



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Oct 16, 2018 – 04:26 PM EDT

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/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

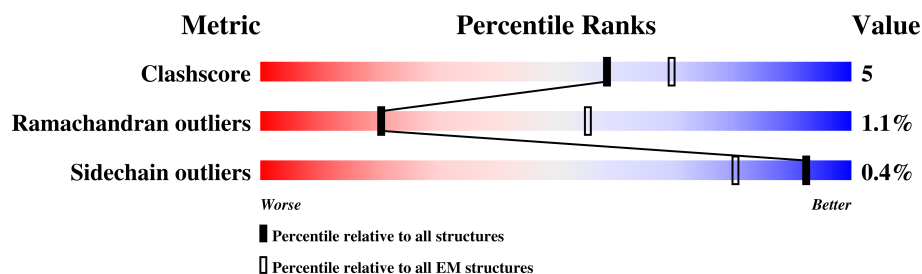
1 Overall quality at a glance

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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	913	37% 58%
1	B	913	36% 5% 58%
1	C	913	35% 7% 58%
1	D	913	35% 5% 58%
1	E	913	37% 5% 58%
1	F	913	36% 5% 58%
1	G	913	13% 84%
1	H	913	14% 84%
1	I	913	13% 84%

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Mol	Chain	Length	Quality of chain	
1	J	913	<div><div></div><div>13%</div><div></div><div></div><div></div></div>	85%
1	K	913	<div><div></div><div>12%</div><div></div><div></div><div></div></div>	85%
1	L	913	<div><div></div><div>13%</div><div></div><div></div><div></div></div>	85%
1	M	913	<div><div></div><div>14%</div><div></div><div></div><div></div></div>	84%
1	N	913	<div><div></div><div>13%</div><div></div><div></div><div></div></div>	85%
1	O	913	<div><div></div><div>12%</div><div></div><div></div><div></div></div>	85%
1	P	913	<div><div></div><div>13%</div><div></div><div></div><div></div></div>	85%
1	Q	913	<div><div></div><div>15%</div><div></div><div></div><div></div></div>	84%
1	R	913	<div><div></div><div>13%</div><div></div><div></div><div></div></div>	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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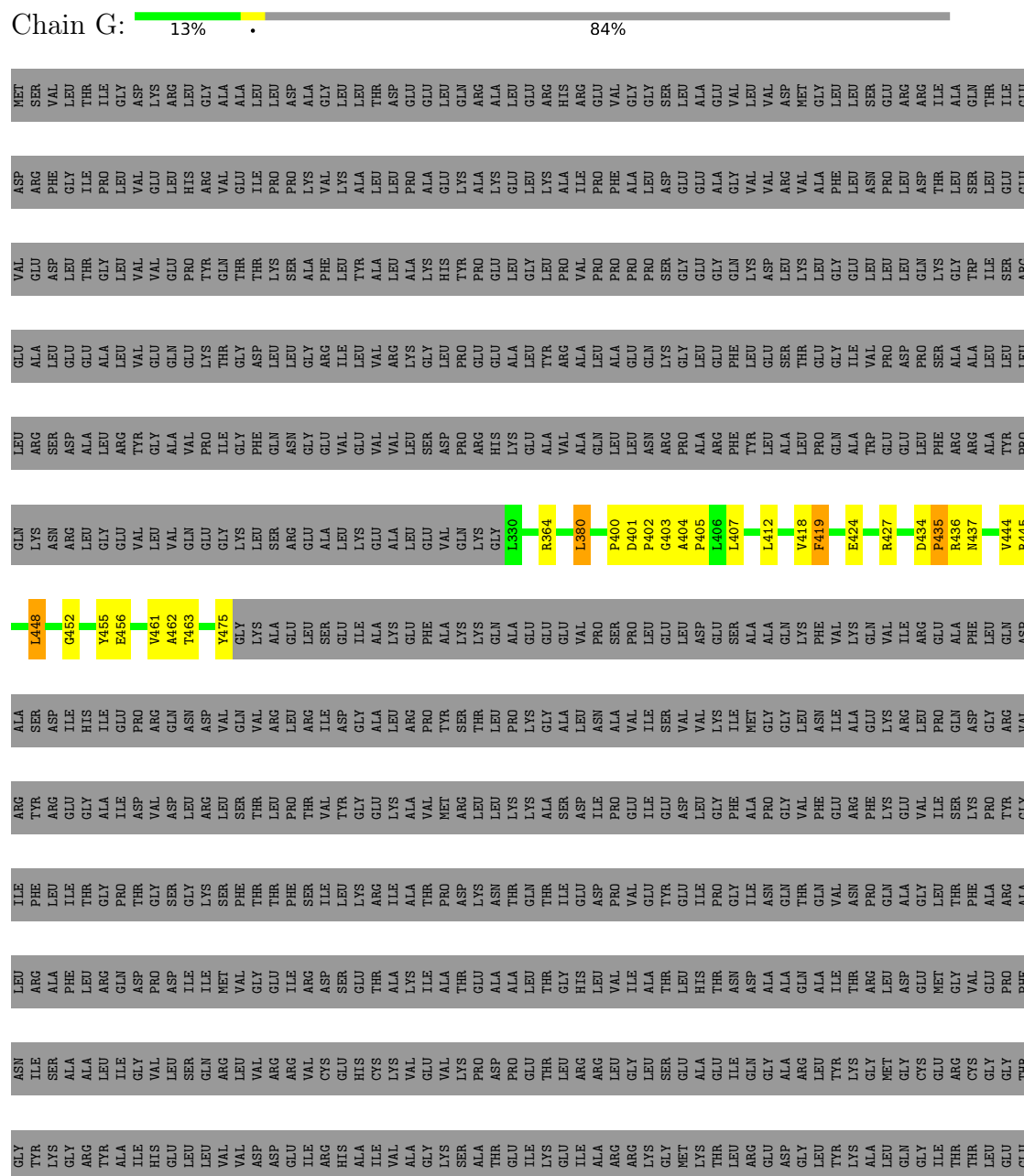
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Chain	Residue	Modelled	Actual	Comment	Reference
F	896	LEU	-	expression tag	UNP Q5SLC9
F	897	VAL	-	expression tag	UNP Q5SLC9
F	898	PRO	-	expression tag	UNP Q5SLC9
F	899	ARG	-	expression tag	UNP Q5SLC9
F	900	GLY	-	expression tag	UNP Q5SLC9
F	901	SER	-	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 and DNA 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. 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. 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



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

- Molecule 1: Type IV pilus assembly protein PilF

Chain J: 13% . 85%

MET	SER	VAL	THR	ILE	ASP	LYS	ARG	LEU	GLY	ALA	ALA	LEU	LEU	ASP	ALA	GLY	LEU	THR	THR	ASP	GLU	GLU	LEU	GLN	ARG	ALA	LEU	GLU	GLU	VAL	GLY	GLY	SER	SER	SER	GLU	GLU	ARG	ARG	ILE	ALA	GLN	THR	THR
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ASP	ARG	ARG	PHE	GLY	ILE	PRO	VAL	VAL	GLU	LEU	HIS	ARG	VAL	GLU	ILE	PRO	PRO	LYS	VAL	LYS	ALA	LEU	PRO	ALA	GLY	LEU	LYS	ALA	LYS	GLU	LEU	LYS	ALA	ILE	PRO	PHE	ALA	LEU	ASP	GLU	ALA	GLY	VAL	VAL	ARG	VAL	ALA	ALA	ASN	LEU	PRO	LEU	ASP	THR	LEU	LEU	LEU	GLY	GLU
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VAL	GLU	ASP	LEU	THR	GLY	LEU	VAL	VAL	PRO	PRO	TYR	GLN	THR	THR	LYS	SER	ALA	PHE	LEU	ALA	ALA	LEU	LEU	ALA	LYS	LEU	THR	TYR	PRO	GLU	GLU	LEU	GLY	LEU	PRO	PRO	PRO	PRO	SER	SER	GLY	GLU	GLU	GLY	G163	K167	L168	G169	L172	I178	V202	R203	L206	L211	G212	P213
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Y248
G249
A250
E259
L264
K270
V273
L276
P287
P288
R297
A298
Y299

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

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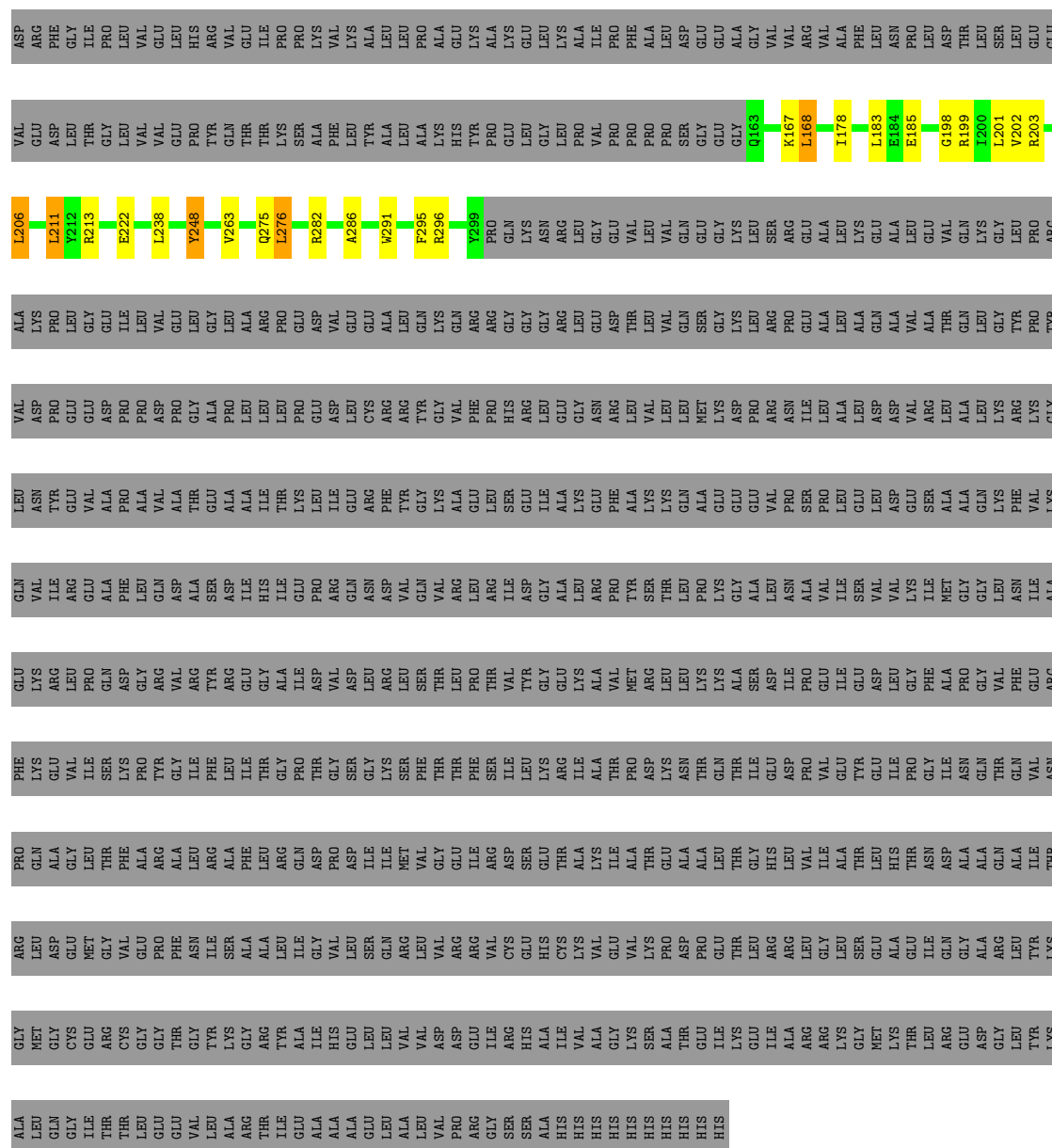
CYS	GLY	THR	GLY	TYR	LYS	GLY	ARG	ALA	ILE	HIS	LEU	LEU	VAL	VAL	ASP	ASP	GLU	ILE	ILE	ARG	HIS	ALA	ILE	VAL	VAL	GLY	LYS	SER	ALA	ALA	ALA	ARG	ARG	LYS	GLY	GLY	LYS	THR	THR	LEU	ARG	GLU	GLY	LEU	LYS	ALA	GLN	GLY	ILE	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----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

[illegible]

- Molecule 1: Type IV pilus assembly protein PilF

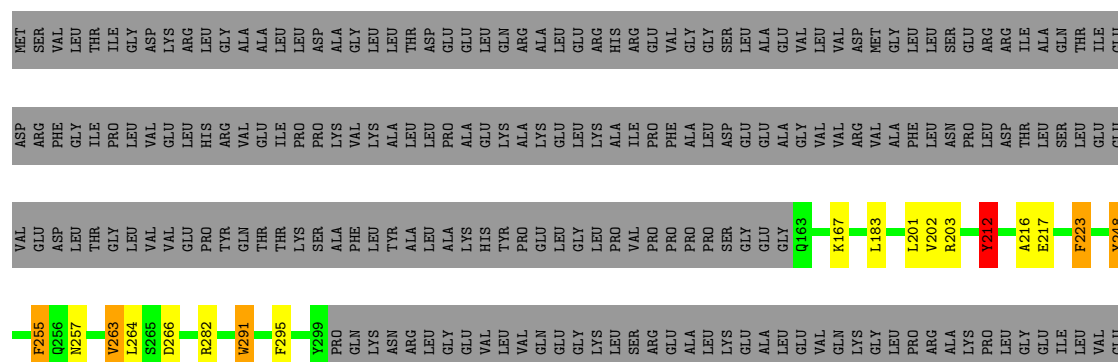
Chain K: 12% .. 85%

MET	SER	VAL	THR	LEU	ILE	GLY	ASP	LYS	ARG	LEU	GLY	ALA	ALA	LEU	LEU	ASP	ALA	GLY	THR	ASP	GLU	GLU	LEU	GLN	ARG	ALA	LEU	GLU	GLU	VAL	GLY	GLY	SER	SER	GLY	MET	GLY	LEU	LEU	ASP	VAL	VAL	LEU	GLU	GLN	THR	ILE	THR
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- Molecule 1: Type IV pilus assembly protein PilF

Chain L: 13% .. 85%



[illegible]

- Molecule 1: Type IV pilus assembly protein PilF

Chain H:  14% • 84%

[illegible]

[illegible]

- Molecule 1: Type IV pilus assembly protein PilF

Chain I:  13% 84%

[illegible]

[illegible]

- Molecule 1: Type IV pilus assembly protein PilF

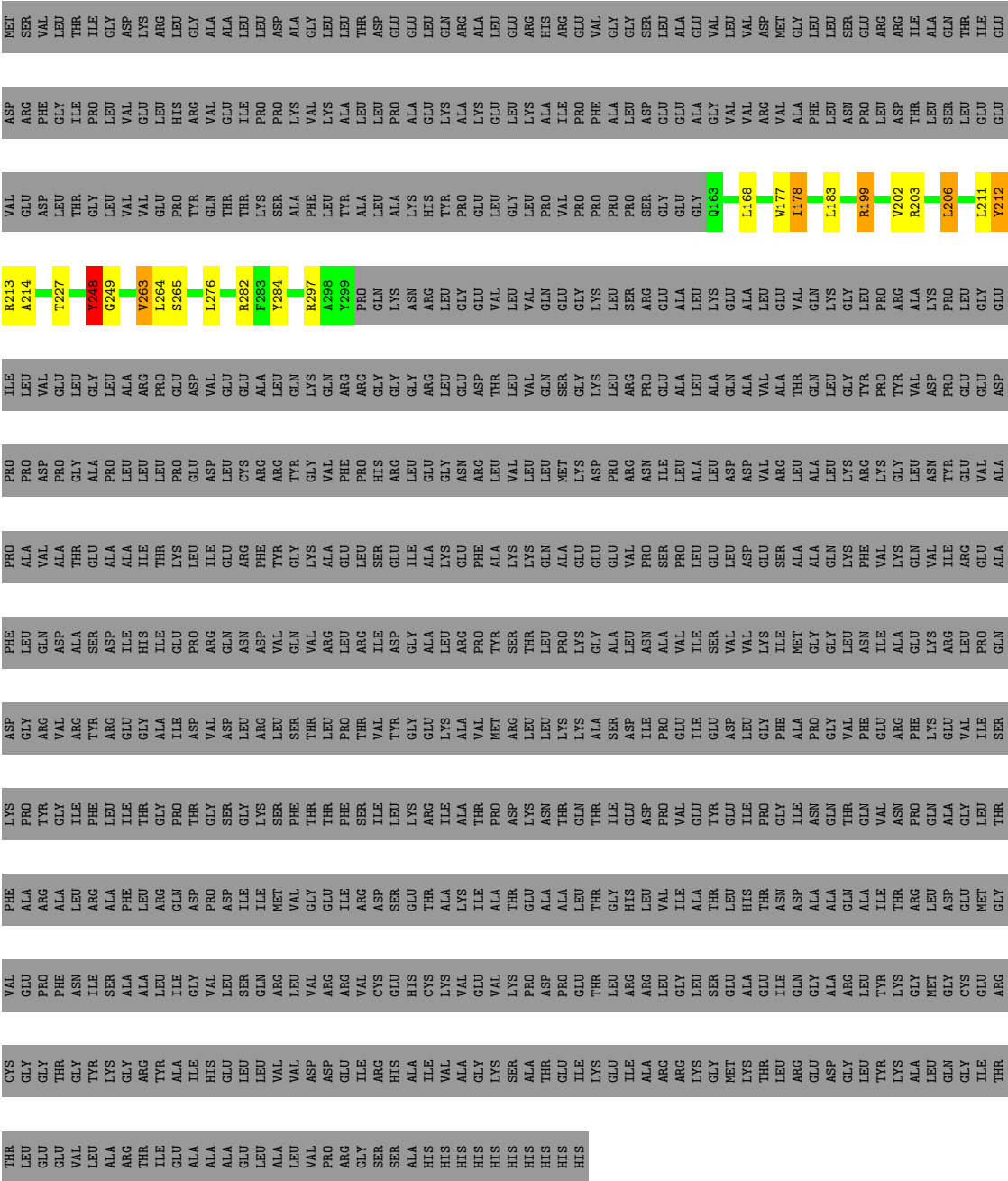
Chain M: 14% • 84%

[illegible]

LEU
VAL
PRO
ARG
GLY
SER
SER
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS

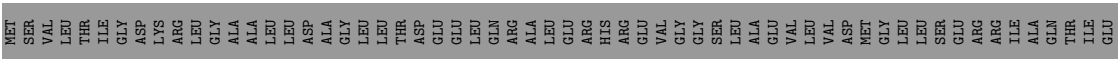
● Molecule 1: Type IV pilus assembly protein PilF

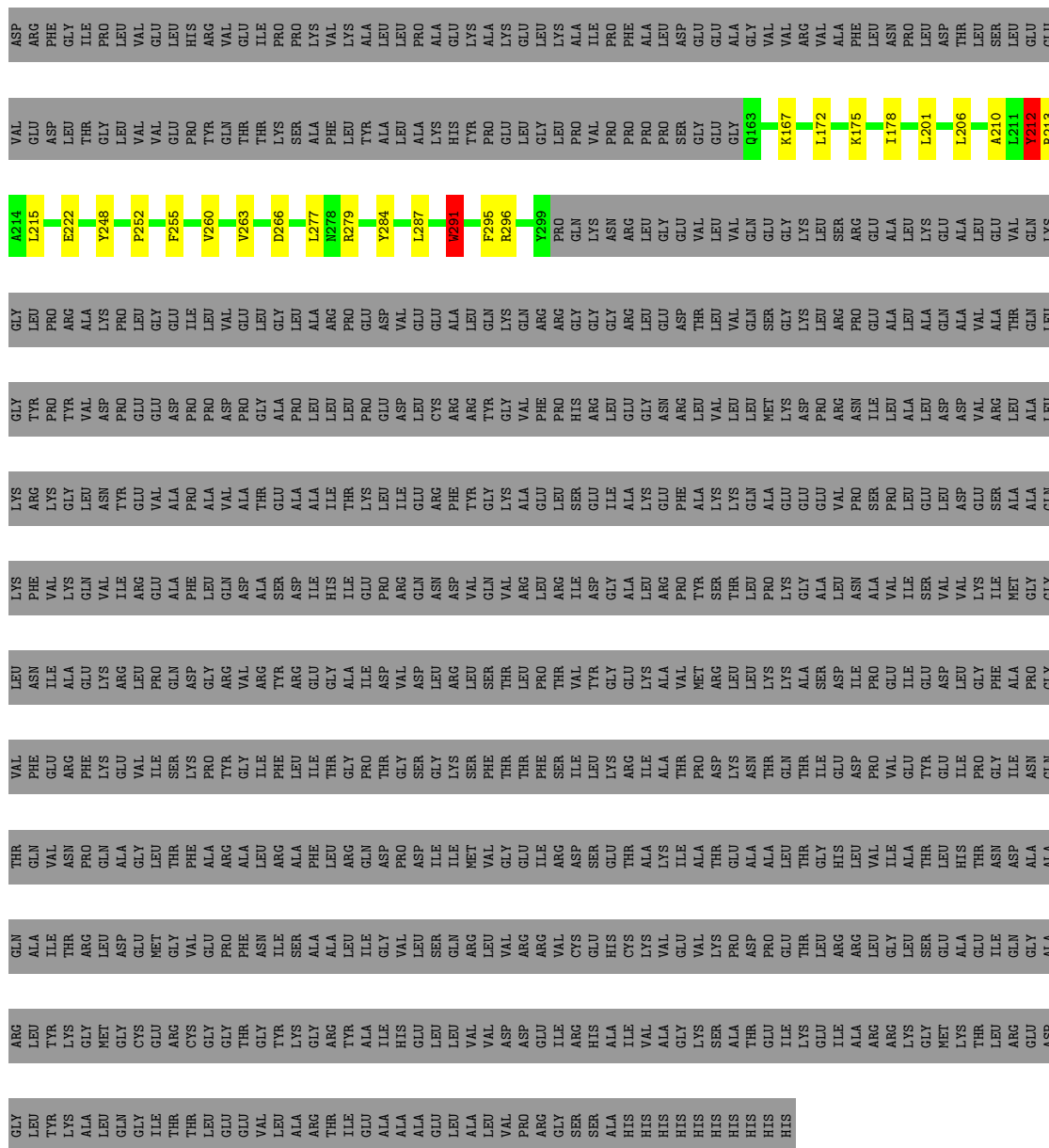
Chain N: 13% .. 85%



● Molecule 1: Type IV pilus assembly protein PilF

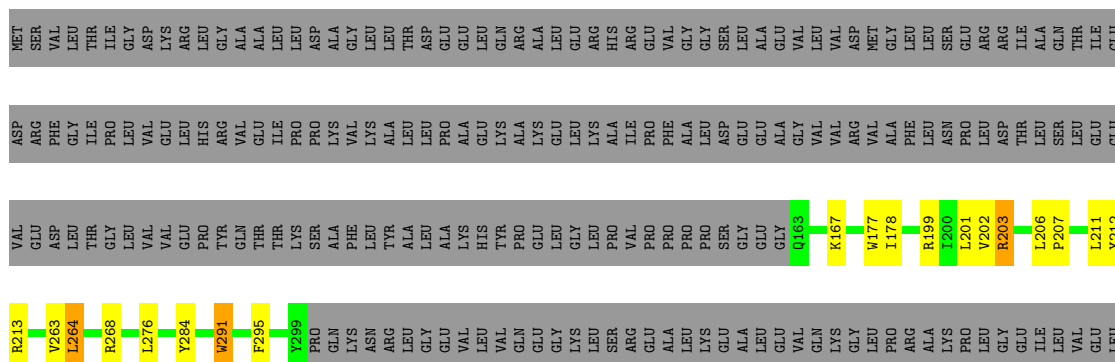
Chain O: 12% . 85%





- Molecule 1: Type IV pilus assembly protein PilF

Chain P:  13% . 85%



[illegible]

- Molecule 1: Type IV pilus assembly protein PilF

Chain Q:  15% . 84%

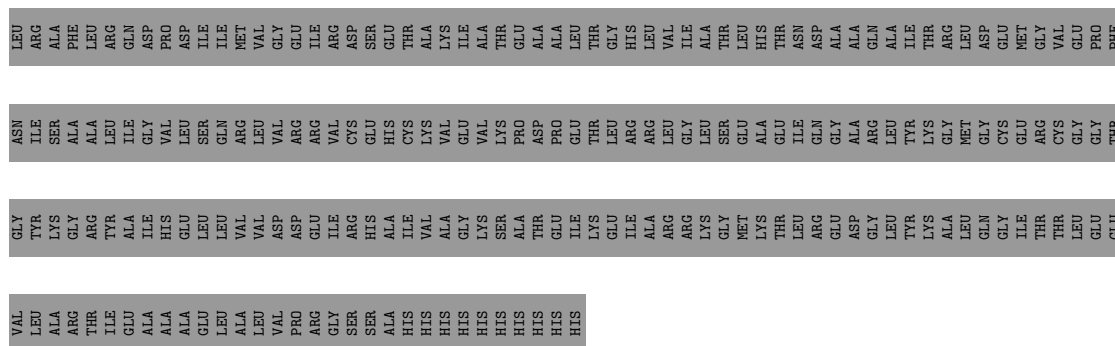
GLU	ILE	ALA	ASN	ARG	GLN	LEU	GLU	VAL	GLU	VAL	ASP	MET
ILE	ALA	ASN	SER	ARG	LYS	ARG	ALA	ALA	LEU	GLU	ARG	SER
LYS	GLU	ARG	ASP	ALA	LEU	ALA	GLU	GLU	THR	LEU	GLY	THR
PHE	ALA	GLY	LEU	LEU	GLY	LEU	ALA	GLY	GLY	PRO	ILE	ILE
ALA	LYS	VAL	TYR	ARG	GLU	ARG	LEU	VAL	LEU	VAL	LEU	ASP
GLY	LYS	VAL	GLY	GLY	GLU	GLY	GLU	VAL	VAL	GLY	GLY	ASP
ALA	GLN	VAL	ALA	VAL	GLN	VAL	GLN	VAL	GLU	GLY	GLY	ARG
GLU	GLU	PRO	ILE	PRO	GLY	ILE	THR	TYR	GLN	VAL	VAL	ALA
GLU	LYS	GLY	PHE	PHE	LYS	ASP	GLY	THR	THR	ILE	GLU	ALA
PRO	SER	SER	GLN	ASN	LEU	LEU	LEU	LYS	SER	PRO	PRO	ASP
PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PHE	ALA	LYS	LYS	GLY
LEU	LEU	VAL	VAL	GLU	ARG	ARG	ARG	THR	ALA	VAL	VAL	GLY
GLU	LEU	LYS	GLU	GLU	LYS	VAL	ILE	LEU	LEU	LYS	LYS	LEU
ASP	ASP	GLU	VAL	VAL	GLU	VAL	VAL	TYR	ALA	ALA	ALA	LEU
GLU	ALA	ALA	VAL	VAL	ALA	VAL	ARG	LEU	LEU	LEU	ASP	THR
SER	SER	LEU	SER	LEU	LEU	LEU	LYS	LYS	ALA	ALA	PRO	GLU
ALA	ALA	VAL	ASP	ASP	GLU	GLY	GLY	GLY	LYS	LYS	ALA	GLU
GLN	GLN	VAL	PRO	PRO	GLN	PRO	PRO	TYR	HIS	GLY	GLY	LEU
LYS	PHE	GLY	HIS	HIS	GLY	GLY	ALA	GLU	GLU	GLU	GLY	ALA
VAL	VAL	L330	LYS	LYS	GLU	GLY	LEU	LEU	LEU	GLY	LEU	LEU
LYS	GLN	L336	ALA	ALA	ALA	TYR	GLY	GLY	GLY	LYS	LEU	GLU
ILE	ILE	L340	VAL	VAL	VAL	ARG	ALA	VAL	PRO	ILE	ALA	ARG
ARG	ARG	E366	GLN	GLN	LEU	LEU	ALA	PRO	PRO	PHE	PRO	GLY
GLU	GLU	E378	ASN	ASN	GLN	GLU	GLU	PRO	PRO	ALA	PHE	VAL
PHE	PHE	V393	ARG	ARG	LYS	LYS	GLN	SER	SER	ASP	GLY	GLY
LEU	LEU	L408	PRO	PRO	ALA	LEU	GLY	GLY	GLY	GLU	GLU	LEU
ASN	ASN	C413	ALA	ALA	ARG	ALA	GLU	GLY	GLY	ALA	ALA	ALA
GLN	GLN	R414	TYR	TYR	PHE	PHE	PHE	GLN	GLY	GLY	GLY	GLU
ILE	ILE	F419	LEU	LEU	LEU	LEU	THR	LYS	LYS	VAL	MET	MET
PRO	PRO	E466	GLN	GLN	PRO	PRO	GLU	LEU	LEU	ALA	ALA	GLY
ARG	ARG	W457	ALA	ALA	TRP	TRP	ILE	GLU	GLU	PHE	PHE	LEU
GLN	GLN	L470	GLY	GLY	GLU	GLU	ASP	LEU	LEU	ASN	ASN	SER
ASN	ASN	Y475	GLU	GLU	GLY	GLY	PRO	LEU	LEU	PRO	PRO	GLY
VAL	VAL	GLY	LEU	LEU	LEU	LEU	PRO	GLN	GLN	ASP	ASP	ARG
GLN	GLN	LYS	PHE	PHE	GLY	PHE	SER	LYS	LYS	THR	THR	ILE
VAL	VAL	ARG	ARG	ARG	ALA	ALA	ALA	GLY	GLY	LEU	LEU	ALA
LEU	LEU	GLU	ALA	ALA	GLU	GLU	ALA	TRP	TRP	SER	SER	GLN
ARG	ARG	LEU	TYR	TYR	LEU	LEU	LEU	ILE	ILE	LEU	LEU	THR
ILE	ILE	SER	PRO	PRO	SER	PRO	LEU	ARG	ARG	GLY	GLY	ILE

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

- Molecule 1: Type IV pilus assembly protein PilF

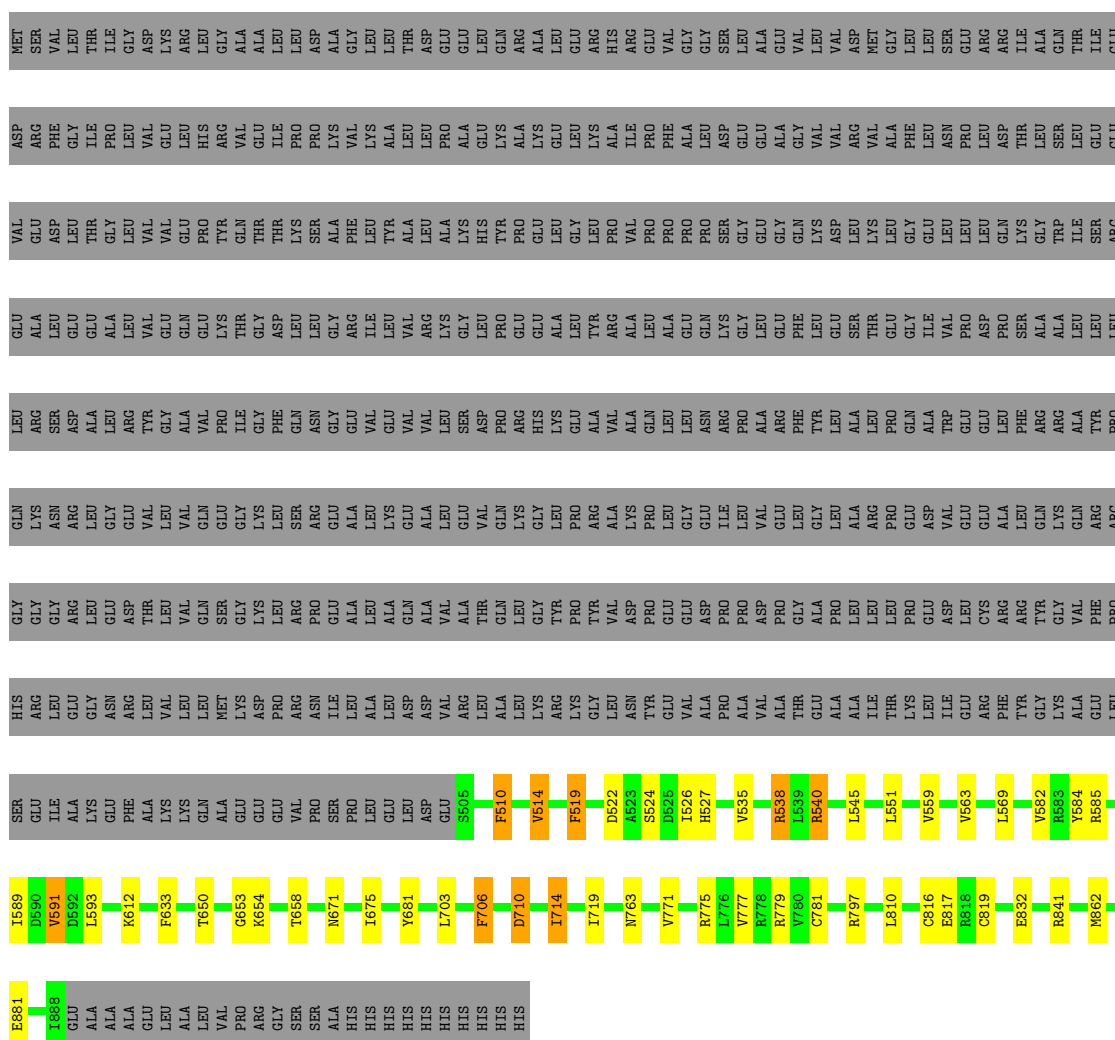
Chain R: 13% . 84%

[illegible]



- Molecule 1: Type IV pilus assembly protein PilF

Chain A:  37% 2% 58%



- Molecule 1: Type IV pilus assembly protein PilF

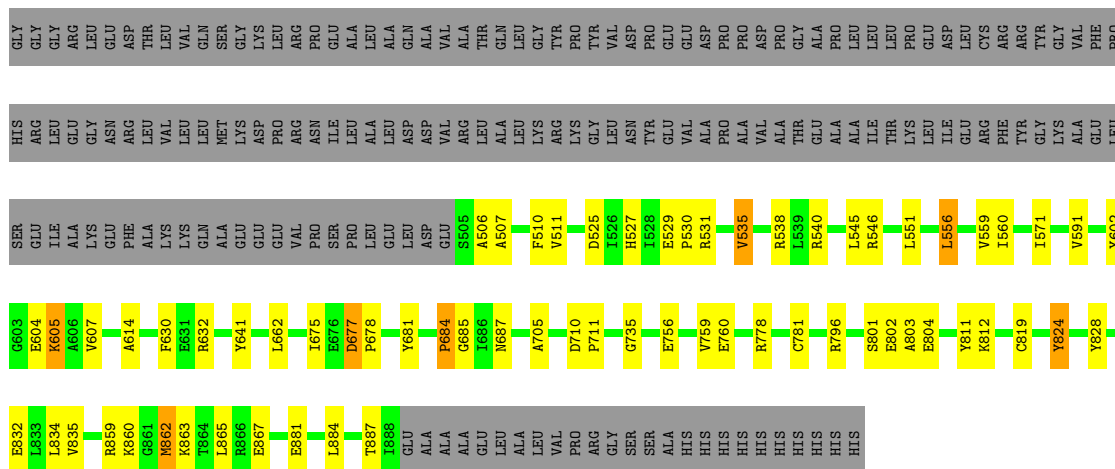
Chain B: 36% 5% 58%

ILE	F644	SER	HIS	GLY	GLN	LEU	GLU	VAL	ASP	MET
GLU		GLU	ARG	GLY	LYS	ARG	ALA	GLU	VAL	ARG
ALA	T650	ILE	LEU	GLY	ASN	SER	LEU	ASP	PHE	SER
ALA		ALA	GLU	ARG	LEU	ASP	GLU	GLU	GLY	LEU
ALA	K654	LYS	LEU	LEU	GLY	ALA	GLU	THR	ILE	THR
GLU	S655	GLU	ASN	GLU	GLY	LEU	ALA	LEU	PRO	ILE
LEU	F656	PHE	ARG	ASP	GLU	ARG	LEU	LEU	LEU	GLY
ALA		ALA	LEU	THR	VAL	TYR	VAL	VAL	VAL	ASP
LEU	F659	LYS	VAL	LEU	LEU	GLY	GLN	GLU	LYS	ARG
VAL		LYS	LEU	VAL	VAL	ALA	GLN	GLU	LEU	ARG
PRO	L662	GLN	LEU	GLN	GLN	VAL	GLU	PRO	HIS	LEU
ARG		ALA	MET	SER	GLU	PRO	LYS	TYR	ARG	GLY
GLY	A666	GLU	LYS	GLY	GLY	ILE	THR	GLN	VAL	ALA
SER		GLU	ASP	LYS	LYS	PHE	GLY	THR	GLU	LEU
SER	M671	GLU	PRO	LEU	LEU	GLN	ASP	THR	ILE	ALA
ALA		VAL	ARG	SER	SER	ASN	LEU	PRO	PRO	LEU
HIS	T674	PRO	ASN	PRO	ARG	ASN	LEU	SER	LEU	ASP
HIS	I675	SER	ILE	GLU	GLU	GLY	GLY	ALA	LYS	ALA
HIS	E676	PRO	LEU	ALA	ALA	GLU	ARG	PHE	VAL	GLY
HIS	D677	LEU	ALA	LEU	LEU	VAL	ILE	LEU	LYS	LEU
HIS	P678	GLU	LEU	ALA	LYS	GLU	LEU	TYR	ALA	THR
HIS	V679	LEU	ASP	GLN	GLU	VAL	VAL	ALA	LEU	ASP
HIS		ASP	ASP	ALA	ALA	VAL	ARG	LEU	LEU	GLU
HIS	I686	GLU	VAL	VAL	LEU	LEU	LYS	ALA	PRO	GLU
HIS		S695	ARG	ALA	GLU	SER	GLY	LYS	ALA	GLU
HIS	V691		LEU	THR	VAL	PRO	LEU	HIS	GLU	LEU
	N692	F510	ALA	GLN	GLN	ASP	PRO	TYR	LYS	GLN
		Y511	LEU	LEU	LYS	ARG	PRO	PRO	ALA	ARG
	R720		LYS	GLY	GLY	HIS	GLU	GLU	LYS	ALA
		S524	ARG	TYR	LEU	LYS	ALA	LEU	GLU	LEU
	H743		LYS	PRO	PRO	GLU	LEU	GLY	LEU	GLU
		H527	GLY	TYR	ARG	ALA	TYR	LEU	LYS	ARG
	E760	I528	LEU	VAL	ALA	VAL	ARG	PRO	ILE	HIS
	P761	E529	ASN	ASP	ALA	ALA	ALA	VAL	ALA	ARG
	F762	P530	TYR	PRO	PRO	GLN	LEU	PRO	PRO	GLU
			GLU	GLU	LEU	LEU	ALA	PRO	PHE	VAL
	V777	V535	VAL	GLU	GLY	LEU	GLU	PRO	GLY	GLY
			ALA	ASP	GLU	ASN	GLN	PRO	LEU	ALA
	C784	R540	PRO	PRO	ILE	ARG	LYS	SER	ASP	SER
			ALA	PRO	LEU	PRO	GLY	GLY	LEU	ALA
	P790	L551	VAL	ASP	VAL	ALA	LEU	GLU	GLU	GLU
			ALA	PRO	GLU	ARG	GLU	GLY	ALA	GLU
	L795	L556	THR	GLY	LEU	PHE	PHE	GLN	VAL	VAL
	R796		GLU	ALA	GLY	TYR	GLY	LYS	VAL	VAL
	R797	I560	ALA	PRO	LEU	LEU	GLU	ASP	VAL	ASP
			ALA	LEU	ALA	ALA	SER	LYS	ARG	MET
	C816	L576	ILE	LEU	ARG	LEU	THR	LEU	VAL	GLY
			THR	LEU	PRO	PRO	GLU	LEU	ALA	LEU
	C819	V582	LYS	PRO	GLU	GLN	GLY	GLY	PHE	GLY
			ILE	GLU	ASP	ALA	ILE	GLU	LEU	LEU
	R827	V591	LEU	ASP	VAL	TRP	VAL	VAL	ASN	SER
	Y828		LEU	LEU	GLU	GLU	GLU	LEU	PRO	GLU
		L595	ARG	CYS	GLU	GLU	ASP	LEU	LEU	ARG
			GLU	ARG	ALA	LEU	PRO	GLN	ASP	ARG
	L833		PHE	ARG	ALA	LEU	PRO	LYS	THR	ILE
		M608	TYR	TYR	LEU	PHE	SER	GLY	ALA	GLN
	M862		GLY	TYR	GLN	ARG	ALA	TRP	SER	GLN
		R632	LYS	VAL	GLN	ALA	LEU	ILE	THR	THR
	E882		ALA	VAL	GLN	ALA	LEU	ILE	LEU	GLN
		Y641	LEU	PHE	ARG	TYR	LEU	ARG	GLU	ILE
	T887		THR	PRO	ASN	PRO	LEU	ARG	GLU	GLU

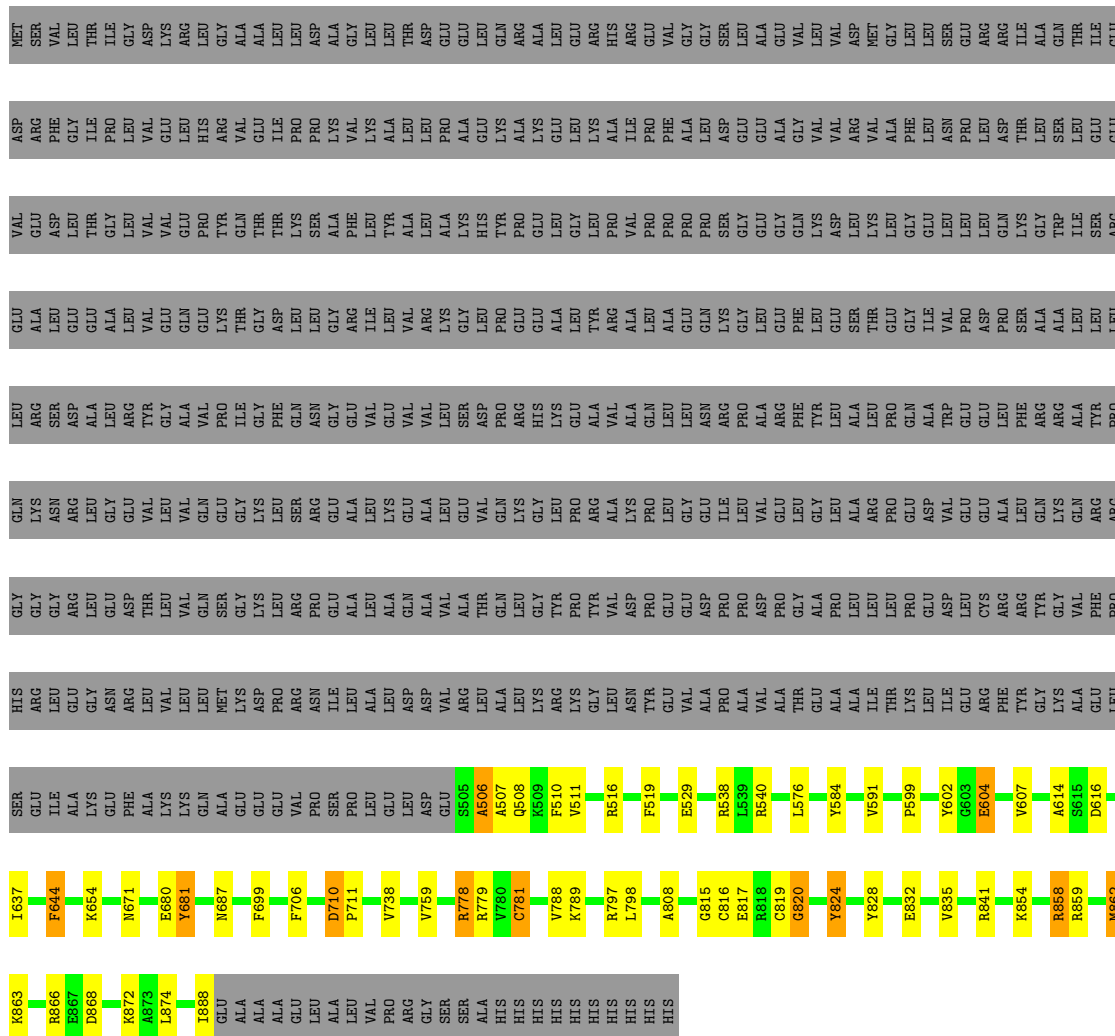
- Molecule 1: Type IV pilus assembly protein PilF

Chain C: 35% 7% 58%

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



- Molecule 1: Type IV pilus assembly protein PilF



- Molecule 1: Type IV pilus assembly protein PilF

Chain E:

[illegible]

- Molecule 1: Type IV pilus assembly protein PilF

Chain F:



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

4885	GLY	HIS	SER	GLY	HIS	GLY	GLN
R886	GLY	ARG	GLU	GLY	LEU	GLY	LEU
T887	ARG	LEU	ILE	ASN	GLU	ARG	ASN
I888	ARG	GLY	LYS	ASN	GLY	LEU	LEU
	ALA	ARG	PHE	LEU	ASP	GLY	GLY
	ALA	LEU	ALA	VAL	THR	VAL	VAL
	GLU	LEU	LYS	LEU	VAL	VAL	VAL
	ALA	GLN	GLN	LEU	SER	GLY	GLN
	LEU	ALA	MET	LEU	GLY	GLY	GLY
	VAL	GLY	LYS	ASP	LYS	LYS	LYS
	PRO	GLY	GLU	PRO	LEU	LEU	LEU
	ARG	GLY	VAL	ARG	ARG	SER	SER
	GLY	VAL	VAL	PRO	PRO	ARG	ARG
	SER	ILE	SER	ILE	GLU	GLU	GLU
	SER	LEU	PRO	LEU	ALA	ALA	ALA
	ALA	LEU	LEU	ALA	LEU	LEU	LEU
	HIS	GLU	GLU	ASP	ALA	ALA	LYS
	HIS	ASP	ASP	ASP	GLN	GLN	GLN
	HIS	VAL	VAL	VAL	ALA	ALA	ALA
	HIS	GLU	GLU	ARG	VAL	VAL	LEU
	HIS	S505	ARG	LEU	ALA	ALA	GLY
	HIS	D710	LEU	ALA	THR	THR	VAL
	HIS	F711	ALA	ALA	GLN	GLN	VAL
	HIS	D712	LEU	LEU	LEU	LEU	GLN
	HIS	R720	LYS	LYS	GLY	GLY	LYS
	HIS	D721	ARG	TYR	TYR	TYR	LEU
	HIS	L733	LYS	LYS	PRO	PRO	PRO
	HIS	T734	GLY	GLY	TYR	TYR	ARG
	HIS	G735	LEU	LEU	VAL	VAL	ALA
	HIS	H743	VAL	VAL	GLU	GLU	LYS
	HIS	S765	ALA	ALA	VAL	GLY	GLY
	HIS	A766	PRO	PRO	ALA	GLU	GLY
	HIS	R775	ALA	ALA	PRO	LEU	LEU
	HIS	R778	THR	THR	GLY	ALA	LEU
	HIS	G807	ALA	ALA	PRO	LEU	LEU
	HIS	C819	ILE	ILE	LEU	ALA	ALA
	HIS	D837	THR	THR	LEU	LEU	ARG
	HIS	R841	LYS	LYS	PRO	GLY	PRO
	HIS	K860	LEU	LEU	ASP	ASP	ASP
	HIS	L870	ILE	ILE	VAL	VAL	VAL
	HIS	E882	L598	L598	GLU	GLU	GLU
	HIS	V883	P599	P599	LEU	LEU	LEU
	HIS	L884	T600	T600	CYS	CYS	GLY
	HIS		V601	V601	ARG	ARG	ALA
	HIS		Y602	Y602	ARG	ARG	ALA
	HIS		R609	R609	TYR	TYR	LEU
	HIS		K613	K613	GLY	GLY	GLN
	HIS				VAL	VAL	LYS
	HIS				PHE	PHE	GLN
	HIS				PRO	PRO	ARG
	HIS				LEU	LEU	ARG

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
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	Depositor
Image detector	GATAN K2 BASE (4k x 4k)	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	$\# Z > 2$	RMSZ	$\# Z > 2$
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:O	1:F:683:ILE:HG22	1.50	1.06
1:Q:336:LEU:HD13	1:Q:336:LEU:C	1.78	1.02
1:B:679:VAL:O	1:B:679:VAL:HG12	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%)	43 81
1	B	381/913 (42%)	369 (97%)	10 (3%)	2 (0%)	31 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	382/913 (42%)	368 (96%)	8 (2%)	6 (2%)	11	50
1	D	382/913 (42%)	366 (96%)	13 (3%)	3 (1%)	21	65
1	E	382/913 (42%)	367 (96%)	13 (3%)	2 (0%)	31	74
1	F	382/913 (42%)	367 (96%)	13 (3%)	2 (0%)	31	74
1	G	144/913 (16%)	133 (92%)	6 (4%)	5 (4%)	4	32
1	H	144/913 (16%)	132 (92%)	9 (6%)	3 (2%)	8	43
1	I	144/913 (16%)	137 (95%)	6 (4%)	1 (1%)	24	67
1	J	135/913 (15%)	123 (91%)	10 (7%)	2 (2%)	11	51
1	K	135/913 (15%)	126 (93%)	7 (5%)	2 (2%)	11	51
1	L	135/913 (15%)	123 (91%)	9 (7%)	3 (2%)	7	42
1	M	144/913 (16%)	133 (92%)	8 (6%)	3 (2%)	8	43
1	N	135/913 (15%)	128 (95%)	6 (4%)	1 (1%)	24	67
1	O	135/913 (15%)	124 (92%)	10 (7%)	1 (1%)	24	67
1	P	135/913 (15%)	130 (96%)	3 (2%)	2 (2%)	11	51
1	Q	144/913 (16%)	135 (94%)	8 (6%)	1 (1%)	24	67
1	R	144/913 (16%)	135 (94%)	7 (5%)	2 (1%)	12	52
All	All	3965/16434 (24%)	3770 (95%)	153 (4%)	42 (1%)	20	58

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%)	93	96
1	B	315/751 (42%)	313 (99%)	2 (1%)	87	93
1	C	317/751 (42%)	317 (100%)	0	100	100
1	D	317/751 (42%)	315 (99%)	2 (1%)	87	93
1	E	317/751 (42%)	317 (100%)	0	100	100
1	F	317/751 (42%)	316 (100%)	1 (0%)	93	96
1	G	120/751 (16%)	119 (99%)	1 (1%)	83	92
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%)	81	90
1	L	112/751 (15%)	110 (98%)	2 (2%)	62	82
1	M	120/751 (16%)	120 (100%)	0	100	100
1	N	112/751 (15%)	111 (99%)	1 (1%)	81	90
1	O	112/751 (15%)	110 (98%)	2 (2%)	62	82
1	P	112/751 (15%)	111 (99%)	1 (1%)	81	90
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%)	92	95

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

Mol	Chain	Res	Type
1	O	291	TRP
1	P	291	TRP
1	D	644	PHE
1	O	212	TYR
1	B	833	LEU

Some 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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.