



Full wwPDB/EMDataBank EM Map/Model Validation 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 Full wwPDB/EMDataBank EM Map/Model Validation 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

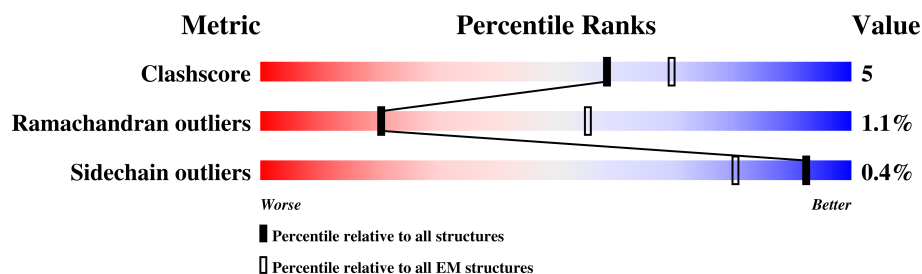
1 Overall quality at a glance

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

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

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31239 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Type IV pilus assembly protein PilF.

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

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

There are 432 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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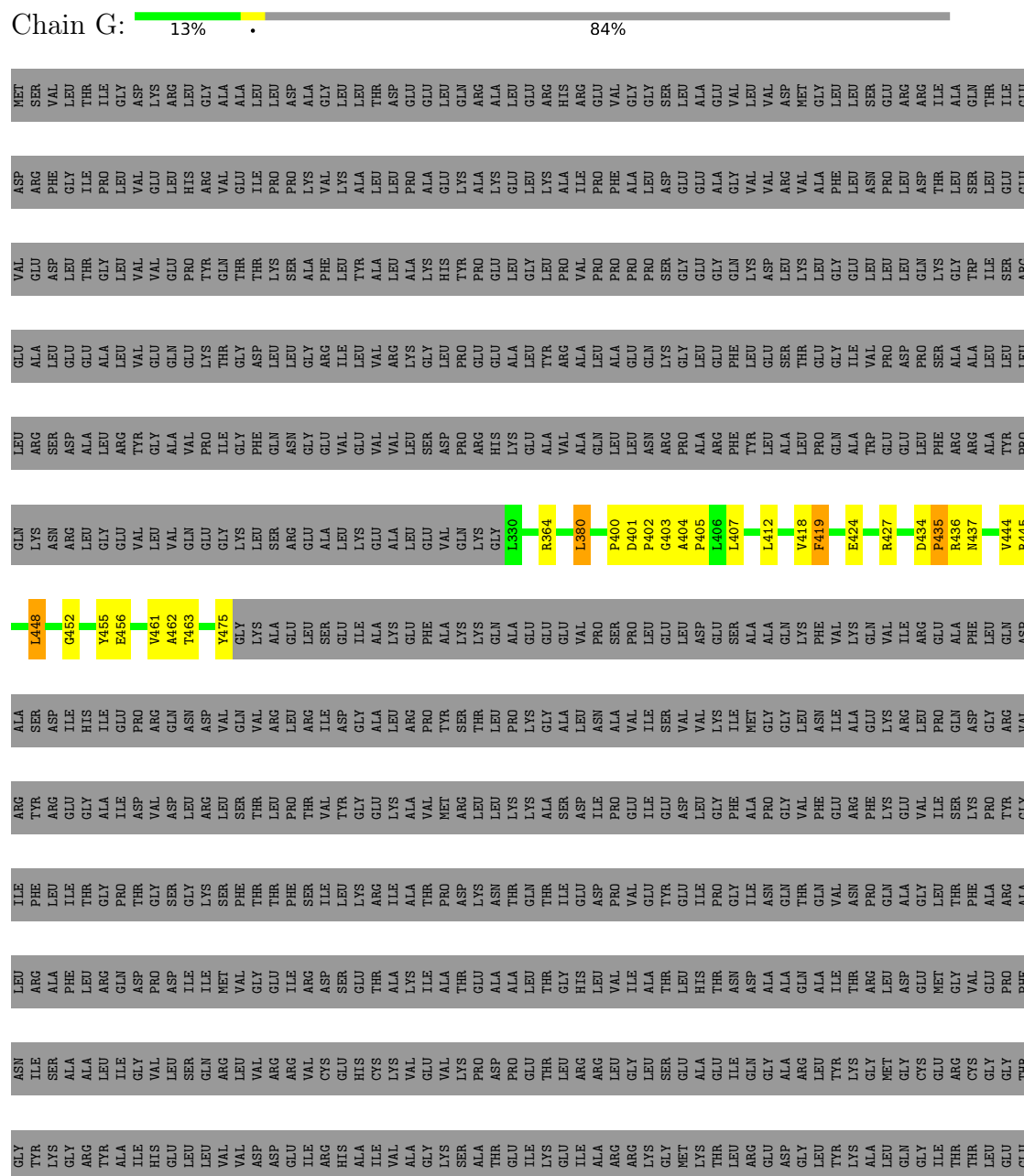
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Chain	Residue	Modelled	Actual	Comment	Reference
F	896	LEU	-	expression tag	UNP Q5SLC9
F	897	VAL	-	expression tag	UNP Q5SLC9
F	898	PRO	-	expression tag	UNP Q5SLC9
F	899	ARG	-	expression tag	UNP Q5SLC9
F	900	GLY	-	expression tag	UNP Q5SLC9
F	901	SER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

3 Residue-property plots

These plots are drawn for all protein, RNA 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.

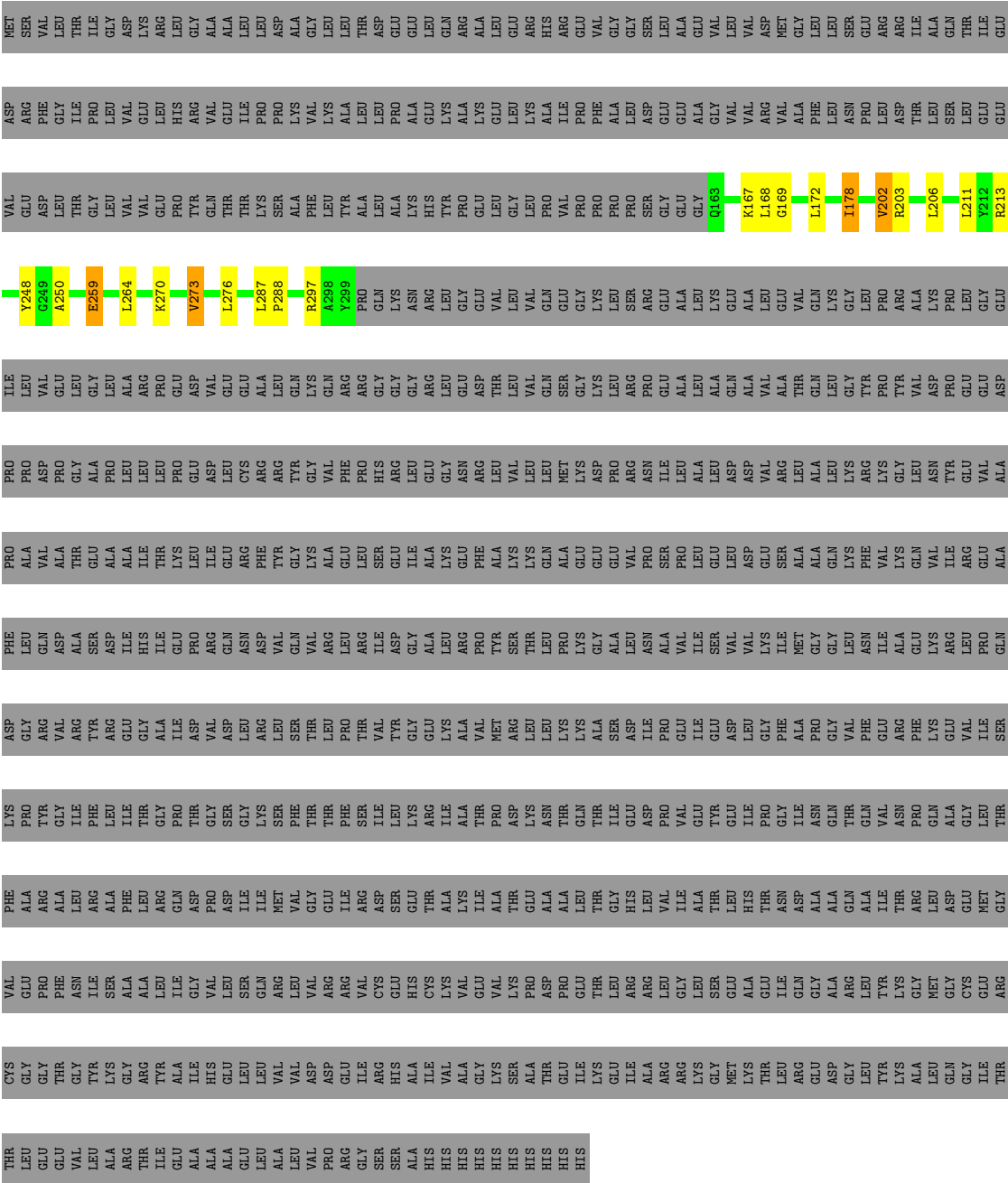
- Molecule 1: Type IV pilus assembly protein PilF



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

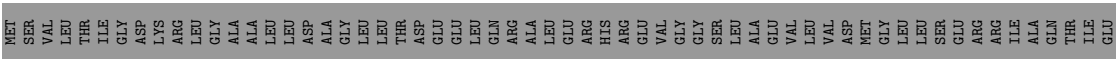
● Molecule 1: Type IV pilus assembly protein PilF

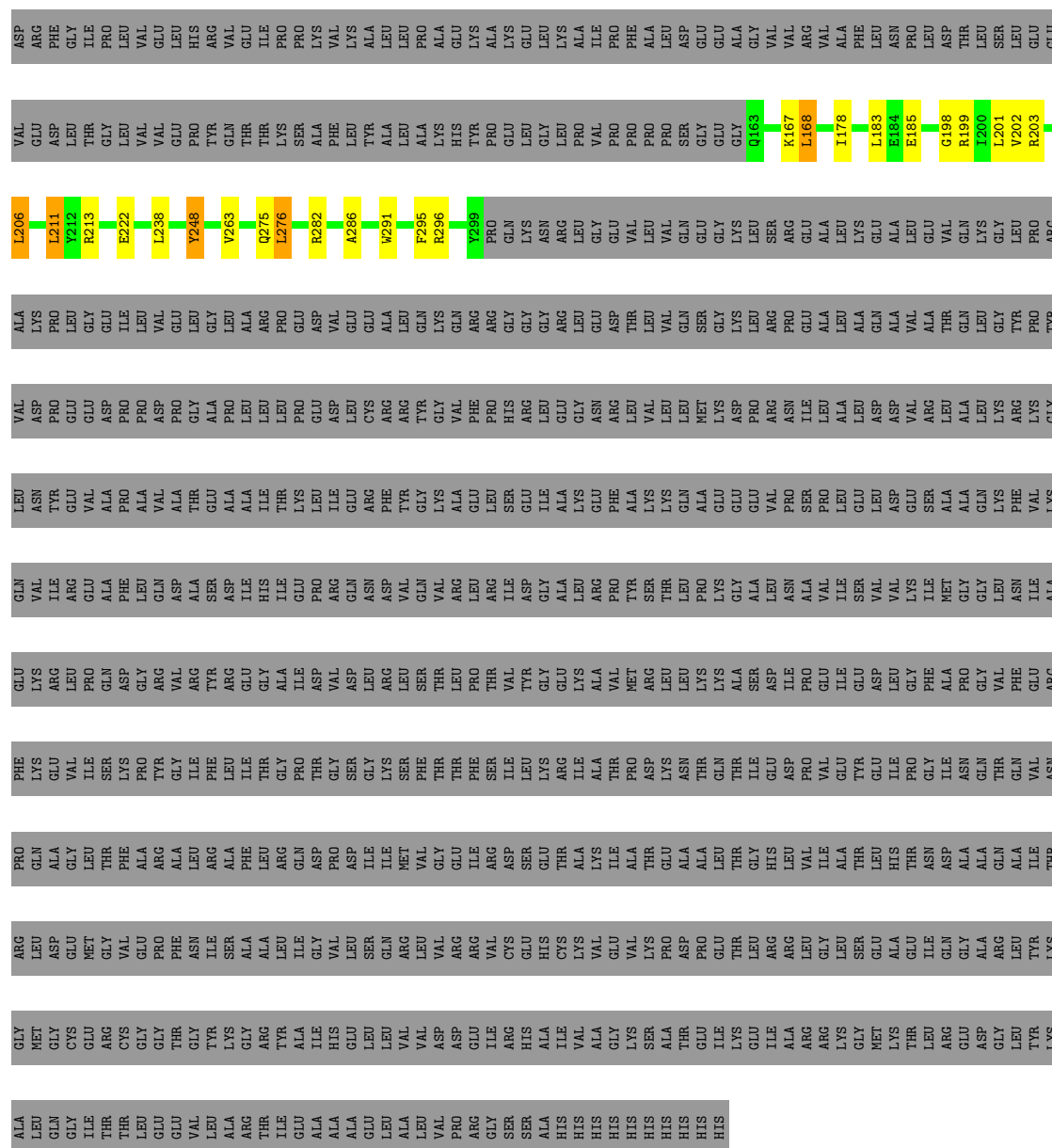
Chain J: 13% 85%



● Molecule 1: Type IV pilus assembly protein PilF

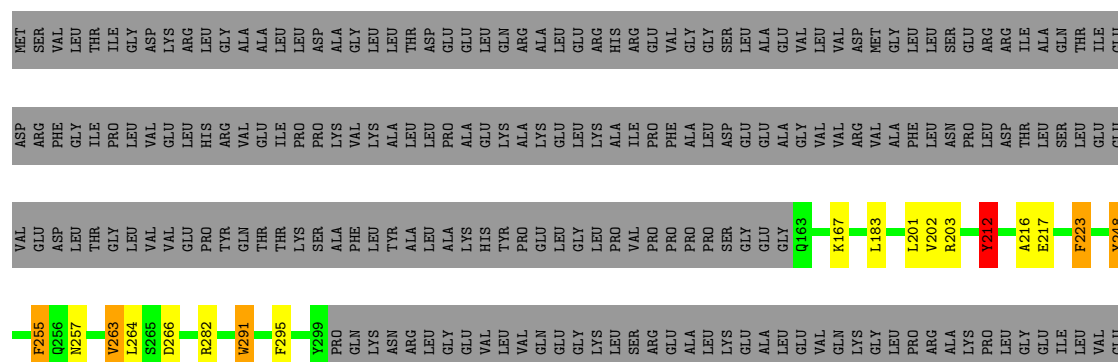
Chain K: 12% 85%





- Molecule 1: Type IV pilus assembly protein PilF

Chain L: 13% .. 85%





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

- Molecule 1: Type IV pilus assembly protein PilF

Chain I:  13% 84%

[illegible]

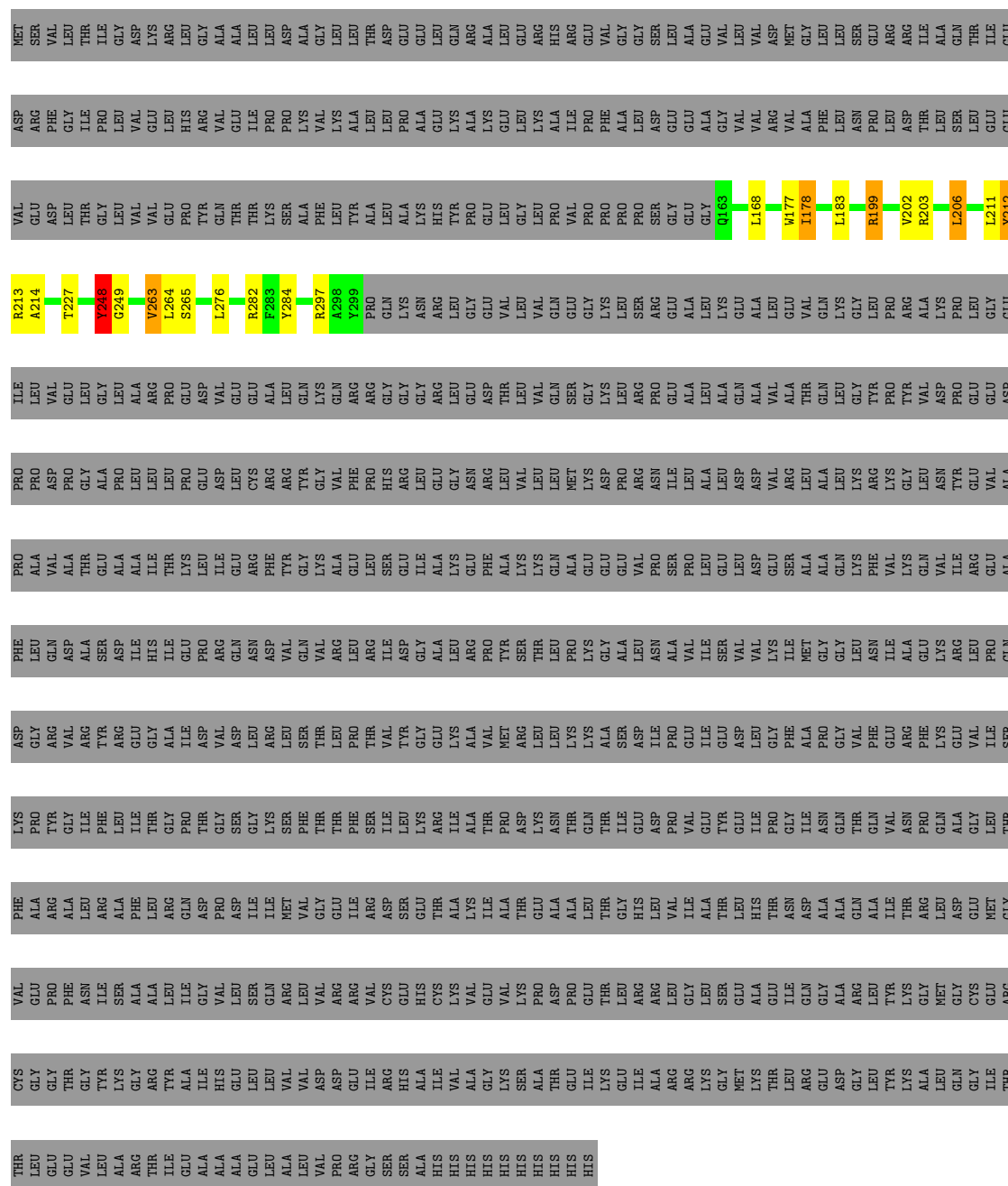
[illegible]

- Molecule 1: Type IV pilus assembly protein PilF

Chain M: 14% 84%

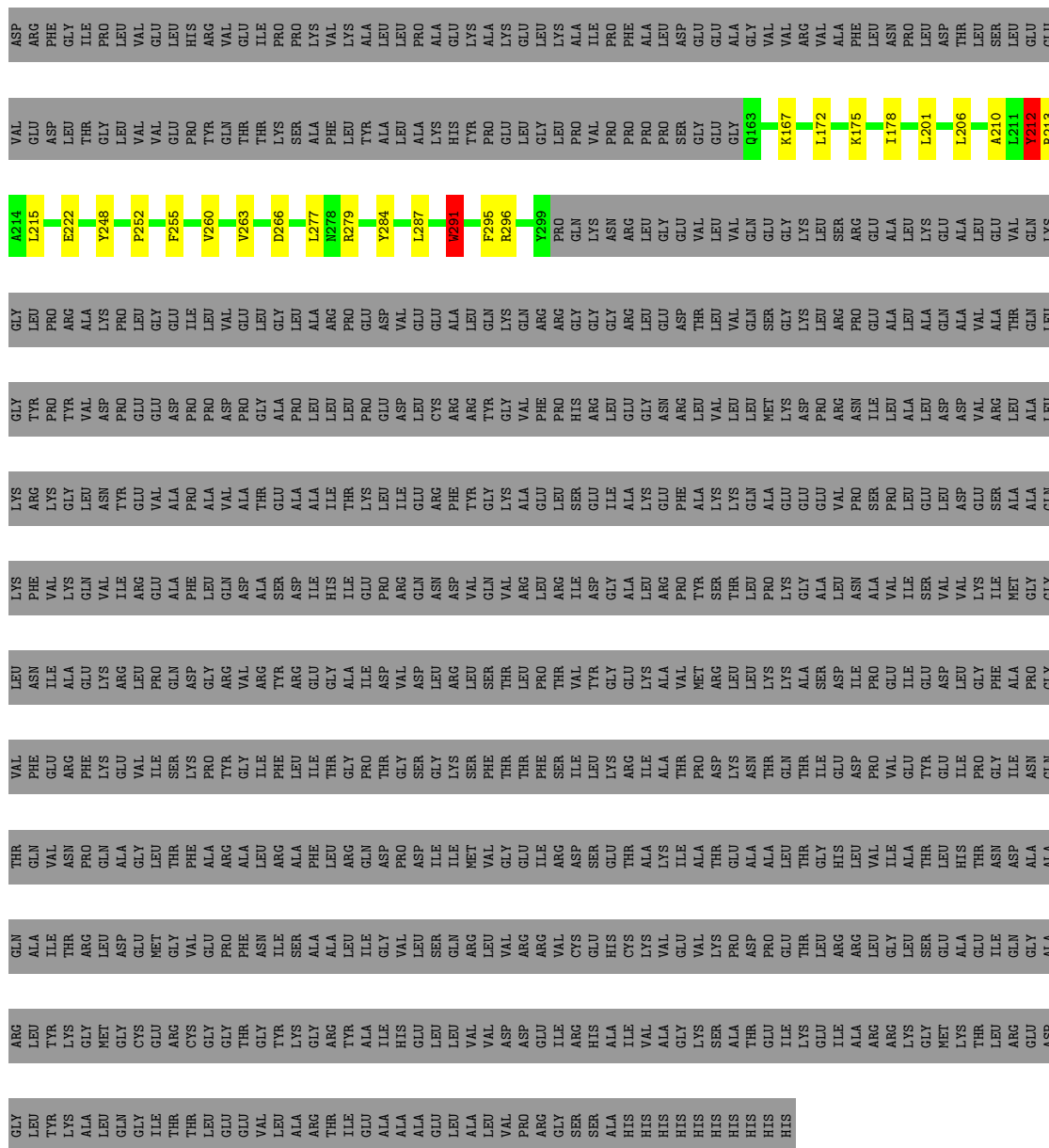
[illegible]

Chain N: 13% .. 85%



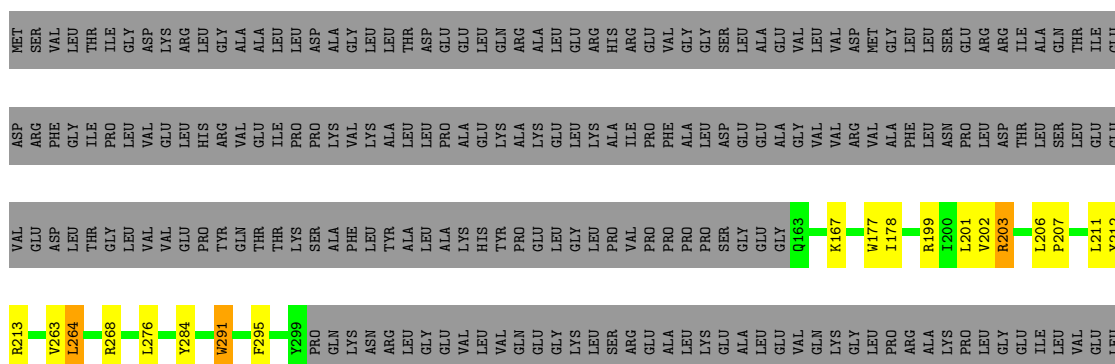
Chain 0: 12% 85%





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

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

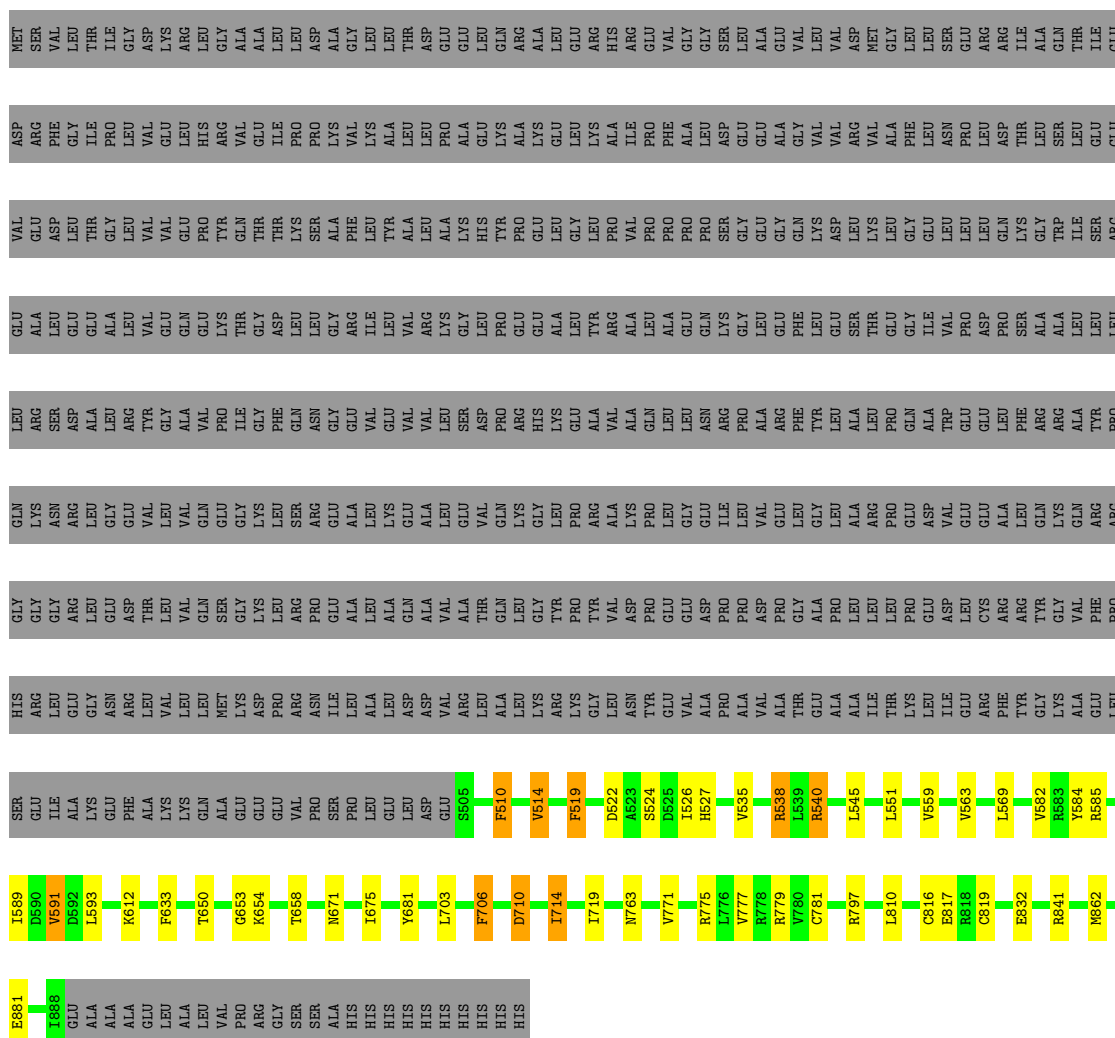
- Molecule 1: Type IV pilus assembly protein PilF

Chain R: 13% 84%

[illegible]



- Molecule 1: Type IV pilus assembly protein PilF

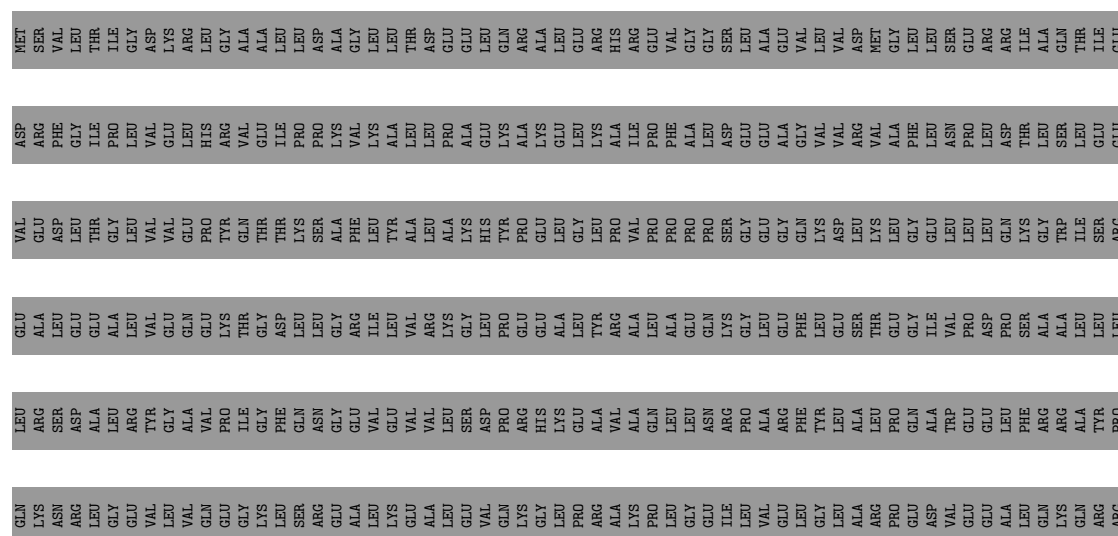


- Molecule 1: Type IV pilus assembly protein PilF





- Molecule 1: Type IV pilus assembly protein PilF



58%

58%

LEU	ARG	ARG	ASP	ALA	LEU	ARG	TYR	GLY	GLY	VAL	PRO	ILE	GLY	PHE	GLN	ASN	GLY	GLU	VAL	GLU	VAL	VAL	LEU	SER	ASP	PRO	PRO	ARG	HIS	LYS	GLU	ALA	GLU	VAL	VAL	GLN	LEU	LEU	LEU	ASN	ARG	PRO	ALA	ALA	LEU	PRO	GLN	ALA	ALA	TRP	GLU	GLU	LEU	LEU	PRO	GLN	PHE	TYR	ARG	ALA	ARG	ALA	TYR
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A885	F630	SER	HIS	GLY	GLN
R886	K634	ILE	ARG	GLY	LYS
T887		ALA	LEU	GLY	ASN
I888	F656	ALA	GLY	ARG	ARG
GLU		GLU	ASN	GLU	LEU
ALA	K670	PHE	ARG	ASP	GLY
ALA		ALA	LEU	THR	VAL
GLU	Q673	LYS	VAL	LEU	LEU
LEU	T674	LYS	LEU	VAL	VAL
ALA	I675	GLN	LEU	GLN	GLN
LEU		ALA	MET	SER	GLN
VAL	E680	GLU	LYS	GLY	GLY
PRO	Y681	GLU	ASP	LYS	GLY
ARG	E682	GLU	PRO	LEU	LEU
GLY	I683	VAL	ARG	ARG	SER
SER		PRO	ASN	PRO	ARG
SER	Q688	SER	ILE	GLU	GLU
ALA		PRO	LEU	ALA	ALA
HIS	L697	LEU	ALA	LEU	LEU
HIS		GLU	LEU	ALA	LYS
HIS	R704	LEU	ASP	GLN	GLY
HIS	A705	GLU	ASP	GLN	GLY
HIS	F706	ASP	ASP	ALA	ALA
HIS		GLU	VAL	VAL	LEU
HIS	D710	S506	ARG	ALA	GLU
HIS	P711	A523	LEU	THR	VAL
HIS	D712		ALA	GLN	GLN
HIS		E529	LEU	GLY	LYS
	R720		ARG	TYR	LEU
	D721	N533	LYS	PRO	PRO
			GLY	TYR	ARG
	L733	I541	LEU	ALA	ALA
	T734	D542	ASN	ASP	LYS
	G735	K564	TYR	PRO	PRO
			GLU	GLU	LEU
	H743		VAL	GLU	GLY
		E573	ALA	ASP	LEU
	S765		PRO	PRO	ILE
	A766	P577	ALA	PRO	LEU
			VAL	ASP	VAL
	R775	Y582	ALA	PRO	GLU
		R583	THR	GLY	LEU
	R778	Y584	GLU	ALA	GLY
		R585	ALA	PRO	LEU
	G807		ALA	LEU	ALA
		D590	ILE	LEU	ARG
	C819		THR	LEU	PRO
		L595	LYS	PRO	GLU
	D837		LEU	GLU	ASP
		L598	ILE	ASP	VAL
	R841	P599	GLU	LEU	GLU
		T600	ARG	CYS	GLY
	K860	Y601	PHE	ARG	ALA
		Y602	TYR	ARG	LEU
			GLY	TYR	GLN
	L870		LYS	VAL	GLN
	E882	R609	ALA	VAL	ARG
	R883		GLU	PHE	ARG
	I884	K613	LEU	PRO	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

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: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
1:O:291:TRP:HA	1:O:291:TRP:HE3	1.32	0.94
1:O:291:TRP:CE3	1:O:291:TRP:HA	2.01	0.91
1:D:832:GLU:O	1:D:832:GLU:HG3	1.72	0.89
1:L:248:TYR:O	1:L:248:TYR:HD1	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:CA	1:O:291:TRP:CE3	2.68	0.76
1:G:401:ASP:O	1:G:401:ASP:OD1	2.04	0.76
1:L:291:TRP:HE3	1:L:291:TRP:HA	1.50	0.76
1:C:862:MET:HG2	1:C:862:MET:O	1.86	0.74
1:B:679:VAL:CG1	1:B:679:VAL:O	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:HA	1:P:291:TRP:CE3	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:HA	1:K:291:TRP:HE3	1.56	0.71
1:F:710:ASP:OD2	1:F:710:ASP:O	2.08	0.71
1:A:519:PHE:HD1	1:A:519:PHE:N	1.89	0.70
1:B:650:THR:O	1:B:650:THR:HG23	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:HE3	1:P:291:TRP:HA	1.58	0.68
1:P:263:VAL:O	1:P:263:VAL:HG23	1.94	0.68
1:O:263:VAL:HG23	1:O:263:VAL:O	1.94	0.66
1:O:212:TYR:CD1	1:O:212:TYR:C	2.67	0.66
1:G:412:LEU:C	1:G:412:LEU:HD23	2.16	0.66
1:D:888:ILE:O	1:D:888:ILE:HG22	1.96	0.66
1:H:419:PHE:CD2	1:H:419:PHE:O	2.49	0.65
1:L:291:TRP:CA	1:L:291:TRP:CE3	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:HD23	1:N:276:LEU:C	2.17	0.64
1:A:519:PHE:CD1	1:A:519:PHE:N	2.65	0.64
1:O:295:PHE:N	1:O:295:PHE:CD1	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:HD12	1:R:407:LEU:O	2.00	0.62
1:R:401:ASP:OD1	1:R:401:ASP:O	2.16	0.62
1:M:410:GLU:H	1:M:410:GLU:CD	2.03	0.61
1:F:595:LEU:HD12	1:F:595:LEU:N	2.16	0.61
1:K:248:TYR:C	1:K:248:TYR:HD1	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:O	1:O:178:ILE:HG23	2.01	0.60
1:F:710:ASP:CG	1:F:710:ASP:O	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:O	1:E:582:VAL:HG13	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:HE3	1:D:862:MET:O	2.04	0.58
1:B:686:ILE:O	1:B:686:ILE:HG23	2.03	0.57
1:B:677:ASP:OD1	1:B:677:ASP:C	2.42	0.57
1:K:263:VAL:CG2	1:K:263:VAL:O	2.42	0.57
1:J:287:LEU:N	1:J:287:LEU:HD12	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:HE3	1:C:862:MET:O	2.06	0.55
1:F:837:ASP:OD2	1:F:860:LYS:NZ	2.40	0.55
1:A:862:MET:HG2	1:A:862:MET:O	2.06	0.55
1:I:336:LEU:C	1:I:336:LEU:HD13	2.26	0.55
1:Q:408:LEU:C	1:Q:408:LEU:HD23	2.27	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:HG	1:O:277:LEU:O	2.07	0.54
1:R:401:ASP:O	1:R:403:GLY:N	2.40	0.54
1:D:644:PHE:HD1	1:D:644:PHE:C	2.12	0.54
1:D:781:CYS:SG	1:D:781:CYS:O	2.63	0.53
1:P:202:VAL:O	1:P:203:ARG:CB	2.55	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:O	1:R:451:LYS:HG3	2.08	0.53
1:D:519:PHE:HD1	1:D:519:PHE:N	2.05	0.53
1:D:519:PHE:CD1	1:D:519:PHE:N	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:B:641:TYR:OH	1:C:812:LYS:NZ	2.31	0.52
1:L:255:PHE:C	1:L:255:PHE:CD2	2.80	0.52
1:J:259:GLU:HG2	1:J:259:GLU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:212:TYR:C	1:L:212:TYR:CD1	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:D:576:LEU:C	1:D:576:LEU:HD12	2.31	0.52
1:I:375:LEU:C	1:I:375:LEU:HD12	2.30	0.52
1:J:276:LEU:C	1:J:276:LEU:CD2	2.78	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:O	1:L:255:PHE:CD2	2.64	0.51
1:B:677:ASP:HB2	1:B:678:PRO:HD2	1.93	0.51
1:E:710:ASP:O	1:E:710:ASP:CG	2.49	0.51
1:C:710:ASP:O	1:C:710:ASP:CG	2.48	0.50
1:O:212:TYR:HD1	1:O:212:TYR:C	2.13	0.50
1:A:650:THR:HG23	1:A:650:THR:O	2.10	0.50
1:K:291:TRP:CA	1:K:291:TRP:CE3	2.94	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:O	1:I:463:THR:HG23	2.10	0.50
1:D:644:PHE:CD1	1:D:644:PHE:C	2.85	0.50
1:N:183:LEU:HD23	1:N:183:LEU:C	2.32	0.50
1:C:677:ASP:HB3	1:C:678:PRO:CD	2.41	0.49
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:D:614:ALA:HA	1:D:681:TYR:CD2	2.47	0.49
1:G:401:ASP:O	1:G:403:GLY:N	2.45	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:B:659:PHE:CD1	1:B:659:PHE:N	2.80	0.49
1:G:401:ASP:C	1:G:401:ASP:OD1	2.50	0.49
1:C:862:MET:O	1:C:863:LYS:C	2.48	0.49
1:O:266:ASP:O	1:O:266:ASP:OD1	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:HG23	1:Q:393:VAL:O	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:E:746:ASP:OD1	1:E:747:ALA:N	2.46	0.48
1:P:202:VAL:O	1:P:203:ARG:HB3	2.14	0.48
1:H:336:LEU:C	1:H:336:LEU:HD13	2.33	0.47
1:F:600:THR:HG22	1:F:602:TYR:H	1.79	0.47
1:F:590:ASP:OD1	1:F:613:LYS:NZ	2.47	0.47
1:H:335:PRO:O	1:H:338:GLU:N	2.47	0.47
1:N:168:LEU:H	1:N:168:LEU:HD23	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:B:510:PHE:CD2	1:B:510:PHE:C	2.85	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: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:B:677:ASP:HB2	1:B:678:PRO:CD	2.45	0.46
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:O	1:O:212:TYR:HD1	1.98	0.46
1:B:790:PRO:HG2	1:B:795:LEU:HD11	1.97	0.46
1:D:835:VAL:HG13	1:D:835:VAL:O	2.14	0.46
1:M:463:THR:O	1:M:465:ALA:N	2.48	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:HD13	1:F:675:ILE:HG21	1.63	0.46
1:C:859:ARG:O	1:C:860:LYS:CB	2.64	0.46
1:D:671:ASN:C	1:D:671:ASN:OD1	2.54	0.46
1:H:461:VAL:O	1:H:461:VAL:HG13	2.15	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:C:551:LEU:N	1:C:551:LEU:HD12	2.31	0.45
1:I:400:PRO:O	1:I:401:ASP:C	2.54	0.45
1:B:686:ILE:O	1:B:686:ILE:CG2	2.61	0.45
1:C:760:GLU:H	1:C:760:GLU:CD	2.19	0.45
1:A:569:LEU:HD12	1:A:569:LEU:N	2.32	0.45
1:Q:419:PHE:CE2	1:Q:470:LEU:HB3	2.50	0.45
1:C:778:ARG:HB3	1:C:824:TYR:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:202:VAL:HG13	1:K:202:VAL:O	2.16	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:N	1:D:824:TYR:CD1	2.85	0.45
1:O:291:TRP:N	1:O:291:TRP:CE3	2.84	0.45
1:C:834:LEU:N	1:C:834:LEU:CD1	2.80	0.45
1:M:419:PHE:O	1:M:419:PHE:CD1	2.70	0.44
1:D:808:ALA:HB1	1:D:874:LEU:HD22	1.99	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:HG	1:P:211:LEU:O	2.16	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:G:400:PRO:O	1:G:401:ASP:C	2.55	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: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:C:862:MET:CE	1:C:862:MET:O	2.65	0.44
1:J:250:ALA:HB2	1:J:264:LEU:HA	2.00	0.44
1:Q:336:LEU:HA	1:Q:336:LEU:HD22	1.57	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:H:455:TYR:O	1:H:456:GLU:CB	2.66	0.44
1:D:506:ALA:HA	1:D:508:GLN:N	2.33	0.44
1:K:275:GLN:O	1:K:276:LEU:CB	2.64	0.44
1:B:662:LEU:O	1:B:666:ALA:N	2.48	0.44
1:D:817:GLU:H	1:D:817:GLU:CD	2.14	0.44
1:H:401:ASP:O	1:H:405:PRO:HD2	2.18	0.44
1:Q:419:PHE:O	1:Q:419:PHE:HD1	2.00	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: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:I:394:ASP:C	1:I:394:ASP:OD1	2.56	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:419:PHE:O	1:M:419:PHE:HD1	2.02	0.43
1:N:248:TYR:O	1:N:248:TYR:HD1	2.00	0.43
1:B:560:ILE:HD13	1:B:560:ILE:HA	1.78	0.43
1:C:884:LEU:HA	1:C:884:LEU:HD23	1.70	0.43
1:M:419:PHE:CE2	1:M:470:LEU:HG	2.54	0.43
1:F:743:HIS:ND1	1:F:743:HIS:C	2.71	0.43
1:J:178:ILE:HG22	1:J:206:LEU:HB2	2.01	0.43
1:A:671:ASN:OD1	1:A:671:ASN:C	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:H:336:LEU:HB2	1:H:366:GLU:HG3	2.01	0.43
1:E:563:VAL:O	1:E:567:GLY:N	2.52	0.43
1:H:335:PRO:O	1:H:336:LEU:C	2.56	0.43
1:J:178:ILE:HG21	1:J:178:ILE:HD13	1.61	0.43
1:P:268:ARG:HG2	1:P:268:ARG:O	2.18	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:Q:457:VAL:O	1:Q:457:VAL:HG13	2.19	0.43
1:A:710:ASP:OD2	1:D:540:ARG:NE	2.51	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:N	1:E:824:TYR:CD1	2.86	0.42
1:G:419:PHE:CD1	1:G:419:PHE:C	2.92	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:C:865:LEU:HB3	1:C:887:THR:HG22	2.00	0.42
1:A:545:LEU:HB2	1:F:712:ASP:OD2	2.20	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:675:ILE:HG21	1:A:675:ILE:HD13	1.74	0.42
1:N:177:TRP:CE3	1:N:214:ALA:HB2	2.54	0.42
1:Q:336:LEU:CD1	1:Q:336:LEU:O	2.37	0.42
1:E:878:THR:OG1	1:E:879:THR:N	2.52	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:617:ILE:HG21	1:E:617:ILE:HD13	1.73	0.42
1:L:291:TRP:N	1:L:291:TRP:CE3	2.87	0.42
1:O:178:ILE:CG2	1:O:178:ILE:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:357:LYS:O	1:R:361:GLY:N	2.52	0.42
1:A:719:ILE:HG21	1:A:719:ILE:HD13	1.91	0.42
1:C:560:ILE:HD12	1:C:560:ILE:HA	1.52	0.42
1:C:662:LEU:HA	1:C:662:LEU:HD23	1.86	0.42
1:E:675:ILE:HG21	1:E:675:ILE:HD13	1.64	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:C:804:GLU:OE2	1:C:863:LYS:NZ	2.44	0.42
1:K:183:LEU:HD23	1:K:183:LEU:C	2.40	0.42
1:L:201:LEU:C	1:L:202:VAL:O	2.55	0.42
1:B:659:PHE:HD1	1:B:659:PHE:N	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:M:423:LEU:HA	1:M:423:LEU:HD23	1.88	0.41
1:N:202:VAL:O	1:N:203:ARG:HB2	2.20	0.41
1:N:212:TYR:CD1	1:N:212:TYR:N	2.79	0.41
1:R:336:LEU:O	1:R:340:LEU:HG	2.20	0.41
1:C:832:GLU:HB2	1:C:865:LEU:HG	2.02	0.41
1:D:862:MET:CG	1:D:862:MET:O	2.54	0.41
1:E:716:VAL:O	1:E:717:GLY:C	2.56	0.41
1:J:168:LEU:HD23	1:J:168:LEU:H	1.86	0.41
1:K:178:ILE:HB	1:K:206:LEU:HD13	2.02	0.41
1:N:263:VAL:O	1:N:263:VAL:HG23	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: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:K:276:LEU:C	1:K:276:LEU:HD23	2.40	0.41
1:M:456:GLU:HA	1:M:456:GLU:OE1	2.21	0.41
1:O:172:LEU:HD22	1:O:210:ALA:HB1	2.03	0.41
1:C:675:ILE:O	1:C:675:ILE:HG23	2.20	0.41
1:D:798:LEU:HD23	1:D:798:LEU:HA	1.89	0.41
1:A:650:THR:CG2	1:A:650:THR:O	2.69	0.41
1:M:400:PRO:O	1:M:401:ASP:C	2.59	0.41
1:O:215:LEU:HA	1:O:215:LEU:HD23	1.95	0.41
1:R:333:ALA:O	1:R:334:LYS:C	2.59	0.41
1:B:576:LEU:HD23	1:B:576:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:ILE:HA	1:C:571:ILE:HD13	1.80	0.41
1:C:835:VAL:O	1:C:835:VAL:CG2	2.68	0.41
1:D:874:LEU:HD23	1:D:874:LEU:HA	1.89	0.41
1:K:211:LEU:HD23	1:K:211:LEU:HA	1.77	0.41
1:M:404:ALA:N	1:M:405:PRO:CD	2.84	0.41
1:C:710:ASP:N	1:C:711:PRO:CD	2.83	0.41
1:D:788:VAL:O	1:D:789:LYS:C	2.59	0.41
1:F:681:TYR:O	1:F:688:GLN:NE2	2.45	0.41
1:A:714:ILE:HG22	1:A:714:ILE:O	2.20	0.41
1:G:380:LEU:HD13	1:G:380:LEU:HA	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: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:G:462:ALA:O	1:G:463:THR:C	2.59	0.40
1:I:419:PHE:O	1:I:431:LEU:HB3	2.21	0.40
1:L:216:ALA:HB3	1:L:223:PHE:CE1	2.56	0.40
1:P:264:LEU:N	1:P:284:TYR:O	2.53	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:Q:475:TYR:N	1:Q:475:TYR:CD1	2.90	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:HG2	1:E:573:GLU:O	2.21	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:O	1:Q:419:PHE:CD1	2.75	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: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
1:I:376:ARG:HA	1:I:377:PRO:HD3	1.93	0.40
1:J:270:LYS:HA	1:J:273:VAL:HG22	2.04	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%)	43	81
1	B	381/913 (42%)	369 (97%)	10 (3%)	2 (0%)	31	74
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

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

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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%)	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

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

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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

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 [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 carbohydrates 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.