



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 11:32 PM UTC

PDB ID : 6F8L / pdb_00006f8l
EMDB ID : EMD-4194
Title : Thermus thermophilus PilF ATPase (AMPPNP-bound form)
Authors : Derrick, J.P.; Collins, R.F.
Deposited on : 2017-12-13
Resolution : 8.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

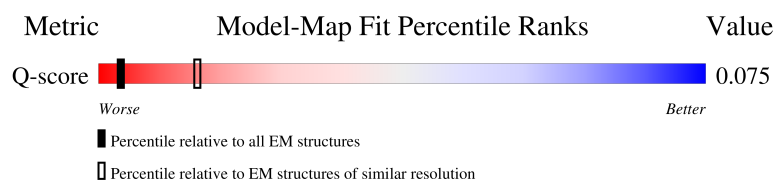
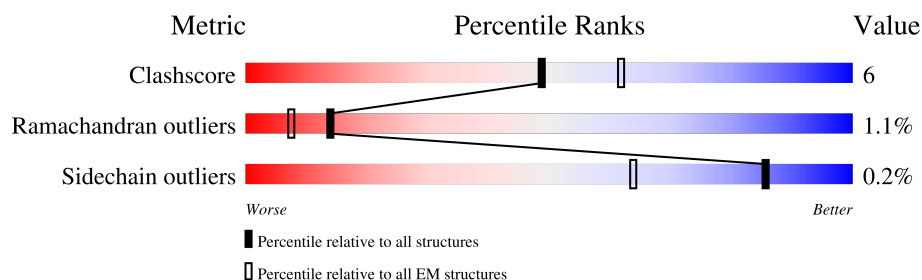
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	913	
1	B	913	
1	C	913	
1	D	913	

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

2 Entry composition

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

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

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

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

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

There are 432 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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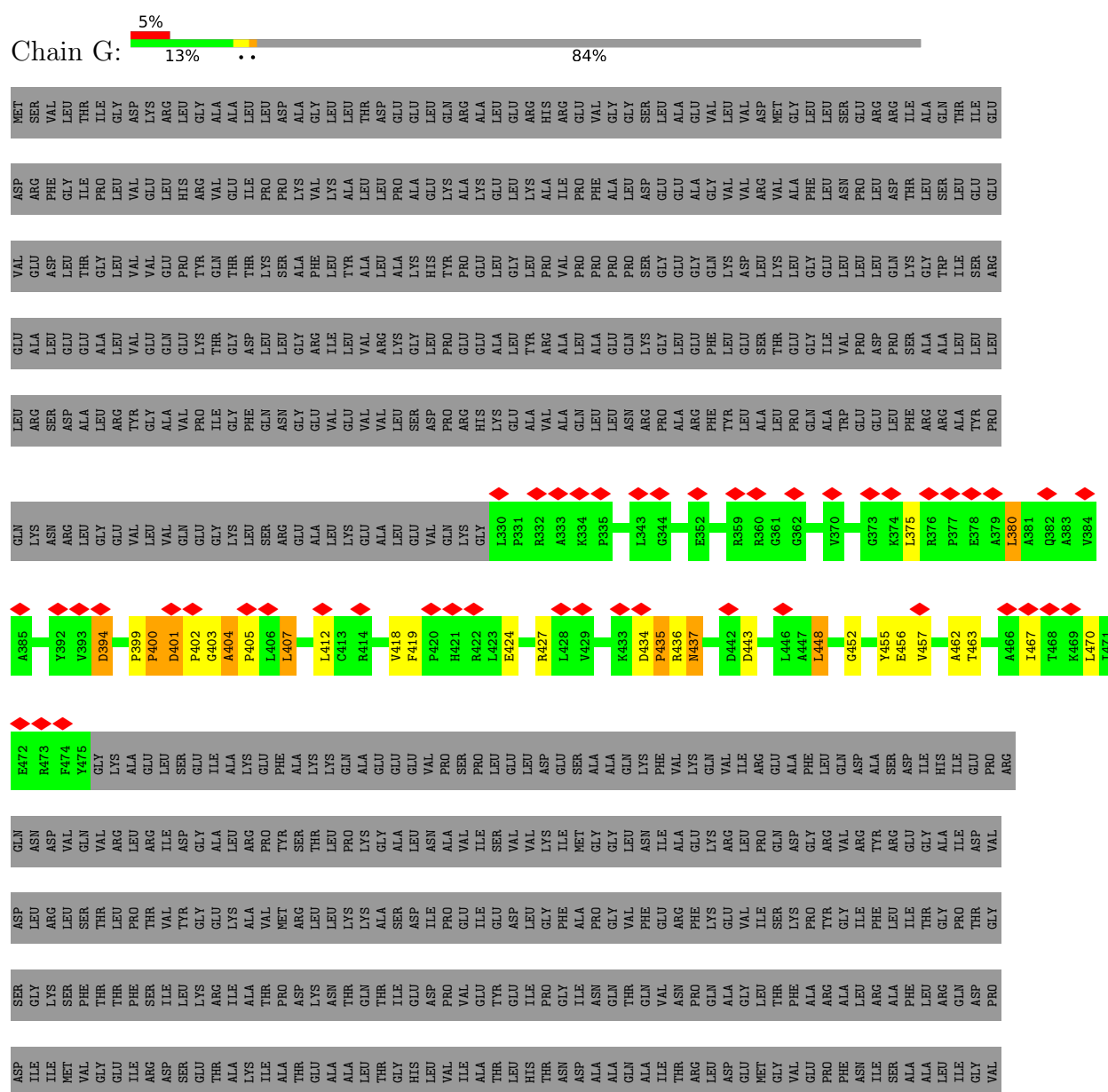
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Chain	Residue	Modelled	Actual	Comment	Reference
F	896	LEU	-	expression tag	UNP Q5SLC9
F	897	VAL	-	expression tag	UNP Q5SLC9
F	898	PRO	-	expression tag	UNP Q5SLC9
F	899	ARG	-	expression tag	UNP Q5SLC9
F	900	GLY	-	expression tag	UNP Q5SLC9
F	901	SER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

3 Residue-property plots

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

- Molecule 1: Type IV pilus assembly protein PilF



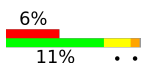
[illegible]

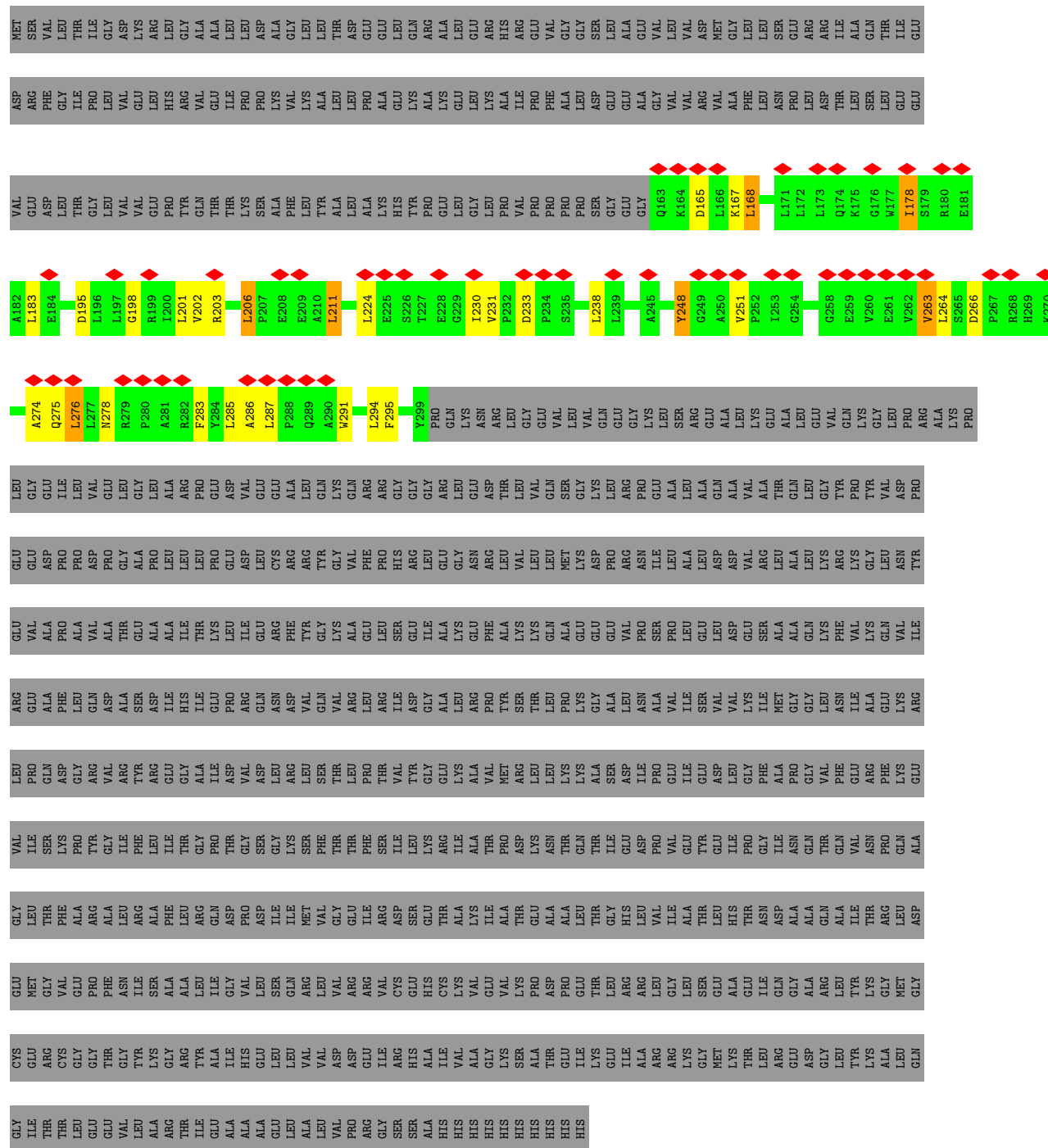
Chain J: 5% 12% 85%

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

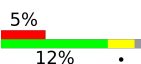
GLY
ILE
THR
THR
GLU
GLU
VAL
LEU
LEU
ARG
THR
ILE
GLU
ALA
ALA
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GLU
LEU
ALA
ALA
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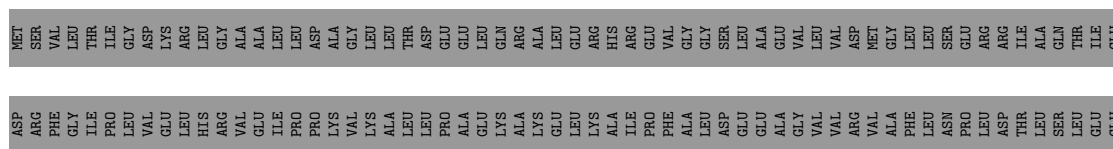
● Molecule 1: Type IV pilus assembly protein PilF

Chain K:  85%



● Molecule 1: Type IV pilus assembly protein PilF

Chain L:  85%







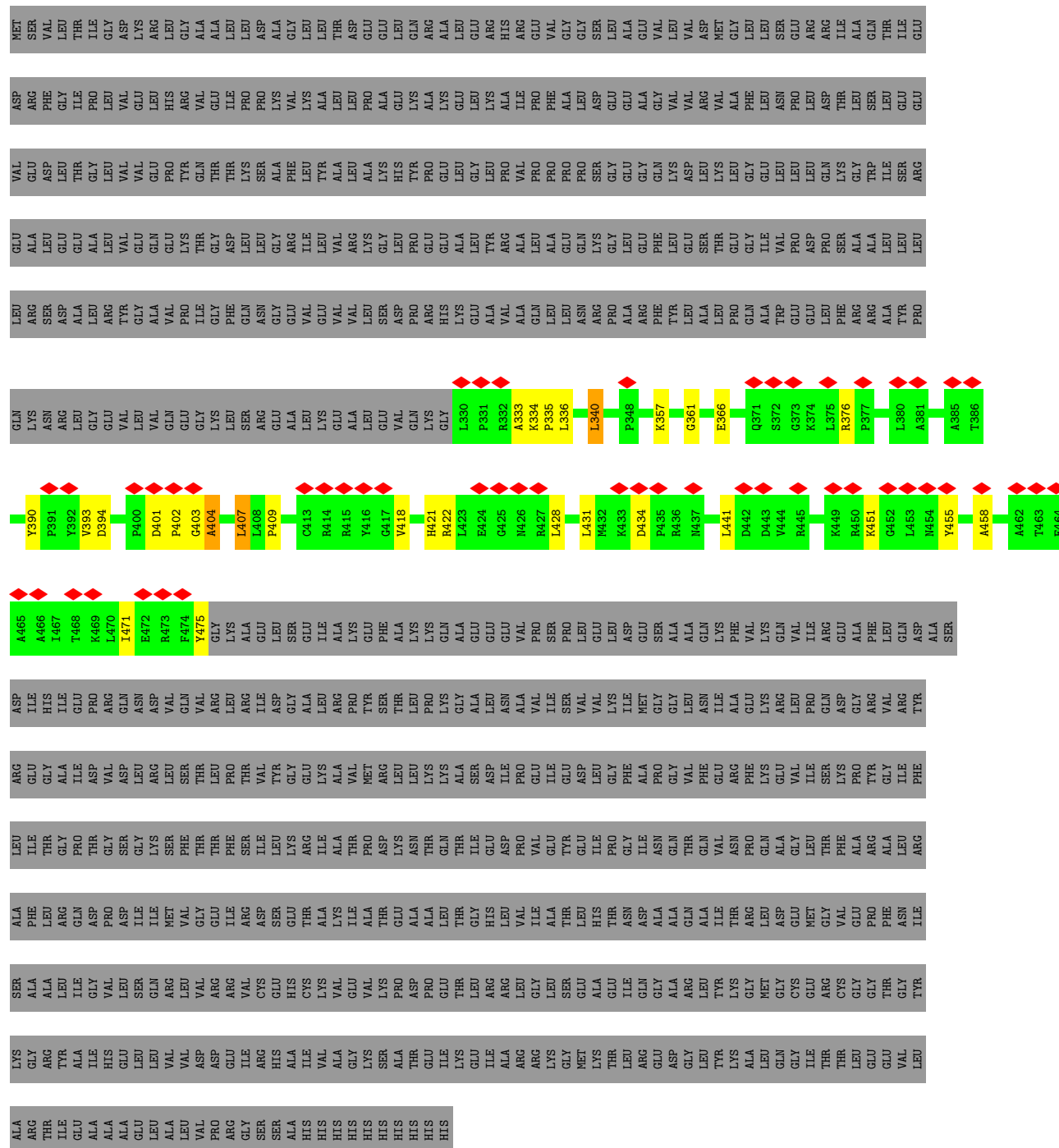


[illegible]

- Molecule 1: Type IV pilus assembly protein PilF

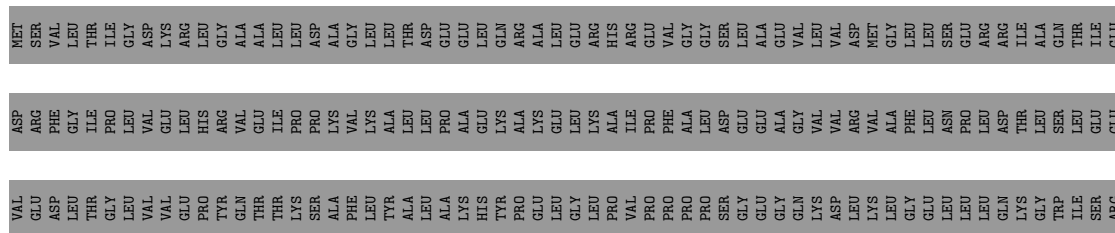
[illegible]

Chain R: 6% 13% 84%



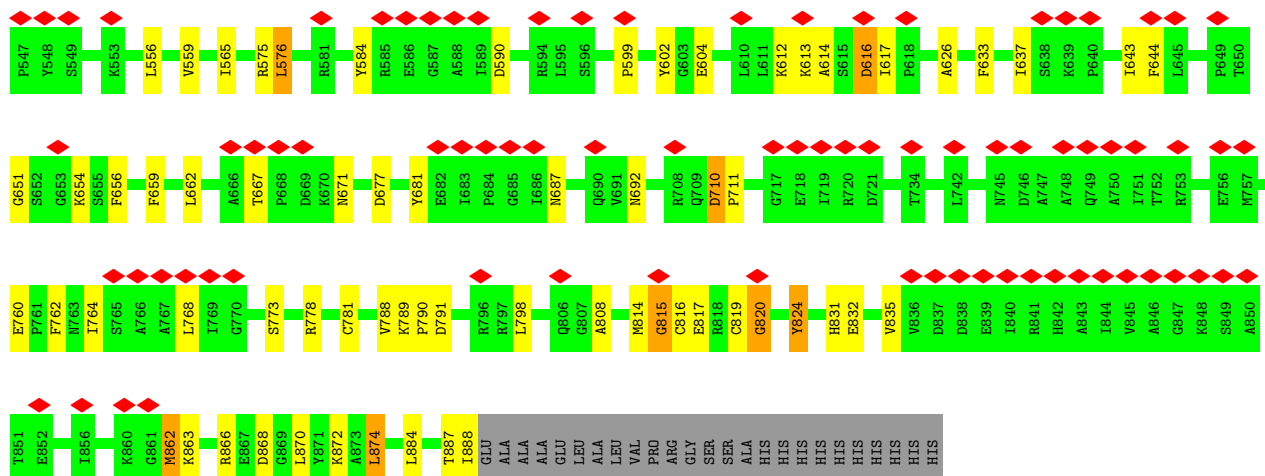
Chain A: 10% 35% 5% 50%

- Molecule 1: Type IV pilus assembly protein PilF

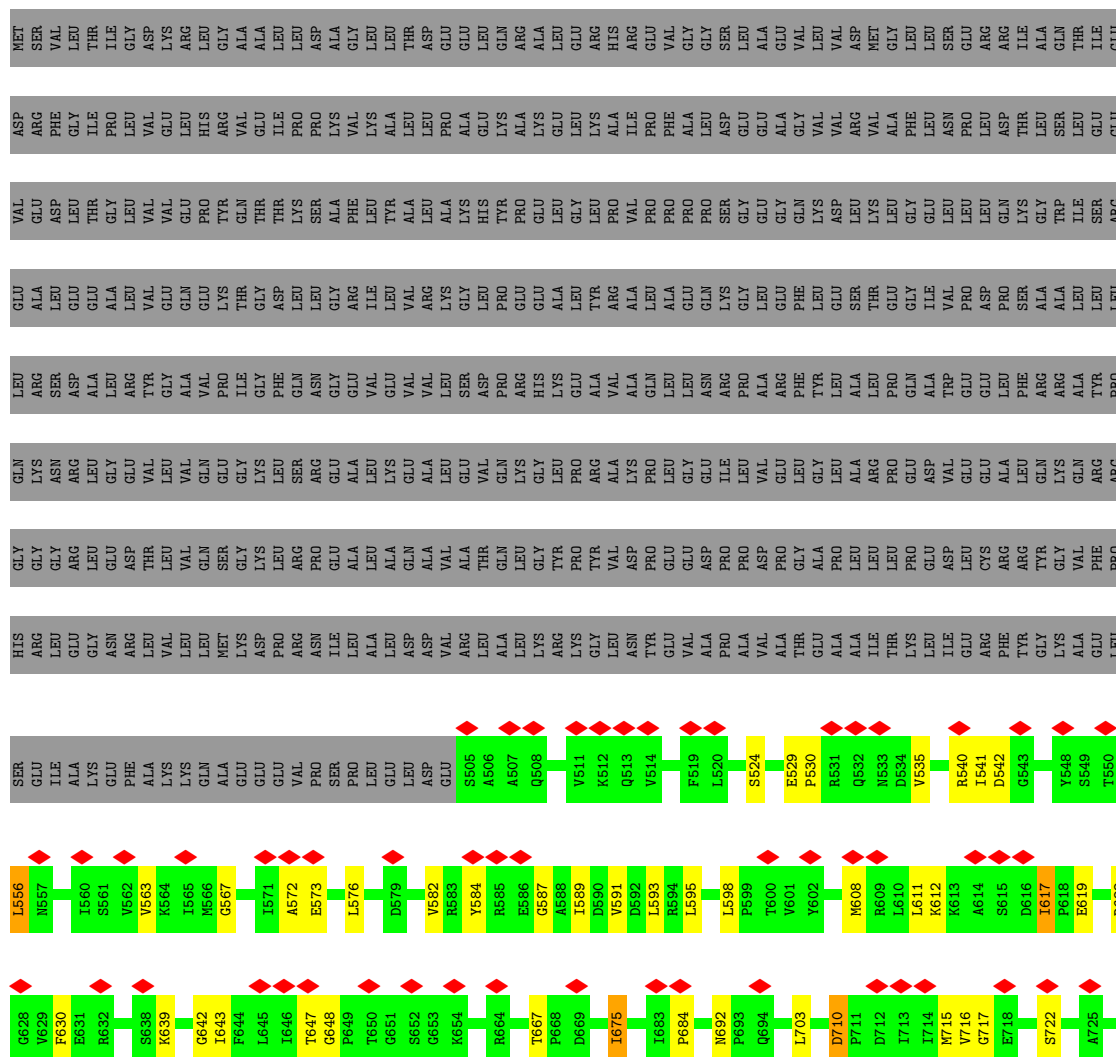
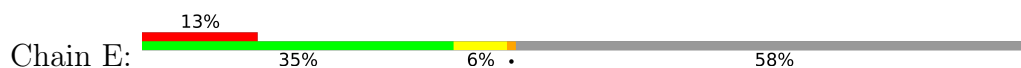








• Molecule 1: Type IV pilus assembly protein PilF



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	450000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	5.398	Depositor
Minimum map value	-4.813	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.290	Depositor
Recommended contour level	1.45	Depositor
Map size ($\text{\AA}$)	341.76, 341.76, 341.76	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.7800001, 1.7800001, 1.7800001	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.34	21/3017 (0.7%)	1.50	44/4073 (1.1%)
1	B	1.32	18/3008 (0.6%)	1.47	43/4061 (1.1%)
1	C	1.33	12/3017 (0.4%)	1.57	53/4073 (1.3%)
1	D	1.33	13/3017 (0.4%)	1.54	50/4073 (1.2%)
1	E	1.26	11/3017 (0.4%)	1.45	46/4073 (1.1%)
1	F	1.29	8/3017 (0.3%)	1.47	43/4073 (1.1%)
1	G	1.23	7/1164 (0.6%)	1.37	13/1580 (0.8%)
1	H	1.22	4/1164 (0.3%)	1.51	20/1580 (1.3%)
1	I	1.24	6/1164 (0.5%)	1.60	26/1580 (1.6%)
1	J	1.21	4/1109 (0.4%)	1.51	20/1499 (1.3%)
1	K	1.29	9/1109 (0.8%)	1.46	22/1499 (1.5%)
1	L	1.24	2/1109 (0.2%)	1.49	16/1499 (1.1%)
1	M	1.19	3/1164 (0.3%)	1.46	19/1580 (1.2%)
1	N	1.25	7/1109 (0.6%)	1.49	17/1499 (1.1%)
1	O	1.23	6/1109 (0.5%)	1.44	18/1499 (1.2%)
1	P	1.25	5/1109 (0.5%)	1.63	24/1499 (1.6%)
1	Q	1.27	6/1164 (0.5%)	1.48	19/1580 (1.2%)
1	R	1.24	3/1164 (0.3%)	1.47	17/1580 (1.1%)
All	All	1.28	145/31731 (0.5%)	1.50	510/42900 (1.2%)

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 (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	527	HIS	CB-CG	-12.62	1.32	1.50
1	F	733	LEU	CB-CG	-11.64	1.30	1.53
1	Q	336	LEU	CB-CG	-11.23	1.30	1.53
1	I	431	LEU	CB-CG	-10.92	1.31	1.53
1	K	211	LEU	CB-CG	-10.69	1.32	1.53
1	R	431	LEU	CB-CG	-10.12	1.33	1.53
1	F	675	ILE	CB-CG1	-9.65	1.34	1.53
1	E	675	ILE	CB-CG1	-9.23	1.34	1.53
1	K	201	LEU	CB-CG	-8.99	1.35	1.53
1	B	675	ILE	CB-CG1	-8.96	1.35	1.53
1	A	810	LEU	CB-CG	-8.48	1.36	1.53
1	J	211	LEU	CB-CG	-8.32	1.36	1.53
1	H	431	LEU	CB-CG	-7.94	1.37	1.53
1	O	201	LEU	CB-CG	-7.94	1.37	1.53
1	J	178	ILE	CB-CG1	-7.86	1.37	1.53
1	C	556	LEU	CB-CG	-7.85	1.37	1.53
1	P	264	LEU	CB-CG	-7.71	1.38	1.53
1	H	340	LEU	CG-CD1	-7.69	1.27	1.52
1	A	776	LEU	CB-CG	-7.63	1.38	1.53
1	E	880	LEU	CB-CG	-7.55	1.38	1.53
1	G	470	LEU	CB-CG	-7.50	1.38	1.53
1	P	178	ILE	CB-CG1	-7.35	1.38	1.53
1	F	673	GLN	CG-CD	-7.24	1.33	1.52
1	H	375	LEU	CB-CG	-7.20	1.39	1.53
1	C	870	LEU	CB-CG	-7.17	1.39	1.53
1	H	336	LEU	CB-CG	-7.13	1.39	1.53
1	N	199	ARG	CD-NE	-7.11	1.36	1.46
1	B	662	LEU	CB-CG	-7.07	1.39	1.53
1	F	733	LEU	CG-CD2	-7.07	1.29	1.52
1	L	264	LEU	CB-CG	-7.06	1.39	1.53
1	A	703	LEU	CB-CG	-7.05	1.39	1.53
1	N	178	ILE	CB-CG2	-6.97	1.29	1.52
1	A	526	ILE	CB-CG1	-6.94	1.39	1.53
1	B	527	HIS	ND1-CE1	-6.94	1.25	1.32
1	A	710	ASP	CA-CB	-6.92	1.46	1.52
1	B	560	ILE	CB-CG1	-6.84	1.39	1.53
1	A	527	HIS	CB-CG	-6.84	1.40	1.50
1	G	407	LEU	CB-CG	-6.81	1.39	1.53
1	N	264	LEU	CB-CG	-6.77	1.40	1.53
1	N	212	TYR	CB-CG	-6.72	1.36	1.51
1	K	294	LEU	CB-CG	-6.70	1.40	1.53
1	C	605	LYS	CE-NZ	-6.70	1.29	1.49
1	I	408	LEU	CB-CG	-6.66	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	800	LEU	CB-CG	-6.49	1.40	1.53
1	M	448	LEU	CB-CG	-6.48	1.40	1.53
1	B	556	LEU	CB-CG	-6.46	1.40	1.53
1	C	545	LEU	CB-CG	-6.46	1.40	1.53
1	D	654	LYS	CE-NZ	-6.46	1.29	1.49
1	R	340	LEU	CB-CG	-6.43	1.40	1.53
1	G	448	LEU	CG-CD2	-6.42	1.31	1.52
1	K	264	LEU	CB-CG	-6.42	1.40	1.53
1	B	510	PHE	CB-CG	-6.42	1.35	1.50
1	D	529	GLU	CG-CD	-6.36	1.36	1.52
1	O	224	LEU	CB-CG	-6.35	1.40	1.53
1	G	448	LEU	CB-CG	-6.31	1.40	1.53
1	C	888	ILE	CB-CG1	-6.29	1.40	1.53
1	F	688	GLN	CG-CD	-6.24	1.36	1.52
1	J	178	ILE	CB-CG2	-6.21	1.32	1.52
1	Q	340	LEU	CG-CD1	-6.21	1.32	1.52
1	D	870	LEU	CB-CG	-6.21	1.41	1.53
1	A	675	ILE	CB-CG1	-6.16	1.41	1.53
1	C	560	ILE	CB-CG1	-6.15	1.41	1.53
1	A	763	ASN	CB-CG	-6.14	1.36	1.52
1	C	661	ILE	CB-CG1	-6.14	1.41	1.53
1	D	662	LEU	CB-CG	-6.07	1.41	1.53
1	P	201	LEU	CB-CG	-6.06	1.41	1.53
1	A	751	ILE	CB-CG1	-6.00	1.41	1.53
1	E	715	MET	CG-SD	-5.98	1.65	1.80
1	A	714	ILE	CB-CG1	-5.94	1.41	1.53
1	E	591	VAL	CB-CG1	-5.94	1.32	1.52
1	C	529	GLU	CG-CD	-5.92	1.37	1.52
1	E	541	ILE	CB-CG1	-5.88	1.41	1.53
1	O	206	LEU	CB-CG	-5.86	1.41	1.53
1	B	686	ILE	CB-CG1	-5.84	1.41	1.53
1	D	687	ASN	CB-CG	-5.84	1.37	1.52
1	R	471	ILE	CB-CG1	-5.84	1.41	1.53
1	K	206	LEU	CG-CD2	-5.83	1.33	1.52
1	F	582	VAL	CB-CG2	-5.83	1.33	1.52
1	P	178	ILE	CB-CG2	-5.80	1.33	1.52
1	I	408	LEU	CG-CD2	-5.78	1.33	1.52
1	O	178	ILE	CB-CG1	-5.78	1.41	1.53
1	I	369	LEU	CB-CG	-5.77	1.42	1.53
1	B	703	LEU	CB-CG	-5.74	1.42	1.53
1	A	830	ILE	CB-CG1	-5.74	1.42	1.53
1	Q	421	HIS	CB-CG	-5.71	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	710	ASP	CB-CG	5.70	1.66	1.52
1	B	671	ASN	CA-C	-5.68	1.46	1.53
1	G	467	ILE	CB-CG1	-5.67	1.42	1.53
1	Q	431	LEU	CB-CG	-5.65	1.42	1.53
1	E	643	ILE	CB-CG1	-5.65	1.42	1.53
1	D	764	ILE	CB-CG1	-5.64	1.42	1.53
1	B	686	ILE	CG1-CD1	-5.60	1.29	1.51
1	E	703	LEU	CB-CG	-5.57	1.42	1.53
1	D	874	LEU	CG-CD2	-5.55	1.34	1.52
1	N	178	ILE	CB-CG1	-5.54	1.42	1.53
1	M	448	LEU	CG-CD1	-5.53	1.34	1.52
1	L	201	LEU	CB-CG	-5.52	1.42	1.53
1	B	810	LEU	CB-CG	-5.52	1.42	1.53
1	P	197	LEU	CB-CG	-5.51	1.42	1.53
1	B	751	ILE	CB-CG1	-5.50	1.42	1.53
1	Q	421	HIS	CG-CD2	-5.50	1.29	1.35
1	K	294	LEU	CG-CD2	-5.49	1.34	1.52
1	D	556	LEU	CB-CG	-5.49	1.42	1.53
1	D	540	ARG	CD-NE	-5.49	1.38	1.46
1	B	545	LEU	CB-CG	-5.48	1.42	1.53
1	G	448	LEU	CG-CD1	-5.44	1.34	1.52
1	I	420	PRO	N-CD	-5.43	1.40	1.47
1	A	514	VAL	CB-CG2	-5.43	1.34	1.52
1	Q	475	TYR	CB-CG	-5.42	1.39	1.51
1	B	784	CYS	CB-SG	-5.41	1.63	1.81
1	C	527	HIS	CB-CG	-5.40	1.42	1.50
1	N	199	ARG	CZ-NH2	-5.40	1.26	1.33
1	G	375	LEU	CB-CG	-5.39	1.42	1.53
1	C	607	VAL	CB-CG2	-5.39	1.34	1.52
1	I	448	LEU	CB-CG	-5.37	1.42	1.53
1	D	602	TYR	CB-CG	-5.32	1.40	1.51
1	C	687	ASN	CB-CG	-5.32	1.38	1.52
1	J	288	PRO	N-CD	-5.29	1.40	1.47
1	F	710	ASP	CB-CG	-5.27	1.38	1.52
1	O	201	LEU	CG-CD2	-5.27	1.35	1.52
1	E	595	LEU	CG-CD2	-5.26	1.35	1.52
1	A	510	PHE	CB-CG	-5.24	1.38	1.50
1	A	648	GLY	CA-C	5.23	1.59	1.51
1	C	800	LEU	CB-CG	-5.23	1.43	1.53
1	K	178	ILE	CB-CG1	-5.22	1.43	1.53
1	A	686	ILE	CB-CG1	-5.22	1.43	1.53
1	A	658	THR	CB-CG2	-5.22	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	617	ILE	CB-CG1	-5.20	1.43	1.53
1	D	824	TYR	CB-CG	-5.18	1.40	1.51
1	B	511	VAL	CB-CG2	-5.17	1.35	1.52
1	E	831	HIS	CB-CG	-5.15	1.43	1.50
1	M	431	LEU	CB-CG	-5.12	1.43	1.53
1	K	285	LEU	CG-CD2	-5.12	1.35	1.52
1	B	675	ILE	CA-CB	-5.11	1.48	1.54
1	B	795	LEU	CB-CG	-5.11	1.43	1.53
1	A	710	ASP	CB-CG	-5.10	1.39	1.52
1	A	540	ARG	CA-C	-5.08	1.46	1.52
1	N	284	TYR	CB-CG	-5.08	1.40	1.51
1	D	884	LEU	CB-CG	-5.07	1.43	1.53
1	F	673	GLN	CB-CG	-5.07	1.37	1.52
1	A	551	LEU	CB-CG	-5.06	1.43	1.53
1	A	683	ILE	CB-CG1	-5.05	1.43	1.53
1	O	284	TYR	CB-CG	-5.03	1.40	1.51
1	K	206	LEU	CB-CG	-5.02	1.43	1.53
1	A	665	ILE	CB-CG1	-5.01	1.43	1.53

All (510) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	394	ASP	CA-C-N	12.46	132.03	119.82
1	I	394	ASP	C-N-CA	12.46	132.03	119.82
1	J	278	ASN	N-CA-C	-12.21	98.48	113.50
1	A	648	GLY	CA-C-N	11.38	132.85	120.11
1	A	648	GLY	C-N-CA	11.38	132.85	120.11
1	H	419	PHE	CA-CB-CG	-11.19	102.61	113.80
1	L	202	VAL	N-CA-C	-10.66	98.16	110.21
1	L	266	ASP	CA-C-N	10.21	129.98	119.56
1	L	266	ASP	C-N-CA	10.21	129.98	119.56
1	M	394	ASP	CA-C-N	10.07	129.69	119.82
1	M	394	ASP	C-N-CA	10.07	129.69	119.82
1	N	204	LYS	N-CA-C	-9.92	101.74	114.04
1	Q	408	LEU	CA-C-N	9.57	130.16	119.92
1	Q	408	LEU	C-N-CA	9.57	130.16	119.92
1	H	394	ASP	CA-C-N	9.52	129.26	119.56
1	H	394	ASP	C-N-CA	9.52	129.26	119.56
1	F	630	PHE	CA-CB-CG	-9.46	104.34	113.80
1	M	398	ASP	CA-C-N	9.30	129.96	120.38
1	M	398	ASP	C-N-CA	9.30	129.96	120.38
1	E	648	GLY	CA-C-N	9.17	130.79	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	648	GLY	C-N-CA	9.17	130.79	120.98
1	A	789	LYS	CA-C-N	9.12	129.25	120.31
1	A	789	LYS	C-N-CA	9.12	129.25	120.31
1	B	648	GLY	CA-C-N	9.06	131.17	119.84
1	B	648	GLY	C-N-CA	9.06	131.17	119.84
1	C	630	PHE	CA-CB-CG	-8.84	104.96	113.80
1	R	390	TYR	CA-C-N	8.77	128.63	120.21
1	R	390	TYR	C-N-CA	8.77	128.63	120.21
1	A	710	ASP	CA-C-N	8.76	128.61	120.21
1	A	710	ASP	C-N-CA	8.76	128.61	120.21
1	D	506	ALA	CA-C-O	-8.70	110.67	121.89
1	H	408	LEU	CA-C-N	8.64	129.17	119.92
1	H	408	LEU	C-N-CA	8.64	129.17	119.92
1	P	266	ASP	CA-C-N	8.64	128.85	119.87
1	P	266	ASP	C-N-CA	8.64	128.85	119.87
1	I	399	PRO	N-CA-C	8.62	119.81	110.58
1	F	648	GLY	CA-C-N	8.62	130.20	120.98
1	F	648	GLY	C-N-CA	8.62	130.20	120.98
1	C	710	ASP	CB-CA-C	-8.45	102.76	110.71
1	H	474	PHE	N-CA-C	8.31	122.99	113.02
1	J	211	LEU	CB-CA-C	-8.29	97.86	110.88
1	C	617	ILE	CA-C-N	8.20	128.34	120.31
1	C	617	ILE	C-N-CA	8.20	128.34	120.31
1	F	755	ASP	CA-CB-CG	8.16	120.76	112.60
1	O	278	ASN	N-CA-C	-8.12	104.52	114.75
1	K	233	ASP	CA-C-N	8.12	127.84	119.56
1	K	233	ASP	C-N-CA	8.12	127.84	119.56
1	I	434	ASP	CA-C-N	8.08	127.81	119.56
1	I	434	ASP	C-N-CA	8.08	127.81	119.56
1	C	659	PHE	CA-CB-CG	-8.05	105.75	113.80
1	C	859	ARG	N-CA-C	-8.03	99.43	110.35
1	Q	334	LYS	N-CA-C	-7.97	98.60	110.24
1	N	200	ILE	N-CA-C	-7.92	105.00	111.81
1	D	656	PHE	CA-CB-CG	7.85	121.65	113.80
1	P	233	ASP	CA-C-N	7.84	129.64	119.84
1	P	233	ASP	C-N-CA	7.84	129.64	119.84
1	P	264	LEU	N-CA-C	7.80	121.50	110.50
1	Q	474	PHE	N-CA-C	7.79	123.74	113.30
1	E	887	THR	N-CA-C	7.77	120.22	109.18
1	B	710	ASP	CA-C-N	7.75	127.70	120.03
1	B	710	ASP	C-N-CA	7.75	127.70	120.03
1	M	434	ASP	CA-C-N	7.74	127.41	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	434	ASP	C-N-CA	7.74	127.41	119.82
1	B	789	LYS	CA-C-N	7.71	127.66	120.03
1	B	789	LYS	C-N-CA	7.71	127.66	120.03
1	D	576	LEU	CA-C-N	7.71	127.66	120.03
1	D	576	LEU	C-N-CA	7.71	127.66	120.03
1	G	457	VAL	N-CA-C	7.69	119.92	108.46
1	E	762	PHE	CA-CB-CG	-7.66	106.14	113.80
1	E	760	GLU	CA-C-N	7.64	128.33	119.47
1	E	760	GLU	C-N-CA	7.64	128.33	119.47
1	P	213	ARG	N-CA-C	-7.62	103.06	111.36
1	C	684	PRO	CA-C-O	-7.59	112.37	122.08
1	D	617	ILE	CA-C-N	7.55	127.71	120.31
1	D	617	ILE	C-N-CA	7.55	127.71	120.31
1	P	256	GLN	N-CA-C	-7.54	100.81	110.53
1	I	471	ILE	CB-CA-C	-7.46	102.27	112.04
1	I	398	ASP	CA-C-N	7.45	125.02	119.66
1	I	398	ASP	C-N-CA	7.45	125.02	119.66
1	K	266	ASP	CA-C-N	7.42	127.05	119.56
1	K	266	ASP	C-N-CA	7.42	127.05	119.56
1	A	687	ASN	CA-CB-CG	-7.40	105.20	112.60
1	D	575	ARG	N-CA-C	-7.40	102.90	112.23
1	D	820	GLY	CA-C-O	-7.37	111.33	122.54
1	R	434	ASP	CA-C-N	7.35	127.05	119.56
1	R	434	ASP	C-N-CA	7.35	127.05	119.56
1	J	178	ILE	CB-CA-C	-7.34	101.13	111.19
1	E	630	PHE	CA-CB-CG	-7.34	106.46	113.80
1	C	525	ASP	CA-CB-CG	-7.31	105.29	112.60
1	C	526	ILE	N-CA-CB	-7.28	102.18	111.64
1	D	762	PHE	CA-CB-CG	-7.28	106.52	113.80
1	C	862	MET	CB-CA-C	-7.26	100.22	111.83
1	F	692	ASN	CA-C-N	7.25	126.96	119.56
1	F	692	ASN	C-N-CA	7.25	126.96	119.56
1	R	394	ASP	CA-C-N	7.24	128.89	119.84
1	R	394	ASP	C-N-CA	7.24	128.89	119.84
1	P	202	VAL	N-CA-C	-7.24	99.60	109.37
1	F	733	LEU	CB-CA-C	-7.21	98.81	110.79
1	L	233	ASP	CA-C-N	7.20	128.84	119.84
1	L	233	ASP	C-N-CA	7.20	128.84	119.84
1	B	760	GLU	CA-C-N	7.17	126.87	119.56
1	B	760	GLU	C-N-CA	7.17	126.87	119.56
1	L	285	LEU	N-CA-C	7.15	121.16	109.72
1	D	659	PHE	CA-CB-CG	-7.11	106.69	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	278	ASN	N-CA-C	-7.09	103.10	114.09
1	M	457	VAL	N-CA-C	7.03	118.61	108.48
1	D	590	ASP	N-CA-C	7.03	119.88	110.88
1	J	226	SER	N-CA-C	-7.01	101.48	110.53
1	P	285	LEU	N-CA-C	6.96	120.86	109.24
1	A	526	ILE	N-CA-C	6.95	117.87	107.80
1	C	648	GLY	CA-C-N	6.94	126.92	119.78
1	C	648	GLY	C-N-CA	6.94	126.92	119.78
1	L	264	LEU	N-CA-C	6.92	119.67	110.53
1	D	612	LYS	N-CA-C	6.90	120.22	110.50
1	G	401	ASP	CB-CA-C	-6.88	106.32	111.20
1	B	529	GLU	CA-C-N	6.86	128.41	119.84
1	B	529	GLU	C-N-CA	6.86	128.41	119.84
1	Q	458	ALA	CA-C-N	6.80	126.74	120.21
1	Q	458	ALA	C-N-CA	6.80	126.74	120.21
1	B	643	ILE	CB-CA-C	-6.80	102.48	110.91
1	F	617	ILE	CA-C-N	6.80	126.72	119.85
1	F	617	ILE	C-N-CA	6.80	126.72	119.85
1	F	533	ASN	CA-C-O	-6.80	113.53	122.03
1	D	506	ALA	N-CA-C	6.79	118.59	110.44
1	A	760	GLU	CA-C-N	6.76	126.45	119.56
1	A	760	GLU	C-N-CA	6.76	126.45	119.56
1	B	741	THR	N-CA-C	6.76	119.95	109.07
1	O	285	LEU	N-CA-C	6.75	120.52	109.24
1	I	376	ARG	CA-C-N	6.75	128.28	119.84
1	I	376	ARG	C-N-CA	6.75	128.28	119.84
1	C	667	THR	CA-C-N	6.75	126.44	119.56
1	C	667	THR	C-N-CA	6.75	126.44	119.56
1	I	418	VAL	N-CA-C	6.70	119.78	108.86
1	R	404	ALA	CA-C-N	6.68	126.38	119.56
1	R	404	ALA	C-N-CA	6.68	126.38	119.56
1	J	231	VAL	CA-C-N	6.68	126.64	120.03
1	J	231	VAL	C-N-CA	6.68	126.64	120.03
1	B	527	HIS	N-CA-C	6.65	119.66	108.02
1	C	683	ILE	CA-C-N	6.64	126.61	120.03
1	C	683	ILE	C-N-CA	6.64	126.61	120.03
1	H	401	ASP	CA-C-N	6.64	127.17	119.47
1	H	401	ASP	C-N-CA	6.64	127.17	119.47
1	N	287	LEU	CA-C-N	6.62	126.21	119.19
1	N	287	LEU	C-N-CA	6.62	126.21	119.19
1	E	647	THR	N-CA-C	6.62	119.49	109.23
1	N	264	LEU	N-CA-C	6.61	119.48	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	398	ASP	CA-CB-CG	6.60	119.20	112.60
1	C	506	ALA	CA-C-O	-6.58	113.35	120.92
1	F	647	THR	N-CA-C	6.57	119.88	109.50
1	M	399	PRO	CA-C-N	6.53	128.01	119.84
1	M	399	PRO	C-N-CA	6.53	128.01	119.84
1	P	263	VAL	N-CA-C	6.53	116.02	106.55
1	O	244	ASP	CA-CB-CG	6.53	119.12	112.60
1	C	576	LEU	CA-C-N	6.49	126.41	119.85
1	C	576	LEU	C-N-CA	6.49	126.41	119.85
1	J	266	ASP	CA-C-N	6.46	127.92	119.84
1	J	266	ASP	C-N-CA	6.46	127.92	119.84
1	O	247	ARG	CA-C-N	6.44	128.82	120.44
1	O	247	ARG	C-N-CA	6.44	128.82	120.44
1	P	230	ILE	CA-C-N	-6.43	117.96	122.59
1	P	230	ILE	C-N-CA	-6.43	117.96	122.59
1	D	565	ILE	CB-CA-C	-6.43	103.46	112.14
1	P	195	ASP	N-CA-C	-6.43	102.24	110.53
1	P	283	PHE	CA-CB-CG	6.42	120.22	113.80
1	D	556	LEU	CB-CA-C	-6.41	100.82	110.88
1	A	833	LEU	N-CA-C	6.38	120.52	107.69
1	G	404	ALA	CA-C-N	6.37	127.81	119.84
1	G	404	ALA	C-N-CA	6.37	127.81	119.84
1	F	682	GLU	CA-C-N	6.35	133.88	122.13
1	F	682	GLU	C-N-CA	6.35	133.88	122.13
1	O	177	TRP	N-CA-C	6.35	119.19	111.82
1	R	418	VAL	N-CA-C	6.35	119.43	108.95
1	D	760	GLU	CA-C-N	6.35	126.83	119.47
1	D	760	GLU	C-N-CA	6.35	126.83	119.47
1	A	556	LEU	CB-CA-C	-6.34	100.83	110.92
1	H	390	TYR	CA-C-N	6.34	127.76	119.84
1	H	390	TYR	C-N-CA	6.34	127.76	119.84
1	B	833	LEU	N-CA-C	6.33	119.26	109.07
1	K	165	ASP	CA-CB-CG	6.32	118.92	112.60
1	M	334	LYS	CA-C-N	6.31	126.32	119.89
1	M	334	LYS	C-N-CA	6.31	126.32	119.89
1	D	710	ASP	CA-C-N	6.31	126.27	120.21
1	D	710	ASP	C-N-CA	6.31	126.27	120.21
1	F	589	ILE	N-CA-C	6.30	117.67	108.53
1	J	279	ARG	CA-C-N	6.29	126.31	119.89
1	J	279	ARG	C-N-CA	6.29	126.31	119.89
1	C	836	VAL	N-CA-C	6.29	116.92	108.11
1	F	710	ASP	N-CA-C	6.29	123.71	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	616	ASP	CA-C-N	-6.27	118.08	122.59
1	D	616	ASP	C-N-CA	-6.27	118.08	122.59
1	J	260	VAL	N-CA-C	-6.27	101.50	109.58
1	E	692	ASN	CA-C-N	6.25	125.87	119.56
1	E	692	ASN	C-N-CA	6.25	125.87	119.56
1	A	692	ASN	CA-C-N	6.24	126.71	119.47
1	A	692	ASN	C-N-CA	6.24	126.71	119.47
1	P	165	ASP	CA-CB-CG	6.24	118.84	112.60
1	G	394	ASP	CA-C-N	6.24	127.63	119.84
1	G	394	ASP	C-N-CA	6.24	127.63	119.84
1	D	612	LYS	CA-C-N	6.23	131.40	120.87
1	D	612	LYS	C-N-CA	6.23	131.40	120.87
1	D	559	VAL	CB-CA-C	-6.23	103.86	112.02
1	E	617	ILE	CA-C-N	6.22	126.13	119.85
1	E	617	ILE	C-N-CA	6.22	126.13	119.85
1	I	347	ARG	CA-C-N	6.21	125.89	119.56
1	I	347	ARG	C-N-CA	6.21	125.89	119.56
1	B	617	ILE	CA-C-N	6.21	126.12	119.85
1	B	617	ILE	C-N-CA	6.21	126.12	119.85
1	C	607	VAL	N-CA-C	6.20	117.70	108.46
1	O	266	ASP	N-CA-C	6.20	117.69	108.76
1	A	510	PHE	CA-CB-CG	-6.20	107.60	113.80
1	P	201	LEU	CA-C-N	-6.20	112.39	120.63
1	P	201	LEU	C-N-CA	-6.20	112.39	120.63
1	I	396	GLU	N-CA-C	-6.19	104.53	111.28
1	N	285	LEU	N-CA-C	6.19	118.48	108.34
1	A	582	VAL	CB-CA-C	-6.17	102.52	110.98
1	I	390	TYR	CA-C-N	6.17	126.52	119.92
1	I	390	TYR	C-N-CA	6.17	126.52	119.92
1	D	667	THR	CA-C-N	6.16	125.85	119.56
1	D	667	THR	C-N-CA	6.16	125.85	119.56
1	P	197	LEU	N-CA-C	6.16	118.78	111.33
1	E	878	THR	N-CA-C	6.15	116.40	108.34
1	M	401	ASP	CA-C-N	6.13	127.50	119.84
1	M	401	ASP	C-N-CA	6.13	127.50	119.84
1	N	165	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	687	ASN	CA-CB-CG	-6.12	106.48	112.60
1	I	449	LYS	N-CA-C	-6.12	105.97	113.50
1	A	710	ASP	CB-CA-C	-6.12	104.96	110.71
1	O	263	VAL	N-CA-C	6.11	115.41	106.55
1	D	692	ASN	CA-C-N	6.11	127.48	119.84
1	D	692	ASN	C-N-CA	6.11	127.48	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	195	ASP	N-CA-C	-6.11	102.65	110.53
1	E	789	LYS	CA-C-N	6.09	127.45	119.84
1	E	789	LYS	C-N-CA	6.09	127.45	119.84
1	N	260	VAL	N-CA-C	6.09	116.89	108.12
1	D	677	ASP	CB-CA-C	-6.08	103.08	110.81
1	F	529	GLU	CA-C-N	6.08	127.44	119.84
1	F	529	GLU	C-N-CA	6.08	127.44	119.84
1	I	428	LEU	N-CA-C	6.07	118.42	108.52
1	D	643	ILE	CB-CA-C	-6.07	103.39	110.91
1	B	677	ASP	CA-C-N	6.06	127.41	119.84
1	B	677	ASP	C-N-CA	6.06	127.41	119.84
1	I	363	GLY	N-CA-C	-6.05	104.97	111.93
1	A	783	HIS	CA-CB-CG	6.05	119.85	113.80
1	C	533	ASN	N-CA-C	-6.05	106.88	114.56
1	A	715	MET	CA-C-N	-6.04	115.02	122.93
1	A	715	MET	C-N-CA	-6.04	115.02	122.93
1	F	675	ILE	CB-CA-C	-6.03	102.16	110.96
1	J	287	LEU	N-CA-C	6.02	117.39	109.93
1	K	224	LEU	N-CA-C	6.02	119.36	109.85
1	C	661	ILE	CB-CA-C	-6.01	104.28	111.97
1	J	284	TYR	N-CA-C	-6.01	100.36	109.85
1	B	644	PHE	CA-CB-CG	-6.01	107.79	113.80
1	D	831	HIS	N-CA-C	6.01	118.54	109.23
1	E	529	GLU	CA-C-N	6.01	125.77	119.76
1	E	529	GLU	C-N-CA	6.01	125.77	119.76
1	C	678	PRO	N-CA-C	-5.98	102.48	111.57
1	Q	394	ASP	CA-C-N	5.97	126.40	119.47
1	Q	394	ASP	C-N-CA	5.97	126.40	119.47
1	H	434	ASP	CA-C-N	5.97	127.30	119.84
1	H	434	ASP	C-N-CA	5.97	127.30	119.84
1	J	287	LEU	CA-C-N	5.96	125.50	119.19
1	J	287	LEU	C-N-CA	5.96	125.50	119.19
1	A	611	LEU	N-CA-C	-5.96	101.64	110.46
1	K	274	ALA	N-CA-C	-5.96	104.79	111.28
1	D	525	ASP	N-CA-C	5.95	118.33	108.99
1	F	582	VAL	N-CA-C	5.95	117.33	108.46
1	C	532	GLN	N-CA-C	5.95	117.77	111.28
1	E	556	LEU	CB-CA-C	-5.94	101.47	110.92
1	A	653	GLY	N-CA-C	-5.93	106.98	115.64
1	K	287	LEU	CA-C-N	5.93	125.61	119.56
1	K	287	LEU	C-N-CA	5.93	125.61	119.56
1	G	401	ASP	CA-C-N	5.92	127.24	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	401	ASP	C-N-CA	5.92	127.24	119.84
1	D	862	MET	CB-CA-C	-5.90	102.38	111.83
1	C	527	HIS	N-CA-C	5.90	118.06	108.26
1	R	458	ALA	CA-C-N	5.90	125.85	119.78
1	R	458	ALA	C-N-CA	5.90	125.85	119.78
1	A	791	ASP	CA-C-N	5.89	125.56	119.56
1	A	791	ASP	C-N-CA	5.89	125.56	119.56
1	A	626	ALA	CA-C-N	5.87	126.02	119.32
1	A	626	ALA	C-N-CA	5.87	126.02	119.32
1	M	419	PHE	CA-CB-CG	-5.87	107.93	113.80
1	K	263	VAL	N-CA-CB	-5.86	106.38	112.06
1	E	831	HIS	N-CA-C	5.85	118.74	109.50
1	L	255	PHE	CA-CB-CG	-5.85	107.95	113.80
1	A	746	ASP	CA-CB-CG	5.84	118.44	112.60
1	N	289	GLN	N-CA-C	-5.83	105.00	111.36
1	D	643	ILE	N-CA-CB	5.83	117.07	110.72
1	A	526	ILE	CB-CA-C	-5.83	102.45	110.96
1	B	671	ASN	CB-CA-C	-5.83	101.94	111.50
1	N	231	VAL	CA-C-N	5.82	125.73	119.85
1	N	231	VAL	C-N-CA	5.82	125.73	119.85
1	E	782	GLU	N-CA-C	5.82	118.37	111.33
1	K	201	LEU	N-CA-C	5.82	117.62	111.28
1	E	667	THR	CA-C-N	5.80	125.48	119.56
1	E	667	THR	C-N-CA	5.80	125.48	119.56
1	C	789	LYS	CA-C-N	5.80	125.78	120.03
1	C	789	LYS	C-N-CA	5.80	125.78	120.03
1	N	266	ASP	CA-C-N	5.80	125.90	119.87
1	N	266	ASP	C-N-CA	5.80	125.90	119.87
1	A	527	HIS	N-CA-C	5.80	118.41	109.07
1	I	457	VAL	N-CA-C	5.80	116.71	108.42
1	C	710	ASP	CA-C-N	5.79	125.76	120.03
1	C	710	ASP	C-N-CA	5.79	125.76	120.03
1	F	534	ASP	CA-C-N	5.77	128.83	120.98
1	F	534	ASP	C-N-CA	5.77	128.83	120.98
1	B	686	ILE	N-CA-C	5.76	118.15	108.81
1	F	743	HIS	N-CA-C	5.76	117.69	108.41
1	C	831	HIS	N-CA-C	5.76	118.16	109.23
1	J	264	LEU	N-CA-C	5.76	118.71	110.24
1	O	287	LEU	CA-C-N	5.75	125.61	119.28
1	O	287	LEU	C-N-CA	5.75	125.61	119.28
1	H	419	PHE	CA-C-N	5.75	127.03	119.84
1	H	419	PHE	C-N-CA	5.75	127.03	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	669	ASP	CA-CB-CG	5.75	118.34	112.60
1	O	264	LEU	N-CA-C	5.71	119.56	109.96
1	R	393	VAL	N-CA-C	5.71	115.49	108.53
1	K	264	LEU	N-CA-C	5.70	118.92	110.48
1	Q	473	ARG	N-CA-C	5.70	117.57	111.36
1	D	815	GLY	O-C-N	-5.69	116.73	122.54
1	C	641	TYR	N-CA-C	5.69	117.49	108.79
1	E	755	ASP	CA-CB-CG	5.67	118.28	112.60
1	C	760	GLU	CA-C-N	5.67	125.52	119.28
1	C	760	GLU	C-N-CA	5.67	125.52	119.28
1	H	401	ASP	CA-CB-CG	5.67	118.27	112.60
1	F	667	THR	CA-C-N	5.66	125.34	119.56
1	F	667	THR	C-N-CA	5.66	125.34	119.56
1	C	598	LEU	CA-C-N	5.66	125.94	119.83
1	C	598	LEU	C-N-CA	5.66	125.94	119.83
1	E	598	LEU	CA-C-N	5.66	125.57	119.85
1	E	598	LEU	C-N-CA	5.66	125.57	119.85
1	K	251	VAL	CA-C-N	5.66	125.59	119.76
1	K	251	VAL	C-N-CA	5.66	125.59	119.76
1	A	514	VAL	CB-CA-C	-5.64	104.43	112.22
1	A	617	ILE	CA-C-N	5.63	125.61	120.03
1	A	617	ILE	C-N-CA	5.63	125.61	120.03
1	Q	398	ASP	CB-CA-C	5.62	119.10	109.82
1	O	233	ASP	CA-C-N	5.62	126.86	119.84
1	O	233	ASP	C-N-CA	5.62	126.86	119.84
1	A	776	LEU	N-CA-C	5.62	118.97	109.76
1	K	283	PHE	CA-CB-CG	5.62	119.42	113.80
1	A	741	THR	N-CA-C	5.61	118.11	109.07
1	D	790	PRO	CB-CA-C	-5.61	103.60	110.95
1	P	231	VAL	CA-C-N	5.61	125.51	119.85
1	P	231	VAL	C-N-CA	5.61	125.51	119.85
1	A	670	LYS	N-CA-C	5.61	118.61	108.69
1	C	812	LYS	CA-C-N	-5.60	114.59	120.31
1	C	812	LYS	C-N-CA	-5.60	114.59	120.31
1	E	684	PRO	N-CA-C	-5.60	102.34	110.80
1	C	862	MET	N-CA-C	5.60	118.27	108.52
1	L	283	PHE	CA-CB-CG	5.59	119.39	113.80
1	H	404	ALA	CA-C-N	5.59	125.95	119.47
1	H	404	ALA	C-N-CA	5.59	125.95	119.47
1	F	712	ASP	CA-CB-CG	5.59	118.19	112.60
1	J	285	LEU	N-CA-C	5.59	118.56	109.06
1	F	836	VAL	N-CA-C	5.59	115.37	106.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	GLN	N-CA-C	5.58	117.37	111.28
1	C	678	PRO	CA-C-N	-5.58	113.39	120.98
1	C	678	PRO	C-N-CA	-5.58	113.39	120.98
1	E	675	ILE	CB-CA-C	-5.57	102.83	110.96
1	E	642	GLY	N-CA-C	5.56	117.75	111.85
1	A	649	PRO	N-CA-C	5.55	119.27	111.33
1	B	509	LYS	N-CA-C	-5.55	105.23	111.28
1	O	287	LEU	N-CA-CB	-5.55	102.55	110.04
1	L	197	LEU	N-CA-C	5.53	117.75	111.11
1	R	376	ARG	N-CA-C	-5.53	102.24	110.20
1	R	407	LEU	N-CA-C	5.51	120.49	113.55
1	B	575	ARG	N-CA-C	-5.51	104.80	112.45
1	E	639	LYS	CA-C-N	5.50	126.72	119.84
1	E	639	LYS	C-N-CA	5.50	126.72	119.84
1	D	654	LYS	CB-CA-C	-5.50	102.49	110.96
1	B	791	ASP	CA-C-N	5.50	125.33	119.28
1	B	791	ASP	C-N-CA	5.50	125.33	119.28
1	B	510	PHE	CA-CB-CG	-5.48	108.32	113.80
1	Q	386	THR	CA-C-N	5.47	127.56	120.44
1	Q	386	THR	C-N-CA	5.47	127.56	120.44
1	E	722	SER	N-CA-C	5.47	116.92	111.07
1	F	682	GLU	CA-C-O	-5.47	112.69	120.51
1	F	760	GLU	CA-C-N	5.47	125.81	119.47
1	F	760	GLU	C-N-CA	5.47	125.81	119.47
1	E	551	LEU	CA-C-N	5.45	125.43	120.03
1	E	551	LEU	C-N-CA	5.45	125.43	120.03
1	L	253	ILE	N-CA-C	5.45	115.83	107.77
1	M	458	ALA	CA-C-N	5.44	125.35	119.85
1	M	458	ALA	C-N-CA	5.44	125.35	119.85
1	E	622	ASP	CA-CB-CG	5.44	118.04	112.60
1	E	710	ASP	N-CA-C	5.44	121.82	109.81
1	F	585	ARG	N-CA-C	5.42	117.51	108.99
1	O	251	VAL	CA-C-N	5.42	125.34	119.76
1	O	251	VAL	C-N-CA	5.42	125.34	119.76
1	C	764	ILE	CB-CA-C	-5.41	105.04	111.97
1	G	399	PRO	N-CA-C	-5.41	105.28	110.47
1	D	584	TYR	CB-CA-C	-5.39	103.71	111.91
1	E	809	ARG	N-CA-C	-5.38	103.99	110.44
1	G	400	PRO	CA-C-N	-5.37	117.71	124.21
1	G	400	PRO	C-N-CA	-5.37	117.71	124.21
1	P	177	TRP	CB-CG-CD2	5.37	134.32	126.80
1	C	692	ASN	CA-C-N	5.37	125.04	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	692	ASN	C-N-CA	5.37	125.04	119.56
1	E	788	VAL	N-CA-C	5.36	116.62	112.12
1	G	443	ASP	N-CA-C	-5.36	105.60	111.82
1	B	519	PHE	CA-CB-CG	5.35	119.15	113.80
1	B	751	ILE	CB-CA-C	-5.35	105.01	112.02
1	B	878	THR	N-CA-C	5.35	115.19	108.45
1	D	791	ASP	CA-C-N	5.34	125.67	119.47
1	D	791	ASP	C-N-CA	5.34	125.67	119.47
1	B	639	LYS	CA-C-N	5.34	125.01	119.56
1	B	639	LYS	C-N-CA	5.34	125.01	119.56
1	J	283	PHE	CA-CB-CG	-5.34	108.46	113.80
1	L	231	VAL	CA-C-N	5.34	125.32	120.03
1	L	231	VAL	C-N-CA	5.34	125.32	120.03
1	I	406	LEU	N-CA-C	-5.34	105.03	112.45
1	E	591	VAL	CA-C-N	-5.34	113.29	120.87
1	E	591	VAL	C-N-CA	-5.34	113.29	120.87
1	A	738	VAL	N-CA-C	5.33	115.53	107.80
1	A	751	ILE	CB-CA-C	-5.32	105.05	112.02
1	E	576	LEU	CA-C-N	5.32	125.08	119.76
1	E	576	LEU	C-N-CA	5.32	125.08	119.76
1	C	656	PHE	CA-CB-CG	5.31	119.11	113.80
1	D	764	ILE	CB-CA-C	-5.31	105.06	112.02
1	O	287	LEU	N-CA-C	5.31	118.00	110.24
1	R	409	PRO	CB-CA-C	-5.31	104.81	111.56
1	C	506	ALA	O-C-N	-5.31	117.00	123.16
1	R	471	ILE	CB-CA-C	-5.31	105.07	112.02
1	J	233	ASP	CA-C-N	5.30	126.47	119.84
1	J	233	ASP	C-N-CA	5.30	126.47	119.84
1	F	831	HIS	N-CA-C	5.30	117.03	108.34
1	B	529	GLU	N-CA-C	5.30	116.60	109.24
1	C	619	GLU	N-CA-C	-5.30	103.03	110.50
1	I	408	LEU	CA-C-N	5.29	125.29	120.21
1	I	408	LEU	C-N-CA	5.29	125.29	120.21
1	K	168	LEU	CB-CA-C	5.29	118.48	109.53
1	B	678	PRO	CA-C-N	5.29	131.49	121.97
1	B	678	PRO	C-N-CA	5.29	131.49	121.97
1	F	576	LEU	CA-C-N	5.28	125.19	119.85
1	F	576	LEU	C-N-CA	5.28	125.19	119.85
1	Q	434	ASP	CA-C-N	5.28	124.99	119.82
1	Q	434	ASP	C-N-CA	5.28	124.99	119.82
1	B	532	GLN	N-CA-C	5.27	117.03	111.28
1	Q	428	LEU	N-CA-C	5.27	116.98	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	683	ILE	N-CA-CB	5.25	118.56	111.21
1	F	592	ASP	N-CA-C	5.25	117.84	110.23
1	P	290	ALA	N-CA-C	-5.24	105.65	111.36
1	G	400	PRO	CB-CA-C	-5.24	106.03	112.89
1	P	295	PHE	CA-CB-CG	5.24	119.04	113.80
1	A	831	HIS	N-CA-C	5.24	117.98	109.24
1	M	412	LEU	N-CA-C	-5.22	105.67	111.36
1	A	639	LYS	CA-C-N	5.22	124.88	119.56
1	A	639	LYS	C-N-CA	5.22	124.88	119.56
1	O	295	PHE	CA-CB-CG	-5.21	108.59	113.80
1	D	506	ALA	O-C-N	-5.21	114.91	121.83
1	N	233	ASP	CA-C-N	5.20	126.34	119.84
1	N	233	ASP	C-N-CA	5.20	126.34	119.84
1	E	542	ASP	CA-CB-CG	-5.20	107.41	112.60
1	I	456	GLU	N-CA-C	-5.19	99.74	110.80
1	B	526	ILE	CB-CA-C	-5.19	103.87	110.98
1	F	704	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	F	610	LEU	N-CA-C	5.18	117.54	108.52
1	E	626	ALA	N-CA-C	-5.18	102.93	110.08
1	R	428	LEU	N-CA-C	5.18	116.85	108.41
1	A	856	ILE	CB-CA-C	-5.17	105.35	111.97
1	B	763	ASN	N-CA-C	-5.17	107.04	113.55
1	C	712	ASP	N-CA-C	-5.16	106.14	112.90
1	B	712	ASP	N-CA-C	-5.16	107.05	113.55
1	C	507	ALA	N-CA-C	5.16	121.78	110.80
1	F	835	VAL	CA-C-N	-5.16	116.56	122.95
1	F	835	VAL	C-N-CA	-5.16	116.56	122.95
1	D	651	GLY	N-CA-C	-5.14	107.89	114.37
1	M	474	PHE	CA-CB-CG	-5.13	108.67	113.80
1	B	525	ASP	N-CA-C	5.13	117.05	108.99
1	K	230	ILE	N-CA-C	5.12	111.69	106.21
1	M	422	ARG	N-CA-C	5.12	118.29	110.20
1	E	540	ARG	N-CA-CB	5.12	118.06	110.49
1	C	674	THR	N-CA-C	5.11	117.77	109.24
1	E	619	GLU	N-CA-C	-5.10	104.13	110.41
1	B	772	LEU	CB-CA-C	-5.09	102.63	110.78
1	P	264	LEU	CB-CA-C	-5.09	100.17	109.54
1	F	791	ASP	CA-C-N	5.09	124.88	119.28
1	F	791	ASP	C-N-CA	5.09	124.88	119.28
1	F	611	LEU	N-CA-C	-5.09	103.32	110.50
1	K	266	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	831	HIS	N-CA-C	5.07	117.52	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	419	PHE	N-CA-CB	5.07	118.04	111.40
1	N	212	TYR	CA-CB-CG	-5.07	104.78	113.90
1	N	233	ASP	CA-CB-CG	5.07	117.67	112.60
1	D	633	PHE	N-CA-C	-5.07	105.65	111.07
1	B	592	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	768	LEU	N-CA-C	5.06	117.73	109.59
1	H	458	ALA	CA-C-N	5.05	126.15	119.84
1	H	458	ALA	C-N-CA	5.05	126.15	119.84
1	E	524	SER	N-CA-C	-5.05	107.25	113.41
1	C	833	LEU	N-CA-C	5.04	116.63	108.41
1	K	231	VAL	CA-C-N	5.04	125.02	120.03
1	K	231	VAL	C-N-CA	5.04	125.02	120.03
1	I	386	THR	CA-C-N	5.04	126.99	120.44
1	I	386	THR	C-N-CA	5.04	126.99	120.44
1	D	773	SER	N-CA-C	-5.04	101.94	109.95
1	L	196	LEU	CA-C-N	5.04	127.34	120.54
1	L	196	LEU	C-N-CA	5.04	127.34	120.54
1	Q	401	ASP	CA-C-N	5.04	126.14	119.84
1	Q	401	ASP	C-N-CA	5.04	126.14	119.84
1	D	626	ALA	CA-C-N	5.04	125.06	119.32
1	D	626	ALA	C-N-CA	5.04	125.06	119.32
1	F	579	ASP	CA-CB-CG	5.04	117.64	112.60
1	D	527	HIS	CA-C-N	-5.02	116.45	122.22
1	D	527	HIS	C-N-CA	-5.02	116.45	122.22
1	Q	360	ARG	N-CA-C	-5.02	108.18	114.56
1	L	172	LEU	N-CA-C	-5.01	105.82	111.28
1	C	625	PHE	CA-CB-CG	5.01	118.81	113.80
1	C	686	ILE	CB-CA-C	-5.01	104.03	110.84

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	506	ALA	Peptide,Mainchain
1	C	684	PRO	Peptide,Mainchain
1	D	506	ALA	Peptide,Mainchain
1	D	815	GLY	Peptide,Mainchain
1	D	819	CYS	Peptide,Mainchain
1	D	820	GLY	Peptide,Mainchain
1	E	587	GLY	Peptide,Mainchain
1	F	533	ASN	Peptide,Mainchain
1	F	682	GLU	Peptide,Mainchain

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	28	0
1	B	2966	0	3066	28	0
1	C	2975	0	3080	41	0
1	D	2975	0	3080	34	0
1	E	2975	0	3080	20	0
1	F	2975	0	3078	29	0
1	G	1143	0	1182	19	0
1	H	1143	0	1182	15	0
1	I	1143	0	1182	13	0
1	J	1090	0	1117	13	0
1	K	1090	0	1117	21	0
1	L	1090	0	1117	18	0
1	M	1143	0	1182	13	0
1	N	1090	0	1117	16	0
1	O	1090	0	1117	24	0
1	P	1090	0	1117	13	0
1	Q	1143	0	1182	16	0
1	R	1143	0	1182	14	0
All	All	31239	0	32258	368	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 6.

All (368) 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:Q:336:LEU:HD13	1:Q:336:LEU:C	1.78	1.07
1:F:683:ILE:HG22	1:F:683:ILE:O	1.50	1.06
1:B:679:VAL:HG12	1:B:679:VAL:O	1.58	1.01
1:K:263:VAL:HG23	1:K:263:VAL:O	1.63	0.96
1:O:291:TRP:HE3	1:O:291:TRP:HA	1.32	0.94
1:O:291:TRP:HA	1:O:291:TRP:CE3	2.01	0.91
1:D:832:GLU:O	1:D:832:GLU:HG3	1.72	0.89
1:L:248:TYR:HD1	1:L:248:TYR:O	1.63	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:336:LEU:C	1:Q:336:LEU:CD1	2.50	0.82
1:L:291:TRP:HA	1:L:291:TRP:CE3	2.18	0.79
1:C:525:ASP:OD1	1:C:525:ASP:C	2.26	0.78
1:O:291:TRP:CE3	1:O:291:TRP:CA	2.68	0.76
1:J:276:LEU:C	1:J:276:LEU:HD23	2.11	0.76
1:G:401:ASP:OD1	1:G:401:ASP:O	2.04	0.76
1:L:291:TRP:HA	1:L:291:TRP:HE3	1.50	0.76
1:C:862:MET:O	1:C:862:MET:HG2	1.86	0.74
1:B:679:VAL:O	1:B:679:VAL:CG1	2.33	0.74
1:L:248:TYR:CD1	1:L:248:TYR:C	2.65	0.74
1:C:525:ASP:OD1	1:C:525:ASP:O	2.06	0.74
1:P:291:TRP:CE3	1:P:291:TRP:HA	2.25	0.71
1:D:862:MET:O	1:D:862:MET:HG2	1.91	0.71
1:K:291:TRP:HE3	1:K:291:TRP:HA	1.56	0.71
1:F:710:ASP:O	1:F:710:ASP:OD2	2.08	0.71
1:G:412:LEU:C	1:G:412:LEU:HD23	2.16	0.71
1:A:519:PHE:HD1	1:A:519:PHE:N	1.89	0.70
1:B:650:THR:HG23	1:B:650:THR:O	1.90	0.70
1:K:291:TRP:HA	1:K:291:TRP:CE3	2.27	0.70
1:O:212:TYR:C	1:O:212:TYR:CD1	2.67	0.70
1:Q:419:PHE:CD1	1:Q:419:PHE:C	2.70	0.69
1:N:276:LEU:C	1:N:276:LEU:HD23	2.17	0.69
1:P:291:TRP:HA	1:P:291:TRP:HE3	1.58	0.68
1:P:263:VAL:HG23	1:P:263:VAL:O	1.94	0.68
1:M:410:GLU:CD	1:M:410:GLU:H	2.03	0.66
1:D:888:ILE:HG22	1:D:888:ILE:O	1.96	0.66
1:K:248:TYR:HD1	1:K:248:TYR:C	2.04	0.66
1:H:419:PHE:O	1:H:419:PHE:CD2	2.49	0.65
1:L:291:TRP:CE3	1:L:291:TRP:CA	2.79	0.65
1:L:248:TYR:O	1:L:248:TYR:CD1	2.48	0.65
1:H:419:PHE:CD2	1:H:419:PHE:C	2.74	0.65
1:F:710:ASP:O	1:F:710:ASP:CG	2.30	0.65
1:K:248:TYR:C	1:K:248:TYR:CD1	2.73	0.65
1:O:263:VAL:HG23	1:O:263:VAL:O	1.94	0.65
1:G:412:LEU:HD23	1:G:412:LEU:O	1.97	0.65
1:A:519:PHE:N	1:A:519:PHE:CD1	2.65	0.64
1:O:295:PHE:CD1	1:O:295:PHE:N	2.61	0.63
1:M:419:PHE:CD1	1:M:419:PHE:C	2.76	0.63
1:D:832:GLU:O	1:D:832:GLU:CG	2.40	0.63
1:L:248:TYR:HD1	1:L:248:TYR:C	2.05	0.63
1:K:178:ILE:HG23	1:K:178:ILE:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:407:LEU:O	1:R:407:LEU:HD12	2.00	0.62
1:R:401:ASP:OD1	1:R:401:ASP:O	2.16	0.62
1:B:677:ASP:C	1:B:677:ASP:OD1	2.42	0.62
1:F:595:LEU:N	1:F:595:LEU:HD12	2.16	0.61
1:O:178:ILE:HG23	1:O:178:ILE:O	2.01	0.60
1:B:691:VAL:O	1:B:692:ASN:C	2.45	0.60
1:K:248:TYR:HD1	1:K:248:TYR:O	1.84	0.60
1:J:276:LEU:HD23	1:J:276:LEU:O	2.01	0.60
1:Q:408:LEU:C	1:Q:408:LEU:HD23	2.27	0.59
1:I:336:LEU:HD13	1:I:336:LEU:C	2.26	0.59
1:E:582:VAL:HG13	1:E:582:VAL:O	2.03	0.59
1:F:884:LEU:C	1:F:884:LEU:HD23	2.28	0.58
1:D:644:PHE:C	1:D:644:PHE:HD1	2.12	0.58
1:G:435:PRO:O	1:G:436:ARG:C	2.47	0.58
1:B:686:ILE:O	1:B:686:ILE:HG23	2.03	0.57
1:K:263:VAL:O	1:K:263:VAL:CG2	2.42	0.57
1:J:287:LEU:HD12	1:J:287:LEU:N	2.19	0.57
1:L:255:PHE:C	1:L:255:PHE:CD2	2.80	0.57
1:L:212:TYR:CD1	1:L:212:TYR:C	2.82	0.56
1:E:584:TYR:CD1	1:E:584:TYR:C	2.83	0.56
1:J:276:LEU:C	1:J:276:LEU:CD2	2.78	0.56
1:L:263:VAL:O	1:L:263:VAL:HG23	2.03	0.56
1:I:375:LEU:C	1:I:375:LEU:HD12	2.30	0.56
1:A:714:ILE:O	1:A:714:ILE:CG2	2.52	0.56
1:D:576:LEU:C	1:D:576:LEU:HD12	2.31	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:D:862:MET:O	1:D:863:LYS:C	2.48	0.56
1:N:276:LEU:HD23	1:N:276:LEU:O	2.06	0.56
1:C:527:HIS:ND1	1:C:605:LYS:NZ	2.54	0.55
1:O:212:TYR:C	1:O:212:TYR:HD1	2.13	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:R:404:ALA:O	1:R:475:TYR:OH	2.24	0.54
1:N:183:LEU:C	1:N:183:LEU:HD23	2.32	0.54
1:R:422:ARG:O	1:R:422:ARG:HG3	2.07	0.54
1:O:277:LEU:O	1:O:277:LEU:HG	2.07	0.54
1:R:401:ASP:O	1:R:403:GLY:N	2.40	0.54
1:G:401:ASP:OD1	1:G:401:ASP:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:202:VAL:O	1:P:203:ARG:CB	2.55	0.53
1:C:710:ASP:CG	1:C:710:ASP:O	2.48	0.53
1:D:781:CYS:O	1:D:781:CYS:SG	2.63	0.53
1:A:817:GLU:H	1:A:817:GLU:CD	2.15	0.53
1:C:859:ARG:O	1:C:860:LYS:HB2	2.09	0.53
1:E:710:ASP:CG	1:E:710:ASP:O	2.49	0.53
1:K:238:LEU:HD12	1:K:238:LEU:C	2.33	0.53
1:H:336:LEU:HD13	1:H:336:LEU:C	2.33	0.53
1:N:178:ILE:HG22	1:N:206:LEU:HB2	1.90	0.53
1:R:451:LYS:HG3	1:R:451:LYS:O	2.08	0.53
1:L:183:LEU:HD23	1:L:183:LEU:C	2.34	0.53
1:D:519:PHE:HD1	1:D:519:PHE:N	2.05	0.53
1:D:519:PHE:N	1:D:519:PHE:CD1	2.76	0.53
1:D:778:ARG:HB3	1:D:824:TYR:HB3	1.90	0.52
1:C:801:SER:O	1:C:803:ALA:N	2.42	0.52
1:B:641:TYR:OH	1:C:812:LYS:NZ	2.31	0.52
1:G:434:ASP:O	1:G:435:PRO:C	2.53	0.52
1:J:259:GLU:O	1:J:259:GLU:HG2	2.10	0.52
1:H:408:LEU:C	1:H:408:LEU:HD23	2.35	0.52
1:B:510:PHE:CD2	1:B:510:PHE:C	2.85	0.52
1:D:644:PHE:C	1:D:644:PHE:CD1	2.85	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:B:650:THR:O	1:B:650:THR:CG2	2.54	0.51
1:C:862:MET:O	1:C:863:LYS:C	2.48	0.51
1:L:255:PHE:CD2	1:L:255:PHE:O	2.64	0.51
1:B:677:ASP:HB2	1:B:678:PRO:HD2	1.93	0.51
1:D:671:ASN:OD1	1:D:671:ASN:C	2.54	0.51
1:F:765:SER:OG	1:F:766:ALA:N	2.44	0.51
1:K:291:TRP:CE3	1:K:291:TRP:CA	2.94	0.50
1:P:276:LEU:HD23	1:P:276:LEU:C	2.37	0.50
1:A:650:THR:O	1:A:650:THR:HG23	2.10	0.50
1:H:336:LEU:HD22	1:H:336:LEU:C	2.35	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:I:400:PRO:O	1:I:401:ASP:C	2.54	0.50
1:A:522:ASP:OD1	1:A:612:LYS:NZ	2.43	0.50
1:C:760:GLU:CD	1:C:760:GLU:H	2.19	0.50
1:L:202:VAL:O	1:L:203:ARG:HB3	2.12	0.50
1:I:463:THR:HG23	1:I:463:THR:O	2.10	0.50
1:I:408:LEU:HD23	1:I:408:LEU:C	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:287:LEU:N	1:J:287:LEU:CD1	2.75	0.49
1:K:202:VAL:O	1:K:203:ARG:HB2	2.12	0.49
1:C:677:ASP:HB3	1:C:678:PRO:CD	2.41	0.49
1:G:401:ASP:O	1:G:403:GLY:N	2.45	0.49
1:D:614:ALA:HA	1:D:681:TYR:CD2	2.47	0.49
1:K:168:LEU:HD21	1:K:198:GLY:H	1.77	0.49
1:G:400:PRO:O	1:G:401:ASP:C	2.55	0.49
1:H:334:LYS:O	1:H:335:PRO:C	2.56	0.49
1:A:653:GLY:O	1:A:654:LYS:C	2.55	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:O:266:ASP:OD1	1:O:266:ASP:O	2.31	0.49
1:A:510:PHE:CZ	1:A:551:LEU:HD11	2.48	0.48
1:A:519:PHE:CE2	1:A:591:VAL:HB	2.47	0.48
1:A:524:SER:N	1:A:540:ARG:O	2.46	0.48
1:N:276:LEU:C	1:N:276:LEU:CD2	2.85	0.48
1:Q:393:VAL:O	1:Q:393:VAL:HG23	2.13	0.48
1:D:817:GLU:H	1:D:817:GLU:CD	2.14	0.48
1:I:394:ASP:OD1	1:I:394:ASP:C	2.56	0.48
1:C:862:MET:O	1:C:862:MET:CG	2.44	0.48
1:E:582:VAL:O	1:E:582:VAL:CG1	2.56	0.48
1:E:788:VAL:O	1:E:789:LYS:C	2.57	0.48
1:P:202:VAL:O	1:P:203:ARG:HB3	2.14	0.48
1:E:746:ASP:OD1	1:E:747:ALA:N	2.46	0.48
1:F:743:HIS:ND1	1:F:743:HIS:C	2.71	0.48
1:H:335:PRO:O	1:H:336:LEU:C	2.56	0.47
1:D:814:MET:HA	1:D:814:MET:HE2	1.96	0.47
1:H:335:PRO:O	1:H:338:GLU:N	2.47	0.47
1:N:168:LEU:HD23	1:N:168:LEU:H	1.79	0.47
1:A:671:ASN:OD1	1:A:671:ASN:C	2.54	0.47
1:F:590:ASP:OD1	1:F:613:LYS:NZ	2.47	0.47
1:F:600:THR:HG22	1:F:602:TYR:H	1.79	0.47
1:G:419:PHE:C	1:G:419:PHE:CD1	2.92	0.47
1:O:175:LYS:NZ	1:Q:378:GLU:OE1	2.46	0.47
1:G:418:VAL:O	1:G:418:VAL:HG23	2.15	0.47
1:K:286:ALA:HB3	1:K:291:TRP:CZ2	2.50	0.47
1:I:350:ASP:HB3	1:I:374:LYS:HB3	1.96	0.47
1:P:201:LEU:O	1:P:202:VAL:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:334:LYS:O	1:I:335:PRO:C	2.58	0.47
1:G:404:ALA:N	1:G:405:PRO:CD	2.77	0.46
1:G:424:GLU:HB3	1:G:427:ARG:HB3	1.97	0.46
1:O:212:TYR:HD1	1:O:212:TYR:O	1.98	0.46
1:B:677:ASP:HB2	1:B:678:PRO:CD	2.45	0.46
1:K:183:LEU:C	1:K:183:LEU:HD23	2.40	0.46
1:B:790:PRO:HG2	1:B:795:LEU:HD11	1.97	0.46
1:C:510:PHE:O	1:C:511:VAL:C	2.57	0.46
1:M:463:THR:O	1:M:465:ALA:N	2.48	0.46
1:D:835:VAL:HG13	1:D:835:VAL:O	2.14	0.46
1:B:535:VAL:HB	1:B:551:LEU:HB2	1.97	0.46
1:D:868:ASP:OD1	1:D:872:LYS:NZ	2.49	0.46
1:R:401:ASP:OD1	1:R:401:ASP:C	2.59	0.46
1:F:675:ILE:HG21	1:F:675:ILE:HD13	1.63	0.46
1:K:276:LEU:HD23	1:K:276:LEU:C	2.40	0.46
1:H:461:VAL:O	1:H:461:VAL:HG13	2.15	0.46
1:A:710:ASP:CG	1:A:710:ASP:O	2.56	0.46
1:C:859:ARG:O	1:C:860:LYS:CB	2.64	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:M:400:PRO:O	1:M:401:ASP:C	2.59	0.46
1:R:333:ALA:O	1:R:334:LYS:C	2.59	0.46
1:C:551:LEU:N	1:C:551:LEU:HD12	2.31	0.45
1:B:686:ILE:O	1:B:686:ILE:CG2	2.61	0.45
1:D:788:VAL:O	1:D:789:LYS:C	2.59	0.45
1:E:716:VAL:O	1:E:717:GLY:C	2.56	0.45
1:G:462:ALA:O	1:G:463:THR:C	2.59	0.45
1:Q:419:PHE:CE2	1:Q:470:LEU:HB3	2.50	0.45
1:A:569:LEU:HD12	1:A:569:LEU:N	2.32	0.45
1:C:778:ARG:HB3	1:C:824:TYR:CB	2.46	0.45
1:N:202:VAL:HG23	1:N:202:VAL:O	2.15	0.45
1:O:287:LEU:HA	1:O:287:LEU:HD23	1.70	0.45
1:D:510:PHE:O	1:D:511:VAL:C	2.59	0.45
1:D:798:LEU:O	1:D:866:ARG:NE	2.50	0.45
1:D:824:TYR:CD1	1:D:824:TYR:N	2.85	0.45
1:L:279:ARG:O	1:L:280:PRO:C	2.58	0.45
1:O:291:TRP:CE3	1:O:291:TRP:N	2.84	0.45
1:R:334:LYS:O	1:R:335:PRO:C	2.58	0.45
1:C:834:LEU:N	1:C:834:LEU:CD1	2.80	0.45
1:M:419:PHE:CD1	1:M:419:PHE:O	2.70	0.44
1:O:183:LEU:C	1:O:183:LEU:HD23	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:407:LEU:HD12	1:G:407:LEU:HA	1.77	0.44
1:P:211:LEU:O	1:P:211:LEU:HG	2.16	0.44
1:D:808:ALA:HB1	1:D:874:LEU:HD22	1.99	0.44
1: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:412:LEU:C	1:G:412:LEU:CD2	2.88	0.44
1:K:202:VAL:O	1:K:202:VAL:HG13	2.16	0.44
1:O:291:TRP:HB3	1:O:295:PHE:CZ	2.53	0.44
1:B:524:SER:N	1:B:540:ARG:O	2.48	0.44
1:C:613:LYS:O	1:C:614:ALA:C	2.60	0.44
1:F:673:GLN:HG3	1:F:706:PHE:CE2	2.52	0.44
1:J:250:ALA:HB2	1:J:264:LEU:HA	2.00	0.44
1:Q:336:LEU:HD22	1:Q:336:LEU:HA	1.57	0.44
1:C:862:MET:O	1:C:862:MET:CE	2.65	0.44
1:L:201:LEU:C	1:L:202:VAL:O	2.55	0.44
1:H:455:TYR:O	1:H:456:GLU:CB	2.66	0.44
1:E:589:ILE:O	1:E:589:ILE:HG23	2.17	0.44
1:K:275:GLN:O	1:K:276:LEU:CB	2.64	0.44
1:D:506:ALA:HA	1:D:508:GLN:N	2.33	0.44
1:D:887:THR:O	1:D:888:ILE:C	2.60	0.44
1:B:662:LEU:O	1:B:666:ALA:N	2.48	0.44
1:H:401:ASP:O	1:H:405:PRO:HD2	2.18	0.44
1:Q:419:PHE:HD1	1:Q:419:PHE:O	2.00	0.44
1:J:202:VAL:O	1:J:203:ARG:HB2	2.19	0.43
1:I:364:ARG:O	1:I:365:LEU:C	2.59	0.43
1:P:206:LEU:HA	1:P:207:PRO:HD2	1.96	0.43
1:G:436:ARG:O	1:G:437:ASN:C	2.61	0.43
1:A:510:PHE:CD2	1:A:510:PHE:C	2.92	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:F:789:LYS:HB2	1:F:790:PRO:C	2.44	0.43
1:M:394:ASP:OD1	1:M:394:ASP:C	2.62	0.43
1:A:535:VAL:HB	1:A:551:LEU:HB2	1.98	0.43
1:C:535:VAL:HB	1:C:551:LEU:HB2	2.00	0.43
1:M:419:PHE:O	1:M:419:PHE:HD1	2.02	0.43
1:N:248:TYR:HD1	1:N:248:TYR:O	2.00	0.43
1:E:791:ASP:HB2	1:E:793:GLU:N	2.33	0.43
1:M:419:PHE:CE2	1:M:470:LEU:HG	2.54	0.43
1:B:560:ILE:HD13	1:B:560:ILE:HA	1.78	0.43
1:C:884:LEU:HD23	1:C:884:LEU:HA	1.70	0.43
1:J:178:ILE:HG22	1:J:206:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:LEU:O	1:L:207:PRO:C	2.62	0.43
1:H:336:LEU:HB2	1:H:366:GLU:HG3	2.01	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:C:862:MET:O	1:C:862:MET:HE3	2.18	0.43
1:F:542:ASP:HB3	1:F:778:ARG:HG2	2.01	0.43
1:J:178:ILE:HG21	1:J:178:ILE:HD13	1.61	0.43
1:C:828:TYR:CD2	1:C:828:TYR:C	2.97	0.43
1:E:563:VAL:O	1:E:567:GLY:N	2.52	0.43
1:Q:457:VAL:O	1:Q:457:VAL:HG13	2.19	0.43
1:R:441:LEU:C	1:R:441:LEU:HD23	2.43	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:392:TYR:CD1	1:Q:392:TYR:C	2.97	0.42
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:CD1	1:E:824:TYR:N	2.86	0.42
1:F:837:ASP:C	1:F:837:ASP:OD1	2.62	0.42
1:E:535:VAL:HB	1:E:551:LEU:HB2	2.01	0.42
1:F:634:LYS:HE3	1:F:634:LYS:HB3	1.88	0.42
1:K:291:TRP:HB3	1:K:295:PHE:CZ	2.54	0.42
1:N:249:GLY:O	1:N:265:SER:N	2.53	0.42
1:N:199:ARG:HA	1:N:199:ARG:HD3	1.47	0.42
1:A:545:LEU:HB2	1:F:712:ASP:OD2	2.20	0.42
1:C:865:LEU:HB3	1:C:887:THR:HG22	2.00	0.42
1:N:177:TRP:CE3	1:N:214:ALA:HB2	2.54	0.42
1:O:266:ASP:OD1	1:O:266:ASP:C	2.62	0.42
1:Q:336:LEU:O	1:Q:336:LEU:CD1	2.37	0.42
1:A:675:ILE:HG21	1:A:675:ILE:HD13	1.74	0.42
1:G:448:LEU:O	1:G:452:GLY:N	2.48	0.42
1:O:178:ILE:HD13	1:O:178:ILE:HG21	1.83	0.42
1:P:268:ARG:O	1:P:268:ARG:HG2	2.18	0.42
1:E:878:THR:OG1	1:E:879:THR:N	2.52	0.42
1:L:291:TRP:CE3	1:L:291:TRP:N	2.87	0.42
1:O:178:ILE:O	1:O:178:ILE:CG2	2.68	0.42
1:R:357:LYS:O	1:R:361:GLY:N	2.52	0.42
1:A:692:ASN:OD1	1:A:692:ASN:C	2.63	0.42
1:E:617:ILE:HD13	1:E:617:ILE:HG21	1.73	0.42
1:P:202:VAL:O	1:P:202:VAL:HG13	2.20	0.42
1:A:719:ILE:HD13	1:A:719:ILE:HG21	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:ILE:HD12	1:C:560:ILE:HA	1.52	0.42
1:C:662:LEU:HD23	1:C:662:LEU:HA	1.86	0.42
1:C:864:THR:O	1:C:865:LEU:C	2.61	0.42
1:E:675:ILE:HD13	1:E:675:ILE:HG21	1.64	0.42
1:B:698:THR:O	1:B:699:PHE:C	2.61	0.42
1:C:804:GLU:OE2	1:C:863:LYS:NZ	2.44	0.42
1:M:423:LEU:HD23	1:M:423:LEU:HA	1.88	0.41
1:N:202:VAL:O	1:N:203:ARG:HB2	2.20	0.41
1:N:212:TYR:N	1:N:212:TYR:CD1	2.79	0.41
1:O:291:TRP:O	1:O:292:GLU:C	2.61	0.41
1:R:336:LEU:O	1:R:340:LEU:HG	2.20	0.41
1:B:659:PHE:N	1:B:659:PHE:HD1	2.18	0.41
1:F:870:LEU:HD23	1:F:870:LEU:HA	1.84	0.41
1:C:779:ARG:O	1:C:780:VAL:C	2.61	0.41
1:C:832:GLU:HB2	1:C:865:LEU:HG	2.02	0.41
1:D:862:MET:O	1:D:862:MET:CG	2.54	0.41
1:E:611:LEU:O	1:E:612:LYS:C	2.63	0.41
1:J:168:LEU:H	1:J:168:LEU:HD23	1.86	0.41
1:K:178:ILE:HB	1:K:206:LEU:HD13	2.02	0.41
1:N:263:VAL:HG23	1:N:263:VAL:O	2.19	0.41
1:Q:408:LEU:HD23	1:Q:408:LEU:O	2.20	0.41
1:G:394:ASP:OD1	1:G:394:ASP:C	2.64	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:421:HIS:O	1:R:422:ARG:C	2.63	0.41
1:M:456:GLU:OE1	1:M:456:GLU:HA	2.21	0.41
1:O:172:LEU:HD22	1:O:210:ALA:HB1	2.03	0.41
1:A:538:ARG:NH1	1:F:670:LYS:O	2.54	0.41
1:B:674:THR:OG1	1:B:686:ILE:HD11	2.21	0.41
1:F:692:ASN:C	1:F:692:ASN:OD1	2.62	0.41
1:F:697:LEU:O	1:F:697:LEU:HG	2.20	0.41
1:I:397:GLU:O	1:I:398:ASP:C	2.62	0.41
1:C:675:ILE:O	1:C:675:ILE:HG23	2.20	0.41
1:D:798:LEU:HA	1:D:798:LEU:HD23	1.89	0.41
1:O:215:LEU:HD23	1:O:215:LEU:HA	1.95	0.41
1:K:211:LEU:HA	1:K:211:LEU:HD23	1.77	0.41
1:M:404:ALA:N	1:M:405:PRO:CD	2.84	0.41
1:B:576:LEU:HA	1:B:576:LEU:HD23	1.88	0.41
1:C:571:ILE:HA	1:C:571:ILE:HD13	1.80	0.41
1:C:710:ASP:N	1:C:711:PRO:CD	2.83	0.41
1:C:835:VAL:O	1:C:835:VAL:CG2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:874:LEU:HA	1:D:874:LEU:HD23	1.89	0.41
1:F:681:TYR:O	1:F:688:GLN:NE2	2.45	0.41
1:G:380:LEU:HA	1:G:380:LEU:HD13	1.73	0.41
1:O:206:LEU:HA	1:O:206:LEU:HD12	1.92	0.41
1:P:291:TRP:HB3	1:P:295:PHE:CZ	2.56	0.41
1:A:714:ILE:O	1:A:714:ILE:HG22	2.20	0.41
1:L:216:ALA:HB3	1:L:223:PHE:CE1	2.56	0.40
1:I:419:PHE:O	1:I:431:LEU:HB3	2.21	0.40
1:P:264:LEU:N	1:P:284:TYR:O	2.53	0.40
1:D:599:PRO:HA	1:D:604:GLU:HA	2.04	0.40
1:D:613:LYS:O	1:D:614:ALA:C	2.64	0.40
1:E:530:PRO:HB3	1:E:556:LEU:CD2	2.51	0.40
1:Q:475:TYR:CD1	1:Q:475:TYR:N	2.90	0.40
1:C:684:PRO:HA	1:C:685:GLY:HA2	1.93	0.40
1:F:775:ARG:NH1	1:F:883:VAL:O	2.54	0.40
1:J:169:GLY:H	1:J:172:LEU:HD12	1.86	0.40
1:H:333:ALA:O	1:H:334:LYS:C	2.64	0.40
1:N:206:LEU:HD21	1:N:211:LEU:HB2	2.03	0.40
1:Q:419:PHE:CD1	1:Q:419:PHE:O	2.75	0.40
1:A:510:PHE:CZ	1:A:514:VAL:HG21	2.55	0.40
1:D:637:ILE:HD13	1:D:637:ILE:HG21	1.89	0.40
1:E:573:GLU:O	1:E:573:GLU:HG2	2.21	0.40
1:H:395:PRO:O	1:H:396:GLU:C	2.61	0.40
1:I:366:GLU:H	1:I:366:GLU:CD	2.29	0.40
1:A:703:LEU:HD23	1:A:703:LEU:HA	1.80	0.40
1:F:583:ARG:HD2	1:F:583:ARG:N	2.36	0.40
1:F:598:LEU:HA	1:F:599:PRO:HD2	1.89	0.40
1:J:270:LYS:HA	1:J:273:VAL:HG22	2.04	0.40
1:I:376:ARG:HA	1:I:377:PRO:HD3	1.93	0.40
1:A:582:VAL:HB	1:A:593:LEU:HB2	2.04	0.40
1:D:710:ASP:N	1:D:711:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	382/913 (42%)	374 (98%)	7 (2%)	1 (0%)	36	72
1	B	381/913 (42%)	369 (97%)	10 (3%)	2 (0%)	24	63
1	C	382/913 (42%)	368 (96%)	8 (2%)	6 (2%)	7	38
1	D	382/913 (42%)	366 (96%)	13 (3%)	3 (1%)	16	54
1	E	382/913 (42%)	367 (96%)	13 (3%)	2 (0%)	24	63
1	F	382/913 (42%)	367 (96%)	13 (3%)	2 (0%)	24	63
1	G	144/913 (16%)	133 (92%)	6 (4%)	5 (4%)	3	20
1	H	144/913 (16%)	132 (92%)	9 (6%)	3 (2%)	5	30
1	I	144/913 (16%)	137 (95%)	6 (4%)	1 (1%)	18	56
1	J	135/913 (15%)	123 (91%)	10 (7%)	2 (2%)	8	40
1	K	135/913 (15%)	126 (93%)	7 (5%)	2 (2%)	8	40
1	L	135/913 (15%)	123 (91%)	9 (7%)	3 (2%)	5	29
1	M	144/913 (16%)	133 (92%)	8 (6%)	3 (2%)	5	30
1	N	135/913 (15%)	128 (95%)	6 (4%)	1 (1%)	18	56
1	O	135/913 (15%)	124 (92%)	10 (7%)	1 (1%)	18	56
1	P	135/913 (15%)	130 (96%)	3 (2%)	2 (2%)	8	40
1	Q	144/913 (16%)	135 (94%)	8 (6%)	1 (1%)	18	56
1	R	144/913 (16%)	135 (94%)	7 (5%)	2 (1%)	9	40
All	All	3965/16434 (24%)	3770 (95%)	153 (4%)	42 (1%)	14	46

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
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

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Mol	Chain	Res	Type
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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/751 (42%)	316 (100%)	1 (0%)	86	86
1	B	315/751 (42%)	314 (100%)	1 (0%)	86	86
1	C	317/751 (42%)	317 (100%)	0	100	100
1	D	317/751 (42%)	317 (100%)	0	100	100
1	E	317/751 (42%)	317 (100%)	0	100	100
1	F	317/751 (42%)	316 (100%)	1 (0%)	86	86
1	G	120/751 (16%)	119 (99%)	1 (1%)	73	80
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%)	70	79
1	L	112/751 (15%)	111 (99%)	1 (1%)	70	79
1	M	120/751 (16%)	120 (100%)	0	100	100
1	N	112/751 (15%)	111 (99%)	1 (1%)	70	79
1	O	112/751 (15%)	111 (99%)	1 (1%)	70	79
1	P	112/751 (15%)	112 (100%)	0	100	100
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%)	3284 (100%)	8 (0%)	85	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	380	LEU
1	K	248	TYR
1	L	248	TYR
1	N	248	TYR
1	O	212	TYR
1	A	519	PHE
1	B	833	LEU
1	F	656	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	275	GLN
1	H	358	GLN
1	I	454	ASN
1	O	275	GLN
1	Q	356	GLN
1	R	387	GLN
1	B	736	HIS
1	C	692	ASN
1	C	709	GLN
1	C	842	HIS
1	E	688	GLN
1	E	743	HIS
1	F	774	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

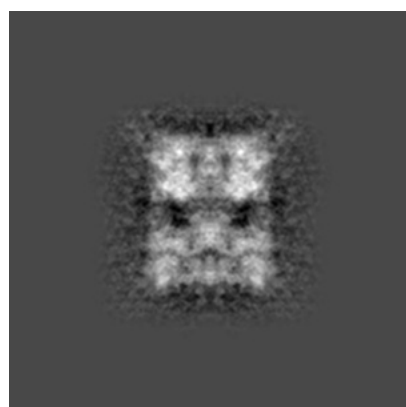
6 Map visualisation [i](#)

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

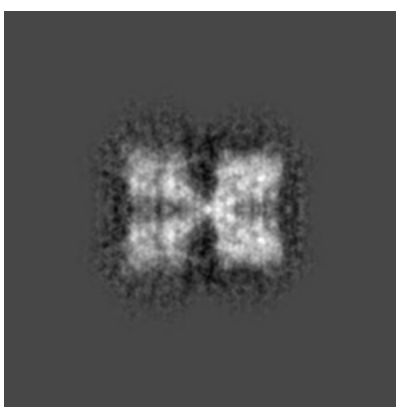
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

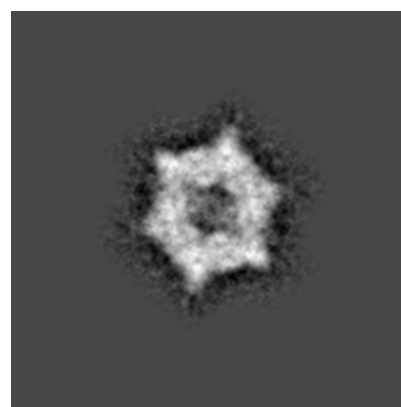
6.1.1 Primary map



X



Y

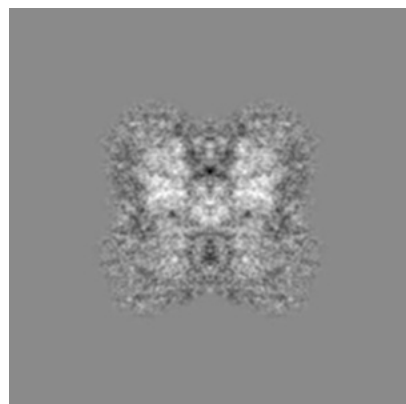


Z

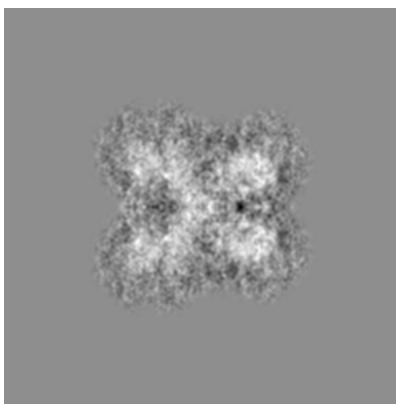
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

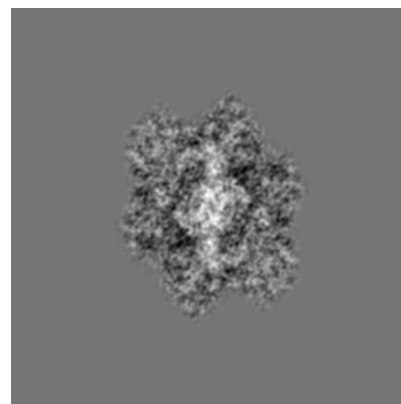
6.2.1 Primary map



X Index: 96



Y Index: 96

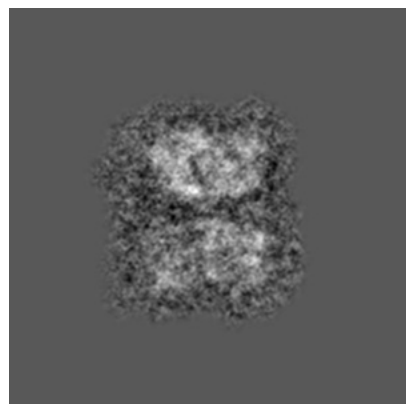


Z Index: 96

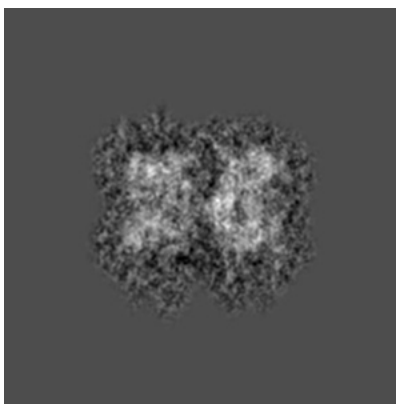
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

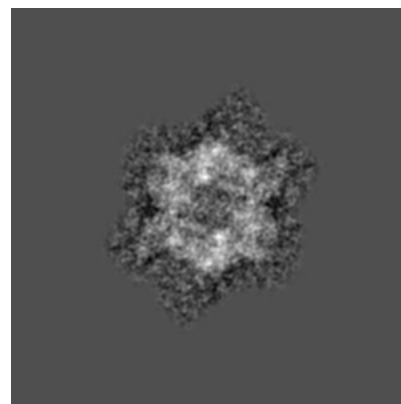
6.3.1 Primary map



X Index: 80



Y Index: 75

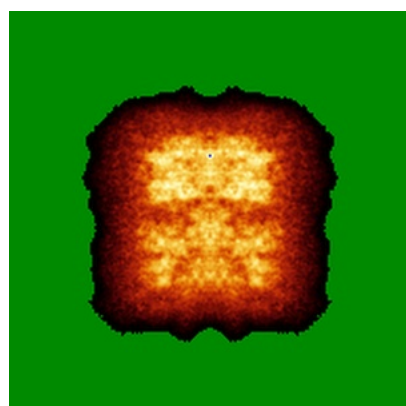


Z Index: 108

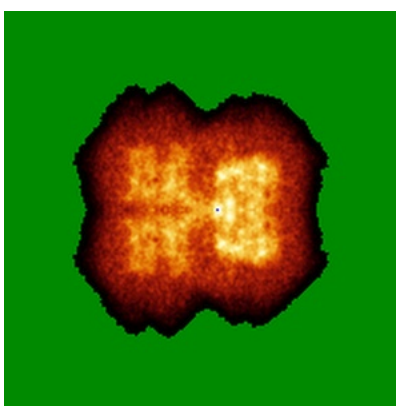
The images above show the largest variance slices of the map in three orthogonal directions.

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

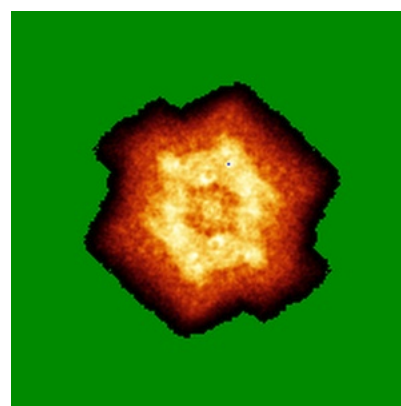
6.4.1 Primary map



X



Y

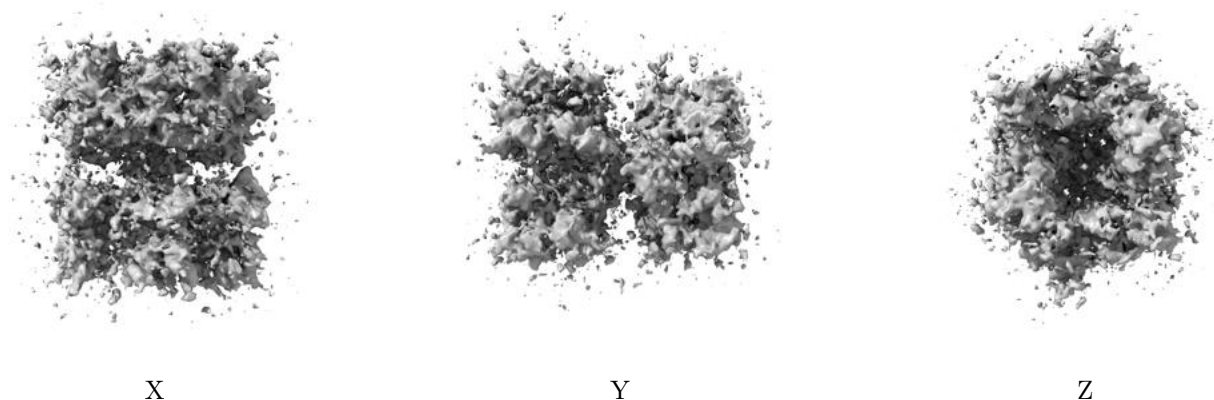


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

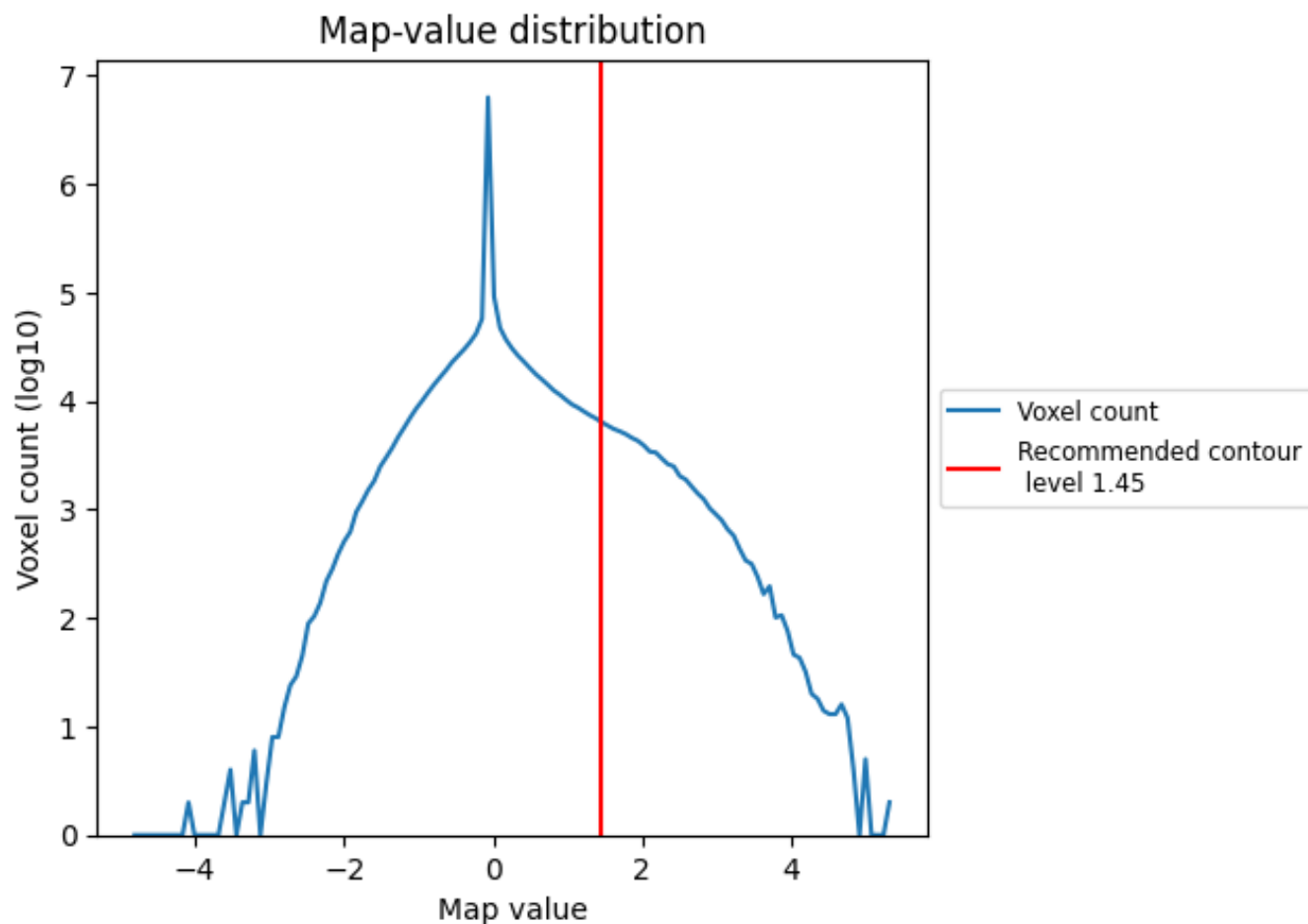
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

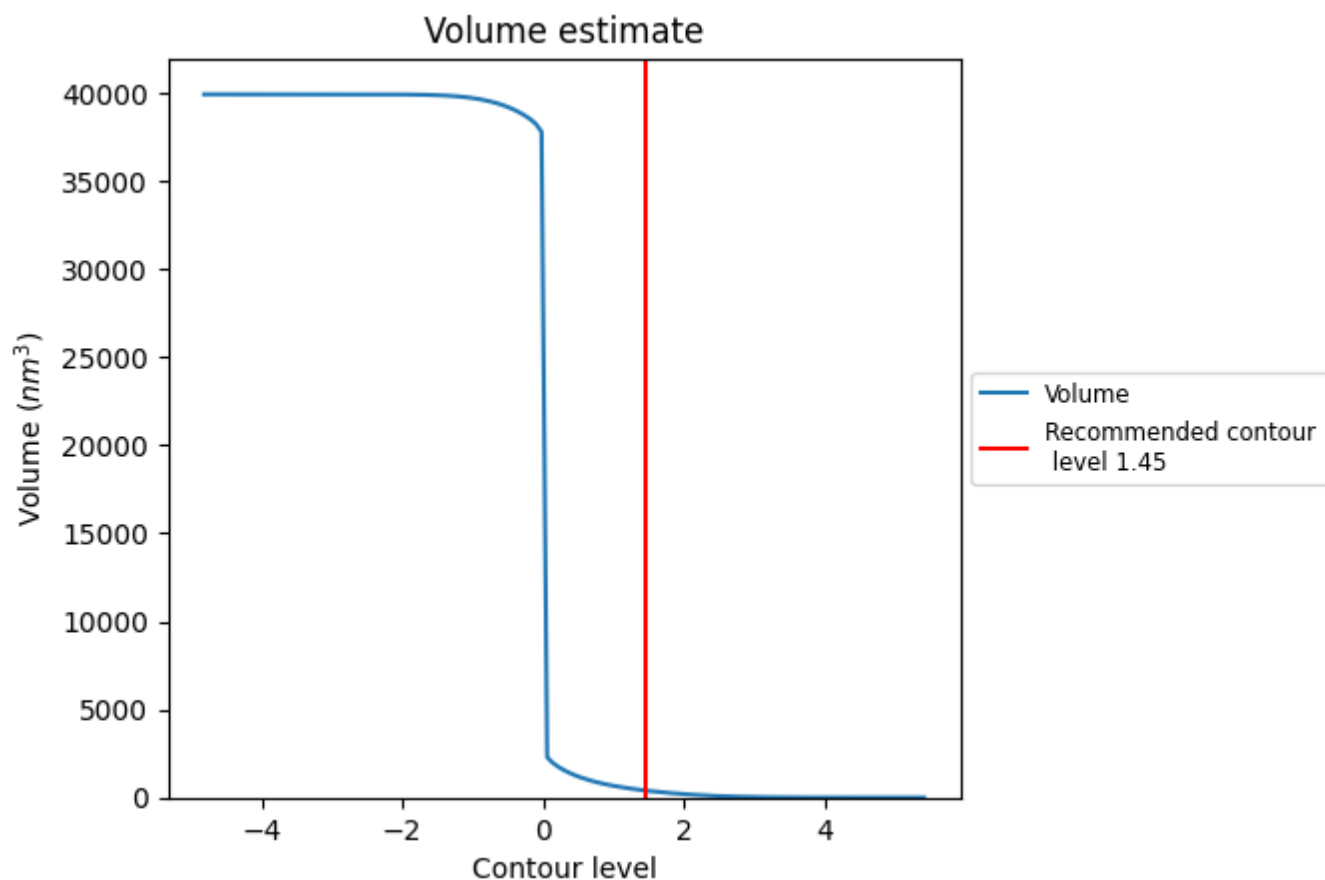
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

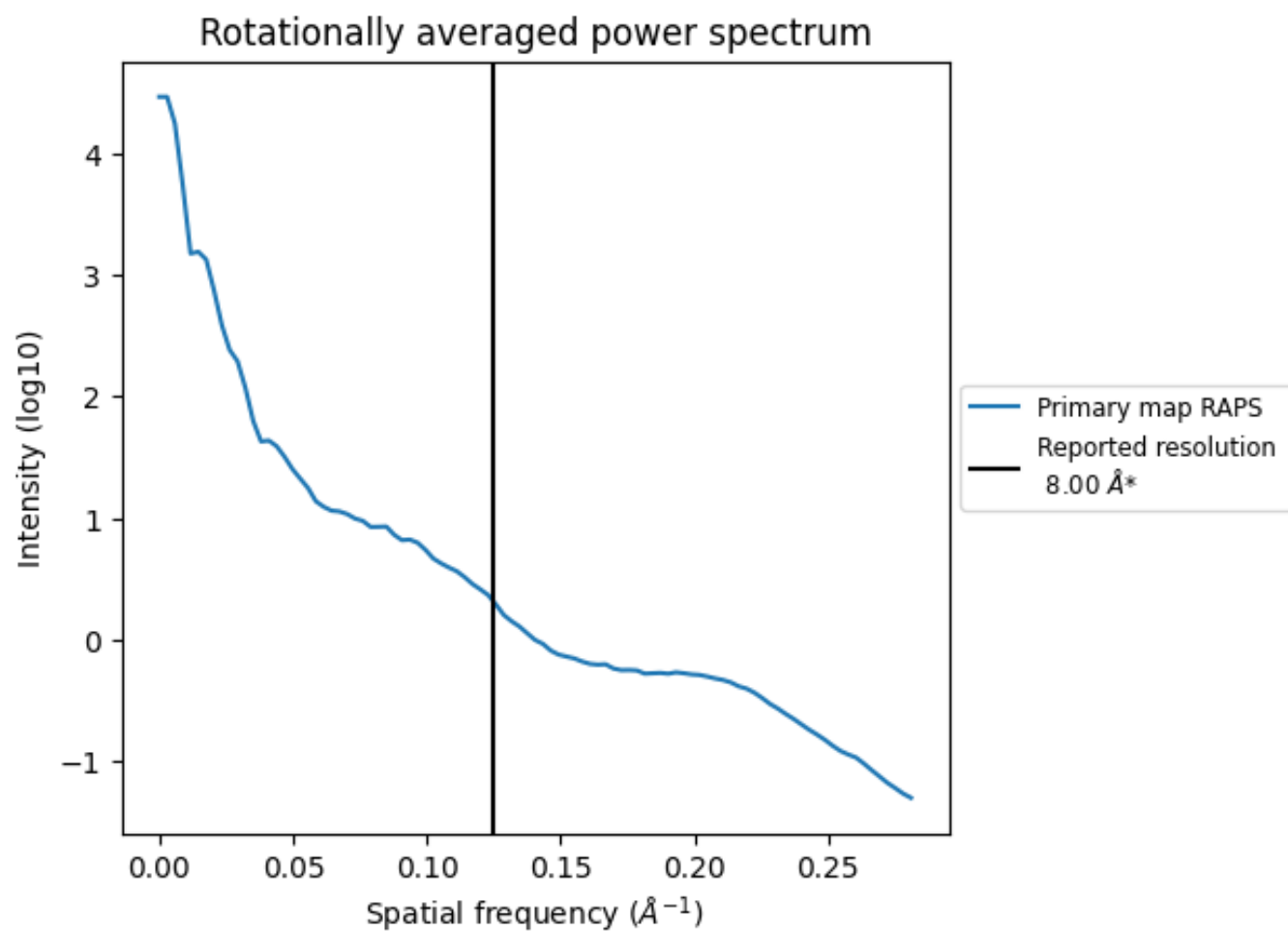
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 398 nm³; this corresponds to an approximate mass of 360 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.125 Å⁻¹

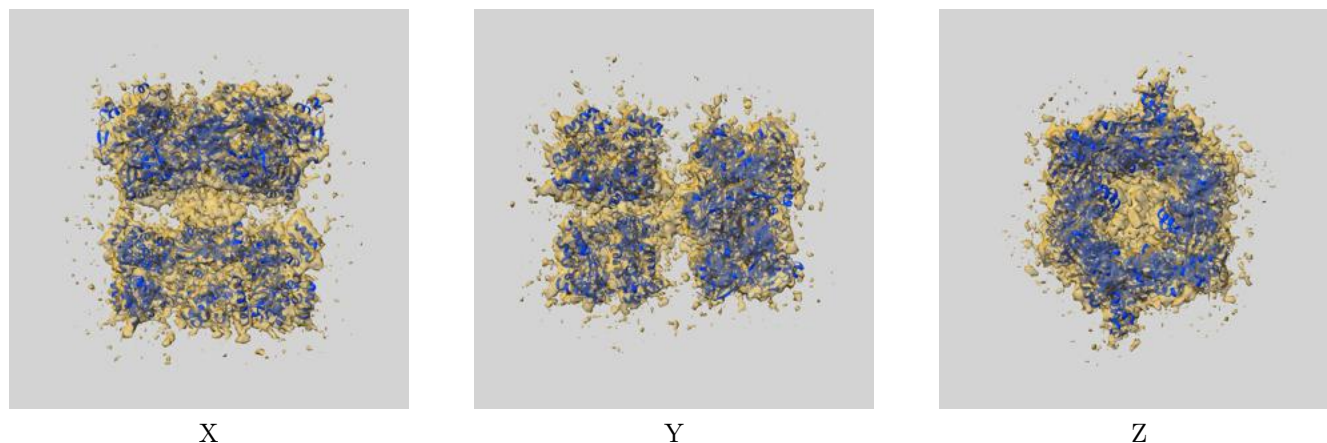
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

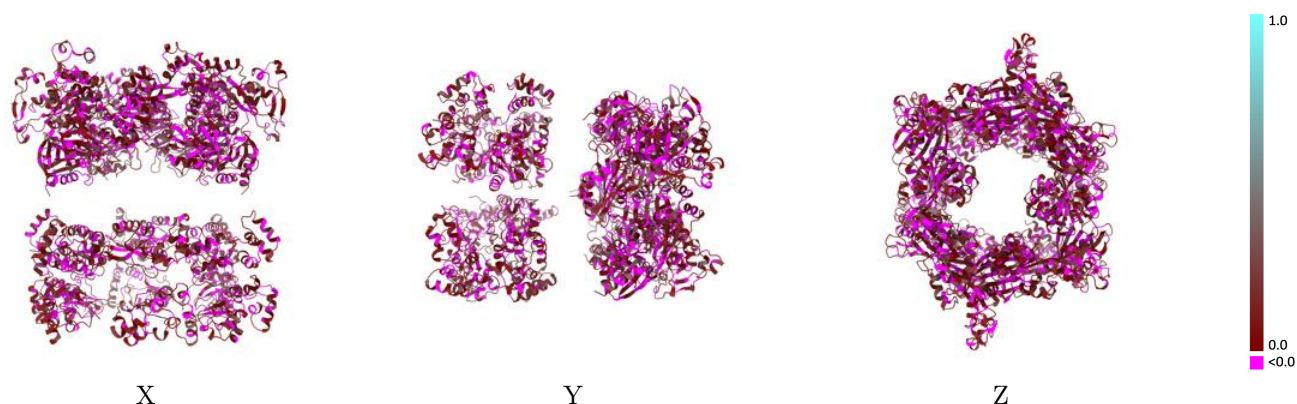
This section contains information regarding the fit between EMDB map EMD-4194 and PDB model 6F8L. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



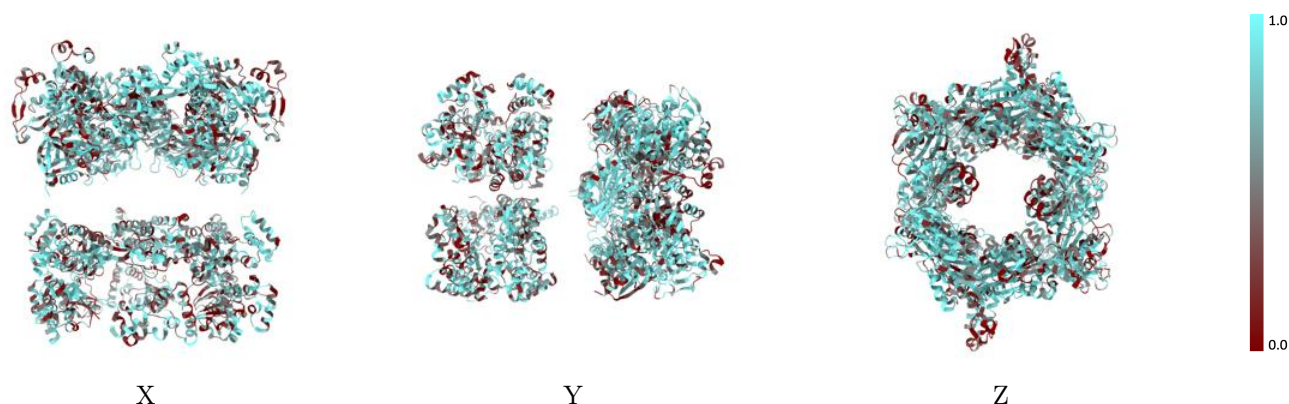
The images above show the 3D surface view of the map at the recommended contour level 1.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



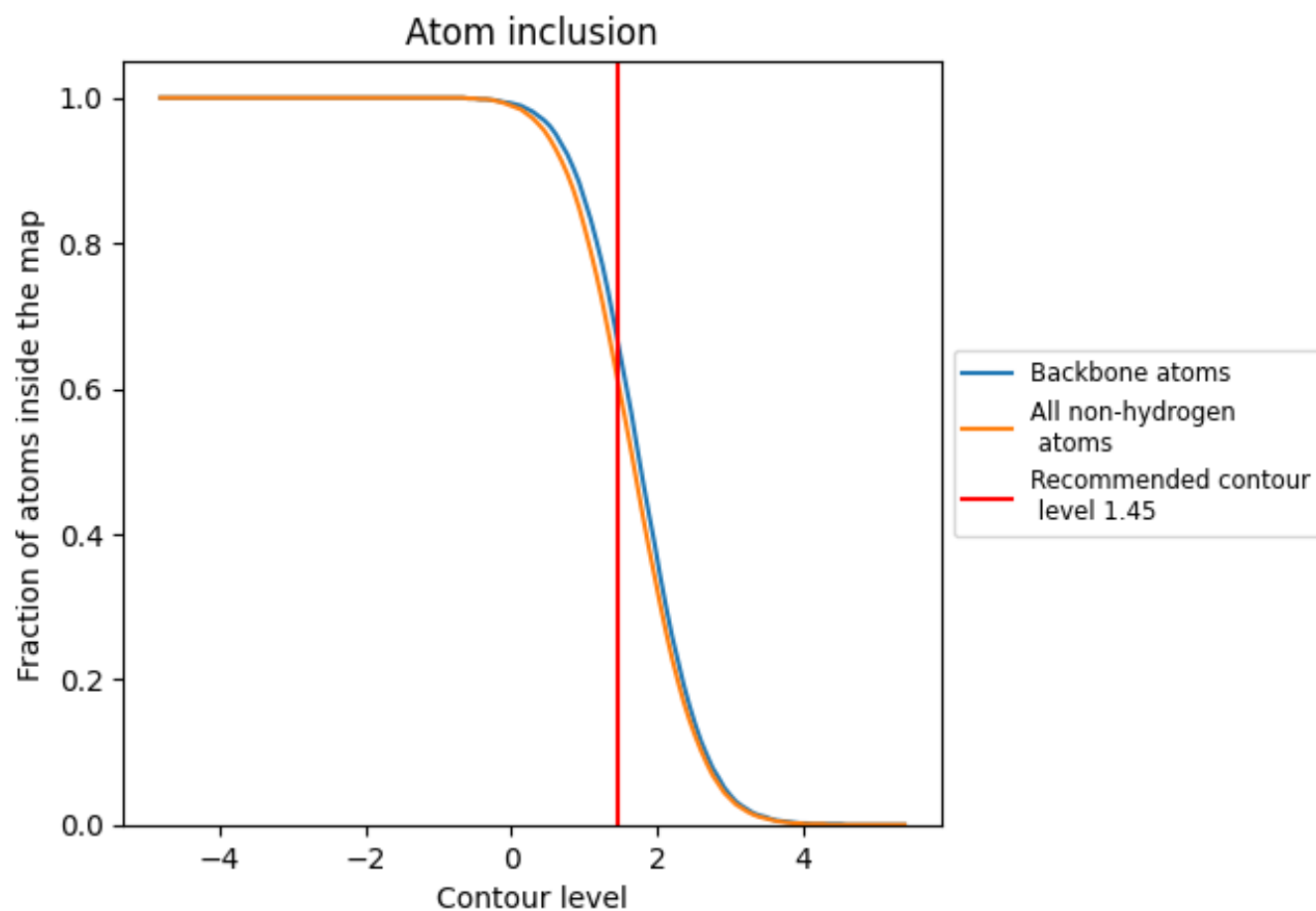
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.45) and Q-score for the entire model and for each chain.

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

