



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:03 AM UTC

PDB ID : 6EJF / pdb_00006ejf
EMDB ID : EMD-3882
Title : Thermus thermophilus PilF ATPase (apoprotein form)
Authors : Derrick, J.P.; Collins, R.F.
Deposited on : 2017-09-21
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

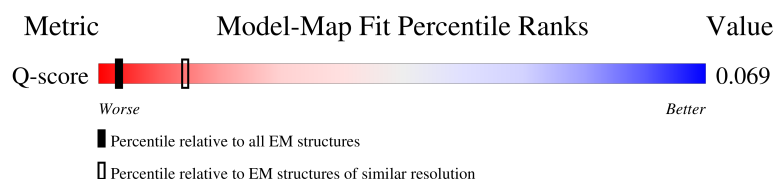
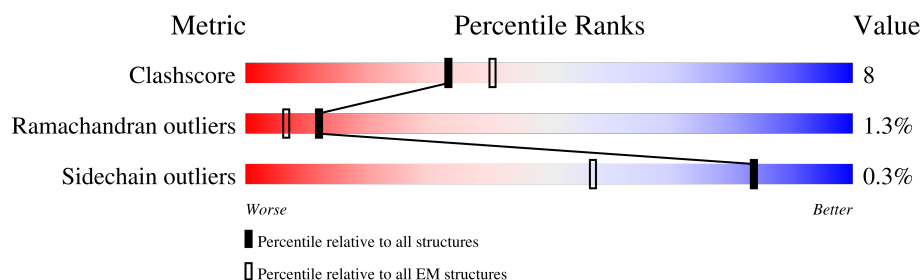
1 Overall quality at a glance

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	G	146	50% 85% 12% •
1	H	146	34% 74% 21% 5%
1	I	146	35% 73% 21% 5%
1	M	146	49% 79% 16% 5% •

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Mol	Chain	Length	Quality of chain
1	Q	146	
1	R	146	
2	J	137	
2	K	137	
2	L	137	
2	N	137	
2	O	137	
2	P	137	
3	A	409	
3	B	409	
3	C	409	
3	D	409	
3	E	409	
3	F	409	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 31260 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
			1144	726	205	211	2		
1	H	146	Total	C	N	O	S	0	0
			1144	726	205	211	2		
1	I	146	Total	C	N	O	S	0	0
			1144	726	205	211	2		
1	M	146	Total	C	N	O	S	0	0
			1144	726	205	211	2		
1	Q	146	Total	C	N	O	S	0	0
			1144	726	205	211	2		
1	R	146	Total	C	N	O	S	0	0
			1144	726	205	211	2		

- Molecule 2 is a protein called Type IV pilus assembly protein PilF.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	J	137	Total	C	N	O	0	0
			1091	699	190	202		
2	K	137	Total	C	N	O	0	0
			1091	699	190	202		
2	L	137	Total	C	N	O	0	0
			1091	699	190	202		
2	N	137	Total	C	N	O	0	0
			1091	699	190	202		
2	O	137	Total	C	N	O	0	0
			1091	699	190	202		
2	P	137	Total	C	N	O	0	0
			1091	699	190	202		

- Molecule 3 is a protein called Type IV pilus assembly protein PilF.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	383	Total	C	N	O	S	0	0
			2966	1868	534	554	10		
3	C	384	Total	C	N	O	S	0	0
			2975	1874	535	556	10		
3	D	384	Total	C	N	O	S	0	0
			2975	1874	535	556	10		
3	E	384	Total	C	N	O	S	0	0
			2975	1874	535	556	10		
3	F	385	Total	C	N	O	S	0	0
			2984	1879	536	559	10		

There are 144 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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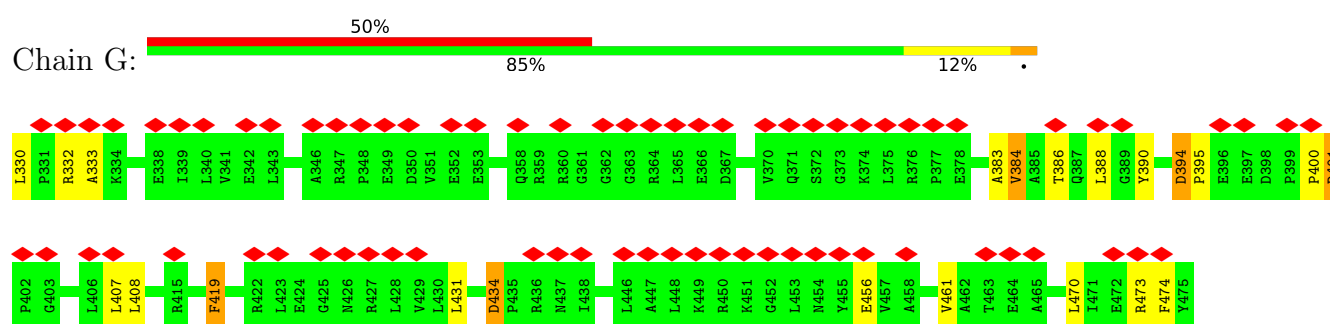
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Chain	Residue	Modelled	Actual	Comment	Reference
E	907	HIS	-	expression tag	UNP Q5SLC9
E	908	HIS	-	expression tag	UNP Q5SLC9
E	909	HIS	-	expression tag	UNP Q5SLC9
E	910	HIS	-	expression tag	UNP Q5SLC9
E	911	HIS	-	expression tag	UNP Q5SLC9
E	912	HIS	-	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
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F	894	LEU	-	expression tag	UNP Q5SLC9
F	895	ALA	-	expression tag	UNP Q5SLC9
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
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F	906	HIS	-	expression tag	UNP Q5SLC9
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F	908	HIS	-	expression tag	UNP Q5SLC9
F	909	HIS	-	expression tag	UNP Q5SLC9
F	910	HIS	-	expression tag	UNP Q5SLC9
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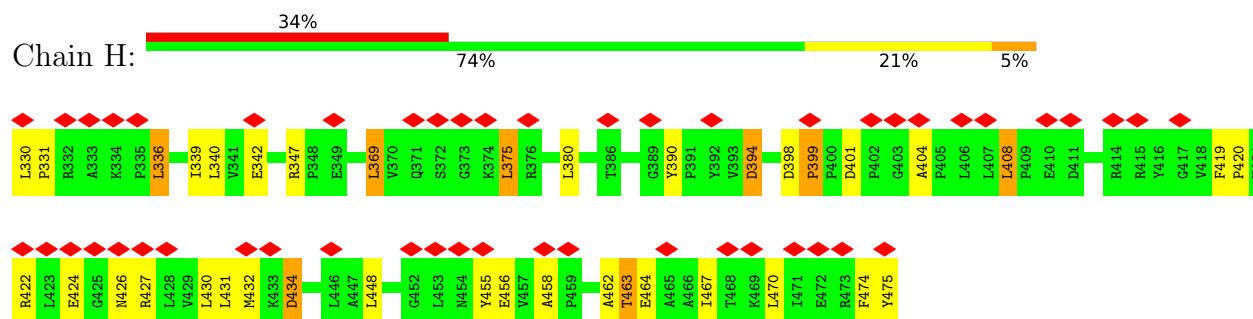
3 Residue-property plots

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.

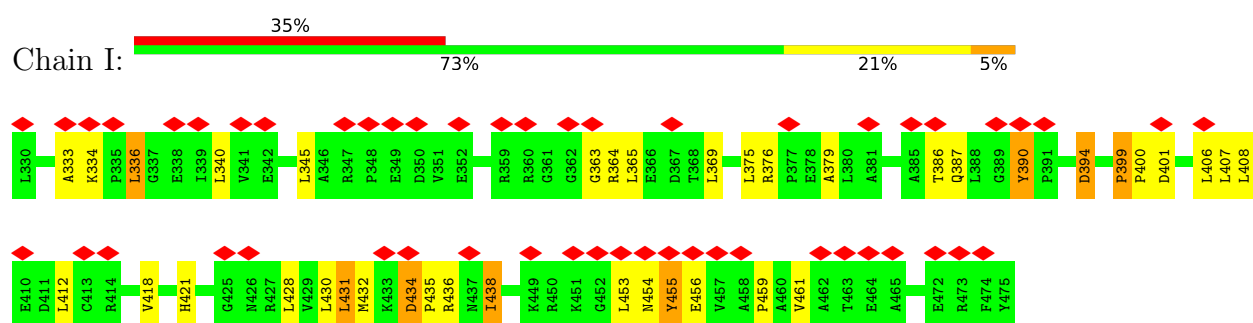
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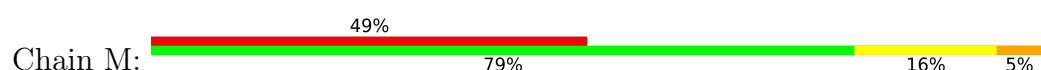
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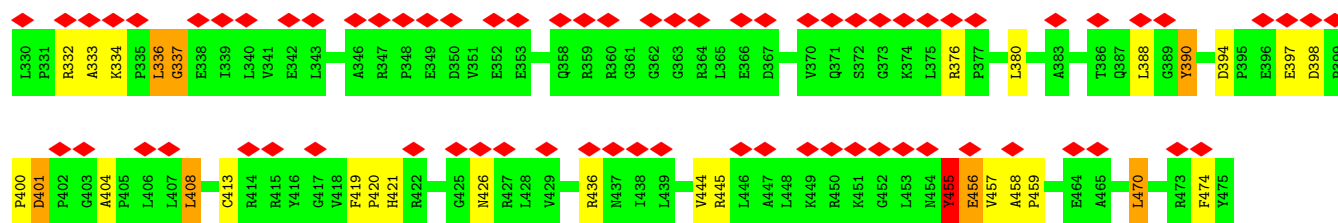


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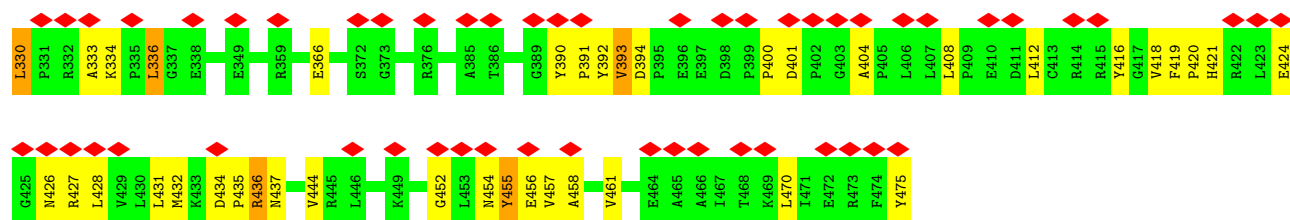
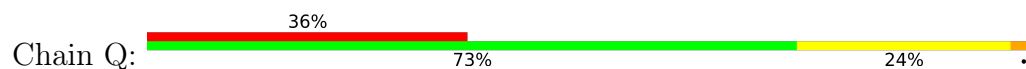


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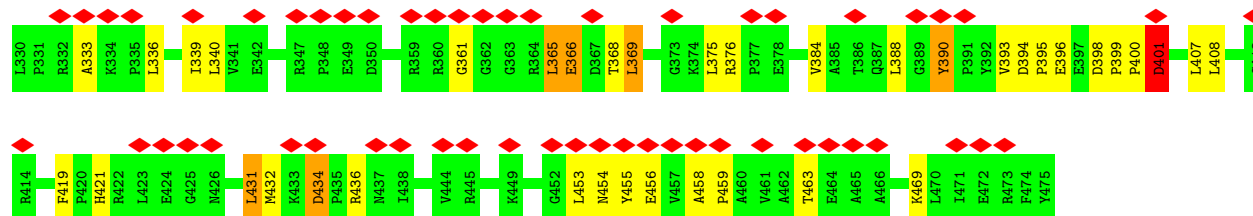
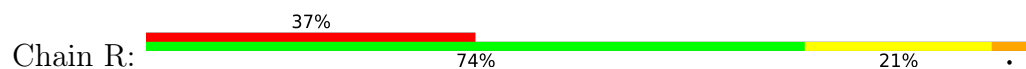




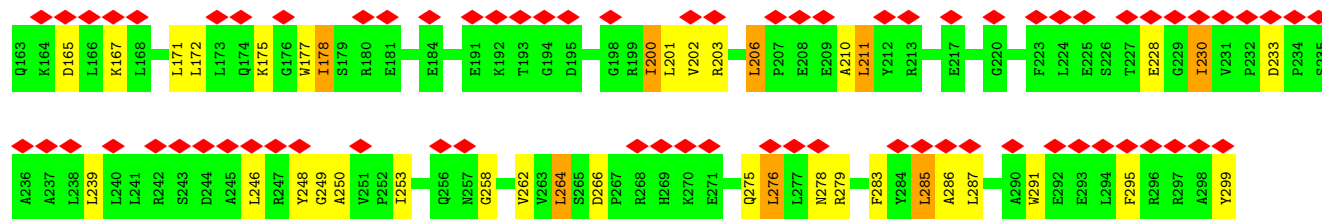
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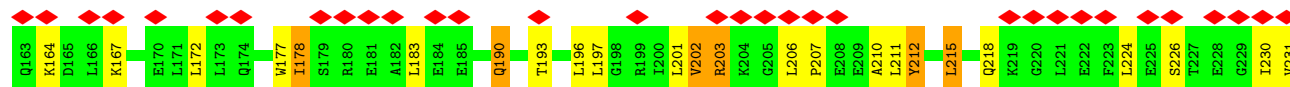
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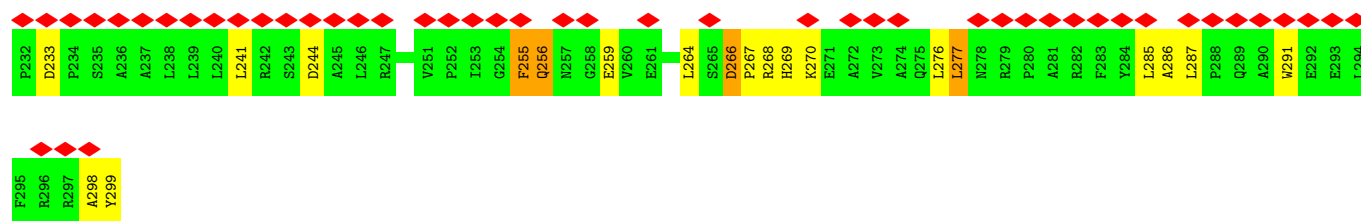


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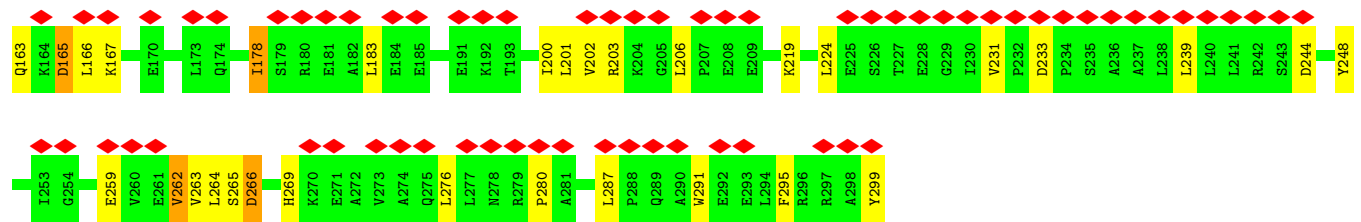
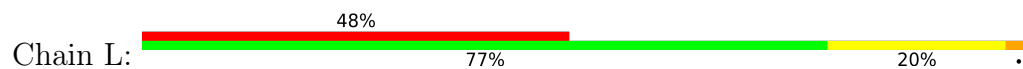


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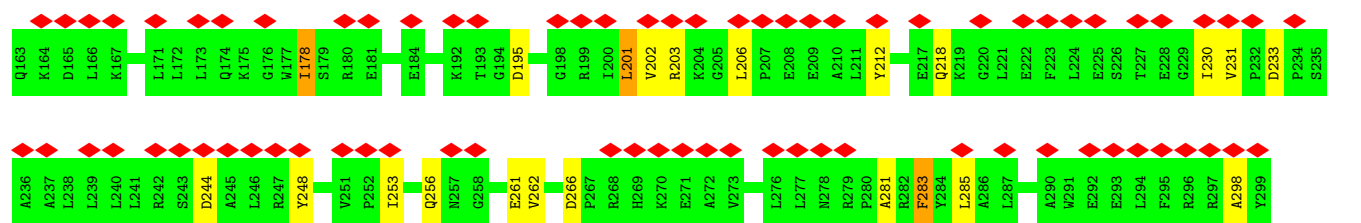
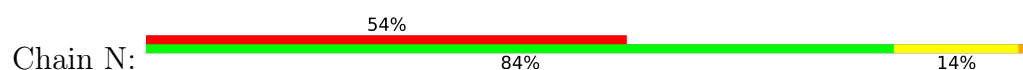




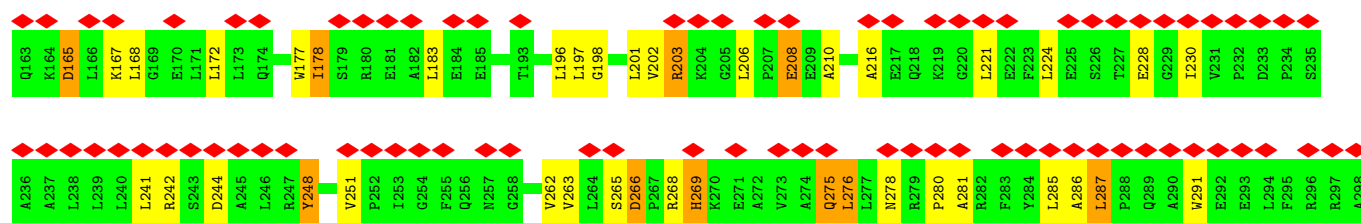
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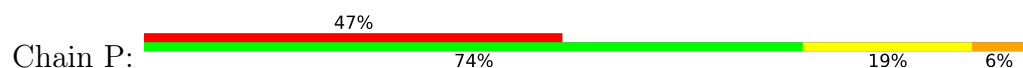
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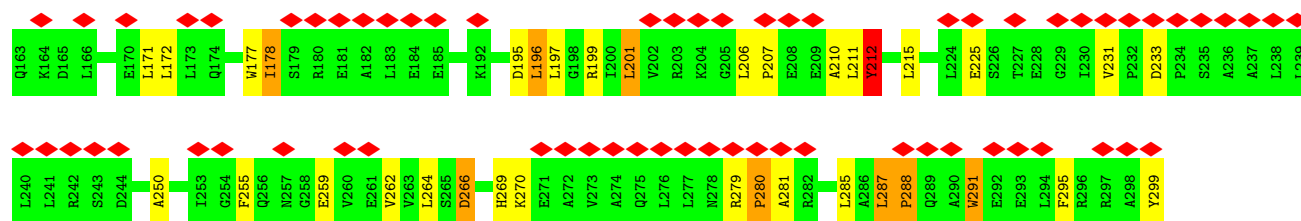


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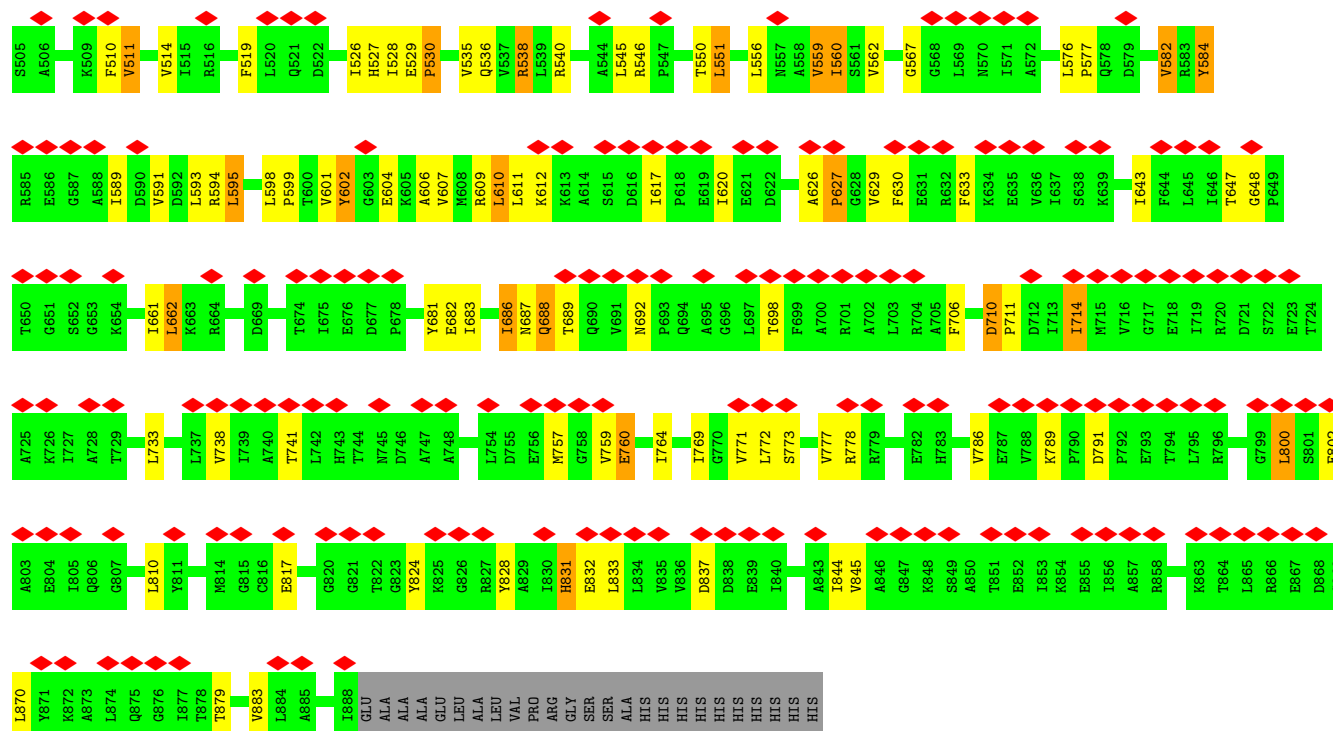
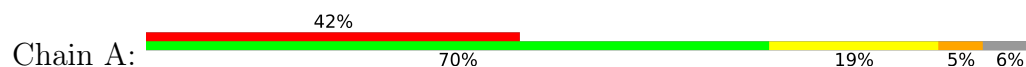


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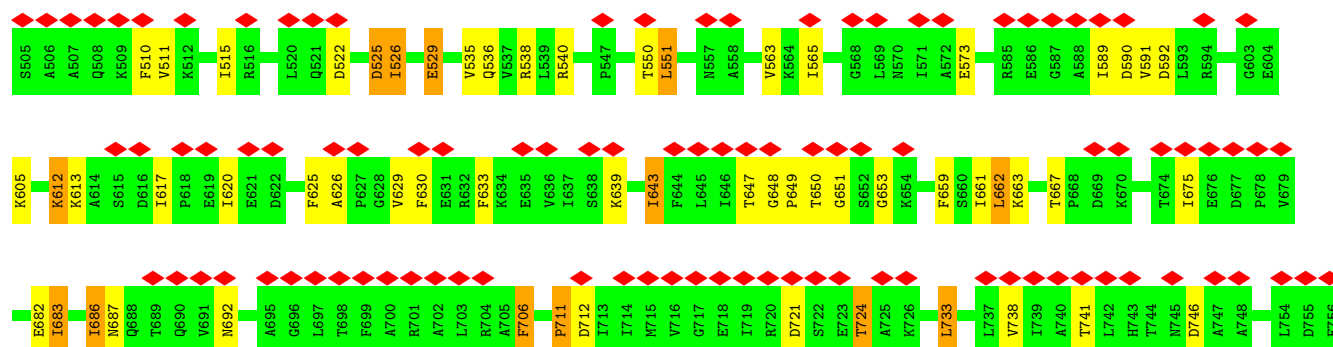
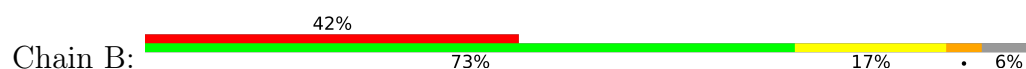


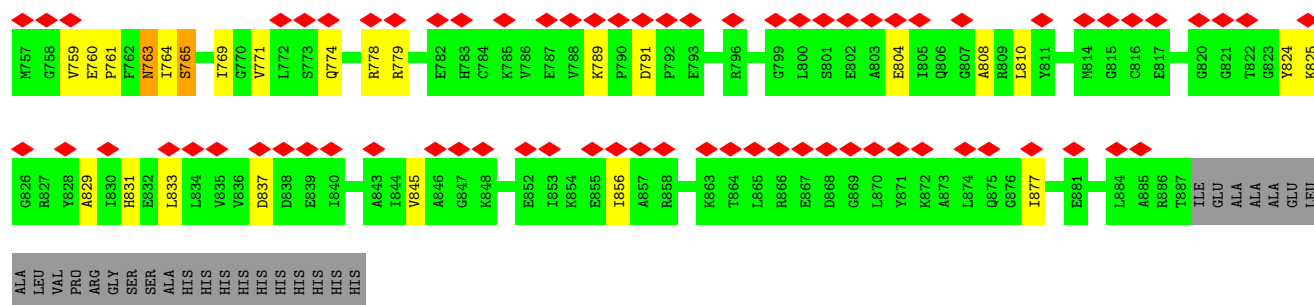


• Molecule 3: Type IV pilus assembly protein PilF

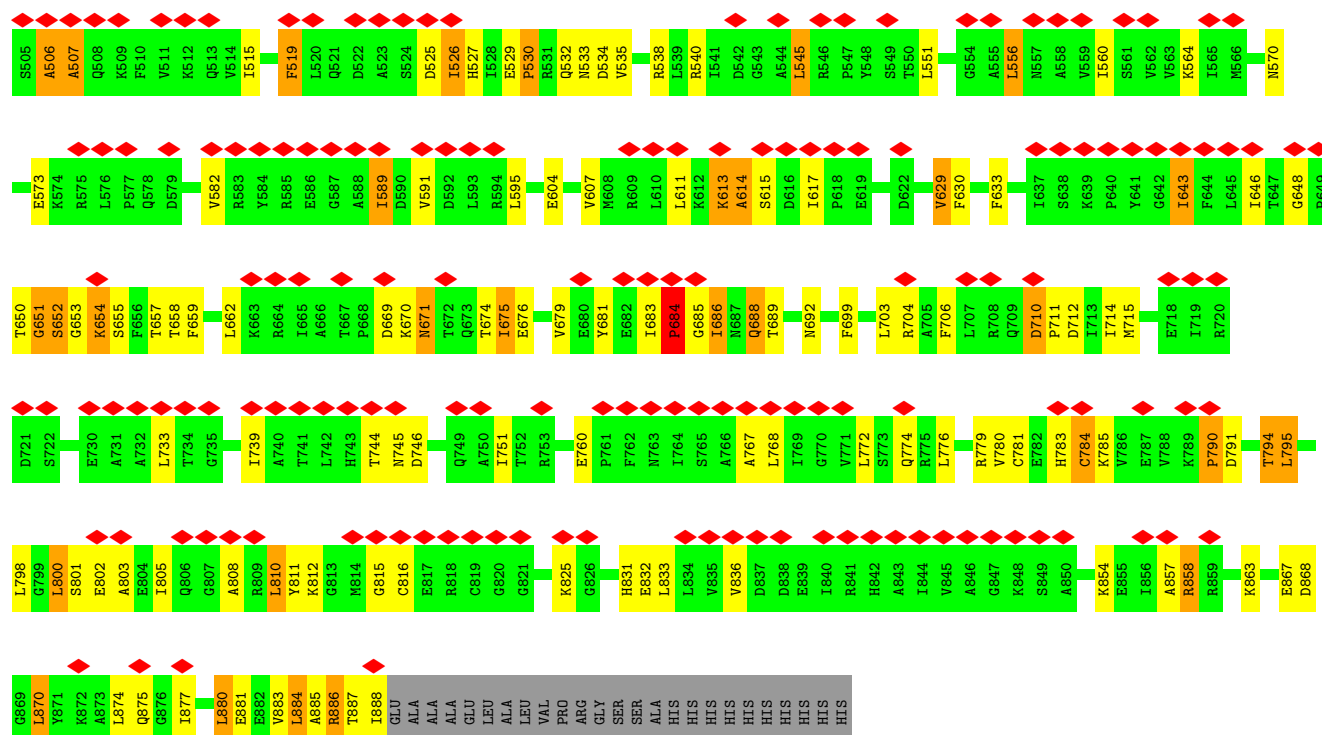
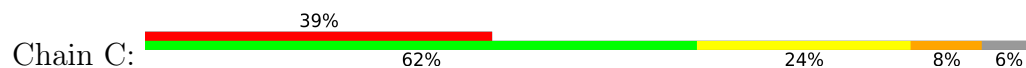


• Molecule 3: Type IV pilus assembly protein PilF

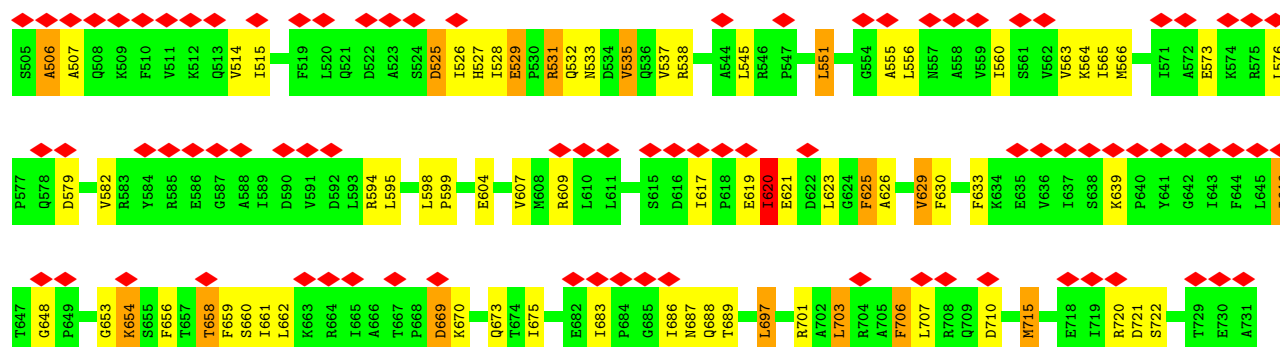
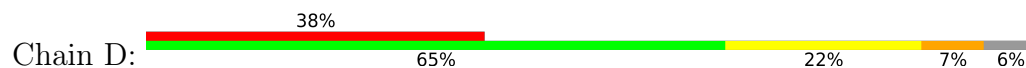




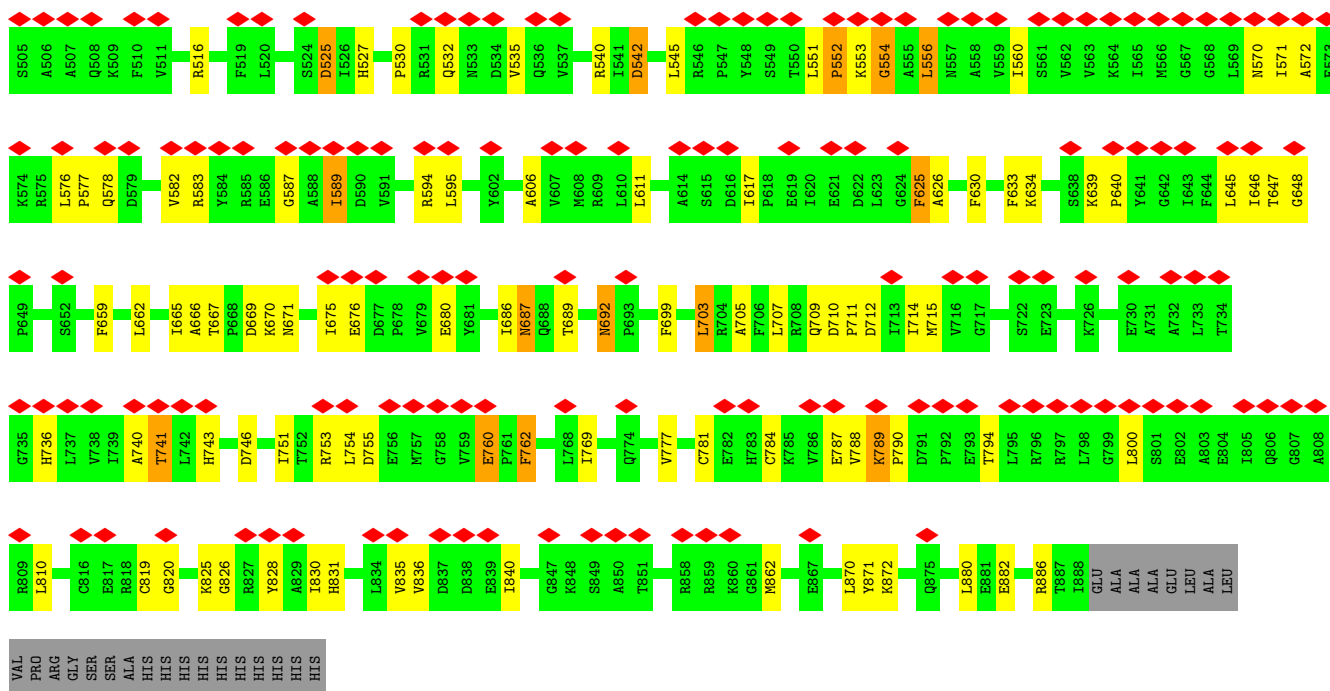
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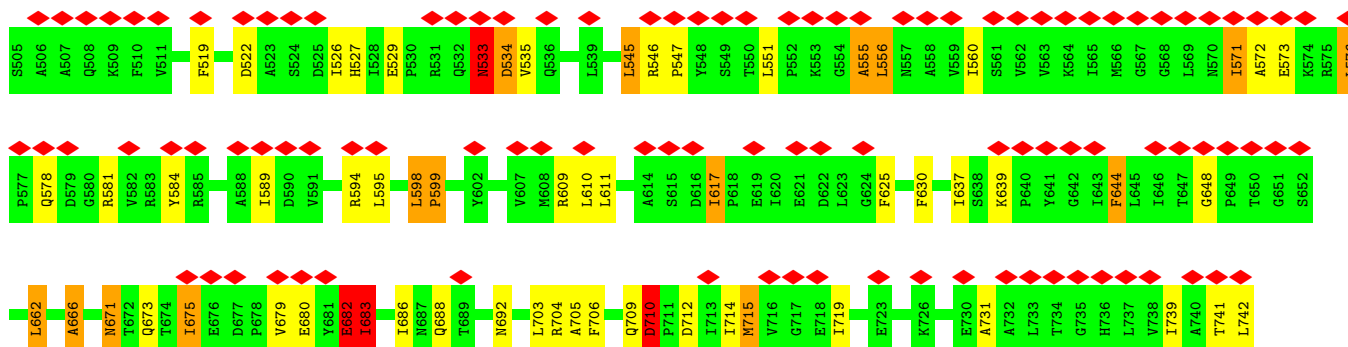
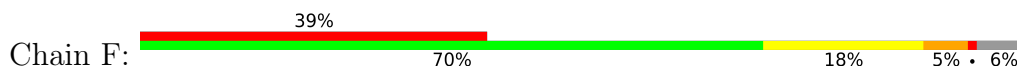
• Molecule 3: Type IV pilus assembly protein PilF

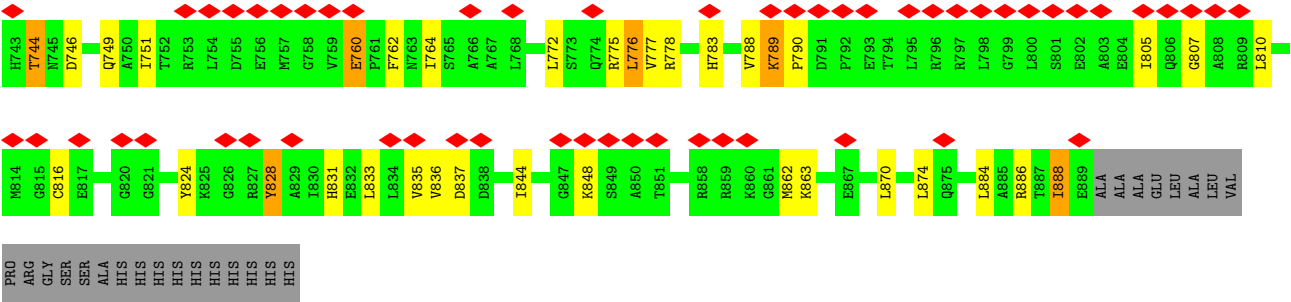


- Molecule 3: Type IV pilus assembly protein PilF



- Molecule 3: 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	45000	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	6.449	Depositor
Minimum map value	-4.043	Depositor
Average map value	0.033	Depositor
Map value standard deviation	0.367	Depositor
Recommended contour level	1.9	Depositor
Map size (Å)	307.2, 307.2, 307.2	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6, 1.6, 1.6	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	G	1.26	4/1165 (0.3%)	1.55	21/1580 (1.3%)
1	H	1.38	8/1165 (0.7%)	1.61	25/1580 (1.6%)
1	I	1.33	5/1165 (0.4%)	1.57	29/1580 (1.8%)
1	M	1.25	2/1165 (0.2%)	1.48	20/1580 (1.3%)
1	Q	1.36	4/1165 (0.3%)	1.55	25/1580 (1.6%)
1	R	1.30	9/1165 (0.8%)	1.54	23/1580 (1.5%)
2	J	1.27	9/1110 (0.8%)	1.61	26/1499 (1.7%)
2	K	1.44	9/1110 (0.8%)	1.57	23/1499 (1.5%)
2	L	1.27	5/1110 (0.5%)	1.54	21/1499 (1.4%)
2	N	1.23	3/1110 (0.3%)	1.50	20/1499 (1.3%)
2	O	1.35	9/1110 (0.8%)	1.63	21/1499 (1.4%)
2	P	1.45	14/1110 (1.3%)	1.56	18/1499 (1.2%)
3	A	1.56	39/3017 (1.3%)	1.63	62/4073 (1.5%)
3	B	1.48	19/3008 (0.6%)	1.64	66/4061 (1.6%)
3	C	1.62	38/3017 (1.3%)	1.70	71/4073 (1.7%)
3	D	1.58	42/3017 (1.4%)	1.70	78/4073 (1.9%)
3	E	1.44	17/3017 (0.6%)	1.59	69/4073 (1.7%)
3	F	1.51	31/3026 (1.0%)	1.62	61/4085 (1.5%)
All	All	1.45	267/31752 (0.8%)	1.61	679/42912 (1.6%)

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	M	0	1
1	Q	0	1
2	P	0	1
3	C	0	4
3	D	0	8
3	E	0	2
3	F	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	23

All (267) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	556	LEU	CB-CG	-13.56	1.26	1.53
3	C	810	LEU	CB-CG	-13.52	1.26	1.53
2	P	285	LEU	CB-CG	-13.11	1.27	1.53
3	A	662	LEU	CB-CG	-10.52	1.32	1.53
3	D	775	ARG	CD-NE	-10.47	1.31	1.46
3	A	686	ILE	CB-CG1	-10.19	1.33	1.53
3	D	675	ILE	CB-CG1	-10.17	1.33	1.53
3	A	511	VAL	CB-CG2	-10.10	1.19	1.52
3	D	703	LEU	CB-CG	-10.05	1.33	1.53
3	D	775	ARG	NE-CZ	-10.00	1.22	1.33
3	C	675	ILE	CB-CG1	-9.84	1.33	1.53
3	F	703	LEU	CB-CG	-9.72	1.34	1.53
1	H	375	LEU	CB-CG	-9.71	1.34	1.53
3	C	800	LEU	CB-CG	-9.50	1.34	1.53
3	F	810	LEU	CB-CG	-9.28	1.34	1.53
3	D	527	HIS	CB-CG	-9.27	1.37	1.50
3	C	880	LEU	CB-CG	-9.21	1.35	1.53
2	J	178	ILE	CB-CG2	-9.01	1.22	1.52
2	K	215	LEU	CB-CG	-8.93	1.35	1.53
3	D	831	HIS	CB-CG	-8.84	1.37	1.50
1	R	340	LEU	CG-CD2	-8.84	1.23	1.52
3	D	810	LEU	CB-CG	-8.83	1.35	1.53
2	K	264	LEU	CB-CG	-8.82	1.35	1.53
3	A	560	ILE	CB-CG1	-8.77	1.35	1.53
2	L	224	LEU	CB-CG	-8.59	1.36	1.53
3	C	662	LEU	CB-CG	-8.47	1.36	1.53
3	E	703	LEU	CB-CG	-8.42	1.36	1.53
3	A	714	ILE	CB-CG2	-8.39	1.24	1.52
3	F	526	ILE	CB-CG1	-8.36	1.36	1.53
3	C	686	ILE	CB-CG1	-8.34	1.36	1.53
1	I	431	LEU	CB-CG	-8.23	1.36	1.53
2	O	196	LEU	CB-CG	-8.23	1.36	1.53
3	D	883	VAL	CA-CB	-8.21	1.43	1.54
3	C	703	LEU	CB-CG	-8.09	1.37	1.53
3	B	551	LEU	CB-CG	-8.06	1.37	1.53
1	R	375	LEU	CG-CD1	-8.04	1.26	1.52
3	C	529	GLU	CG-CD	-7.98	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	201	LEU	CB-CG	-7.96	1.37	1.53
1	Q	431	LEU	CB-CG	-7.93	1.37	1.53
3	F	675	ILE	CB-CG1	-7.92	1.37	1.53
1	I	421	HIS	CB-CG	-7.92	1.39	1.50
3	A	538	ARG	CD-NE	-7.89	1.35	1.46
3	B	810	LEU	CB-CG	-7.84	1.37	1.53
3	E	686	ILE	CB-CG1	-7.83	1.37	1.53
3	D	858	ARG	CD-NE	-7.82	1.35	1.46
3	E	870	LEU	CB-CG	-7.78	1.37	1.53
3	C	884	LEU	CB-CG	-7.74	1.38	1.53
1	I	340	LEU	CB-CG	-7.66	1.38	1.53
1	Q	330	LEU	CB-CG	-7.66	1.38	1.53
3	B	733	LEU	CB-CG	-7.65	1.38	1.53
3	C	858	ARG	CD-NE	-7.61	1.35	1.46
3	A	610	LEU	CB-CG	-7.59	1.38	1.53
3	D	880	LEU	CB-CG	-7.58	1.38	1.53
3	B	675	ILE	CB-CG1	-7.55	1.38	1.53
3	C	538	ARG	CD-NE	-7.53	1.35	1.46
3	B	526	ILE	CB-CG1	-7.52	1.38	1.53
2	K	218	GLN	CG-CD	-7.52	1.33	1.52
3	A	611	LEU	CB-CG	-7.38	1.38	1.53
3	D	865	LEU	CB-CG	-7.35	1.38	1.53
2	L	178	ILE	CB-CG2	-7.29	1.28	1.52
1	H	340	LEU	CB-CG	-7.28	1.38	1.53
3	A	527	HIS	CB-CG	-7.27	1.40	1.50
2	K	178	ILE	CB-CG2	-7.26	1.28	1.52
2	O	285	LEU	CB-CG	-7.24	1.39	1.53
3	D	884	LEU	CB-CG	-7.21	1.39	1.53
3	F	884	LEU	CB-CG	-7.18	1.39	1.53
3	E	800	LEU	CB-CG	-7.16	1.39	1.53
3	D	595	LEU	CB-CG	-7.15	1.39	1.53
3	D	870	LEU	CG-CD1	-7.13	1.29	1.52
1	H	431	LEU	CB-CG	-7.12	1.39	1.53
3	C	714	ILE	CB-CG1	-7.11	1.39	1.53
3	B	625	PHE	CB-CG	-7.05	1.34	1.50
3	F	703	LEU	CG-CD1	-7.03	1.29	1.52
3	A	591	VAL	CB-CG1	-7.02	1.29	1.52
3	F	874	LEU	CG-CD1	-7.00	1.29	1.52
3	D	545	LEU	CB-CG	-6.98	1.39	1.53
3	D	791	ASP	CB-CG	-6.95	1.34	1.52
1	H	369	LEU	CB-CG	-6.94	1.39	1.53
3	A	617	ILE	CB-CG1	-6.93	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	556	LEU	CB-CG	-6.92	1.39	1.53
2	N	218	GLN	CG-CD	-6.90	1.34	1.52
2	L	178	ILE	CB-CG1	-6.88	1.39	1.53
3	E	576	LEU	CA-C	6.88	1.61	1.52
3	C	883	VAL	CA-CB	-6.86	1.45	1.54
1	H	470	LEU	CB-CG	-6.77	1.40	1.53
3	F	775	ARG	CD-NE	-6.76	1.36	1.46
2	P	178	ILE	CB-CG2	-6.73	1.30	1.52
2	O	201	LEU	CB-CG	-6.71	1.40	1.53
3	A	831	HIS	CB-CG	-6.70	1.40	1.50
3	A	560	ILE	CA-CB	-6.70	1.46	1.54
3	F	751	ILE	CB-CG1	-6.69	1.40	1.53
3	C	791	ASP	CB-CG	-6.67	1.35	1.52
3	A	511	VAL	CA-CB	-6.66	1.46	1.54
1	Q	421	HIS	CB-CG	-6.64	1.40	1.50
1	R	339	ILE	CB-CG1	-6.62	1.40	1.53
3	C	688	GLN	CG-CD	-6.59	1.35	1.52
3	D	775	ARG	CB-CG	-6.55	1.32	1.52
2	O	172	LEU	CB-CG	-6.54	1.40	1.53
2	P	171	LEU	CB-CG	-6.53	1.40	1.53
3	D	538	ARG	CZ-NH1	-6.52	1.23	1.32
3	D	620	ILE	CB-CG1	-6.51	1.40	1.53
1	R	407	LEU	CB-CG	-6.51	1.40	1.53
2	J	171	LEU	CB-CG	-6.50	1.40	1.53
3	A	582	VAL	CA-CB	-6.49	1.46	1.53
2	K	285	LEU	CB-CG	-6.48	1.40	1.53
2	J	206	LEU	CG-CD1	-6.46	1.31	1.52
3	A	582	VAL	CA-C	-6.46	1.45	1.53
2	P	212	TYR	CG-CD1	-6.43	1.25	1.39
3	C	643	ILE	CB-CG1	-6.43	1.40	1.53
3	B	617	ILE	CB-CG1	-6.40	1.40	1.53
3	B	662	LEU	CB-CG	-6.36	1.40	1.53
3	B	686	ILE	CB-CG1	-6.36	1.40	1.53
1	R	431	LEU	CB-CG	-6.33	1.40	1.53
2	N	285	LEU	CB-CG	-6.31	1.40	1.53
2	L	264	LEU	CB-CG	-6.30	1.40	1.53
3	F	671	ASN	CA-CB	-6.30	1.44	1.52
3	F	870	LEU	CG-CD2	-6.30	1.31	1.52
2	O	178	ILE	CB-CG1	-6.29	1.40	1.53
2	K	172	LEU	CB-CG	-6.28	1.40	1.53
3	A	800	LEU	CB-CG	-6.27	1.41	1.53
1	M	413	CYS	CB-SG	-6.25	1.60	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	172	LEU	CB-CG	-6.24	1.41	1.53
3	C	675	ILE	CB-CG2	-6.24	1.31	1.52
3	D	529	GLU	CG-CD	-6.20	1.36	1.52
3	A	610	LEU	CG-CD1	-6.19	1.32	1.52
3	F	772	LEU	CB-CG	-6.19	1.41	1.53
3	C	751	ILE	CB-CG2	-6.18	1.32	1.52
3	F	844	ILE	CB-CG1	-6.17	1.41	1.53
3	A	643	ILE	CB-CG1	-6.15	1.41	1.53
3	C	739	ILE	CB-CG1	-6.12	1.41	1.53
3	C	798	LEU	CB-CG	-6.12	1.41	1.53
3	A	584	TYR	CG-CD2	-6.08	1.26	1.39
3	F	527	HIS	CB-CG	-6.06	1.41	1.50
3	A	582	VAL	CB-CG2	-6.04	1.32	1.52
3	A	526	ILE	CB-CG1	-6.02	1.41	1.53
3	F	775	ARG	CG-CD	-6.02	1.34	1.52
3	C	888	ILE	CB-CG1	-6.02	1.41	1.53
3	F	545	LEU	CB-CG	-6.01	1.41	1.53
2	O	178	ILE	CB-CG2	-5.99	1.32	1.52
2	J	264	LEU	CB-CG	-5.99	1.41	1.53
3	F	617	ILE	CB-CG1	-5.99	1.41	1.53
1	H	430	LEU	CB-CG	-5.99	1.41	1.53
3	E	545	LEU	CB-CG	-5.96	1.41	1.53
3	A	810	LEU	CB-CG	-5.95	1.41	1.53
2	P	212	TYR	CB-CG	-5.94	1.38	1.51
2	O	168	LEU	CB-CG	-5.90	1.41	1.53
1	Q	418	VAL	CB-CG1	-5.90	1.33	1.52
3	E	645	LEU	CB-CG	-5.89	1.41	1.53
3	B	563	VAL	CB-CG2	-5.87	1.33	1.52
3	F	776	LEU	CB-CG	-5.87	1.41	1.53
1	G	407	LEU	CB-CG	-5.87	1.41	1.53
2	P	288	PRO	N-CD	-5.87	1.39	1.47
3	E	880	LEU	CB-CG	-5.85	1.41	1.53
3	F	522	ASP	CB-CG	5.84	1.66	1.52
1	R	369	LEU	CG-CD1	-5.83	1.33	1.52
3	F	671	ASN	CB-CG	-5.83	1.37	1.52
3	C	654	LYS	CB-CG	-5.83	1.34	1.52
3	E	617	ILE	CB-CG1	-5.82	1.41	1.53
3	F	715	MET	CG-SD	-5.79	1.66	1.80
3	D	683	ILE	CB-CG1	-5.78	1.41	1.53
1	G	431	LEU	CB-CG	-5.77	1.42	1.53
3	A	551	LEU	CG-CD2	-5.76	1.33	1.52
3	E	525	ASP	CB-CG	-5.76	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	795	LEU	CB-CG	-5.76	1.42	1.53
1	H	380	LEU	CB-CG	-5.75	1.42	1.53
3	D	798	LEU	CB-CG	-5.74	1.42	1.53
3	F	688	GLN	CG-CD	-5.74	1.37	1.52
1	M	470	LEU	CB-CG	-5.74	1.42	1.53
3	A	577	PRO	N-CD	-5.73	1.39	1.47
2	J	230	ILE	CB-CG1	-5.73	1.42	1.53
2	K	201	LEU	CG-CD2	-5.72	1.33	1.52
2	P	215	LEU	CB-CG	-5.71	1.42	1.53
1	R	421	HIS	CB-CG	-5.71	1.42	1.50
3	B	706	PHE	CB-CG	-5.70	1.37	1.50
3	D	703	LEU	CG-CD1	-5.70	1.33	1.52
3	E	751	ILE	CB-CG1	-5.69	1.42	1.53
3	A	589	ILE	CB-CG1	-5.67	1.42	1.53
3	E	769	ILE	CB-CG1	-5.64	1.42	1.53
2	P	178	ILE	CB-CG1	-5.63	1.42	1.53
2	P	197	LEU	CB-CG	-5.60	1.42	1.53
3	D	646	ILE	CB-CG1	-5.59	1.42	1.53
3	E	589	ILE	CG1-CD1	-5.59	1.29	1.51
3	B	661	ILE	CB-CG1	-5.58	1.42	1.53
3	A	538	ARG	CG-CD	-5.58	1.35	1.52
3	D	595	LEU	CG-CD1	-5.58	1.34	1.52
3	D	697	LEU	CG-CD2	-5.57	1.34	1.52
1	G	388	LEU	CB-CG	-5.57	1.42	1.53
3	C	527	HIS	CB-CG	-5.56	1.42	1.50
3	E	527	HIS	CE1-NE2	-5.54	1.27	1.32
3	A	661	ILE	CB-CG1	-5.53	1.42	1.53
3	D	804	GLU	CG-CD	-5.53	1.38	1.52
3	D	746	ASP	CB-CG	-5.52	1.38	1.52
3	D	870	LEU	CG-CD2	-5.51	1.34	1.52
2	L	201	LEU	CB-CG	-5.50	1.42	1.53
2	P	196	LEU	CG-CD1	-5.49	1.34	1.52
3	D	673	GLN	CG-CD	-5.48	1.38	1.52
3	B	686	ILE	CG1-CD1	-5.48	1.30	1.51
3	D	662	LEU	CB-CG	-5.45	1.42	1.53
3	C	772	LEU	CB-CG	5.45	1.64	1.53
3	D	795	LEU	CG-CD2	-5.45	1.34	1.52
3	E	831	HIS	CE1-NE2	-5.45	1.27	1.32
3	A	584	TYR	CB-CG	-5.43	1.39	1.51
3	C	530	PRO	N-CD	-5.43	1.40	1.47
3	D	706	PHE	CG-CD1	-5.42	1.27	1.38
2	J	206	LEU	CG-CD2	-5.41	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	686	ILE	CA-CB	-5.41	1.47	1.55
3	C	681	TYR	CB-CG	-5.39	1.39	1.51
3	B	525	ASP	CB-CG	-5.38	1.38	1.52
3	D	527	HIS	CG-ND1	-5.38	1.32	1.38
1	H	339	ILE	CB-CG1	-5.38	1.42	1.53
3	D	658	THR	CB-CG2	-5.38	1.34	1.52
2	P	291	TRP	CZ3-CH2	-5.37	1.27	1.40
3	A	686	ILE	CB-CG2	-5.37	1.34	1.52
2	O	197	LEU	CG-CD1	-5.37	1.34	1.52
1	R	336	LEU	CB-CG	-5.36	1.42	1.53
3	F	546	ARG	CG-CD	-5.36	1.36	1.52
3	D	790	PRO	CA-C	-5.33	1.48	1.52
3	D	862	MET	SD-CE	-5.33	1.66	1.79
3	F	529	GLU	CG-CD	-5.32	1.38	1.52
2	P	212	TYR	CE1-CZ	-5.31	1.25	1.38
3	A	688	GLN	CG-CD	-5.30	1.38	1.52
3	A	686	ILE	CG1-CD1	-5.29	1.31	1.51
3	F	776	LEU	CA-C	-5.29	1.46	1.52
3	D	531	ARG	CZ-NH2	-5.26	1.26	1.33
3	D	886	ARG	CA-CB	-5.26	1.46	1.54
3	F	744	THR	CB-CG2	-5.26	1.35	1.52
3	F	742	LEU	CA-C	5.25	1.58	1.52
3	C	858	ARG	CG-CD	-5.22	1.36	1.52
3	F	599	PRO	CA-C	-5.22	1.46	1.52
2	J	264	LEU	CG-CD1	-5.22	1.35	1.52
1	I	375	LEU	CG-CD2	-5.22	1.35	1.52
2	P	172	LEU	CB-CG	-5.21	1.43	1.53
2	K	266	ASP	CB-CG	-5.21	1.39	1.52
3	C	545	LEU	CB-CG	-5.21	1.43	1.53
3	D	772	LEU	CG-CD2	-5.21	1.35	1.52
3	F	637	ILE	CB-CG1	-5.20	1.43	1.53
3	A	582	VAL	CB-CG1	-5.20	1.35	1.52
3	C	805	ILE	CG1-CD1	-5.20	1.31	1.51
1	R	375	LEU	CG-CD2	-5.20	1.35	1.52
1	I	369	LEU	CG-CD1	-5.19	1.35	1.52
3	F	764	ILE	CB-CG1	-5.19	1.43	1.53
3	C	595	LEU	CB-CG	-5.19	1.43	1.53
2	N	201	LEU	CB-CG	-5.19	1.43	1.53
3	C	629	VAL	CB-CG1	-5.18	1.35	1.52
3	A	528	ILE	CB-CG2	-5.17	1.35	1.52
3	C	556	LEU	CA-CB	-5.17	1.45	1.53
3	B	526	ILE	CA-CB	-5.16	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	870	LEU	CG-CD1	-5.16	1.35	1.52
3	C	886	ARG	CD-NE	-5.16	1.39	1.46
3	B	711	PRO	N-CD	-5.15	1.40	1.47
3	B	733	LEU	CA-CB	-5.14	1.46	1.53
3	E	617	ILE	CA-C	5.14	1.57	1.53
3	B	831	HIS	CB-CG	-5.13	1.43	1.50
3	A	595	LEU	CB-CG	-5.12	1.43	1.53
3	B	724	THR	CB-CG2	-5.12	1.35	1.52
3	A	610	LEU	CA-C	-5.11	1.46	1.52
2	J	262	VAL	CB-CG2	-5.11	1.35	1.52
2	K	218	GLN	CB-CG	-5.10	1.37	1.52
2	O	276	LEU	CB-CG	-5.10	1.43	1.53
3	E	810	LEU	CG-CD2	-5.09	1.35	1.52
3	A	698	THR	CA-C	-5.09	1.46	1.53
3	D	531	ARG	CD-NE	-5.06	1.39	1.46
3	D	528	ILE	CB-CG1	-5.06	1.43	1.53
3	C	790	PRO	CA-C	-5.05	1.45	1.52
3	A	530	PRO	CA-CB	-5.04	1.46	1.53
1	G	470	LEU	CB-CG	-5.04	1.43	1.53
3	C	715	MET	CB-CG	-5.02	1.37	1.52

All (679) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	625	PHE	CA-CB-CG	14.00	127.80	113.80
3	E	576	LEU	CA-C-N	12.37	132.52	119.90
3	E	576	LEU	C-N-CA	12.37	132.52	119.90
3	C	712	ASP	N-CA-C	-12.05	98.06	113.12
1	H	426	ASN	CA-CB-CG	11.06	123.66	112.60
2	J	278	ASN	N-CA-C	-10.71	100.27	113.97
3	B	763	ASN	N-CA-C	-10.57	96.90	110.53
3	B	687	ASN	CA-CB-CG	-10.46	102.14	112.60
3	B	617	ILE	N-CA-C	10.18	117.39	108.63
1	Q	390	TYR	CA-C-N	9.99	129.92	120.03
1	Q	390	TYR	C-N-CA	9.99	129.92	120.03
2	O	265	SER	N-CA-C	-9.91	101.52	114.31
3	E	630	PHE	CA-CB-CG	-9.90	103.90	113.80
3	B	590	ASP	N-CA-C	-9.71	99.62	113.21
3	A	648	GLY	CA-C-N	9.46	129.88	120.52
3	A	648	GLY	C-N-CA	9.46	129.88	120.52
3	A	710	ASP	CA-C-N	9.40	129.34	120.03
3	A	710	ASP	C-N-CA	9.40	129.34	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	630	PHE	CA-CB-CG	-9.27	104.53	113.80
3	C	805	ILE	CB-CA-C	-9.24	103.85	111.71
1	G	474	PHE	N-CA-C	9.24	123.73	108.49
1	R	458	ALA	CA-C-N	9.16	129.00	120.21
1	R	458	ALA	C-N-CA	9.16	129.00	120.21
1	G	419	PHE	CA-C-N	9.13	129.16	119.76
1	G	419	PHE	C-N-CA	9.13	129.16	119.76
3	C	630	PHE	CA-CB-CG	-9.02	104.78	113.80
2	J	295	PHE	CA-CB-CG	9.00	122.80	113.80
1	M	394	ASP	CA-C-N	8.97	129.88	119.47
1	M	394	ASP	C-N-CA	8.97	129.88	119.47
3	A	630	PHE	CA-CB-CG	-8.83	104.97	113.80
2	L	231	VAL	N-CA-C	8.74	118.36	108.05
3	B	629	VAL	N-CA-C	-8.72	101.49	111.00
3	B	648	GLY	CA-C-N	8.65	129.18	119.92
3	B	648	GLY	C-N-CA	8.65	129.18	119.92
2	N	178	ILE	CB-CA-C	-8.63	97.52	110.82
1	Q	431	LEU	N-CA-C	-8.60	97.29	110.10
3	F	644	PHE	CA-CB-CG	-8.52	105.28	113.80
1	H	394	ASP	CA-C-N	8.49	130.45	119.84
1	H	394	ASP	C-N-CA	8.49	130.45	119.84
2	L	262	VAL	N-CA-C	8.45	120.28	108.12
2	L	287	LEU	N-CA-C	8.44	120.55	109.83
2	L	266	ASP	CA-C-N	8.33	127.99	119.82
2	L	266	ASP	C-N-CA	8.33	127.99	119.82
3	D	819	CYS	CA-C-O	-8.32	113.09	118.33
3	C	648	GLY	CA-C-N	8.30	128.33	119.78
3	C	648	GLY	C-N-CA	8.30	128.33	119.78
2	P	212	TYR	CA-CB-CG	-8.27	99.02	113.90
1	Q	434	ASP	CA-C-N	8.27	128.20	119.85
1	Q	434	ASP	C-N-CA	8.27	128.20	119.85
2	O	278	ASN	N-CA-C	-8.24	102.79	113.17
1	Q	432	MET	N-CA-C	8.23	121.92	108.99
3	E	741	THR	N-CA-C	8.19	121.79	109.25
3	D	506	ALA	CA-C-O	-8.10	111.44	121.89
3	B	591	VAL	N-CA-C	-8.09	98.21	109.21
2	P	287	LEU	N-CA-C	8.08	120.09	109.83
2	P	233	ASP	CA-C-N	8.04	127.76	119.56
2	P	233	ASP	C-N-CA	8.04	127.76	119.56
3	F	576	LEU	CA-C-N	8.04	127.97	119.85
3	F	576	LEU	C-N-CA	8.04	127.97	119.85
1	I	394	ASP	CA-C-N	8.03	129.88	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	394	ASP	C-N-CA	8.03	129.88	119.84
1	H	458	ALA	CA-C-N	7.96	127.92	120.03
1	H	458	ALA	C-N-CA	7.96	127.92	120.03
3	A	687	ASN	CA-CB-CG	-7.90	104.70	112.60
2	P	225	GLU	N-CA-C	7.87	120.36	109.18
1	I	376	ARG	N-CA-C	-7.79	99.33	110.08
2	J	178	ILE	CB-CA-C	-7.72	99.40	110.82
3	D	686	ILE	N-CA-C	7.70	119.20	108.12
3	D	648	GLY	CA-C-N	7.67	127.68	119.78
3	D	648	GLY	C-N-CA	7.67	127.68	119.78
3	E	617	ILE	CA-C-N	7.65	128.10	119.92
3	E	617	ILE	C-N-CA	7.65	128.10	119.92
2	P	264	LEU	N-CA-C	7.60	121.60	108.76
1	R	394	ASP	CA-C-N	7.57	127.28	119.56
1	R	394	ASP	C-N-CA	7.57	127.28	119.56
1	H	426	ASN	N-CA-C	-7.56	104.56	114.31
3	B	589	ILE	CA-C-N	7.53	132.01	119.35
3	B	589	ILE	C-N-CA	7.53	132.01	119.35
3	C	686	ILE	N-CA-C	7.53	119.44	108.53
2	P	287	LEU	CA-C-N	7.51	128.19	119.47
2	P	287	LEU	C-N-CA	7.51	128.19	119.47
1	I	390	TYR	CA-C-N	7.51	127.44	119.85
1	I	390	TYR	C-N-CA	7.51	127.44	119.85
3	D	545	LEU	N-CA-C	7.51	120.44	110.53
3	F	630	PHE	CA-CB-CG	-7.50	106.30	113.80
2	L	263	VAL	CB-CA-C	-7.50	101.89	110.96
2	J	253	ILE	N-CA-C	7.48	118.89	108.12
3	F	648	GLY	CA-C-N	7.44	127.88	119.92
3	F	648	GLY	C-N-CA	7.44	127.88	119.92
3	A	559	VAL	CB-CA-C	-7.44	102.45	111.97
2	O	208	GLU	N-CA-C	7.42	119.16	111.14
3	B	653	GLY	N-CA-C	-7.41	104.98	115.43
3	A	530	PRO	N-CA-C	7.33	122.40	111.41
3	C	692	ASN	CA-C-N	7.31	127.95	119.47
3	C	692	ASN	C-N-CA	7.31	127.95	119.47
3	C	589	ILE	N-CA-CB	-7.30	102.67	111.00
3	D	808	ALA	N-CA-C	7.29	119.94	108.79
2	O	275	GLN	N-CA-C	-7.29	100.91	110.53
3	E	639	LYS	CA-C-N	7.28	127.91	119.47
3	E	639	LYS	C-N-CA	7.28	127.91	119.47
3	A	771	VAL	N-CA-C	7.24	118.74	108.17
3	F	571	ILE	N-CA-C	7.24	113.96	106.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	684	PRO	CA-C-O	-7.23	112.82	122.08
3	A	833	LEU	N-CA-C	7.22	120.18	108.41
3	F	589	ILE	N-CA-C	7.22	119.00	108.53
3	D	656	PHE	CA-CB-CG	7.19	120.99	113.80
1	H	398	ASP	CA-C-N	7.19	127.78	120.38
1	H	398	ASP	C-N-CA	7.19	127.78	120.38
3	C	768	LEU	N-CA-C	7.18	120.72	109.96
2	K	231	VAL	CA-C-N	7.17	127.09	120.21
2	K	231	VAL	C-N-CA	7.17	127.09	120.21
3	F	760	GLU	CA-C-N	7.16	127.77	119.47
3	F	760	GLU	C-N-CA	7.16	127.77	119.47
3	D	768	LEU	N-CA-C	7.15	120.59	110.23
3	C	711	PRO	CB-CA-C	-7.14	101.62	110.98
2	K	269	HIS	CA-CB-CG	-7.14	106.66	113.80
3	A	738	VAL	N-CA-C	7.13	118.14	107.80
3	E	617	ILE	N-CA-C	7.13	115.75	107.77
3	C	506	ALA	CA-C-O	-7.13	112.93	121.05
3	C	651	GLY	N-CA-C	-7.13	98.37	111.34
2	O	266	ASP	CA-C-N	7.10	127.25	119.87
2	O	266	ASP	C-N-CA	7.10	127.25	119.87
3	E	746	ASP	CA-CB-CG	7.08	119.69	112.60
1	G	394	ASP	CA-C-N	7.08	128.69	119.84
1	G	394	ASP	C-N-CA	7.08	128.69	119.84
3	F	805	ILE	CB-CA-C	-7.07	102.75	112.02
3	E	667	THR	CA-C-N	7.06	126.74	119.82
3	E	667	THR	C-N-CA	7.06	126.74	119.82
3	D	710	ASP	CA-C-N	7.05	126.98	120.21
3	D	710	ASP	C-N-CA	7.05	126.98	120.21
1	I	434	ASP	CA-C-N	7.04	128.65	119.84
1	I	434	ASP	C-N-CA	7.04	128.65	119.84
3	C	791	ASP	CA-CB-CG	-7.01	105.58	112.60
3	F	617	ILE	CA-C-N	7.01	126.94	120.21
3	F	617	ILE	C-N-CA	7.01	126.94	120.21
3	A	789	LYS	CA-C-N	7.00	126.92	119.85
3	A	789	LYS	C-N-CA	7.00	126.92	119.85
2	J	262	VAL	CB-CA-C	-7.00	101.89	110.99
2	L	233	ASP	CA-C-N	6.99	127.58	119.47
2	L	233	ASP	C-N-CA	6.99	127.58	119.47
1	R	454	ASN	N-CA-C	-6.98	104.07	112.59
3	F	712	ASP	CA-CB-CG	6.96	119.56	112.60
2	L	231	VAL	CA-C-N	6.94	126.86	119.85
2	L	231	VAL	C-N-CA	6.94	126.86	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	764	ILE	N-CA-C	-6.94	103.76	110.42
1	I	454	ASN	N-CA-C	-6.92	104.14	112.59
1	M	390	TYR	CA-C-N	6.92	128.49	119.84
1	M	390	TYR	C-N-CA	6.92	128.49	119.84
3	F	884	LEU	CB-CA-C	-6.92	100.02	110.88
3	B	589	ILE	N-CA-C	6.91	119.00	108.71
3	B	617	ILE	CA-C-N	6.89	126.85	120.03
3	B	617	ILE	C-N-CA	6.89	126.85	120.03
2	K	264	LEU	N-CA-C	6.88	120.21	110.23
3	F	692	ASN	CA-C-N	6.88	126.58	119.56
3	F	692	ASN	C-N-CA	6.88	126.58	119.56
1	M	458	ALA	CA-C-N	6.86	127.25	119.92
1	M	458	ALA	C-N-CA	6.86	127.25	119.92
3	E	788	VAL	N-CA-C	6.85	117.88	112.12
2	J	233	ASP	CA-C-N	6.83	128.38	119.84
2	J	233	ASP	C-N-CA	6.83	128.38	119.84
3	E	819	CYS	N-CA-C	-6.83	102.34	110.41
1	M	474	PHE	N-CA-C	6.83	120.92	112.59
3	D	794	THR	N-CA-C	-6.82	103.78	111.14
3	D	767	ALA	N-CA-C	6.78	118.47	111.14
3	D	689	THR	N-CA-C	6.78	121.35	109.96
3	C	790	PRO	N-CA-C	-6.77	100.62	111.38
2	P	259	GLU	N-CA-C	6.75	119.40	108.32
3	A	562	VAL	CB-CA-C	-6.72	103.37	111.97
3	D	556	LEU	CB-CA-C	-6.72	100.33	110.88
1	Q	458	ALA	CA-C-N	6.71	126.68	119.76
1	Q	458	ALA	C-N-CA	6.71	126.68	119.76
3	E	835	VAL	CA-C-N	-6.71	114.50	122.22
3	E	835	VAL	C-N-CA	-6.71	114.50	122.22
2	J	178	ILE	N-CA-C	6.70	118.59	108.80
3	A	647	THR	N-CA-C	6.70	120.45	109.06
3	F	715	MET	CG-SD-CE	-6.69	86.19	100.90
3	A	595	LEU	N-CA-C	6.68	120.17	110.28
2	N	281	ALA	N-CA-C	6.67	119.00	108.79
2	N	283	PHE	CA-CB-CG	-6.66	107.14	113.80
2	K	178	ILE	CB-CA-C	-6.66	100.43	110.55
2	O	196	LEU	N-CA-C	6.66	120.38	109.06
1	H	434	ASP	CA-C-N	6.65	126.34	119.82
1	H	434	ASP	C-N-CA	6.65	126.34	119.82
3	E	762	PHE	CA-CB-CG	-6.62	107.18	113.80
3	A	686	ILE	N-CA-C	6.62	117.88	108.42
3	F	682	GLU	CA-C-O	-6.61	113.39	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	195	ASP	N-CA-C	-6.58	101.22	110.50
3	F	533	ASN	CA-C-O	-6.58	113.75	122.44
3	B	831	HIS	N-CA-C	6.58	119.89	109.50
2	J	248	TYR	N-CA-C	-6.57	104.74	112.89
2	O	165	ASP	CA-CB-CG	-6.56	106.04	112.60
3	D	582	VAL	N-CA-C	6.55	118.22	108.46
3	C	781	CYS	CA-C-N	6.55	129.94	120.38
3	C	781	CYS	C-N-CA	6.55	129.94	120.38
3	F	560	ILE	N-CA-C	-6.54	103.95	110.62
3	D	532	GLN	N-CA-C	6.53	118.39	111.28
3	D	529	GLU	N-CA-C	6.50	118.27	109.24
3	D	753	ARG	N-CA-C	6.49	119.18	111.33
3	F	546	ARG	CA-C-N	6.48	127.94	119.84
3	F	546	ARG	C-N-CA	6.48	127.94	119.84
1	Q	408	LEU	CA-C-N	6.47	126.85	119.92
1	Q	408	LEU	C-N-CA	6.47	126.85	119.92
3	D	598	LEU	CA-C-N	6.46	126.81	119.83
3	D	598	LEU	C-N-CA	6.46	126.81	119.83
3	E	687	ASN	CA-CB-CG	-6.46	106.14	112.60
2	N	298	ALA	N-CA-C	6.46	118.11	111.14
3	E	630	PHE	N-CA-CB	6.46	119.37	110.01
3	B	738	VAL	N-CA-C	6.45	118.07	108.46
3	F	704	ARG	N-CA-C	-6.43	104.19	111.07
3	E	551	LEU	CB-CA-C	6.43	119.52	108.91
2	L	165	ASP	CA-CB-CG	-6.42	106.18	112.60
1	H	399	PRO	N-CA-C	6.42	118.53	110.70
2	O	244	ASP	CA-CB-CG	6.40	119.00	112.60
1	M	336	LEU	N-CA-C	-6.40	104.38	111.36
3	E	583	ARG	NE-CZ-NH2	6.40	124.96	119.20
2	J	285	LEU	N-CA-C	6.39	119.92	109.24
1	R	390	TYR	CA-C-N	6.39	126.84	120.52
1	R	390	TYR	C-N-CA	6.39	126.84	120.52
3	F	848	LYS	N-CA-C	6.39	119.50	110.50
1	G	408	LEU	CA-C-N	6.38	126.36	119.78
1	G	408	LEU	C-N-CA	6.38	126.36	119.78
1	M	332	ARG	N-CA-C	-6.36	99.66	109.14
3	E	659	PHE	CA-CB-CG	-6.36	107.44	113.80
3	A	769	ILE	N-CA-C	-6.36	106.34	111.81
3	A	791	ASP	CA-C-N	6.35	126.84	119.47
3	A	791	ASP	C-N-CA	6.35	126.84	119.47
1	I	399	PRO	N-CA-C	6.35	118.45	110.70
1	R	453	LEU	CB-CA-C	-6.35	107.20	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	669	ASP	CA-CB-CG	6.35	118.95	112.60
1	M	334	LYS	N-CA-C	-6.35	100.87	110.39
3	C	784	CYS	N-CA-C	-6.34	103.72	112.03
3	A	802	GLU	N-CA-C	6.33	118.71	111.11
3	F	571	ILE	CB-CA-C	-6.33	106.13	113.22
3	F	675	ILE	CB-CA-C	-6.33	102.23	110.84
3	C	831	HIS	CA-CB-CG	-6.33	107.47	113.80
3	C	533	ASN	N-CA-C	-6.32	106.53	114.56
3	E	692	ASN	CA-C-N	6.31	126.00	119.56
3	E	692	ASN	C-N-CA	6.31	126.00	119.56
3	D	607	VAL	N-CA-C	6.30	116.94	108.11
3	F	639	LYS	CA-C-N	6.30	125.92	119.56
3	F	639	LYS	C-N-CA	6.30	125.92	119.56
1	Q	426	ASN	N-CA-C	-6.30	106.56	114.56
3	E	689	THR	N-CA-C	6.28	119.18	109.07
1	I	406	LEU	CA-C-N	6.27	128.59	120.44
1	I	406	LEU	C-N-CA	6.27	128.59	120.44
3	D	576	LEU	CA-C-N	6.27	126.03	119.76
3	D	576	LEU	C-N-CA	6.27	126.03	119.76
1	H	401	ASP	CA-C-N	6.25	125.87	119.56
1	H	401	ASP	C-N-CA	6.25	125.87	119.56
1	M	408	LEU	CA-C-N	6.25	126.22	119.78
1	M	408	LEU	C-N-CA	6.25	126.22	119.78
3	C	654	LYS	CB-CA-C	-6.24	101.35	110.96
1	M	401	ASP	CA-C-N	6.24	126.70	119.47
1	M	401	ASP	C-N-CA	6.24	126.70	119.47
1	H	474	PHE	CA-CB-CG	-6.23	107.57	113.80
3	C	812	LYS	CA-C-N	-6.23	114.31	120.60
3	C	812	LYS	C-N-CA	-6.23	114.31	120.60
2	P	266	ASP	N-CA-C	6.23	117.73	108.76
2	K	285	LEU	N-CA-C	6.23	118.64	108.55
1	G	384	VAL	CB-CA-C	-6.22	103.63	112.22
3	D	529	GLU	CA-C-N	6.22	127.62	119.84
3	D	529	GLU	C-N-CA	6.22	127.62	119.84
3	B	538	ARG	N-CA-C	6.21	119.15	109.52
3	D	579	ASP	N-CA-C	6.21	117.32	108.74
3	B	682	GLU	CA-C-N	6.21	133.61	122.13
3	B	682	GLU	C-N-CA	6.21	133.61	122.13
3	B	765	SER	N-CA-C	-6.20	104.52	111.28
3	F	617	ILE	CB-CA-C	-6.20	105.18	110.94
2	N	262	VAL	CA-C-N	-6.19	114.98	122.90
2	N	262	VAL	C-N-CA	-6.19	114.98	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	625	PHE	N-CA-C	6.18	119.22	110.50
1	R	401	ASP	CA-C-N	6.18	127.57	119.84
1	R	401	ASP	C-N-CA	6.18	127.57	119.84
3	C	810	LEU	N-CA-C	6.18	118.89	110.55
3	E	789	LYS	CA-C-N	6.18	127.56	119.84
3	E	789	LYS	C-N-CA	6.18	127.56	119.84
1	H	375	LEU	N-CA-C	6.17	119.88	109.76
3	F	581	ARG	N-CA-C	6.17	118.54	108.55
1	G	401	ASP	CA-C-N	6.16	127.54	119.84
1	G	401	ASP	C-N-CA	6.16	127.54	119.84
3	C	710	ASP	CA-C-N	6.16	126.07	119.85
3	C	710	ASP	C-N-CA	6.16	126.07	119.85
3	C	831	HIS	N-CA-C	6.15	120.29	109.96
3	D	777	VAL	N-CA-C	-6.14	99.72	109.17
3	B	789	LYS	CA-C-N	6.12	126.09	120.03
3	B	789	LYS	C-N-CA	6.12	126.09	120.03
3	B	687	ASN	CA-C-N	6.11	129.39	120.71
3	B	687	ASN	C-N-CA	6.11	129.39	120.71
1	Q	434	ASP	CA-CB-CG	6.11	118.71	112.60
3	C	582	VAL	N-CA-C	6.09	116.64	108.11
2	P	231	VAL	N-CA-C	6.08	113.86	108.63
3	F	555	ALA	CA-C-N	-6.07	112.55	120.44
3	F	555	ALA	C-N-CA	-6.07	112.55	120.44
3	F	741	THR	N-CA-C	6.07	118.19	108.41
1	H	467	ILE	N-CA-C	-6.07	104.59	110.72
3	A	514	VAL	CB-CA-C	-6.06	103.85	112.22
3	C	857	ALA	CA-C-N	6.06	129.00	120.28
3	C	857	ALA	C-N-CA	6.06	129.00	120.28
3	B	565	ILE	CB-CA-C	-6.05	104.23	111.97
3	A	683	ILE	CA-C-N	6.04	126.23	120.31
3	A	683	ILE	C-N-CA	6.04	126.23	120.31
3	E	755	ASP	CA-CB-CG	6.04	118.64	112.60
3	D	831	HIS	N-CA-C	6.03	118.86	109.52
2	N	230	ILE	CB-CA-C	-6.02	105.42	111.80
3	E	647	THR	N-CA-C	6.02	118.56	109.23
3	D	791	ASP	CA-C-N	6.00	125.68	119.56
3	D	791	ASP	C-N-CA	6.00	125.68	119.56
2	N	195	ASP	N-CA-C	-6.00	102.79	110.53
3	E	777	VAL	N-CA-C	-6.00	100.99	109.63
1	G	434	ASP	CA-C-N	6.00	127.34	119.84
1	G	434	ASP	C-N-CA	6.00	127.34	119.84
3	F	683	ILE	N-CA-C	6.00	121.83	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	511	VAL	CB-CA-C	-5.99	104.31	111.97
3	F	551	LEU	CB-CA-C	5.99	118.18	109.20
2	K	224	LEU	N-CA-C	5.97	119.25	110.59
1	G	390	TYR	CA-C-N	5.96	125.94	120.03
1	G	390	TYR	C-N-CA	5.96	125.94	120.03
2	P	285	LEU	N-CA-C	5.96	118.13	108.41
3	D	533	ASN	N-CA-C	-5.95	107.00	114.56
3	D	871	TYR	CA-CB-CG	5.94	124.60	113.90
3	C	655	SER	N-CA-C	-5.94	105.52	112.89
2	O	287	LEU	CA-C-N	5.94	125.62	119.56
2	O	287	LEU	C-N-CA	5.94	125.62	119.56
3	B	639	LYS	CA-C-N	5.94	125.56	119.56
3	B	639	LYS	C-N-CA	5.94	125.56	119.56
3	A	551	LEU	O-C-N	-5.94	117.91	121.71
2	J	246	LEU	N-CA-C	5.93	117.54	111.14
3	B	711	PRO	CB-CA-C	-5.93	103.22	110.98
3	A	511	VAL	CB-CA-C	-5.92	104.14	112.14
3	F	777	VAL	N-CA-C	-5.92	99.73	108.85
1	I	386	THR	CA-C-N	5.92	128.14	120.44
1	I	386	THR	C-N-CA	5.92	128.14	120.44
3	D	819	CYS	N-CA-C	5.92	114.43	108.75
1	R	393	VAL	N-CA-C	5.92	116.16	108.35
3	D	760	GLU	CA-C-N	5.91	125.59	119.56
3	D	760	GLU	C-N-CA	5.91	125.59	119.56
3	D	777	VAL	CA-C-N	-5.91	113.34	122.09
3	D	777	VAL	C-N-CA	-5.91	113.34	122.09
3	F	573	GLU	N-CA-C	5.91	119.09	107.98
2	L	287	LEU	CA-C-N	5.91	125.58	119.56
2	L	287	LEU	C-N-CA	5.91	125.58	119.56
3	B	643	ILE	N-CA-C	5.91	116.99	108.48
2	O	251	VAL	CA-C-N	5.89	126.08	119.90
2	O	251	VAL	C-N-CA	5.89	126.08	119.90
3	A	582	VAL	CB-CA-C	-5.89	104.87	111.23
3	E	648	GLY	CA-C-N	5.89	126.22	119.92
3	E	648	GLY	C-N-CA	5.89	126.22	119.92
3	C	671	ASN	CB-CA-C	-5.88	100.94	110.77
3	E	760	GLU	CA-C-N	5.88	125.75	119.28
3	E	760	GLU	C-N-CA	5.88	125.75	119.28
3	F	529	GLU	CA-C-N	5.88	125.90	119.90
3	F	529	GLU	C-N-CA	5.88	125.90	119.90
3	A	576	LEU	CA-C-N	5.88	125.78	119.85
3	A	576	LEU	C-N-CA	5.88	125.78	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	710	ASP	CA-C-N	5.86	125.77	119.85
3	E	710	ASP	C-N-CA	5.86	125.77	119.85
1	R	401	ASP	CA-CB-CG	5.85	118.45	112.60
3	E	712	ASP	N-CA-C	-5.85	104.32	112.45
3	E	675	ILE	N-CA-CB	5.85	118.83	111.46
3	C	715	MET	N-CA-C	5.84	118.72	109.50
3	E	831	HIS	N-CA-C	5.84	118.41	108.02
3	C	875	GLN	N-CA-C	-5.83	106.51	113.97
3	D	820	GLY	O-C-N	-5.83	115.12	122.70
2	K	233	ASP	CA-C-N	5.81	126.21	119.47
2	K	233	ASP	C-N-CA	5.81	126.21	119.47
3	C	815	GLY	N-CA-C	-5.81	104.11	111.72
2	J	250	ALA	N-CA-C	5.81	117.96	108.55
3	C	836	VAL	N-CA-C	5.81	114.97	106.55
2	P	262	VAL	CA-C-N	-5.80	115.58	123.12
2	P	262	VAL	C-N-CA	-5.80	115.58	123.12
2	P	255	PHE	N-CA-C	5.79	117.81	108.32
3	C	526	ILE	N-CA-C	5.79	116.22	108.11
3	F	710	ASP	N-CA-C	5.79	122.60	109.81
3	C	683	ILE	CA-C-N	5.79	125.76	120.03
3	C	683	ILE	C-N-CA	5.79	125.76	120.03
3	B	741	THR	N-CA-C	5.78	118.82	109.40
3	F	662	LEU	CB-CA-C	-5.78	101.56	110.81
2	K	218	GLN	N-CA-C	5.78	117.58	111.28
2	J	211	LEU	CB-CA-C	-5.77	101.82	110.88
1	H	408	LEU	CA-C-N	5.77	125.75	120.21
1	H	408	LEU	C-N-CA	5.77	125.75	120.21
2	N	231	VAL	CA-C-N	5.77	125.67	119.85
2	N	231	VAL	C-N-CA	5.77	125.67	119.85
3	B	774	GLN	N-CA-C	5.75	117.52	108.96
3	C	532	GLN	N-CA-C	5.73	117.53	111.28
3	E	820	GLY	N-CA-C	-5.73	101.36	112.02
3	A	844	ILE	CB-CA-C	-5.73	104.64	111.97
3	A	617	ILE	CA-C-N	5.73	125.68	119.78
3	A	617	ILE	C-N-CA	5.73	125.68	119.78
2	L	244	ASP	N-CA-C	-5.72	104.65	111.69
3	E	633	PHE	CA-CB-CG	-5.72	108.08	113.80
2	O	230	ILE	N-CA-C	5.72	112.33	106.21
1	Q	391	PRO	N-CA-C	5.72	119.98	111.41
2	N	253	ILE	N-CA-C	5.71	116.23	107.77
1	R	398	ASP	CA-C-N	5.71	126.27	120.38
1	R	398	ASP	C-N-CA	5.71	126.27	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	200	ILE	CB-CA-C	-5.69	104.45	112.14
3	B	525	ASP	CA-CB-CG	-5.69	106.91	112.60
3	A	661	ILE	N-CA-C	-5.69	104.97	110.72
3	B	856	ILE	CB-CA-C	-5.69	104.69	111.97
3	E	554	GLY	N-CA-C	-5.68	105.80	113.24
3	F	617	ILE	N-CA-C	5.68	113.51	108.63
3	B	763	ASN	CA-C-O	-5.67	115.42	121.94
3	C	794	THR	N-CA-C	-5.67	105.00	111.07
3	A	607	VAL	N-CA-C	5.67	116.91	108.46
3	C	790	PRO	CB-CA-C	-5.67	103.56	110.98
3	F	556	LEU	N-CA-C	-5.66	105.01	111.07
3	B	630	PHE	CA-CB-CG	-5.66	108.14	113.80
3	B	692	ASN	CA-C-N	5.66	126.91	119.84
3	B	692	ASN	C-N-CA	5.66	126.91	119.84
1	I	401	ASP	CA-CB-CG	5.66	118.26	112.60
3	A	526	ILE	N-CA-C	5.66	116.00	107.80
3	D	831	HIS	CA-CB-CG	-5.66	108.14	113.80
3	E	617	ILE	CB-CA-C	-5.66	104.28	110.78
3	A	760	GLU	CA-C-N	5.65	125.32	119.56
3	A	760	GLU	C-N-CA	5.65	125.32	119.56
1	Q	461	VAL	CB-CA-C	-5.64	102.92	111.33
1	I	340	LEU	CB-CA-C	-5.64	101.09	110.68
3	B	829	ALA	CA-C-N	5.63	129.43	121.66
3	B	829	ALA	C-N-CA	5.63	129.43	121.66
3	A	546	ARG	CA-C-N	5.63	126.88	119.84
3	A	546	ARG	C-N-CA	5.63	126.88	119.84
1	I	333	ALA	CB-CA-C	-5.63	110.07	116.54
3	A	692	ASN	CA-C-N	5.62	125.30	119.56
3	A	692	ASN	C-N-CA	5.62	125.30	119.56
2	O	224	LEU	N-CA-C	5.62	118.40	110.14
2	J	264	LEU	N-CA-C	5.61	117.93	109.23
3	B	667	THR	CA-C-N	5.61	125.32	119.82
3	B	667	THR	C-N-CA	5.61	125.32	119.82
2	L	166	LEU	CA-C-N	5.61	132.26	121.54
2	L	166	LEU	C-N-CA	5.61	132.26	121.54
3	E	634	LYS	N-CA-C	-5.61	105.06	111.07
3	C	800	LEU	N-CA-C	5.61	117.94	110.53
2	N	266	ASP	CA-C-N	5.60	125.69	119.87
2	N	266	ASP	C-N-CA	5.60	125.69	119.87
1	Q	428	LEU	N-CA-C	5.60	118.56	108.48
3	C	767	ALA	N-CA-C	5.60	120.12	111.56
3	B	791	ASP	CA-C-N	5.59	125.27	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	791	ASP	C-N-CA	5.59	125.27	119.56
2	J	228	GLU	N-CA-C	-5.59	105.33	111.82
3	F	578	GLN	N-CA-C	5.58	117.66	109.24
1	R	408	LEU	CA-C-N	5.58	125.59	119.90
1	R	408	LEU	C-N-CA	5.58	125.59	119.90
3	D	819	CYS	O-C-N	-5.57	117.02	121.65
1	M	459	PRO	CB-CA-C	-5.57	103.93	111.12
3	A	538	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	H	434	ASP	CB-CA-C	-5.57	103.74	110.81
3	B	877	ILE	N-CA-C	-5.56	104.94	111.00
3	D	617	ILE	CA-C-N	5.56	125.76	120.31
3	D	617	ILE	C-N-CA	5.56	125.76	120.31
1	G	473	ARG	N-CA-C	5.56	119.23	112.23
1	I	428	LEU	N-CA-C	5.56	118.53	108.69
1	I	407	LEU	N-CA-C	5.56	117.02	111.07
3	C	704	ARG	N-CA-C	-5.56	105.22	111.28
3	B	712	ASP	N-CA-C	-5.55	105.63	112.90
3	A	662	LEU	CB-CA-C	-5.54	101.59	110.79
3	E	840	ILE	N-CA-C	-5.54	105.71	111.58
1	R	333	ALA	CB-CA-C	-5.54	110.21	116.63
3	E	525	ASP	N-CA-C	5.54	116.55	108.14
1	I	453	LEU	N-CA-C	5.53	117.92	109.95
3	F	863	LYS	N-CA-C	-5.53	101.86	110.10
3	B	650	THR	N-CA-C	-5.53	101.67	109.96
3	C	760	GLU	CA-C-N	5.52	125.19	119.56
3	C	760	GLU	C-N-CA	5.52	125.19	119.56
3	E	578	GLN	N-CA-C	5.52	117.57	109.24
3	F	598	LEU	CA-C-N	5.52	125.83	119.93
3	F	598	LEU	C-N-CA	5.52	125.83	119.93
3	C	611	LEU	CA-C-N	-5.51	113.04	120.82
3	C	611	LEU	C-N-CA	-5.51	113.04	120.82
2	P	250	ALA	N-CA-C	5.51	117.64	108.99
1	Q	431	LEU	CA-C-N	-5.51	112.09	121.85
1	Q	431	LEU	C-N-CA	-5.51	112.09	121.85
1	Q	394	ASP	CA-C-N	5.51	125.86	119.47
1	Q	394	ASP	C-N-CA	5.51	125.86	119.47
3	D	654	LYS	CA-CB-CG	5.50	125.11	114.10
3	E	589	ILE	N-CA-C	5.50	116.50	108.58
1	M	333	ALA	N-CA-C	5.50	117.45	108.76
3	A	714	ILE	CB-CA-C	-5.50	102.03	110.50
3	C	646	ILE	N-CA-C	5.50	116.65	108.46
1	Q	431	LEU	CA-C-O	-5.50	114.66	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	612	LYS	N-CA-C	-5.49	103.24	110.43
3	C	688	GLN	CA-CB-CG	-5.48	103.13	114.10
3	C	570	ASN	CA-C-N	5.48	127.47	120.56
3	C	570	ASN	C-N-CA	5.48	127.47	120.56
3	E	676	GLU	CA-C-N	-5.48	116.08	122.00
3	E	676	GLU	C-N-CA	-5.48	116.08	122.00
3	F	836	VAL	N-CA-C	5.48	114.50	106.55
3	C	654	LYS	N-CA-C	5.48	116.94	110.97
3	D	772	LEU	N-CA-CB	5.47	119.28	110.85
3	D	858	ARG	NE-CZ-NH2	5.47	124.12	119.20
3	D	617	ILE	N-CA-CB	-5.47	103.55	111.21
3	F	835	VAL	CA-C-N	-5.47	115.93	122.22
3	F	835	VAL	C-N-CA	-5.47	115.93	122.22
2	L	280	PRO	CB-CA-C	5.47	118.50	111.56
1	I	363	GLY	N-CA-C	-5.47	105.64	111.93
3	A	689	THR	N-CA-C	5.46	119.14	109.96
3	C	699	PHE	CA-CB-CG	5.46	119.27	113.80
3	C	589	ILE	CA-CB-CG2	5.46	119.78	110.50
3	A	791	ASP	N-CA-C	5.46	117.52	109.50
3	B	526	ILE	N-CA-CB	-5.45	103.89	111.41
3	A	594	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	I	418	VAL	N-CA-C	5.45	117.94	108.95
3	D	656	PHE	N-CA-C	-5.44	105.04	110.97
3	B	659	PHE	CA-CB-CG	-5.44	108.36	113.80
2	K	226	SER	N-CA-C	5.43	116.93	110.19
1	I	375	LEU	CA-C-N	-5.43	112.43	120.68
1	I	375	LEU	C-N-CA	-5.43	112.43	120.68
1	Q	437	ASN	CA-CB-CG	5.42	118.02	112.60
2	K	202	VAL	N-CA-C	-5.42	101.68	108.84
1	H	347	ARG	CA-C-N	5.42	125.76	119.47
1	H	347	ARG	C-N-CA	5.42	125.76	119.47
2	K	196	LEU	CB-CA-C	-5.42	100.72	109.72
3	F	534	ASP	CA-C-N	5.42	127.83	120.63
3	F	534	ASP	C-N-CA	5.42	127.83	120.63
3	F	666	ALA	CB-CA-C	-5.42	103.68	111.91
3	E	707	LEU	N-CA-C	-5.41	105.46	111.36
3	E	556	LEU	CB-CA-C	-5.41	102.39	110.88
3	A	883	VAL	CB-CA-C	-5.40	105.06	111.97
3	F	679	VAL	N-CA-C	5.40	116.66	109.37
3	E	665	ILE	N-CA-CB	-5.39	105.15	112.16
3	E	646	ILE	N-CA-CB	-5.38	104.92	110.95
3	B	771	VAL	N-CA-C	5.38	115.87	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	833	LEU	N-CA-C	5.38	117.86	108.76
3	D	525	ASP	N-CA-C	5.38	117.02	108.79
1	M	421	HIS	CB-CA-C	-5.37	108.70	116.54
2	L	259	GLU	N-CA-C	5.37	117.25	108.55
3	B	769	ILE	N-CA-C	-5.37	105.89	111.58
3	A	686	ILE	CB-CG1-CD1	-5.36	102.54	113.80
3	A	764	ILE	CB-CA-C	-5.36	105.11	111.97
3	D	646	ILE	N-CA-C	5.36	116.44	108.46
3	D	791	ASP	CA-CB-CG	-5.36	107.25	112.60
3	E	577	PRO	N-CA-C	5.36	119.61	111.15
3	E	714	ILE	N-CA-CB	5.35	118.42	111.83
2	N	233	ASP	CA-C-N	5.35	125.68	119.47
2	N	233	ASP	C-N-CA	5.35	125.68	119.47
3	D	815	GLY	CA-C-N	5.34	131.74	121.54
3	D	815	GLY	C-N-CA	5.34	131.74	121.54
1	M	419	PHE	CA-C-N	5.34	125.76	119.99
1	M	419	PHE	C-N-CA	5.34	125.76	119.99
3	A	527	HIS	N-CA-C	5.34	117.09	108.34
3	F	831	HIS	N-CA-C	5.34	119.71	107.48
1	I	421	HIS	CA-CB-CG	5.34	119.14	113.80
3	B	746	ASP	CA-CB-CG	5.34	117.94	112.60
3	D	661	ILE	CB-CA-C	-5.33	105.14	111.97
3	C	832	GLU	N-CA-C	5.33	117.18	108.55
3	D	739	ILE	CA-C-N	-5.33	112.42	121.85
3	D	739	ILE	C-N-CA	-5.33	112.42	121.85
3	D	721	ASP	CA-CB-CG	5.33	117.93	112.60
3	E	626	ALA	N-CA-C	-5.32	103.43	110.40
3	E	826	GLY	N-CA-C	-5.32	105.98	112.68
3	F	686	ILE	N-CA-C	-5.31	100.67	108.85
3	D	639	LYS	CA-C-N	5.31	126.48	119.84
3	D	639	LYS	C-N-CA	5.31	126.48	119.84
3	E	640	PRO	N-CA-C	5.31	121.51	113.81
1	G	419	PHE	CA-CB-CG	-5.31	108.49	113.80
3	C	816	CYS	N-CA-C	5.31	116.59	108.42
2	O	281	ALA	N-CA-C	5.30	117.13	109.07
3	D	625	PHE	CB-CA-C	-5.30	100.13	109.62
3	E	740	ALA	N-CA-C	5.30	117.13	109.07
3	A	584	TYR	CA-CB-CG	-5.30	104.37	113.90
3	A	617	ILE	N-CA-C	5.29	113.27	107.60
3	A	831	HIS	N-CA-C	5.29	117.70	108.76
2	O	228	GLU	N-CA-C	-5.29	106.60	113.16
3	B	649	PRO	CA-C-N	-5.29	113.55	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	649	PRO	C-N-CA	-5.29	113.55	120.95
3	D	626	ALA	CA-C-N	5.29	125.60	119.47
3	D	626	ALA	C-N-CA	5.29	125.60	119.47
3	E	743	HIS	N-CA-C	5.28	117.24	107.73
2	K	244	ASP	N-CA-C	-5.28	105.61	111.36
3	E	830	ILE	N-CA-C	-5.27	102.25	109.37
1	I	334	LYS	CA-C-N	5.27	125.03	119.76
1	I	334	LYS	C-N-CA	5.27	125.03	119.76
2	N	261	GLU	CA-C-N	-5.27	115.79	122.43
2	N	261	GLU	C-N-CA	-5.27	115.79	122.43
2	P	207	PRO	N-CA-C	-5.27	102.92	111.14
2	K	230	ILE	N-CA-C	5.27	111.85	106.21
3	D	535	VAL	CA-C-N	-5.27	113.06	122.07
3	D	535	VAL	C-N-CA	-5.27	113.06	122.07
2	K	212	TYR	CA-CB-CG	-5.27	104.42	113.90
3	B	647	THR	N-CA-C	5.27	117.39	109.23
1	R	376	ARG	CA-C-N	5.26	125.57	119.47
1	R	376	ARG	C-N-CA	5.26	125.57	119.47
1	I	461	VAL	N-CA-C	5.26	116.15	108.58
1	H	463	THR	N-CA-C	-5.25	102.52	110.24
3	D	722	SER	N-CA-C	-5.25	105.55	111.28
3	A	599	PRO	CB-CA-C	5.25	117.82	111.46
3	C	591	VAL	N-CA-C	5.25	116.22	108.45
3	A	786	VAL	N-CA-C	5.25	115.42	107.75
2	J	239	LEU	CA-C-N	5.25	128.22	120.82
2	J	239	LEU	C-N-CA	5.25	128.22	120.82
3	F	682	GLU	CA-C-N	5.24	131.83	122.13
3	F	682	GLU	C-N-CA	5.24	131.83	122.13
3	B	529	GLU	CA-C-N	5.24	125.22	120.03
3	B	529	GLU	C-N-CA	5.24	125.22	120.03
1	G	386	THR	CA-C-N	5.23	128.02	120.38
1	G	386	THR	C-N-CA	5.23	128.02	120.38
2	K	270	LYS	N-CA-C	5.23	119.14	112.34
1	R	434	ASP	CA-C-N	5.23	126.38	119.84
1	R	434	ASP	C-N-CA	5.23	126.38	119.84
3	F	828	TYR	CB-CA-C	-5.23	102.23	111.22
3	C	833	LEU	CB-CA-C	-5.23	103.12	111.17
3	D	560	ILE	CB-CA-C	-5.23	105.19	111.88
3	E	542	ASP	CA-CB-CG	-5.23	107.37	112.60
2	J	167	LYS	N-CA-C	5.22	117.02	110.91
2	O	285	LEU	N-CA-C	5.21	117.67	108.75
2	J	239	LEU	N-CA-C	-5.21	107.47	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	390	TYR	N-CA-C	-5.21	103.62	110.39
3	A	602	TYR	CA-CB-CG	5.21	123.27	113.90
3	C	617	ILE	CA-C-N	5.21	125.66	120.14
3	C	617	ILE	C-N-CA	5.21	125.66	120.14
3	D	836	VAL	N-CA-C	5.21	115.27	107.51
3	A	617	ILE	CB-CA-C	-5.20	105.20	111.18
3	A	609	ARG	N-CA-CB	5.20	117.61	109.97
3	D	715	MET	CG-SD-CE	-5.19	89.48	100.90
2	K	164	LYS	N-CA-C	5.19	118.07	109.46
3	C	783	HIS	CA-CB-CG	-5.19	108.61	113.80
2	N	178	ILE	N-CA-C	5.18	116.83	108.85
2	K	277	LEU	N-CA-C	5.18	117.53	108.52
1	H	426	ASN	N-CA-CB	5.18	117.78	110.90
1	Q	334	LYS	CA-C-N	5.18	126.31	119.84
1	Q	334	LYS	C-N-CA	5.18	126.31	119.84
3	C	607	VAL	N-CA-C	5.18	115.57	108.12
3	E	836	VAL	CB-CA-C	5.16	118.56	112.68
3	D	815	GLY	CA-C-O	-5.16	113.43	119.72
3	E	552	PRO	N-CA-C	5.16	121.97	112.33
3	D	565	ILE	CB-CA-C	-5.15	105.19	112.14
3	E	777	VAL	CA-C-N	-5.15	114.06	121.42
3	E	777	VAL	C-N-CA	-5.15	114.06	121.42
1	I	408	LEU	CA-C-N	5.14	125.05	119.85
1	I	408	LEU	C-N-CA	5.14	125.05	119.85
3	C	507	ALA	N-CA-C	5.13	121.74	110.80
3	D	545	LEU	CB-CA-C	-5.13	99.16	109.68
2	J	262	VAL	CA-C-N	-5.13	114.02	121.71
2	J	262	VAL	C-N-CA	-5.13	114.02	121.71
3	C	686	ILE	CB-CA-C	-5.13	103.02	110.81
3	C	887	THR	CB-CA-C	-5.13	104.76	112.09
1	M	426	ASN	N-CA-C	-5.12	108.29	114.75
1	G	384	VAL	N-CA-CB	5.12	118.26	110.58
1	Q	457	VAL	CB-CA-C	-5.11	104.23	111.38
3	B	651	GLY	N-CA-C	-5.11	108.07	115.27
2	K	193	THR	N-CA-C	-5.10	107.61	113.88
2	L	295	PHE	CB-CA-C	-5.10	102.65	110.81
3	C	870	LEU	N-CA-C	-5.10	105.72	111.28
3	E	625	PHE	N-CA-C	5.10	117.82	110.28
3	D	629	VAL	N-CA-C	-5.10	107.18	111.56
3	D	675	ILE	CB-CA-C	-5.10	103.53	110.77
2	J	279	ARG	CA-C-N	5.09	125.37	119.92
2	J	279	ARG	C-N-CA	5.09	125.37	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	280	PRO	N-CA-C	-5.09	103.45	111.34
2	N	244	ASP	CA-C-N	5.09	127.10	120.28
2	N	244	ASP	C-N-CA	5.09	127.10	120.28
2	J	266	ASP	CA-C-N	5.09	124.75	119.56
2	J	266	ASP	C-N-CA	5.09	124.75	119.56
3	F	545	LEU	N-CA-C	5.08	117.80	110.28
1	G	383	ALA	CA-C-N	-5.08	113.21	120.42
1	G	383	ALA	C-N-CA	-5.08	113.21	120.42
1	Q	444	VAL	N-CA-C	-5.07	105.45	110.62
3	B	675	ILE	CB-CA-C	-5.07	104.86	111.81
1	R	459	PRO	N-CA-C	5.07	118.31	111.22
2	K	266	ASP	CA-C-N	5.06	124.78	119.82
2	K	266	ASP	C-N-CA	5.06	124.78	119.82
3	D	515	ILE	N-CA-C	-5.06	104.77	111.09
2	L	269	HIS	CA-C-N	5.05	128.39	120.82
2	L	269	HIS	C-N-CA	5.05	128.39	120.82
1	H	448	LEU	N-CA-C	-5.04	105.86	111.36
3	A	538	ARG	N-CA-C	5.04	117.05	109.23
3	B	626	ALA	CA-C-N	5.04	125.06	119.32
3	B	626	ALA	C-N-CA	5.04	125.06	119.32
3	A	741	THR	N-CA-C	5.03	117.95	109.95
3	C	652	SER	N-CA-C	5.03	121.50	110.80
3	B	810	LEU	CA-C-N	-5.02	115.91	122.99
3	B	810	LEU	C-N-CA	-5.02	115.91	122.99
3	D	772	LEU	CB-CA-C	-5.02	100.67	109.71
3	E	595	LEU	N-CA-C	5.01	117.13	109.07
2	K	241	LEU	N-CA-C	-5.00	102.87	110.28
2	O	262	VAL	CA-C-N	-5.00	116.47	122.22
2	O	262	VAL	C-N-CA	-5.00	116.47	122.22
1	R	384	VAL	N-CA-C	-5.00	105.67	110.72
3	C	613	LYS	N-CA-C	-5.00	102.65	110.10

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	506	ALA	Mainchain,Peptide
3	C	684	PRO	Mainchain,Peptide
3	D	506	ALA	Mainchain,Peptide
3	D	815	GLY	Mainchain,Peptide
3	D	819	CYS	Mainchain,Peptide
3	D	820	GLY	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
3	E	587	GLY	Mainchain,Peptide
3	F	533	ASN	Mainchain,Peptide
3	F	682	GLU	Mainchain,Peptide
3	F	888	ILE	Mainchain,Peptide
1	M	455	TYR	Sidechain
2	P	212	TYR	Sidechain
1	Q	416	TYR	Sidechain

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	G	1144	0	1182	10	0
1	H	1144	0	1182	17	0
1	I	1144	0	1182	20	0
1	M	1144	0	1182	13	0
1	Q	1144	0	1182	23	0
1	R	1144	0	1182	14	0
2	J	1091	0	1117	22	0
2	K	1091	0	1117	28	0
2	L	1091	0	1117	22	0
2	N	1091	0	1117	10	0
2	O	1091	0	1117	31	0
2	P	1091	0	1117	19	0
3	A	2975	0	3080	55	0
3	B	2966	0	3066	43	0
3	C	2975	0	3080	69	0
3	D	2975	0	3080	54	0
3	E	2975	0	3080	41	0
3	F	2984	0	3084	43	0
All	All	31260	0	32264	526	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 8.

All (526) 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)
2:J:276:LEU:O	2:J:276:LEU:HD23	1.39	1.17
1:Q:393:VAL:O	1:Q:393:VAL:HG13	1.46	1.05
2:O:263:VAL:HG23	2:O:263:VAL:O	1.73	0.87
2:L:219:LYS:O	2:L:219:LYS:HG3	1.75	0.85
3:F:710:ASP:O	3:F:710:ASP:OD2	1.96	0.82
2:P:266:ASP:OD1	2:P:266:ASP:O	1.98	0.80
3:F:710:ASP:O	3:F:710:ASP:CG	2.22	0.80
2:K:190:GLN:HE21	2:K:190:GLN:C	1.88	0.79
2:O:276:LEU:C	2:O:276:LEU:HD23	2.09	0.78
3:E:662:LEU:HD12	3:E:662:LEU:O	1.83	0.78
2:P:291:TRP:HE3	2:P:291:TRP:HA	1.48	0.78
2:P:212:TYR:N	2:P:212:TYR:CD1	2.50	0.77
2:P:291:TRP:HA	2:P:291:TRP:CE3	2.19	0.77
2:J:276:LEU:HD23	2:J:276:LEU:C	2.10	0.77
3:D:697:LEU:HD23	3:D:697:LEU:C	2.09	0.77
2:O:248:TYR:HD1	2:O:248:TYR:O	1.67	0.77
2:L:291:TRP:HE3	2:L:291:TRP:HA	1.50	0.76
3:D:862:MET:HE3	3:D:862:MET:O	1.87	0.75
1:I:438:ILE:HD13	1:I:438:ILE:O	1.87	0.74
2:L:291:TRP:HA	2:L:291:TRP:CE3	2.22	0.73
3:D:720:ARG:O	3:D:720:ARG:HG2	1.88	0.73
2:L:291:TRP:CE3	2:L:291:TRP:CA	2.74	0.71
2:J:276:LEU:O	2:J:276:LEU:CD2	2.30	0.70
1:I:412:LEU:HD23	1:I:412:LEU:C	2.17	0.70
3:A:714:ILE:HG23	3:A:714:ILE:O	1.91	0.70
2:L:165:ASP:OD1	2:L:165:ASP:O	2.10	0.69
1:Q:412:LEU:C	1:Q:412:LEU:HD23	2.18	0.69
2:N:248:TYR:HD1	2:N:248:TYR:O	1.75	0.69
3:B:540:ARG:O	3:B:540:ARG:HG2	1.93	0.69
1:H:336:LEU:HD22	1:H:336:LEU:O	1.92	0.69
1:Q:366:GLU:H	1:Q:366:GLU:CD	1.98	0.69
3:C:790:PRO:O	3:C:790:PRO:CD	2.40	0.69
3:B:686:ILE:HG23	3:B:686:ILE:O	1.89	0.67
1:Q:392:TYR:HD1	1:Q:392:TYR:O	1.76	0.67
2:L:265:SER:OG	2:L:266:ASP:N	2.26	0.67
1:Q:330:LEU:HD22	1:Q:330:LEU:N	2.10	0.67
1:Q:392:TYR:O	1:Q:392:TYR:CD1	2.47	0.67
3:D:531:ARG:NH1	3:D:531:ARG:HG3	2.10	0.67
2:L:165:ASP:OD1	2:L:165:ASP:C	2.36	0.67
1:Q:412:LEU:HD23	1:Q:412:LEU:O	1.95	0.66
3:B:845:VAL:HG22	3:B:845:VAL:O	1.95	0.66
1:R:436:ARG:O	1:R:436:ARG:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:697:LEU:CD2	3:D:697:LEU:O	2.43	0.66
3:A:530:PRO:HB2	3:A:602:TYR:HB2	1.76	0.66
3:F:571:ILE:O	3:F:571:ILE:HG22	1.96	0.66
1:H:336:LEU:HD22	1:H:336:LEU:C	2.21	0.65
3:B:733:LEU:HB2	3:C:885:ALA:HB2	1.78	0.65
2:K:291:TRP:HA	2:K:291:TRP:CE3	2.31	0.65
2:O:276:LEU:HD23	2:O:276:LEU:O	1.97	0.65
2:P:291:TRP:CE3	2:P:291:TRP:CA	2.80	0.64
1:Q:366:GLU:OE1	1:Q:366:GLU:N	2.27	0.64
1:I:438:ILE:HD13	1:I:438:ILE:C	2.23	0.64
3:F:683:ILE:HG22	3:F:683:ILE:O	1.97	0.63
2:K:183:LEU:HD22	2:K:183:LEU:O	1.98	0.63
2:P:266:ASP:OD1	2:P:266:ASP:C	2.41	0.63
3:D:697:LEU:C	3:D:697:LEU:CD2	2.68	0.63
3:D:697:LEU:O	3:D:697:LEU:HD22	1.99	0.63
3:B:686:ILE:O	3:B:686:ILE:CG2	2.42	0.62
3:D:747:ALA:N	3:D:773:SER:OG	2.32	0.62
1:R:365:LEU:O	1:R:366:GLU:C	2.43	0.62
2:O:165:ASP:OD1	2:O:165:ASP:O	2.19	0.61
3:F:719:ILE:HG22	3:F:719:ILE:O	2.00	0.61
2:O:276:LEU:C	2:O:276:LEU:CD2	2.74	0.61
2:K:190:GLN:C	2:K:190:GLN:NE2	2.58	0.61
2:K:291:TRP:HA	2:K:291:TRP:HE3	1.65	0.61
2:O:165:ASP:OD1	2:O:165:ASP:C	2.40	0.60
3:F:576:LEU:C	3:F:576:LEU:HD12	2.26	0.60
3:C:733:LEU:HD23	3:C:733:LEU:C	2.25	0.60
3:D:594:ARG:HB3	3:D:609:ARG:HB3	1.82	0.60
2:N:178:ILE:HG13	2:N:178:ILE:O	2.01	0.59
2:O:248:TYR:O	2:O:248:TYR:CD1	2.53	0.59
3:C:779:ARG:O	3:C:825:LYS:N	2.36	0.59
3:E:872:LYS:HA	3:E:872:LYS:HE2	1.83	0.59
2:O:291:TRP:HA	2:O:291:TRP:CE3	2.37	0.59
3:A:706:PHE:CZ	3:A:714:ILE:HB	2.38	0.59
3:C:790:PRO:O	3:C:790:PRO:CG	2.51	0.59
2:K:183:LEU:HD22	2:K:183:LEU:C	2.28	0.59
3:F:682:GLU:O	3:F:682:GLU:HG3	2.03	0.59
3:B:763:ASN:O	3:B:765:SER:N	2.36	0.58
1:Q:393:VAL:O	1:Q:393:VAL:CG1	2.27	0.58
1:G:330:LEU:C	1:G:330:LEU:HD12	2.27	0.58
2:L:163:GLN:O	2:L:163:GLN:HG2	2.03	0.58
2:L:183:LEU:HD23	2:L:183:LEU:C	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:535:VAL:HB	3:D:551:LEU:HB2	1.85	0.58
2:J:276:LEU:C	2:J:276:LEU:CD2	2.76	0.58
3:C:774:GLN:HG3	3:C:774:GLN:O	2.03	0.58
3:C:525:ASP:OD1	3:C:525:ASP:C	2.45	0.58
3:D:825:LYS:O	3:D:825:LYS:HG2	2.03	0.58
2:O:299:TYR:CD2	2:O:299:TYR:OXT	2.57	0.57
2:O:183:LEU:C	2:O:183:LEU:HD23	2.28	0.57
2:L:291:TRP:CE3	2:L:291:TRP:N	2.72	0.57
2:L:178:ILE:HG22	2:L:206:LEU:HB2	1.87	0.57
3:C:613:LYS:O	3:C:614:ALA:C	2.46	0.57
3:F:595:LEU:N	3:F:595:LEU:HD12	2.20	0.57
3:D:862:MET:SD	3:D:862:MET:C	2.88	0.57
3:B:711:PRO:CD	3:B:711:PRO:O	2.53	0.57
2:O:263:VAL:O	2:O:263:VAL:CG2	2.49	0.56
1:Q:455:TYR:O	1:Q:456:GLU:C	2.48	0.56
3:C:564:LYS:NZ	3:C:573:GLU:O	2.38	0.56
3:E:662:LEU:HD12	3:E:662:LEU:C	2.26	0.56
2:L:299:TYR:CG	2:L:299:TYR:OXT	2.56	0.56
2:L:200:ILE:HG22	2:L:200:ILE:O	2.05	0.56
3:D:531:ARG:HG3	3:D:531:ARG:HH11	1.71	0.56
2:O:291:TRP:HA	2:O:291:TRP:HE3	1.69	0.55
2:O:268:ARG:O	2:O:269:HIS:C	2.49	0.55
3:B:706:PHE:CD1	3:B:706:PHE:N	2.73	0.55
3:C:744:THR:OG1	3:C:745:ASN:N	2.38	0.55
2:O:208:GLU:N	2:O:208:GLU:OE1	2.38	0.55
1:Q:392:TYR:CD1	1:Q:392:TYR:C	2.85	0.55
1:R:436:ARG:O	1:R:436:ARG:CG	2.54	0.55
3:D:864:THR:O	3:D:868:ASP:N	2.34	0.55
2:O:202:VAL:O	2:O:203:ARG:HB3	2.07	0.55
2:N:248:TYR:CD1	2:N:248:TYR:C	2.85	0.55
2:J:285:LEU:HD12	2:J:285:LEU:N	2.23	0.54
2:P:199:ARG:HD3	2:P:199:ARG:O	2.07	0.54
3:E:862:MET:O	3:E:862:MET:HG2	2.06	0.54
2:J:178:ILE:CG2	2:J:206:LEU:HD13	2.38	0.54
2:N:212:TYR:HD1	2:N:212:TYR:N	2.06	0.54
3:A:582:VAL:CG2	3:A:595:LEU:HB2	2.37	0.53
3:A:510:PHE:CD1	3:A:510:PHE:C	2.86	0.53
3:D:599:PRO:HA	3:D:604:GLU:HA	1.89	0.53
3:F:576:LEU:HD12	3:F:576:LEU:O	2.08	0.53
3:F:744:THR:HG22	3:F:746:ASP:H	1.74	0.53
1:H:475:TYR:CD2	1:H:475:TYR:O	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:564:LYS:NZ	3:D:573:GLU:O	2.41	0.53
1:I:336:LEU:O	1:I:336:LEU:HD22	2.09	0.53
1:H:408:LEU:C	1:H:408:LEU:HD23	2.34	0.53
2:L:202:VAL:O	2:L:203:ARG:HB2	2.08	0.52
2:O:248:TYR:CD1	2:O:248:TYR:C	2.87	0.52
3:D:619:GLU:O	3:D:621:GLU:N	2.42	0.52
1:H:462:ALA:O	1:H:463:THR:C	2.51	0.52
3:C:530:PRO:HB3	3:C:556:LEU:HD21	1.90	0.52
3:C:659:PHE:CD1	3:C:659:PHE:N	2.76	0.52
2:J:287:LEU:HD12	2:J:287:LEU:N	2.24	0.52
2:J:299:TYR:CD2	2:J:299:TYR:OXT	2.63	0.52
3:B:721:ASP:C	3:B:721:ASP:OD1	2.52	0.52
3:D:779:ARG:O	3:D:825:LYS:N	2.42	0.52
3:D:551:LEU:HB3	3:D:555:ALA:HB3	1.89	0.52
2:K:266:ASP:OD1	2:K:266:ASP:C	2.46	0.52
3:A:567:GLY:HA2	3:A:582:VAL:HA	1.91	0.52
3:F:789:LYS:HB3	3:F:790:PRO:HA	1.91	0.52
2:J:165:ASP:OD1	2:J:165:ASP:C	2.53	0.52
3:A:662:LEU:HD22	3:A:686:ILE:HD12	1.91	0.52
3:F:705:ALA:O	3:F:709:GLN:N	2.42	0.52
3:F:662:LEU:O	3:F:666:ALA:N	2.43	0.52
1:Q:412:LEU:C	1:Q:412:LEU:CD2	2.83	0.52
3:C:800:LEU:N	3:C:800:LEU:HD12	2.25	0.52
3:D:798:LEU:HD13	3:D:870:LEU:HD13	1.92	0.52
3:C:535:VAL:HB	3:C:551:LEU:HB2	1.93	0.51
3:B:522:ASP:OD1	3:B:612:LYS:NZ	2.44	0.51
3:C:654:LYS:O	3:C:658:THR:N	2.41	0.51
3:C:669:ASP:OD2	3:C:670:LYS:NZ	2.43	0.51
1:H:394:ASP:C	1:H:394:ASP:OD1	2.54	0.51
1:I:434:ASP:OD1	1:I:434:ASP:C	2.53	0.51
3:B:525:ASP:OD1	3:B:525:ASP:C	2.51	0.51
3:D:706:PHE:HD1	3:D:706:PHE:H	1.59	0.51
3:C:650:THR:O	3:C:651:GLY:C	2.53	0.51
3:B:721:ASP:OD1	3:B:721:ASP:O	2.28	0.51
3:E:671:ASN:ND2	3:E:709:GLN:O	2.44	0.51
3:C:551:LEU:N	3:C:551:LEU:HD12	2.26	0.50
3:E:715:MET:SD	3:E:715:MET:C	2.94	0.50
2:O:202:VAL:O	2:O:203:ARG:CB	2.59	0.50
3:C:651:GLY:O	3:C:653:GLY:N	2.44	0.50
1:G:419:PHE:C	1:G:419:PHE:CD1	2.89	0.50
1:Q:330:LEU:N	1:Q:330:LEU:CD2	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:828:TYR:CD2	3:A:828:TYR:C	2.90	0.50
3:C:534:ASP:OD1	3:C:534:ASP:N	2.41	0.50
3:C:746:ASP:OD2	3:C:854:LYS:NZ	2.42	0.50
2:N:212:TYR:N	2:N:212:TYR:CD1	2.78	0.50
2:P:295:PHE:O	2:P:299:TYR:N	2.45	0.50
3:A:511:VAL:CG2	3:A:559:VAL:HG13	2.42	0.50
2:K:202:VAL:O	2:K:203:ARG:CB	2.60	0.50
3:B:759:VAL:O	3:B:760:GLU:C	2.53	0.50
3:E:828:TYR:C	3:E:828:TYR:CD1	2.90	0.50
3:E:784:CYS:O	3:E:784:CYS:SG	2.67	0.50
1:I:390:TYR:CE2	1:I:435:PRO:HB2	2.47	0.50
1:M:376:ARG:H	1:M:376:ARG:HD3	1.76	0.50
3:A:817:GLU:H	3:A:817:GLU:CD	2.18	0.50
2:K:286:ALA:H	2:K:291:TRP:HE1	1.60	0.50
1:R:463:THR:HG23	1:R:463:THR:O	2.11	0.50
3:B:529:GLU:O	3:B:536:GLN:N	2.45	0.50
3:C:519:PHE:CD1	3:C:519:PHE:N	2.79	0.50
3:D:706:PHE:HD1	3:D:706:PHE:N	2.10	0.49
3:E:787:GLU:OE2	3:E:789:LYS:NZ	2.45	0.49
1:I:364:ARG:O	1:I:365:LEU:C	2.54	0.49
3:E:711:PRO:O	3:E:736:HIS:ND1	2.45	0.49
3:C:613:LYS:O	3:C:615:SER:N	2.46	0.49
2:N:248:TYR:HD1	2:N:248:TYR:C	2.19	0.49
1:I:394:ASP:OD1	1:I:394:ASP:C	2.55	0.49
3:F:862:MET:HG2	3:F:862:MET:O	2.12	0.49
2:P:196:LEU:CD2	2:P:270:LYS:H	2.26	0.49
3:C:790:PRO:O	3:C:790:PRO:HD2	2.12	0.49
1:I:432:MET:HG2	1:I:434:ASP:H	1.77	0.48
3:A:777:VAL:HB	3:A:828:TYR:CE1	2.48	0.48
3:C:675:ILE:HG13	3:C:706:PHE:CE2	2.48	0.48
3:B:733:LEU:O	3:C:886:ARG:NH1	2.45	0.48
3:C:530:PRO:HB3	3:C:556:LEU:CD2	2.43	0.48
3:E:669:ASP:OD2	3:E:670:LYS:NZ	2.43	0.48
3:C:671:ASN:HB2	3:F:545:LEU:HD22	1.94	0.48
3:F:594:ARG:HB3	3:F:609:ARG:HB3	1.95	0.48
2:P:287:LEU:N	2:P:287:LEU:HD12	2.28	0.48
3:C:710:ASP:CG	3:C:710:ASP:O	2.57	0.48
2:P:199:ARG:HD3	2:P:199:ARG:C	2.38	0.48
3:B:761:PRO:HB2	3:B:845:VAL:HA	1.94	0.48
2:K:206:LEU:HD21	2:K:211:LEU:HB2	1.95	0.48
1:Q:400:PRO:O	1:Q:401:ASP:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:800:LEU:CD1	3:A:870:LEU:HD21	2.44	0.48
3:F:778:ARG:HB3	3:F:824:TYR:HB3	1.95	0.48
3:F:625:PHE:CE1	3:F:833:LEU:HB2	2.49	0.48
1:R:366:GLU:OE1	1:R:366:GLU:N	2.45	0.48
1:H:404:ALA:HB1	1:H:420:PRO:HB2	1.96	0.48
2:O:248:TYR:HD1	2:O:248:TYR:C	2.21	0.48
3:A:529:GLU:O	3:A:536:GLN:N	2.47	0.48
3:D:551:LEU:N	3:D:551:LEU:HD12	2.29	0.48
3:E:560:ILE:HD12	3:E:606:ALA:HB3	1.96	0.48
2:K:291:TRP:CE3	2:K:291:TRP:CA	2.96	0.48
2:P:206:LEU:HD21	2:P:211:LEU:HB2	1.96	0.48
3:B:620:ILE:HB	3:B:633:PHE:CE1	2.49	0.48
3:B:662:LEU:O	3:B:663:LYS:C	2.55	0.48
3:C:733:LEU:HD23	3:C:733:LEU:O	2.14	0.47
3:E:552:PRO:O	3:E:554:GLY:N	2.47	0.47
1:I:412:LEU:HD23	1:I:412:LEU:O	2.13	0.47
1:R:432:MET:HG2	1:R:434:ASP:H	1.77	0.47
3:A:759:VAL:O	3:A:760:GLU:C	2.57	0.47
3:A:598:LEU:C	3:A:604:GLU:HG3	2.39	0.47
3:A:778:ARG:HB3	3:A:824:TYR:CB	2.44	0.47
3:E:705:ALA:O	3:E:709:GLN:N	2.47	0.47
2:P:177:TRP:HB3	2:P:210:ALA:HB1	1.97	0.47
3:E:625:PHE:N	3:E:625:PHE:CD1	2.82	0.47
3:F:828:TYR:CD1	3:F:828:TYR:C	2.84	0.47
2:J:283:PHE:CD1	2:J:283:PHE:N	2.83	0.47
1:H:369:LEU:HB3	1:H:375:LEU:HG	1.96	0.47
2:L:291:TRP:N	2:L:291:TRP:CD2	2.80	0.47
3:B:510:PHE:CD1	3:B:510:PHE:C	2.93	0.47
3:B:515:ILE:HG12	3:B:526:ILE:HD13	1.96	0.47
3:B:711:PRO:O	3:B:711:PRO:HD2	2.15	0.47
3:D:525:ASP:OD1	3:D:526:ILE:N	2.48	0.47
2:O:177:TRP:CG	2:O:210:ALA:HB1	2.50	0.47
2:J:230:ILE:O	2:J:230:ILE:HG22	2.14	0.47
3:B:592:ASP:OD2	3:B:613:LYS:NZ	2.48	0.47
3:B:845:VAL:HG21	3:C:794:THR:HA	1.97	0.47
3:A:535:VAL:HB	3:A:551:LEU:HG	1.97	0.47
2:J:275:GLN:O	2:J:276:LEU:CB	2.63	0.46
1:H:475:TYR:O	1:H:475:TYR:CG	2.68	0.46
3:E:525:ASP:OD1	3:E:525:ASP:C	2.56	0.46
3:E:872:LYS:HE2	3:E:872:LYS:CA	2.44	0.46
2:J:249:GLY:O	2:J:264:LEU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:286:ALA:HB3	2:O:291:TRP:CZ2	2.50	0.46
3:C:657:THR:O	3:C:657:THR:HG22	2.14	0.46
3:C:884:LEU:HD23	3:C:884:LEU:HA	1.30	0.46
3:D:862:MET:O	3:D:862:MET:CE	2.62	0.46
3:F:888:ILE:HG22	3:F:888:ILE:O	2.15	0.46
1:H:330:LEU:HB2	1:H:342:GLU:HG3	1.98	0.46
1:I:336:LEU:HD22	1:I:336:LEU:C	2.40	0.46
2:O:263:VAL:HB	2:O:291:TRP:CZ2	2.51	0.46
2:J:177:TRP:HB3	2:J:210:ALA:HB1	1.98	0.46
2:O:287:LEU:HD12	2:O:287:LEU:N	2.29	0.46
1:R:455:TYR:O	1:R:456:GLU:C	2.58	0.46
3:C:659:PHE:HD1	3:C:659:PHE:H	1.62	0.46
3:F:535:VAL:HG21	3:F:556:LEU:HG	1.96	0.46
2:O:266:ASP:OD1	2:O:266:ASP:C	2.59	0.46
2:N:202:VAL:O	2:N:203:ARG:HB2	2.15	0.46
3:E:703:LEU:HA	3:E:703:LEU:HD23	1.67	0.46
3:A:620:ILE:HB	3:A:633:PHE:CE1	2.50	0.46
3:F:715:MET:HB2	3:F:715:MET:HE3	1.67	0.46
2:O:291:TRP:CE3	2:O:291:TRP:CA	2.99	0.46
3:C:808:ALA:HB1	3:C:874:LEU:HD13	1.98	0.46
3:F:760:GLU:OE2	3:F:762:PHE:CD2	2.69	0.46
2:J:202:VAL:O	2:J:203:ARG:HB2	2.15	0.46
3:A:556:LEU:O	3:A:559:VAL:HB	2.15	0.46
3:A:710:ASP:N	3:A:711:PRO:CD	2.78	0.46
1:H:434:ASP:OD1	1:H:434:ASP:C	2.53	0.45
3:B:778:ARG:HB3	3:B:824:TYR:CB	2.46	0.45
3:C:674:THR:O	3:C:689:THR:N	2.48	0.45
2:K:215:LEU:HA	2:K:215:LEU:HD23	1.73	0.45
2:K:276:LEU:HD23	2:K:276:LEU:C	2.41	0.45
3:A:686:ILE:O	3:A:686:ILE:HG23	2.16	0.45
3:B:837:ASP:OD1	3:B:837:ASP:C	2.59	0.45
3:A:540:ARG:O	3:A:540:ARG:HG2	2.16	0.45
3:D:833:LEU:O	3:D:833:LEU:HG	2.16	0.45
3:F:598:LEU:HD12	3:F:599:PRO:HD2	1.98	0.45
1:G:434:ASP:C	1:G:434:ASP:OD1	2.58	0.45
1:M:444:VAL:O	1:M:445:ARG:C	2.59	0.45
3:A:626:ALA:O	3:A:627:PRO:C	2.60	0.45
3:C:540:ARG:O	3:C:540:ARG:HG2	2.17	0.45
1:G:330:LEU:HD12	1:G:330:LEU:O	2.15	0.45
2:O:198:GLY:N	2:O:266:ASP:OD2	2.50	0.45
3:A:610:LEU:N	3:A:610:LEU:HD12	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:206:LEU:HD21	2:J:211:LEU:HB2	1.99	0.45
1:Q:419:PHE:CG	1:Q:420:PRO:HD2	2.52	0.45
2:K:277:LEU:HA	2:K:277:LEU:HD23	1.77	0.45
1:Q:435:PRO:O	1:Q:436:ARG:C	2.59	0.45
3:A:773:SER:HB3	3:A:832:GLU:HB3	1.99	0.45
3:C:785:LYS:HB2	3:C:811:TYR:HB3	1.99	0.45
3:D:706:PHE:N	3:D:706:PHE:CD1	2.80	0.45
2:N:201:LEU:HB3	2:N:206:LEU:HD23	1.98	0.45
2:N:256:GLN:OE1	2:N:256:GLN:HA	2.17	0.45
3:A:535:VAL:O	3:A:550:THR:HA	2.16	0.45
3:A:800:LEU:N	3:A:800:LEU:HD12	2.32	0.45
3:F:673:GLN:HG2	3:F:706:PHE:CE2	2.52	0.45
1:I:430:LEU:O	1:I:459:PRO:HA	2.17	0.45
1:M:376:ARG:HD3	1:M:376:ARG:N	2.32	0.45
1:M:404:ALA:HB1	1:M:420:PRO:HB2	1.99	0.45
2:O:178:ILE:HG22	2:O:206:LEU:HB2	1.98	0.45
3:B:721:ASP:O	3:B:724:THR:OG1	2.35	0.45
3:C:810:LEU:HD23	3:C:810:LEU:HA	1.62	0.45
3:E:741:THR:O	3:E:741:THR:HG22	2.17	0.45
3:A:686:ILE:HD13	3:A:686:ILE:HG21	1.45	0.44
3:B:662:LEU:HD23	3:B:662:LEU:HA	1.68	0.44
3:F:671:ASN:OD1	3:F:671:ASN:C	2.56	0.44
2:K:177:TRP:HB3	2:K:210:ALA:HB1	1.99	0.44
1:H:330:LEU:HB3	1:H:331:PRO:HA	1.99	0.44
1:M:397:GLU:O	1:M:398:ASP:C	2.59	0.44
1:R:400:PRO:O	1:R:401:ASP:C	2.60	0.44
3:A:510:PHE:CE1	3:A:551:LEU:HD23	2.52	0.44
3:A:681:TYR:O	3:A:688:GLN:NE2	2.50	0.44
3:B:711:PRO:O	3:B:711:PRO:CG	2.65	0.44
3:C:519:PHE:N	3:C:519:PHE:HD1	2.15	0.44
3:C:560:ILE:HD13	3:C:604:GLU:HB2	2.00	0.44
3:D:620:ILE:H	3:D:660:SER:HG	1.65	0.44
3:F:837:ASP:C	3:F:837:ASP:OD1	2.60	0.44
2:L:262:VAL:HG11	2:L:276:LEU:HB3	2.00	0.44
3:B:529:GLU:OE2	3:E:687:ASN:N	2.50	0.44
3:D:701:ARG:HD2	3:D:701:ARG:N	2.32	0.44
2:L:183:LEU:HD23	2:L:183:LEU:O	2.18	0.44
1:H:432:MET:HG2	1:H:434:ASP:H	1.83	0.44
3:C:800:LEU:N	3:C:800:LEU:CD1	2.81	0.44
1:I:412:LEU:C	1:I:412:LEU:CD2	2.88	0.44
3:D:791:ASP:OD1	3:D:791:ASP:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:794:THR:O	3:E:794:THR:HG22	2.16	0.44
3:E:871:TYR:N	3:E:871:TYR:CD1	2.85	0.44
2:K:298:ALA:O	2:K:299:TYR:CB	2.66	0.44
1:M:470:LEU:HD12	1:M:470:LEU:HA	1.80	0.44
3:A:519:PHE:CE1	3:A:610:LEU:HG	2.53	0.44
3:A:530:PRO:CB	3:A:602:TYR:HB2	2.46	0.44
3:C:515:ILE:HG12	3:C:526:ILE:HD13	2.00	0.44
1:G:461:VAL:O	1:G:461:VAL:HG13	2.17	0.44
2:K:259:GLU:HG2	2:K:259:GLU:O	2.16	0.44
1:M:336:LEU:O	1:M:337:GLY:C	2.60	0.44
3:A:837:ASP:C	3:A:837:ASP:OD1	2.60	0.44
3:D:669:ASP:OD1	3:D:670:LYS:NZ	2.50	0.44
3:A:535:VAL:N	3:A:551:LEU:O	2.50	0.43
3:C:519:PHE:CD2	3:C:589:ILE:HG23	2.53	0.43
3:C:545:LEU:HA	3:C:545:LEU:HD23	1.76	0.43
3:C:858:ARG:HD2	3:C:867:GLU:HB2	2.00	0.43
1:G:400:PRO:O	1:G:401:ASP:C	2.58	0.43
2:J:201:LEU:HB3	2:J:206:LEU:CD2	2.48	0.43
2:K:215:LEU:HD22	2:K:267:PRO:HD2	1.99	0.43
3:B:573:GLU:O	3:B:573:GLU:HG3	2.18	0.43
1:H:419:PHE:CD1	1:H:420:PRO:HD2	2.53	0.43
3:C:629:VAL:O	3:C:633:PHE:N	2.50	0.43
3:C:801:SER:O	3:C:803:ALA:N	2.51	0.43
3:E:525:ASP:OD1	3:E:540:ARG:HB2	2.18	0.43
2:K:287:LEU:N	2:K:287:LEU:HD12	2.34	0.43
3:A:511:VAL:HG21	3:A:559:VAL:HG13	2.01	0.43
3:B:706:PHE:N	3:B:706:PHE:HD1	2.16	0.43
3:D:514:VAL:HG21	3:D:537:VAL:HG12	2.01	0.43
2:K:268:ARG:O	2:K:268:ARG:HG2	2.18	0.43
2:P:212:TYR:OH	2:P:288:PRO:HD3	2.17	0.43
1:R:388:LEU:HB2	1:R:390:TYR:CE2	2.53	0.43
3:B:633:PHE:CD1	3:B:633:PHE:C	2.96	0.43
3:C:686:ILE:HG21	3:C:686:ILE:HD13	1.72	0.43
3:C:784:CYS:O	3:C:784:CYS:SG	2.75	0.43
1:H:424:GLU:HB2	1:H:427:ARG:HB2	2.00	0.43
2:O:183:LEU:HD23	2:O:183:LEU:O	2.18	0.43
1:Q:404:ALA:HB1	1:Q:420:PRO:HB2	2.00	0.43
3:C:676:GLU:OE2	3:C:688:GLN:NE2	2.52	0.43
3:C:706:PHE:HD1	3:C:706:PHE:HA	1.47	0.43
3:E:530:PRO:HB3	3:E:556:LEU:HD22	2.01	0.43
3:F:662:LEU:HB2	3:F:715:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:400:PRO:O	1:M:401:ASP:C	2.60	0.43
1:M:455:TYR:CZ	1:M:457:VAL:HB	2.54	0.43
2:P:279:ARG:HB2	2:P:280:PRO:HD2	2.01	0.43
2:P:279:ARG:O	2:P:281:ALA:N	2.51	0.43
3:D:720:ARG:O	3:D:720:ARG:CG	2.58	0.43
3:F:584:TYR:CD2	3:F:584:TYR:C	2.94	0.43
3:F:776:LEU:O	3:F:886:ARG:NE	2.52	0.43
1:I:455:TYR:O	1:I:456:GLU:C	2.61	0.43
3:A:559:VAL:HG12	3:A:606:ALA:CB	2.49	0.43
3:C:880:LEU:HA	3:C:880:LEU:HD12	1.70	0.43
3:D:778:ARG:HB3	3:D:824:TYR:HB3	2.01	0.43
2:K:212:TYR:CD2	2:K:212:TYR:N	2.86	0.43
3:A:551:LEU:C	3:A:551:LEU:HD12	2.44	0.43
3:B:778:ARG:HB3	3:B:824:TYR:CG	2.53	0.43
3:C:790:PRO:O	3:C:790:PRO:HG2	2.18	0.43
3:D:623:LEU:O	3:D:831:HIS:NE2	2.52	0.43
2:J:286:ALA:HB3	2:J:291:TRP:CZ2	2.54	0.42
1:I:387:GLN:HE22	1:I:436:ARG:HG2	1.83	0.42
1:Q:454:ASN:O	1:Q:455:TYR:HB3	2.18	0.42
3:E:582:VAL:O	3:E:582:VAL:HG13	2.17	0.42
2:J:201:LEU:HB3	2:J:206:LEU:HD23	2.01	0.42
2:N:283:PHE:CD1	2:N:283:PHE:N	2.86	0.42
1:Q:470:LEU:HD12	1:Q:470:LEU:HA	1.76	0.42
1:R:365:LEU:O	1:R:368:THR:N	2.52	0.42
3:A:582:VAL:HB	3:A:593:LEU:HB2	2.00	0.42
3:B:733:LEU:HD13	3:C:881:GLU:O	2.20	0.42
3:F:644:PHE:CD1	3:F:644:PHE:C	2.97	0.42
2:K:256:GLN:N	2:K:256:GLN:OE1	2.52	0.42
3:D:707:LEU:C	3:D:707:LEU:HD23	2.43	0.42
3:E:699:PHE:N	3:E:699:PHE:CD1	2.87	0.42
1:G:394:ASP:HA	1:G:395:PRO:HD3	1.88	0.42
2:J:200:ILE:O	2:J:200:ILE:HG22	2.15	0.42
3:A:582:VAL:O	3:A:584:TYR:N	2.52	0.42
3:A:845:VAL:H	3:A:845:VAL:HG22	1.55	0.42
3:D:625:PHE:HB3	3:D:629:VAL:HB	2.00	0.42
3:E:753:ARG:O	3:E:754:LEU:C	2.60	0.42
3:F:675:ILE:HD13	3:F:675:ILE:HG21	1.80	0.42
3:F:714:ILE:HD12	3:F:731:ALA:HB1	2.00	0.42
3:C:886:ARG:N	3:C:886:ARG:HD2	2.34	0.42
3:E:781:CYS:HB2	3:E:784:CYS:SG	2.60	0.42
2:K:178:ILE:HG23	2:K:206:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:345:LEU:HB3	1:I:379:ALA:HB2	2.00	0.42
1:I:434:ASP:OD1	1:I:434:ASP:O	2.37	0.42
1:M:408:LEU:HB3	1:M:420:PRO:HG3	2.00	0.42
1:M:436:ARG:O	1:M:436:ARG:HG2	2.19	0.42
1:Q:424:GLU:HB2	1:Q:427:ARG:HB2	2.01	0.42
3:A:733:LEU:HB3	3:D:885:ALA:HA	2.01	0.42
3:C:863:LYS:HD2	3:C:863:LYS:N	2.33	0.42
3:D:633:PHE:CD2	3:D:633:PHE:C	2.98	0.42
3:E:516:ARG:HA	3:E:589:ILE:HD13	2.00	0.42
1:Q:475:TYR:CG	1:Q:475:TYR:O	2.71	0.42
3:A:626:ALA:O	3:A:629:VAL:N	2.53	0.42
3:B:535:VAL:O	3:B:550:THR:HA	2.20	0.42
3:D:870:LEU:HD22	3:D:880:LEU:CD1	2.50	0.42
1:R:396:GLU:OE2	1:R:469:LYS:NZ	2.48	0.42
3:B:643:ILE:HD13	3:B:643:ILE:HG21	1.84	0.42
3:C:870:LEU:O	3:C:874:LEU:HG	2.20	0.42
3:E:532:GLN:N	3:E:532:GLN:CD	2.77	0.42
3:A:529:GLU:CD	3:A:538:ARG:HH22	2.28	0.42
3:B:779:ARG:O	3:B:825:LYS:N	2.53	0.42
3:E:882:GLU:O	3:E:886:ARG:HG2	2.20	0.42
2:O:216:ALA:HA	2:O:221:LEU:HB2	2.01	0.42
3:A:612:LYS:O	3:A:682:GLU:N	2.53	0.42
3:C:776:LEU:O	3:C:886:ARG:NE	2.51	0.42
3:E:542:ASP:OD2	3:E:825:LYS:HD2	2.20	0.42
1:Q:419:PHE:CD1	1:Q:420:PRO:HD2	2.55	0.41
3:C:808:ALA:HB1	3:C:874:LEU:HD22	2.02	0.41
3:D:659:PHE:N	3:D:659:PHE:CD1	2.86	0.41
3:E:594:ARG:HB2	3:E:611:LEU:HD21	2.02	0.41
3:A:757:MET:HB3	3:A:757:MET:HE2	1.79	0.41
3:C:676:GLU:HB2	3:C:679:VAL:HA	2.01	0.41
3:C:810:LEU:HD21	3:C:880:LEU:HB2	2.02	0.41
3:D:563:VAL:O	3:D:566:MET:HG2	2.20	0.41
3:D:715:MET:HB2	3:D:715:MET:HE2	1.87	0.41
3:D:832:GLU:HB2	3:D:865:LEU:N	2.35	0.41
3:F:545:LEU:N	3:F:545:LEU:HD12	2.34	0.41
2:K:255:PHE:CD1	2:K:255:PHE:O	2.74	0.41
2:O:275:GLN:O	2:O:276:LEU:CB	2.69	0.41
1:Q:336:LEU:N	1:Q:336:LEU:CD2	2.82	0.41
3:B:845:VAL:O	3:B:845:VAL:CG2	2.64	0.41
3:F:788:VAL:O	3:F:788:VAL:HG23	2.16	0.41
2:L:178:ILE:CG2	2:L:206:LEU:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:785:LYS:HB2	3:D:811:TYR:HB3	2.01	0.41
1:R:419:PHE:CD2	1:R:419:PHE:C	2.99	0.41
3:C:810:LEU:HD11	3:C:880:LEU:HB2	2.02	0.41
3:D:646:ILE:HB	3:D:658:THR:CG2	2.51	0.41
3:D:745:ASN:O	3:D:775:ARG:NH1	2.51	0.41
3:F:533:ASN:HA	3:F:534:ASP:HA	1.93	0.41
3:A:530:PRO:HA	3:A:535:VAL:HA	2.01	0.41
3:F:746:ASP:O	3:F:749:GLN:N	2.53	0.41
2:K:183:LEU:C	2:K:183:LEU:HD13	2.46	0.41
2:P:178:ILE:HD13	2:P:178:ILE:HG21	1.88	0.41
3:D:529:GLU:O	3:D:535:VAL:HA	2.21	0.41
3:D:864:THR:O	3:D:865:LEU:C	2.54	0.41
3:F:611:LEU:HB3	3:F:680:GLU:HB3	2.02	0.41
2:K:206:LEU:HA	2:K:207:PRO:HD2	1.96	0.41
1:H:463:THR:O	1:H:464:GLU:C	2.63	0.41
2:P:201:LEU:O	2:P:206:LEU:HB3	2.20	0.41
3:A:560:ILE:HD13	3:A:560:ILE:HA	1.65	0.41
3:B:535:VAL:HB	3:B:551:LEU:HB2	2.03	0.41
3:E:611:LEU:HB3	3:E:680:GLU:HA	2.02	0.41
1:G:332:ARG:O	1:G:333:ALA:HB3	2.21	0.41
2:L:178:ILE:HG21	2:L:178:ILE:HD13	1.78	0.41
2:L:202:VAL:O	2:L:203:ARG:CB	2.69	0.41
1:I:438:ILE:C	1:I:438:ILE:CD1	2.91	0.41
1:R:366:GLU:HA	1:R:369:LEU:HD12	2.03	0.41
3:A:560:ILE:HG13	3:A:604:GLU:HB3	2.02	0.41
3:A:601:VAL:O	3:A:601:VAL:HG22	2.20	0.41
3:A:662:LEU:HA	3:A:662:LEU:HD23	1.85	0.41
3:B:515:ILE:HA	3:B:526:ILE:CD1	2.51	0.41
3:C:684:PRO:HA	3:C:685:GLY:HA2	1.93	0.41
3:C:795:LEU:HA	3:C:795:LEU:HD23	1.80	0.41
3:D:687:ASN:OD1	3:D:688:GLN:N	2.54	0.41
3:E:699:PHE:H	3:E:699:PHE:HD1	1.68	0.41
3:E:760:GLU:OE2	3:E:762:PHE:CD2	2.74	0.41
3:F:783:HIS:HB2	3:F:816:CYS:HB2	2.02	0.41
1:I:430:LEU:O	1:I:431:LEU:C	2.59	0.41
1:M:455:TYR:O	1:M:456:GLU:CB	2.68	0.41
3:A:538:ARG:HE	3:A:538:ARG:HB2	1.45	0.41
3:A:800:LEU:HD11	3:A:870:LEU:HD21	2.03	0.41
3:D:884:LEU:HA	3:D:884:LEU:HD23	1.58	0.41
3:E:540:ARG:O	3:E:540:ARG:HG2	2.19	0.41
1:I:399:PRO:HA	1:I:400:PRO:HD2	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:706:PHE:CZ	3:A:711:PRO:CG	3.04	0.40
3:C:780:VAL:N	3:C:877:ILE:O	2.53	0.40
3:D:531:ARG:HH11	3:D:531:ARG:CG	2.29	0.40
3:D:775:ARG:CD	3:D:886:ARG:HB3	2.51	0.40
3:E:662:LEU:O	3:E:666:ALA:N	2.54	0.40
3:E:692:ASN:OD1	3:E:692:ASN:C	2.64	0.40
3:F:617:ILE:HD13	3:F:617:ILE:HG21	1.83	0.40
1:G:384:VAL:O	1:G:384:VAL:HG12	2.18	0.40
2:K:286:ALA:HB3	2:K:291:TRP:CZ2	2.56	0.40
2:L:219:LYS:O	2:L:219:LYS:CG	2.48	0.40
1:M:388:LEU:HB3	1:M:390:TYR:CD2	2.56	0.40
2:P:291:TRP:CE3	2:P:291:TRP:N	2.90	0.40
3:A:545:LEU:HD23	3:A:545:LEU:HA	1.86	0.40
3:A:772:LEU:HD11	3:A:831:HIS:HD1	1.86	0.40
3:B:529:GLU:OE1	3:B:605:LYS:NZ	2.54	0.40
3:B:804:GLU:O	3:B:808:ALA:N	2.54	0.40
3:C:657:THR:O	3:C:657:THR:CG2	2.69	0.40
3:E:535:VAL:HG21	3:E:556:LEU:HB2	2.03	0.40
3:F:555:ALA:O	3:F:556:LEU:C	2.58	0.40
2:L:248:TYR:C	2:L:248:TYR:CD1	2.97	0.40
2:O:241:LEU:O	2:O:242:ARG:C	2.64	0.40
1:R:395:PRO:HB3	1:R:431:LEU:HD23	2.03	0.40
3:C:863:LYS:HB3	3:C:868:ASP:HB2	2.02	0.40
3:E:570:ASN:O	3:E:572:ALA:N	2.54	0.40
3:C:643:ILE:HG21	3:C:643:ILE:HD13	1.86	0.40
1:G:394:ASP:OD2	2:J:175:LYS:NZ	2.54	0.40
2:J:275:GLN:O	2:J:276:LEU:HB3	2.21	0.40
2:K:197:LEU:HB3	2:K:266:ASP:OD2	2.22	0.40
1:H:408:LEU:C	1:H:408:LEU:CD2	2.95	0.40
3:B:683:ILE:O	3:B:686:ILE:HG22	2.22	0.40
3:D:703:LEU:HD23	3:D:703:LEU:HA	1.89	0.40
3:F:519:PHE:CZ	3:F:610:LEU:HG	2.56	0.40
3:F:715:MET:CE	3:F:739:ILE:HB	2.51	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	G	144/146 (99%)	135 (94%)	8 (6%)	1 (1%)	18	56
1	H	144/146 (99%)	132 (92%)	8 (6%)	4 (3%)	4	24
1	I	144/146 (99%)	131 (91%)	12 (8%)	1 (1%)	18	56
1	M	144/146 (99%)	132 (92%)	9 (6%)	3 (2%)	5	30
1	Q	144/146 (99%)	130 (90%)	8 (6%)	6 (4%)	2	17
1	R	144/146 (99%)	126 (88%)	13 (9%)	5 (4%)	3	20
2	J	135/137 (98%)	124 (92%)	9 (7%)	2 (2%)	8	40
2	K	135/137 (98%)	123 (91%)	9 (7%)	3 (2%)	5	29
2	L	135/137 (98%)	118 (87%)	15 (11%)	2 (2%)	8	40
2	N	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
2	O	135/137 (98%)	124 (92%)	8 (6%)	3 (2%)	5	29
2	P	135/137 (98%)	122 (90%)	11 (8%)	2 (2%)	8	40
3	A	382/409 (93%)	365 (96%)	16 (4%)	1 (0%)	36	72
3	B	381/409 (93%)	363 (95%)	16 (4%)	2 (0%)	24	63
3	C	382/409 (93%)	363 (95%)	15 (4%)	4 (1%)	12	49
3	D	382/409 (93%)	361 (94%)	17 (4%)	4 (1%)	12	49
3	E	382/409 (93%)	363 (95%)	16 (4%)	3 (1%)	16	54
3	F	383/409 (94%)	362 (94%)	15 (4%)	6 (2%)	7	38
All	All	3966/4152 (96%)	3700 (93%)	214 (5%)	52 (1%)	12	42

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	456	GLU
2	K	203	ARG
1	H	399	PRO
1	H	422	ARG

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Mol	Chain	Res	Type
1	H	455	TYR
1	H	456	GLU
1	M	456	GLU
2	O	167	LYS
2	O	269	HIS
2	P	269	HIS
1	Q	393	VAL
1	R	366	GLU
3	B	683	ILE
3	B	764	ILE
3	C	614	ALA
3	C	652	SER
3	C	802	GLU
3	D	507	ALA
3	D	620	ILE
3	D	654	LYS
3	E	553	LYS
3	E	571	ILE
3	E	790	PRO
3	F	547	PRO
3	F	572	ALA
2	K	255	PHE
1	M	337	GLY
2	P	280	PRO
1	Q	336	LEU
1	R	399	PRO
2	J	276	LEU
2	L	167	LYS
2	L	239	LEU
1	Q	436	ARG
1	R	361	GLY
1	R	365	LEU
2	J	258	GLY
2	K	167	LYS
3	C	507	ALA
3	F	789	LYS
1	I	455	TYR
1	M	455	TYR
2	O	203	ARG
1	Q	333	ALA
1	Q	455	TYR
3	F	683	ILE

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Mol	Chain	Res	Type
3	F	710	ASP
1	R	401	ASP
3	A	627	PRO
3	F	807	GLY
3	D	653	GLY
1	Q	452	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	120/120 (100%)	120 (100%)	0	100	100
1	H	120/120 (100%)	119 (99%)	1 (1%)	73	80
1	I	120/120 (100%)	118 (98%)	2 (2%)	53	69
1	M	120/120 (100%)	119 (99%)	1 (1%)	73	80
1	Q	120/120 (100%)	120 (100%)	0	100	100
1	R	120/120 (100%)	120 (100%)	0	100	100
2	J	112/112 (100%)	112 (100%)	0	100	100
2	K	112/112 (100%)	110 (98%)	2 (2%)	51	68
2	L	112/112 (100%)	112 (100%)	0	100	100
2	N	112/112 (100%)	112 (100%)	0	100	100
2	O	112/112 (100%)	111 (99%)	1 (1%)	70	79
2	P	112/112 (100%)	112 (100%)	0	100	100
3	A	317/336 (94%)	316 (100%)	1 (0%)	86	86
3	B	315/336 (94%)	315 (100%)	0	100	100
3	C	317/336 (94%)	316 (100%)	1 (0%)	86	86
3	D	317/336 (94%)	316 (100%)	1 (0%)	86	86
3	E	317/336 (94%)	317 (100%)	0	100	100
3	F	318/336 (95%)	318 (100%)	0	100	100
All	All	3293/3408 (97%)	3283 (100%)	10 (0%)	84	86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	190	GLN
2	K	256	GLN
1	H	336	LEU
1	I	336	LEU
1	I	438	ILE
1	M	380	LEU
2	O	248	TYR
3	A	879	THR
3	C	519	PHE
3	D	551	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	454	ASN
2	J	256	GLN
2	J	257	ASN
2	J	269	HIS
2	L	275	GLN
1	H	371	GLN
1	H	454	ASN
2	O	275	GLN
2	P	174	GLN
2	P	275	GLN
3	A	536	GLN
3	A	745	ASN
3	B	527	HIS
3	B	694	GLN
3	C	745	ASN
3	D	532	GLN
3	D	690	GLN
3	D	745	ASN
3	D	783	HIS
3	E	875	GLN

5.3.3 RNA ⓘ

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.

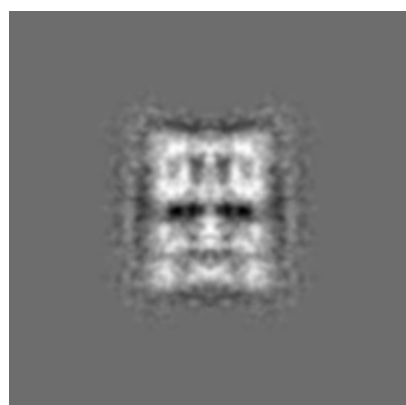
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3882. These allow visual inspection of the internal detail of the map and identification of artifacts.

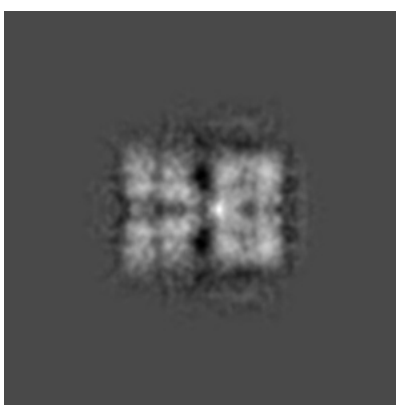
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

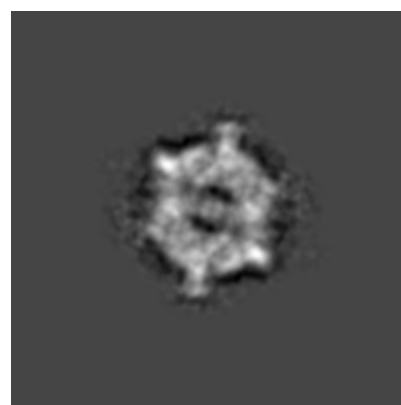
6.1.1 Primary map



X



Y

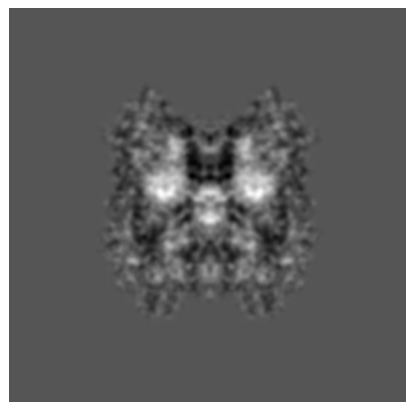


Z

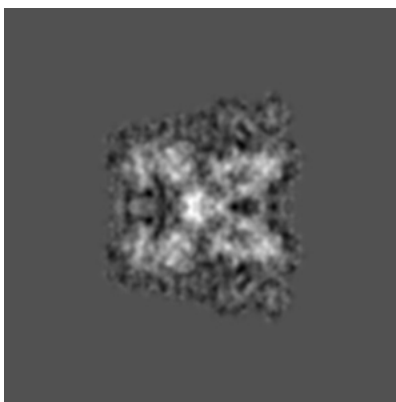
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

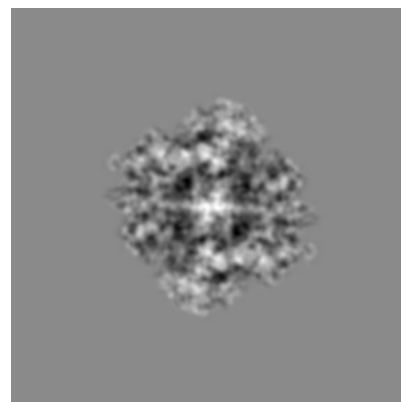
6.2.1 Primary map



X Index: 96



Y Index: 96

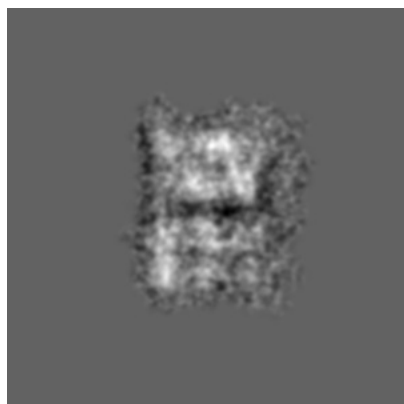


Z Index: 96

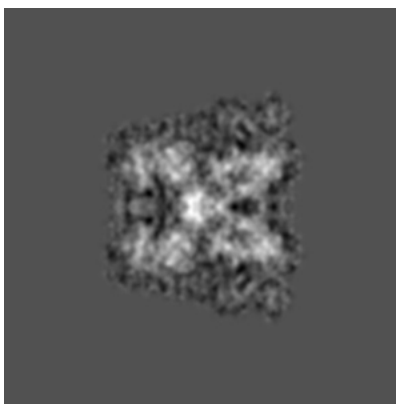
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

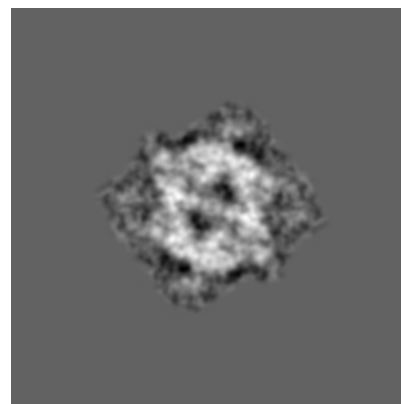
6.3.1 Primary map



X Index: 114



Y Index: 96

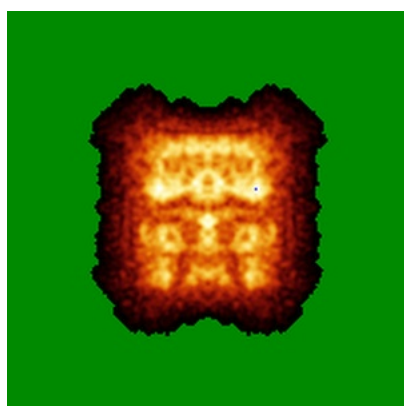


Z Index: 106

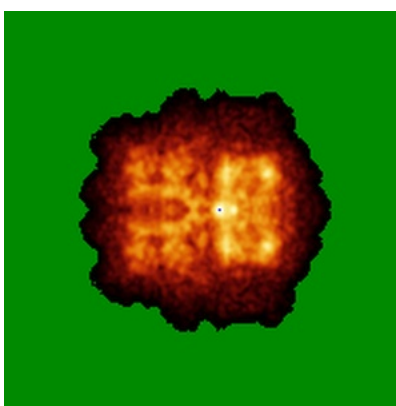
The images above show the largest variance slices of the map in three orthogonal directions.

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

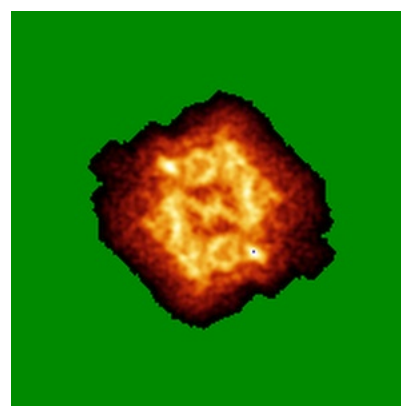
6.4.1 Primary map



X



Y

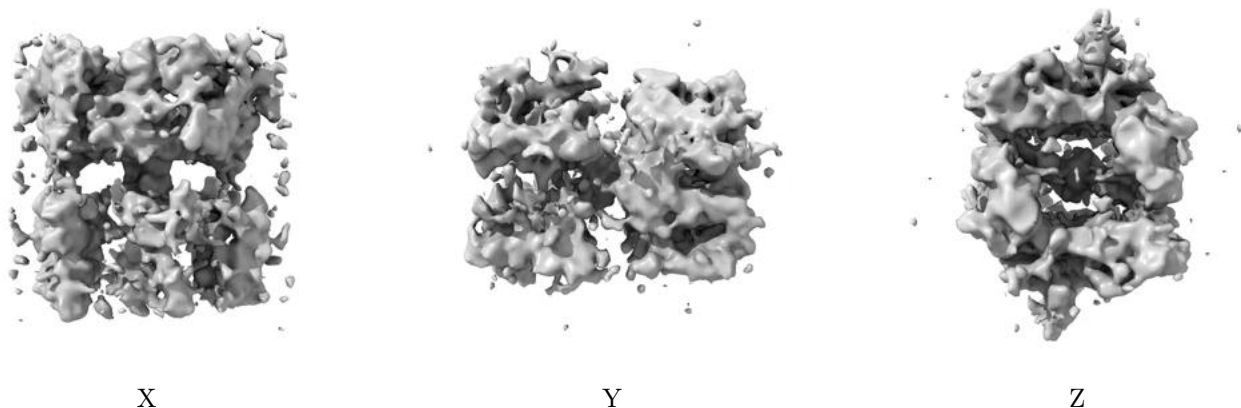


Z

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 1.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

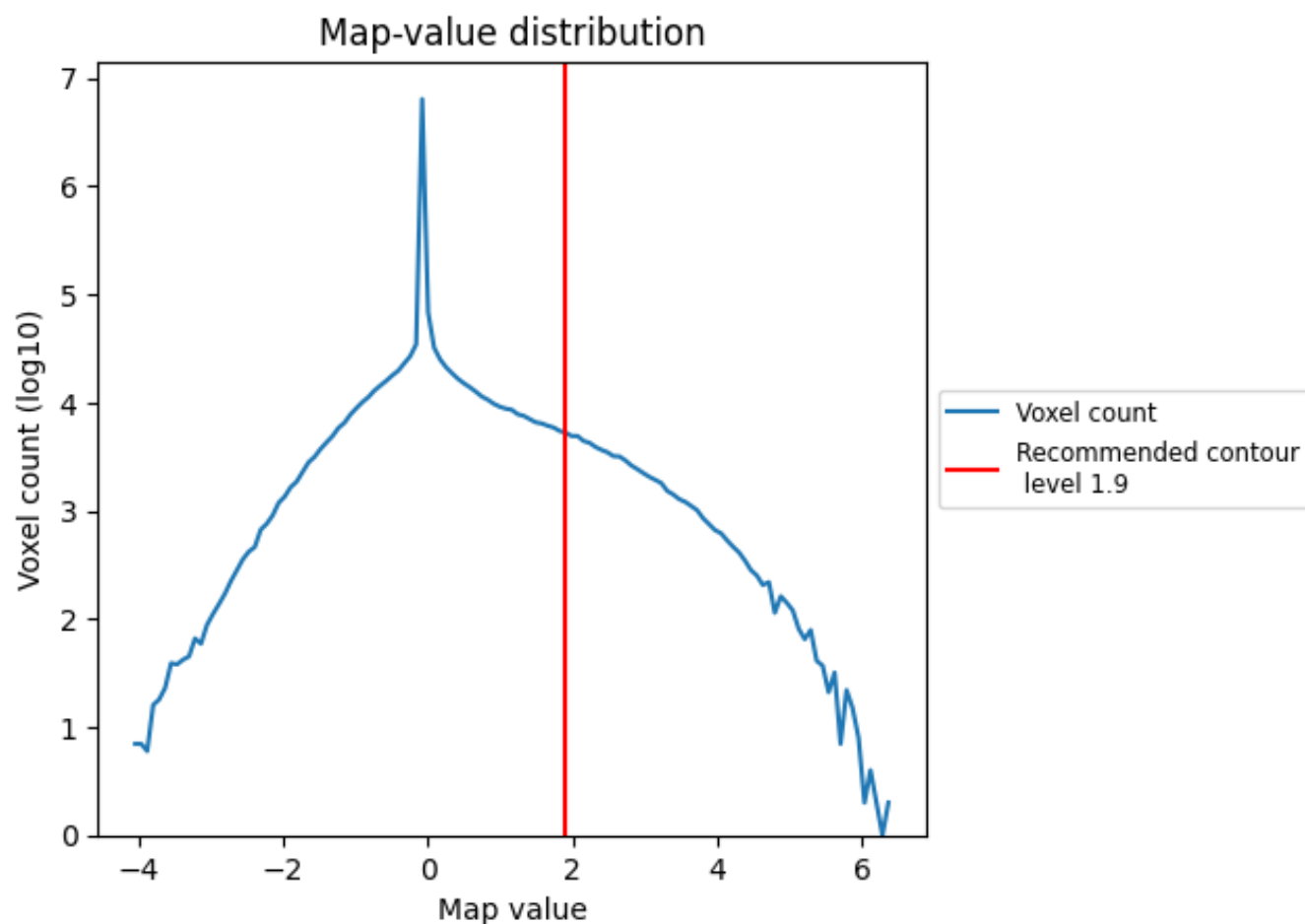
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

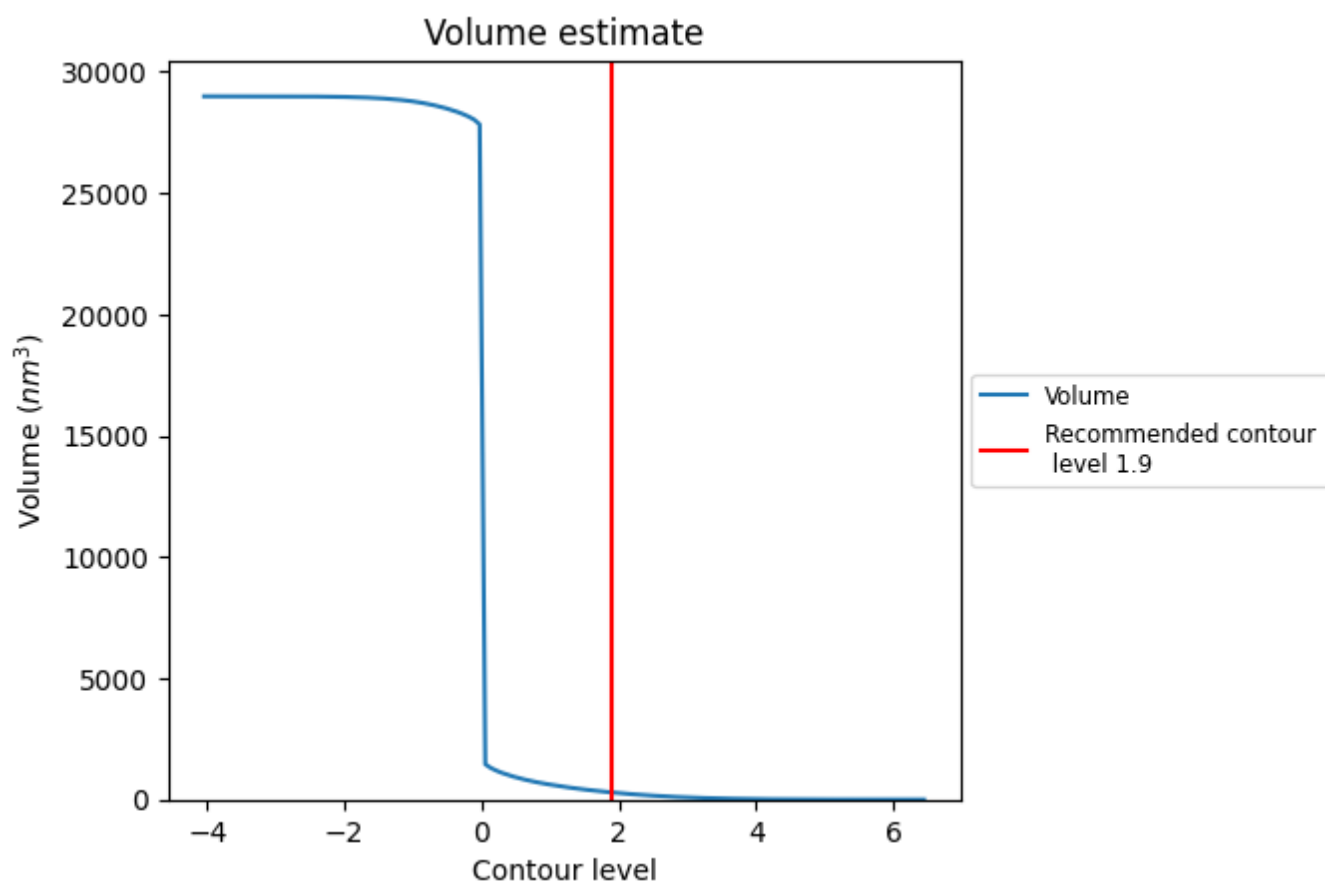
This section contains the results of statistical analysis of the map.

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.

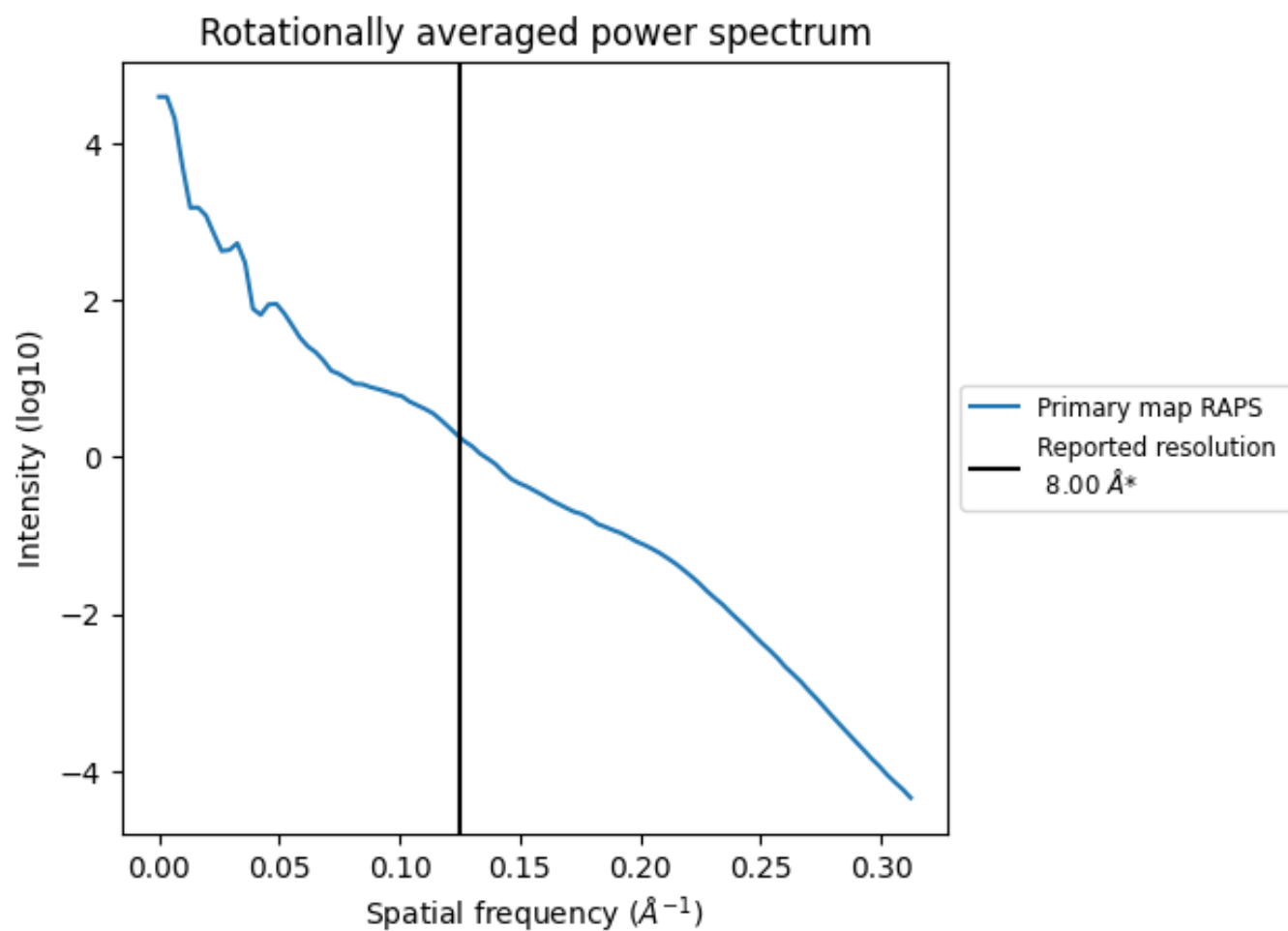
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 294 nm³; this corresponds to an approximate mass of 265 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

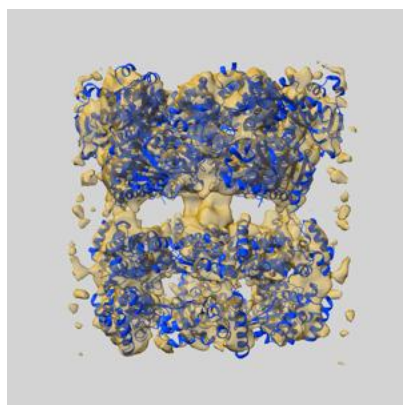
8 Fourier-Shell correlation ⓘ

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

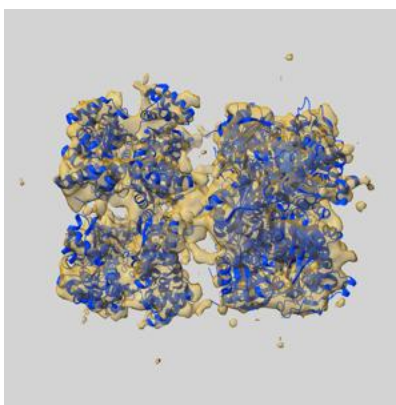
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3882 and PDB model 6EJF. Per-residue inclusion information can be found in section [3](#) on page [9](#).

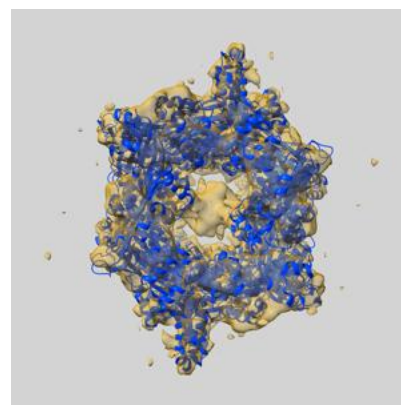
9.1 Map-model overlay [i](#)



X



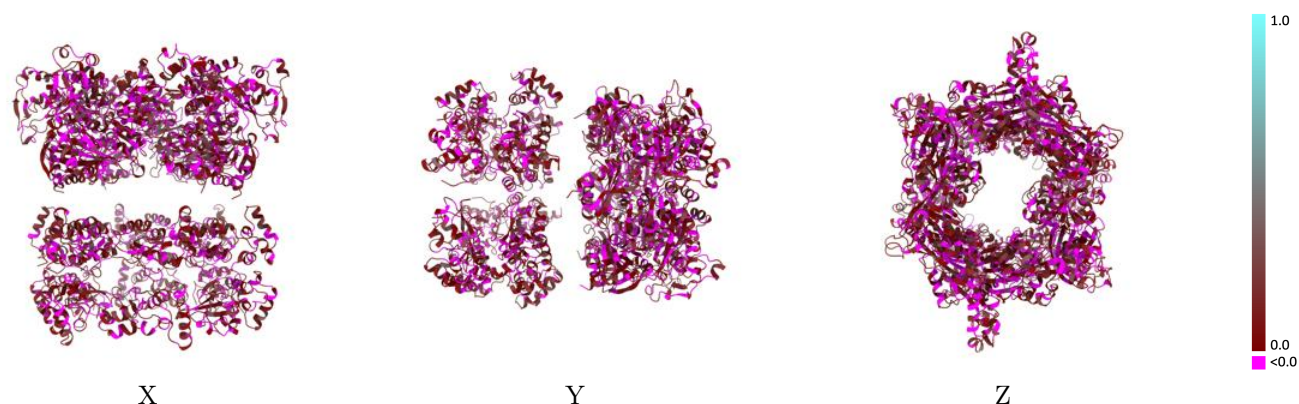
Y



Z

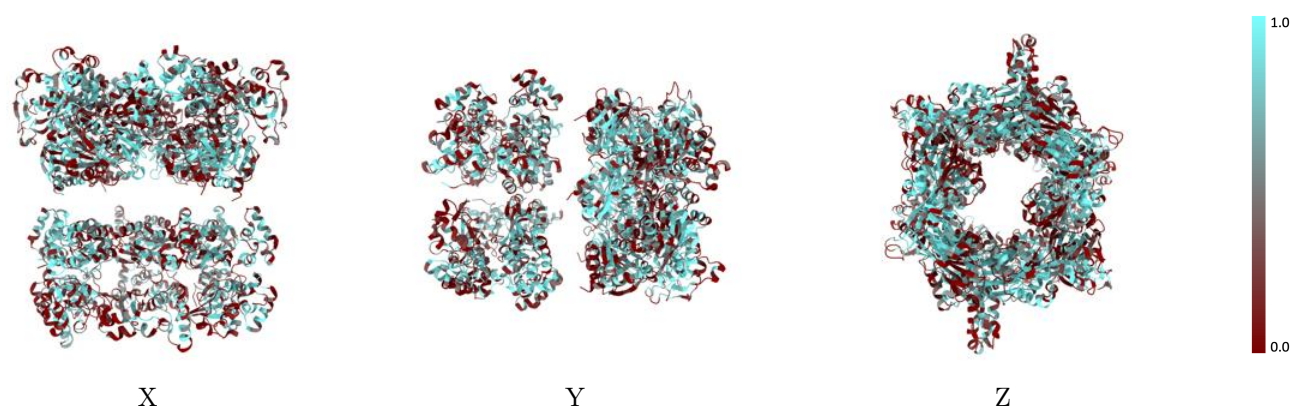
The images above show the 3D surface view of the map at the recommended contour level 1.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



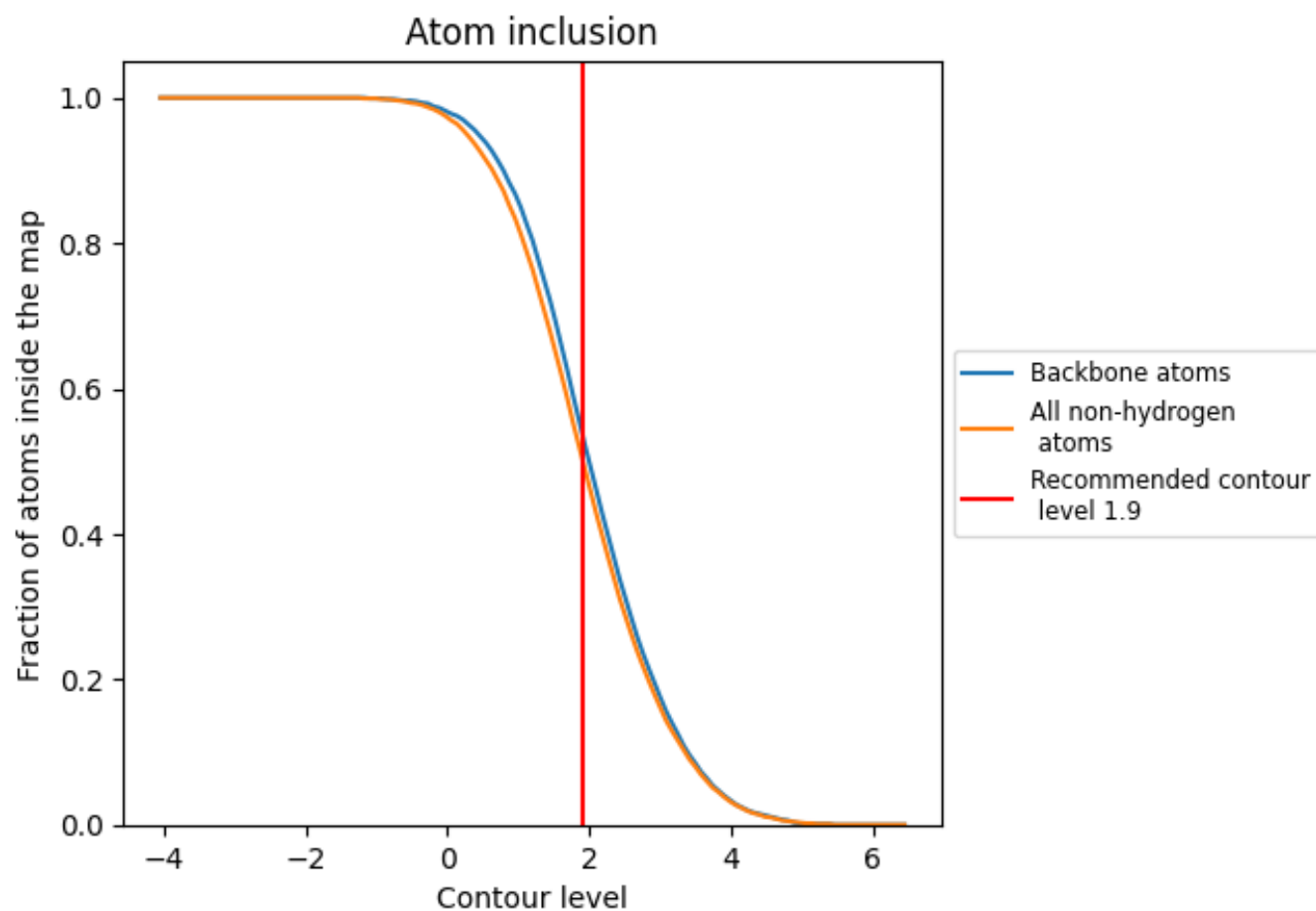
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 50% 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 (1.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5050	0.0690
A	0.5150	0.0660
B	0.5070	0.0510
C	0.5390	0.0640
D	0.5490	0.0700
E	0.5200	0.0570
F	0.5310	0.0580
G	0.4440	0.0870
H	0.5640	0.0760
I	0.5640	0.0800
J	0.3980	0.0840
K	0.3790	0.0730
L	0.4740	0.0730
M	0.4540	0.0830
N	0.4110	0.0920
O	0.3810	0.0740
P	0.4950	0.0690
Q	0.5590	0.0800
R	0.5630	0.0730

1.0

0.0

<0.0