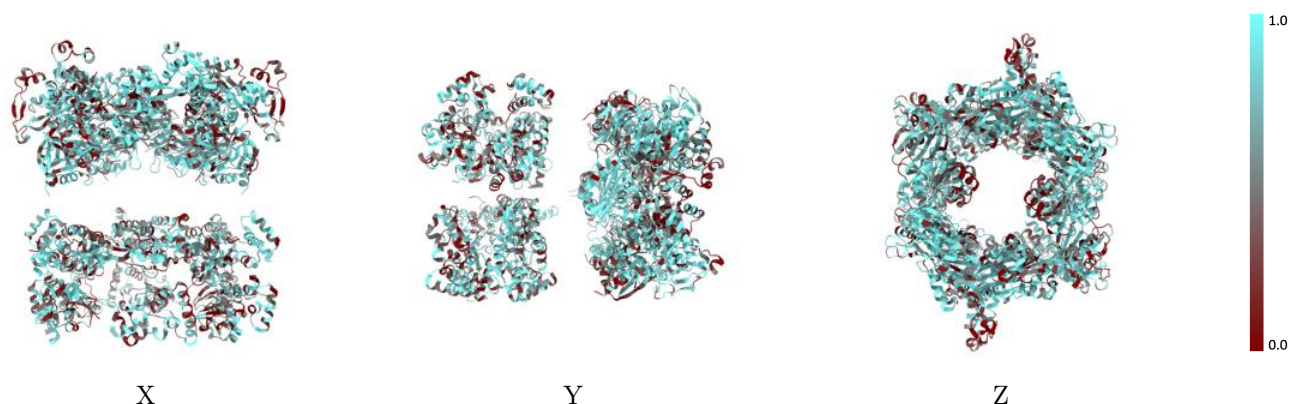
The images above show the 3D surface view of the map at the recommended contour level 1.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

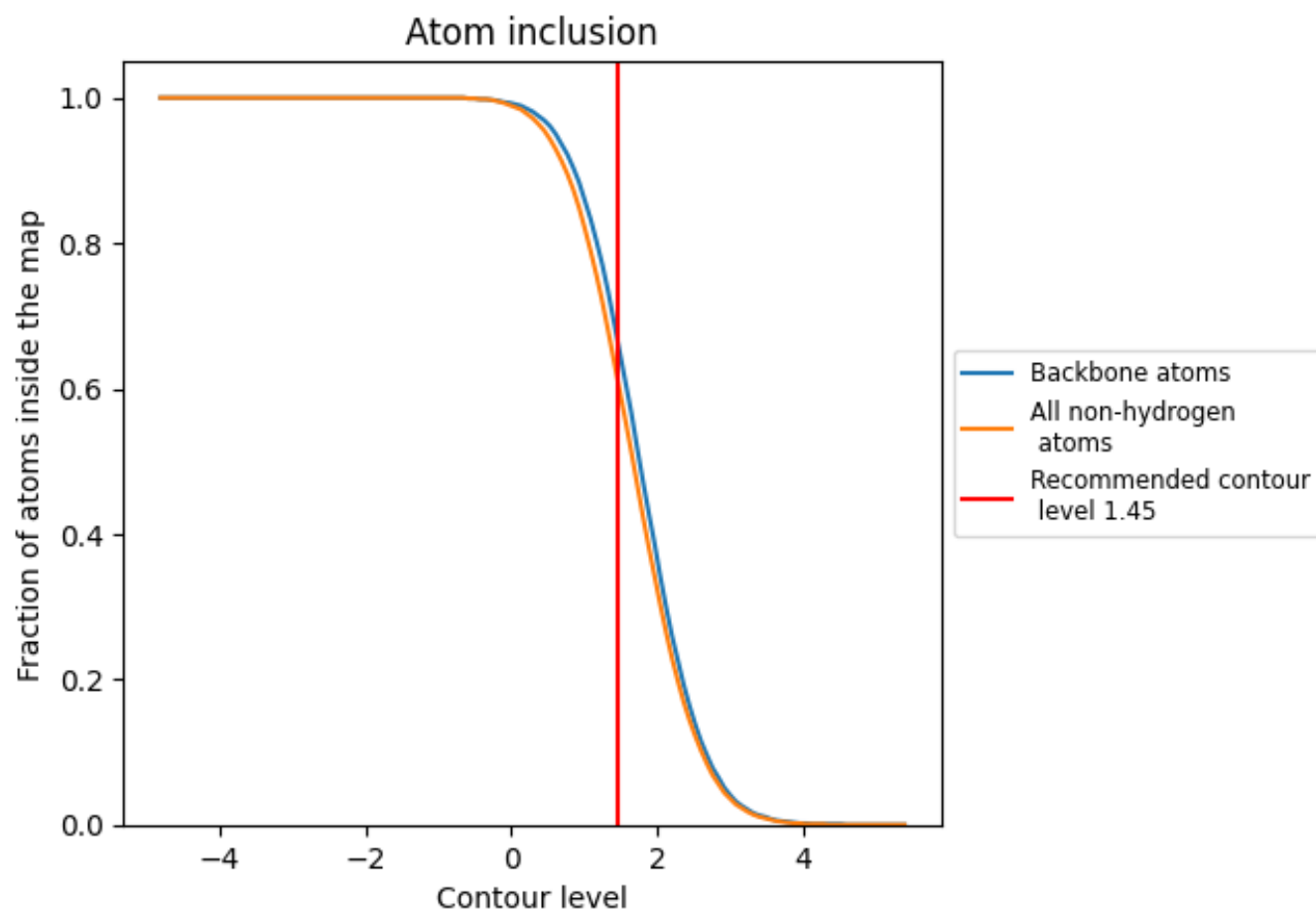
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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

