



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 07:37 pm GMT

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

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

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

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

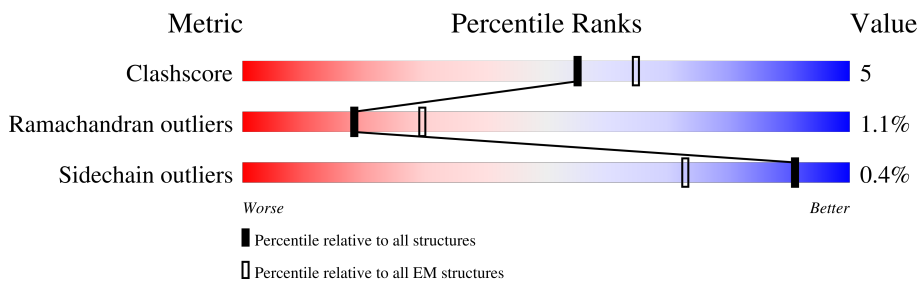
1 Overall quality at a glance i

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.



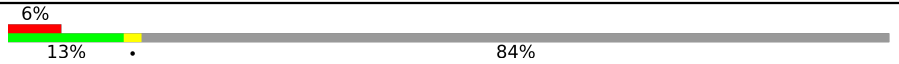





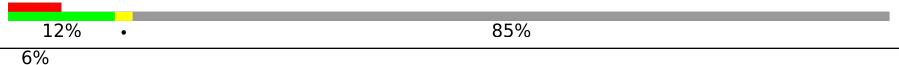



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
1	E	913	
1	F	913	
1	G	913	
1	H	913	

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

2 Entry composition

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

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

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

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

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

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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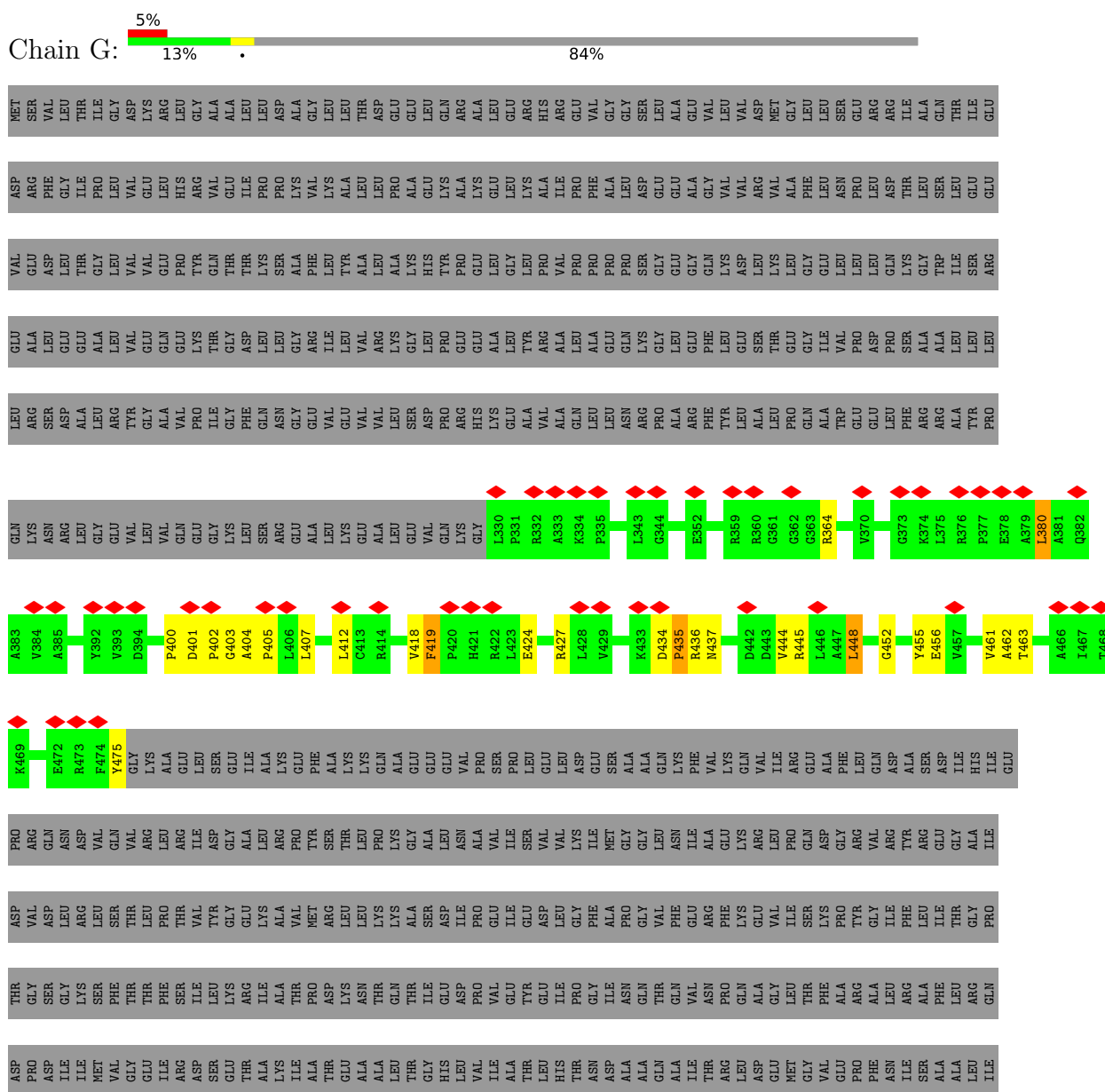
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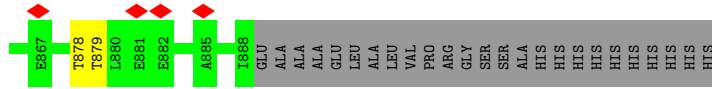
Chain	Residue	Modelled	Actual	Comment	Reference
F	896	LEU	-	expression tag	UNP Q5SLC9
F	897	VAL	-	expression tag	UNP Q5SLC9
F	898	PRO	-	expression tag	UNP Q5SLC9
F	899	ARG	-	expression tag	UNP Q5SLC9
F	900	GLY	-	expression tag	UNP Q5SLC9
F	901	SER	-	expression tag	UNP Q5SLC9
F	902	SER	-	expression tag	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

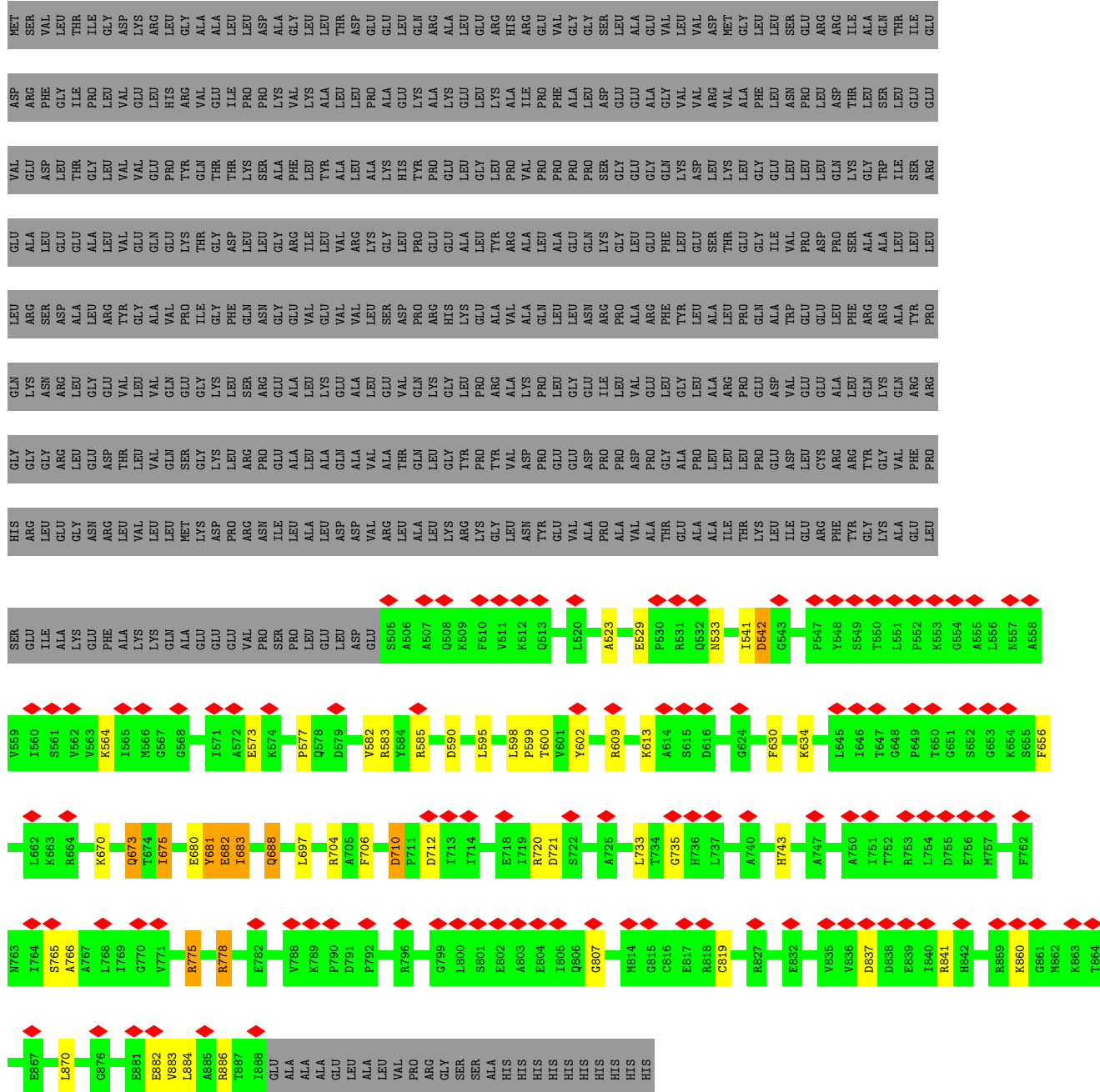
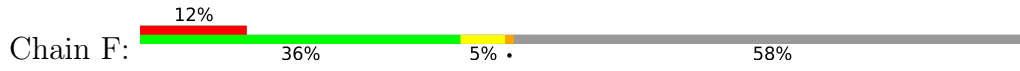
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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





• Molecule 1: Type IV pilus assembly protein PilF



4 Experimental information

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.29	21/3017 (0.7%)	1.10	12/4073 (0.3%)
1	B	1.25	17/3008 (0.6%)	1.03	6/4061 (0.1%)
1	C	1.27	19/3017 (0.6%)	1.11	10/4073 (0.2%)
1	D	1.28	18/3017 (0.6%)	1.13	14/4073 (0.3%)
1	E	1.22	13/3017 (0.4%)	1.07	13/4073 (0.3%)
1	F	1.23	20/3017 (0.7%)	1.07	9/4073 (0.2%)
1	G	1.21	4/1164 (0.3%)	1.03	4/1580 (0.3%)
1	H	1.16	6/1164 (0.5%)	1.12	7/1580 (0.4%)
1	I	1.09	2/1164 (0.2%)	1.09	6/1580 (0.4%)
1	J	1.21	7/1109 (0.6%)	1.08	6/1499 (0.4%)
1	K	1.23	6/1109 (0.5%)	1.06	5/1499 (0.3%)
1	L	1.27	7/1109 (0.6%)	1.07	4/1499 (0.3%)
1	M	1.17	5/1164 (0.4%)	1.00	2/1580 (0.1%)
1	N	1.29	11/1109 (1.0%)	1.17	9/1499 (0.6%)
1	O	1.24	7/1109 (0.6%)	1.08	6/1499 (0.4%)
1	P	1.22	5/1109 (0.5%)	1.11	4/1499 (0.3%)
1	Q	1.28	11/1164 (0.9%)	1.07	1/1580 (0.1%)
1	R	1.19	6/1164 (0.5%)	1.05	4/1580 (0.3%)
All	All	1.24	185/31731 (0.6%)	1.08	122/42900 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	4
1	D	0	8
1	E	0	2
1	F	0	4
All	All	0	18

All (185) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	784	CYS	CB-SG	-11.09	1.63	1.82
1	D	529	GLU	CG-CD	-10.54	1.36	1.51
1	N	212	TYR	CB-CG	-9.85	1.36	1.51
1	C	529	GLU	CG-CD	-9.80	1.37	1.51
1	B	527	HIS	CB-CG	-9.76	1.32	1.50
1	E	591	VAL	CB-CG1	-9.48	1.32	1.52
1	F	582	VAL	CB-CG2	-9.31	1.33	1.52
1	B	510	PHE	CB-CG	-9.10	1.35	1.51
1	A	514	VAL	CB-CG2	-8.68	1.34	1.52
1	C	607	VAL	CB-CG2	-8.62	1.34	1.52
1	B	511	VAL	CB-CG2	-8.27	1.35	1.52
1	A	819	CYS	CB-SG	-8.25	1.68	1.82
1	Q	475	TYR	CB-CG	-7.95	1.39	1.51
1	C	605	LYS	CE-NZ	-7.92	1.29	1.49
1	R	413	CYS	CB-SG	-7.83	1.69	1.82
1	D	602	TYR	CB-CG	-7.81	1.40	1.51
1	F	733	LEU	CB-CG	-7.72	1.30	1.52
1	D	654	LYS	CE-NZ	-7.63	1.29	1.49
1	D	824	TYR	CB-CG	-7.60	1.40	1.51
1	A	591	VAL	CB-CG1	-7.56	1.36	1.52
1	N	178	ILE	CB-CG2	-7.52	1.29	1.52
1	A	510	PHE	CB-CG	-7.50	1.38	1.51
1	N	284	TYR	CB-CG	-7.45	1.40	1.51
1	Q	336	LEU	CB-CG	-7.44	1.30	1.52
1	F	673	GLN	CG-CD	-7.43	1.33	1.51
1	B	777	VAL	CB-CG1	-7.41	1.37	1.52
1	O	284	TYR	CB-CG	-7.38	1.40	1.51
1	E	811	TYR	CG-CD2	-7.25	1.29	1.39
1	I	431	LEU	CB-CG	-7.22	1.31	1.52
1	A	563	VAL	CB-CG2	-7.19	1.37	1.52
1	D	529	GLU	CB-CG	-7.18	1.38	1.52
1	F	675	ILE	CB-CG1	-7.11	1.34	1.54
1	K	211	LEU	CB-CG	-7.07	1.32	1.52
1	E	811	TYR	CG-CD1	-7.01	1.30	1.39
1	C	828	TYR	CB-CG	-6.99	1.41	1.51
1	A	681	TYR	CB-CG	-6.97	1.41	1.51
1	D	710	ASP	CB-CG	6.93	1.66	1.51
1	D	681	TYR	CG-CD1	-6.89	1.30	1.39
1	C	867	GLU	CG-CD	-6.85	1.41	1.51
1	N	212	TYR	CG-CD2	-6.82	1.30	1.39
1	E	675	ILE	CB-CG1	-6.81	1.34	1.54
1	G	419	PHE	CB-CG	-6.80	1.39	1.51
1	L	223	PHE	CB-CG	-6.76	1.39	1.51

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

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

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

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

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	248	TYR	CB-CG-CD2	-11.44	114.13	121.00
1	H	414	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	A	585	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	O	284	TYR	CB-CG-CD2	-9.33	115.40	121.00
1	M	445	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	C	546	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	N	248	TYR	CB-CG-CD1	8.95	126.37	121.00
1	J	213	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	C	796	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	G	445	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	O	213	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	K	213	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	D	841	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	A	797	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	H	475	TYR	CB-CG-CD1	-7.69	116.39	121.00
1	C	546	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	P	213	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	I	445	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	C	632	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	R	414	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	Q	414	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	E	546	ARG	NE-CZ-NH1	7.22	123.91	120.30

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

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

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

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	506	ALA	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 [\(i\)](#)

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2975	0	3080	37	0
1	D	2975	0	3080	32	0
1	E	2975	0	3080	19	0
1	F	2975	0	3078	27	0
1	G	1143	0	1182	16	0
1	H	1143	0	1182	13	0
1	I	1143	0	1182	10	0
1	J	1090	0	1117	13	0
1	K	1090	0	1117	21	0
1	L	1090	0	1117	16	0
1	M	1143	0	1182	12	0
1	N	1090	0	1117	16	0
1	O	1090	0	1117	21	0
1	P	1090	0	1117	13	0
1	Q	1143	0	1182	15	0
1	R	1143	0	1182	11	0
All	All	31239	0	32258	339	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (339) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:336:LEU:HD13	1:Q:336:LEU:O	1.43	1.17
1:F:683:ILE:HG22	1:F:683:ILE:O	1.50	1.06
1:Q:336:LEU:HD13	1:Q:336:LEU:C	1.78	1.02
1:B:679:VAL:HG12	1:B:679:VAL:O	1.58	1.01
1:K:263:VAL:HG23	1:K:263:VAL:O	1.63	0.96
1:O:291:TRP:HE3	1:O:291:TRP:HA	1.32	0.94
1:O:291:TRP:HA	1:O:291:TRP:CE3	2.01	0.91
1:D:832:GLU:O	1:D:832:GLU:HG3	1.72	0.89
1:L:248:TYR:HD1	1:L:248:TYR:O	1.63	0.82
1:L:291:TRP:HA	1:L:291:TRP:CE3	2.18	0.79
1:Q:336:LEU:C	1:Q:336:LEU:CD1	2.50	0.78
1:O:291:TRP:CE3	1:O:291:TRP:CA	2.68	0.76
1:G:401:ASP:OD1	1:G:401:ASP:O	2.04	0.76
1:L:291:TRP:HA	1:L:291:TRP:HE3	1.50	0.76
1:C:862:MET:O	1:C:862:MET:HG2	1.86	0.74
1:B:679:VAL:O	1:B:679:VAL:CG1	2.33	0.74
1:C:525:ASP:OD1	1:C:525:ASP:O	2.06	0.74

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

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

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

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

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

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

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

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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	382/913 (42%)	374 (98%)	7 (2%)	1 (0%)	41	77
1	B	381/913 (42%)	369 (97%)	10 (3%)	2 (0%)	29	69
1	C	382/913 (42%)	368 (96%)	8 (2%)	6 (2%)	9	44
1	D	382/913 (42%)	366 (96%)	13 (3%)	3 (1%)	19	60
1	E	382/913 (42%)	367 (96%)	13 (3%)	2 (0%)	29	69
1	F	382/913 (42%)	367 (96%)	13 (3%)	2 (0%)	29	69
1	G	144/913 (16%)	133 (92%)	6 (4%)	5 (4%)	3	25
1	H	144/913 (16%)	132 (92%)	9 (6%)	3 (2%)	7	36
1	I	144/913 (16%)	137 (95%)	6 (4%)	1 (1%)	22	63
1	J	135/913 (15%)	123 (91%)	10 (7%)	2 (2%)	10	46
1	K	135/913 (15%)	126 (93%)	7 (5%)	2 (2%)	10	46
1	L	135/913 (15%)	123 (91%)	9 (7%)	3 (2%)	6	35
1	M	144/913 (16%)	133 (92%)	8 (6%)	3 (2%)	7	36
1	N	135/913 (15%)	128 (95%)	6 (4%)	1 (1%)	22	63
1	O	135/913 (15%)	124 (92%)	10 (7%)	1 (1%)	22	63
1	P	135/913 (15%)	130 (96%)	3 (2%)	2 (2%)	10	46
1	Q	144/913 (16%)	135 (94%)	8 (6%)	1 (1%)	22	63
1	R	144/913 (16%)	135 (94%)	7 (5%)	2 (1%)	11	46
All	All	3965/16434 (24%)	3770 (95%)	153 (4%)	42 (1%)	18	52

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 [i](#)

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%)	92	95
1	B	315/751 (42%)	313 (99%)	2 (1%)	86	92
1	C	317/751 (42%)	317 (100%)	0	100	100
1	D	317/751 (42%)	315 (99%)	2 (1%)	86	92
1	E	317/751 (42%)	317 (100%)	0	100	100
1	F	317/751 (42%)	316 (100%)	1 (0%)	92	95
1	G	120/751 (16%)	119 (99%)	1 (1%)	81	89
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%)	78	87
1	L	112/751 (15%)	110 (98%)	2 (2%)	59	77
1	M	120/751 (16%)	120 (100%)	0	100	100
1	N	112/751 (15%)	111 (99%)	1 (1%)	78	87
1	O	112/751 (15%)	110 (98%)	2 (2%)	59	77
1	P	112/751 (15%)	111 (99%)	1 (1%)	78	87
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%)	91	94

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

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

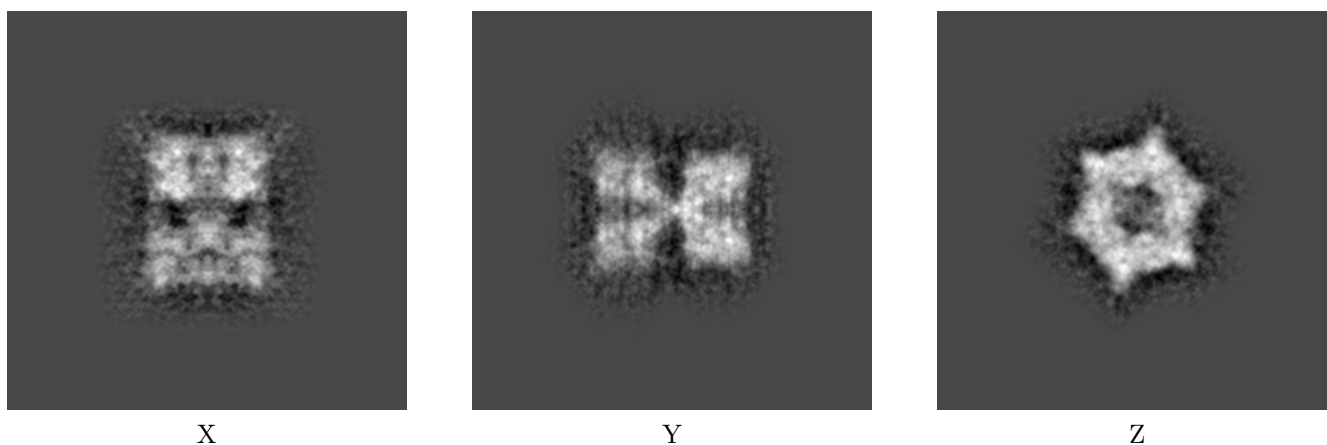
6 Map visualisation [i](#)

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

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

6.1 Orthogonal projections [i](#)

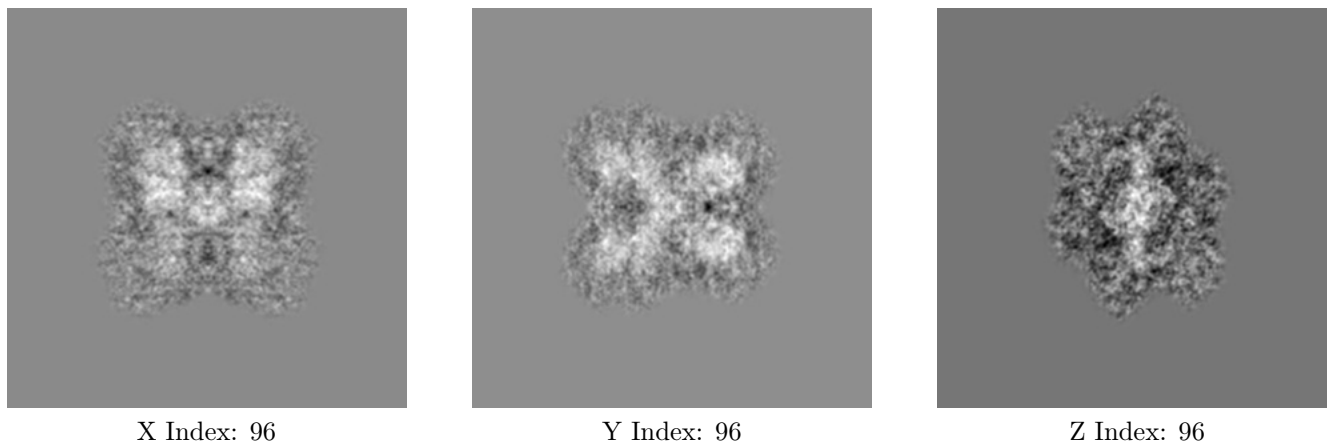
6.1.1 Primary map



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

6.2 Central slices [i](#)

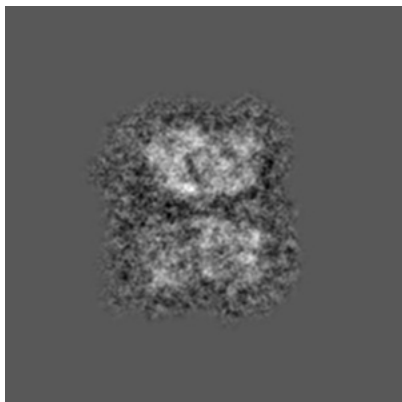
6.2.1 Primary map



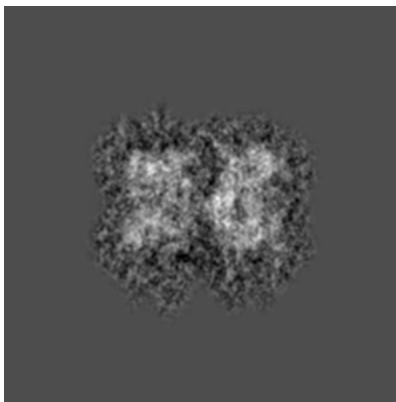
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

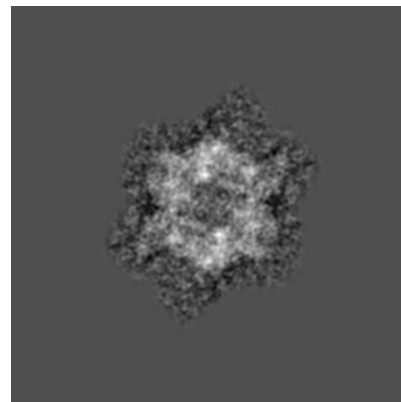
6.3.1 Primary map



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 surface views [i](#)

6.4.1 Primary map



X



Y



Z

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.

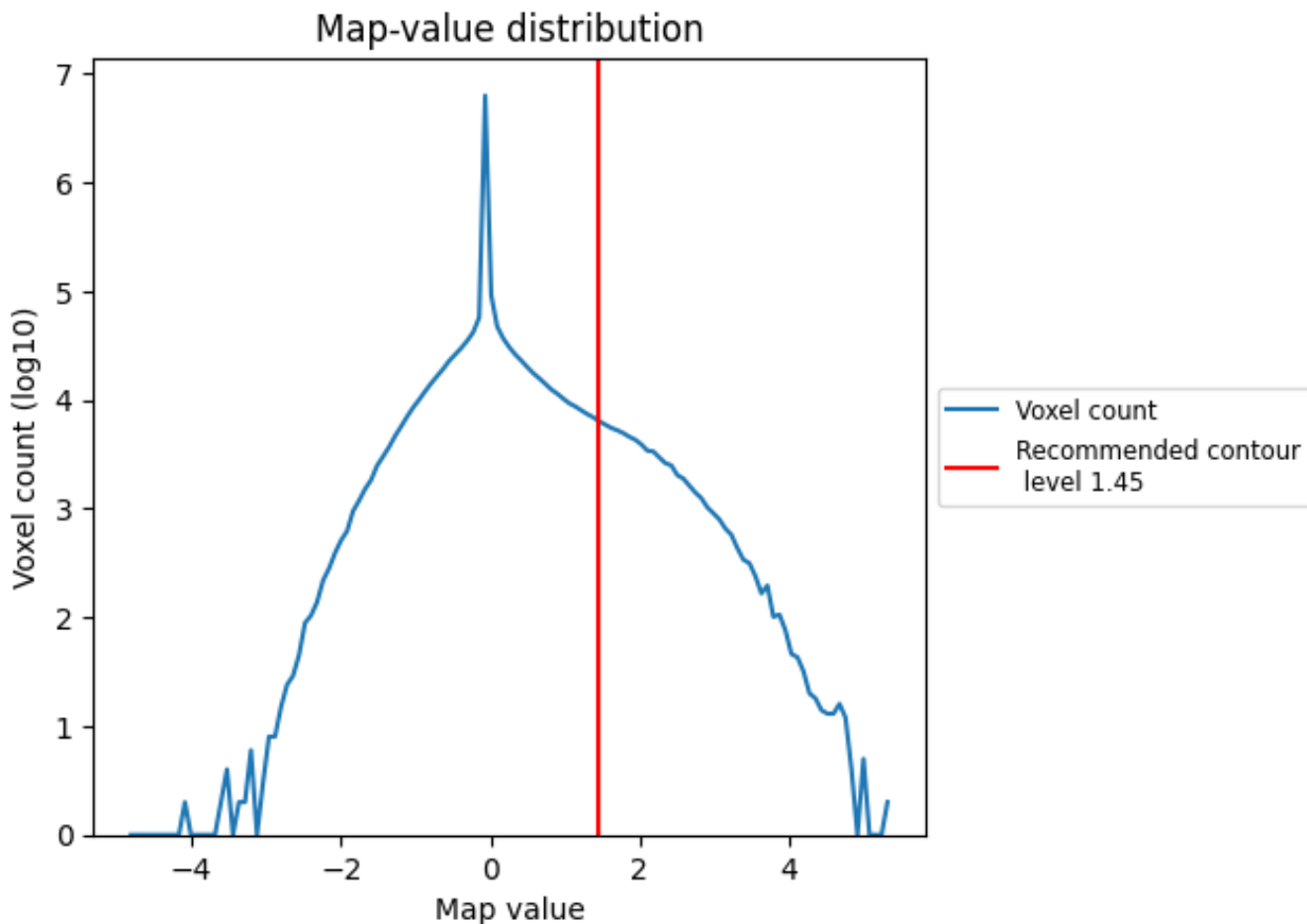
6.5 Mask visualisation

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

7 Map analysis [i](#)

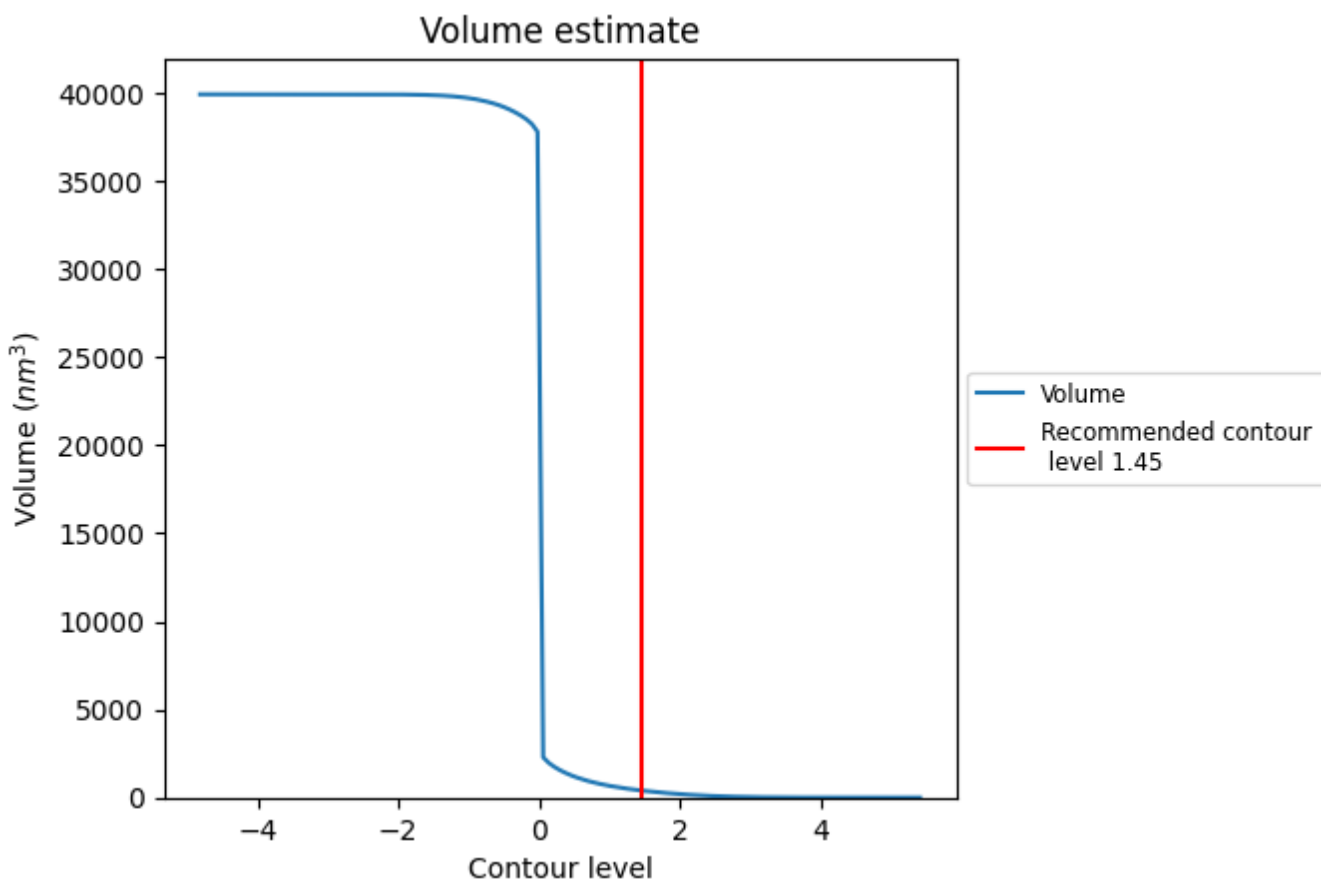
This section contains the results of statistical analysis of the map.

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.

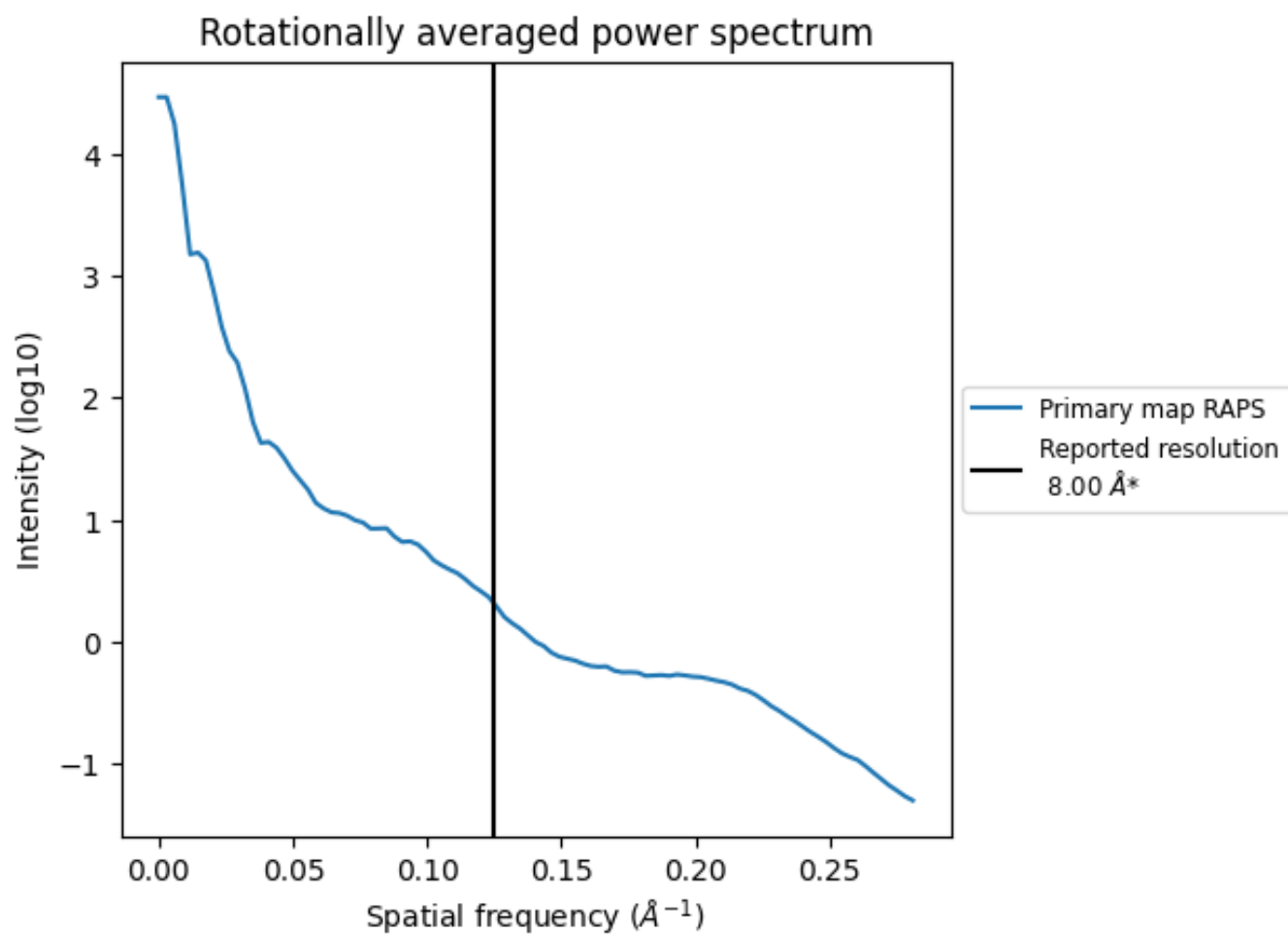
7.2 Volume estimate [i](#)



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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.125\AA^{-1}

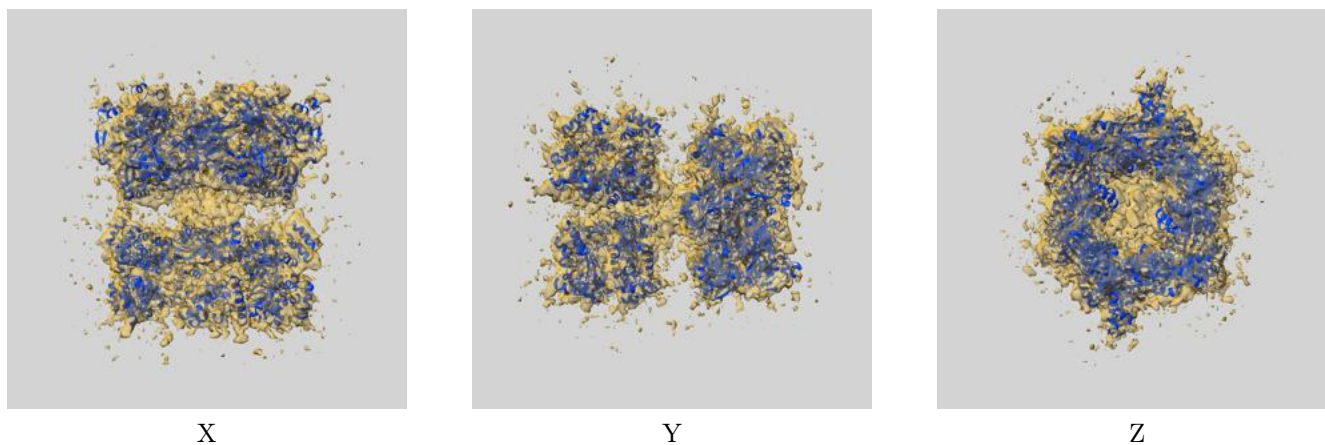
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

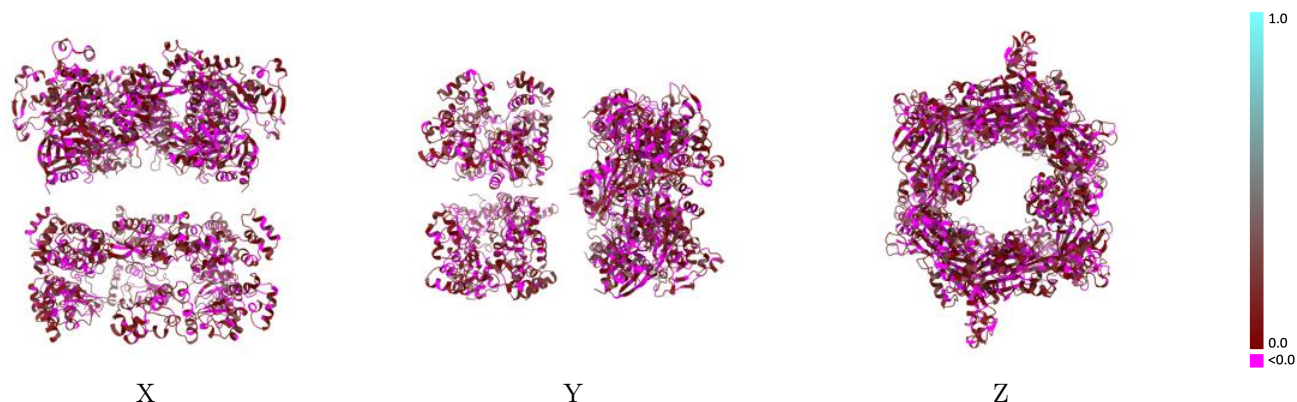
This section contains information regarding the fit between EMDB map EMD-4194 and PDB model 6F8L. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



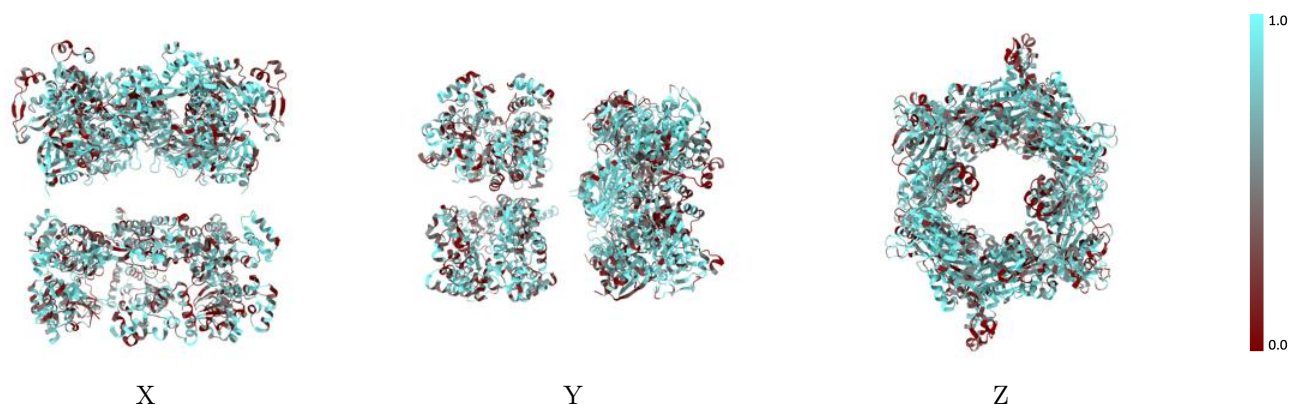
The images above show the 3D surface view of the map at the recommended contour level 1.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



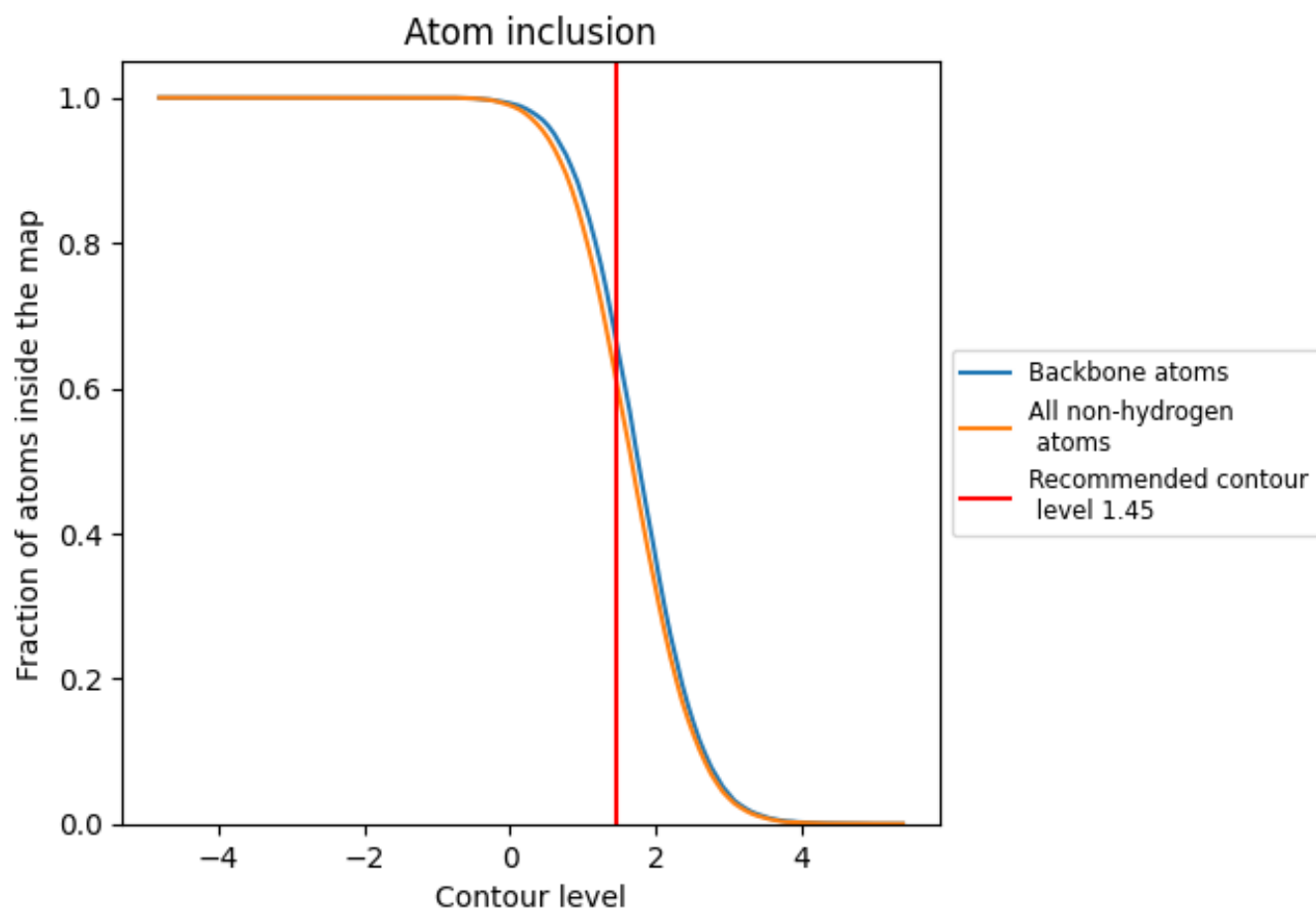
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.6163	 0.0750
A	 0.6660	 0.0610
B	 0.6839	 0.0670
C	 0.6760	 0.0700
D	 0.6722	 0.0730
E	 0.6136	 0.0730
F	 0.6195	 0.0780
G	 0.5288	 0.0720
H	 0.6477	 0.0860
I	 0.5550	 0.0720
J	 0.5556	 0.1040
K	 0.5330	 0.0710
L	 0.5772	 0.0800
M	 0.5568	 0.0840
N	 0.5273	 0.0900
O	 0.5377	 0.0810
P	 0.5546	 0.0850
Q	 0.6514	 0.0890
R	 0.5432	 0.0570

