Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 07:40 pm GMT

PDB ID	:	6EJF
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 (i) 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 (i)) were used in the production of this report:

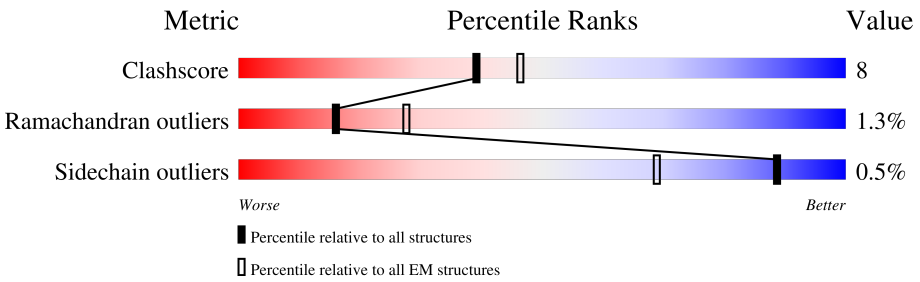
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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% 88% 12%
1	H	146	34% 79% 18% •
1	I	146	35% 84% 16% •
1	M	146	49% 85% 12% • •
1	Q	146	36% 81% 14% • •
1	R	146	37% 84% 12% •
2	J	137	53% 80% 16% •
2	K	137	58% 76% 18% 7%

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Mol	Chain	Length	Quality of chain
2	L	137	48% 80% 18% •
2	N	137	54% 90% 7% •
2	O	137	60% 80% 16% • •
2	P	137	47% 80% 15% • •
3	A	409	42% 75% 13% 6% 6%
3	B	409	42% 78% 12% • 6%
3	C	409	39% 69% 19% 6% 6%
3	D	409	38% 71% 18% 5% 6%
3	E	409	37% 78% 15% • 6%
3	F	409	39% 72% 19% • 6%

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
			Total	C	N	O	S		
1	G	146	1144	726	205	211	2	0	0
1	H	146	1144	726	205	211	2	0	0
1	I	146	1144	726	205	211	2	0	0
1	M	146	1144	726	205	211	2	0	0
1	Q	146	1144	726	205	211	2	0	0
1	R	146	1144	726	205	211	2	0	0

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

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

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

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

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

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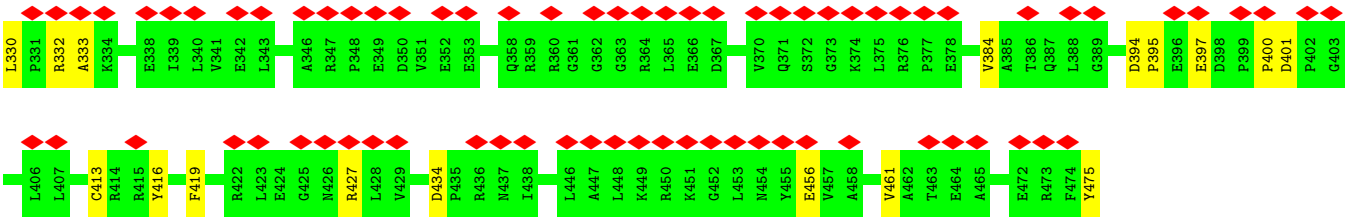
Chain	Residue	Modelled	Actual	Comment	Reference
E	907	HIS	-	expression tag	UNP Q5SLC9
E	908	HIS	-	expression tag	UNP Q5SLC9
E	909	HIS	-	expression tag	UNP Q5SLC9
E	910	HIS	-	expression tag	UNP Q5SLC9
E	911	HIS	-	expression tag	UNP Q5SLC9
E	912	HIS	-	expression tag	UNP Q5SLC9
E	913	HIS	-	expression tag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

3 Residue-property plots (i)

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

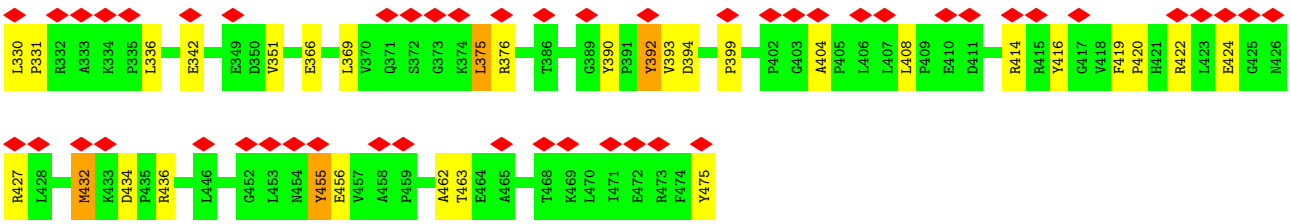
• Molecule 1: Type IV pilus assembly protein PilF

Chain G:



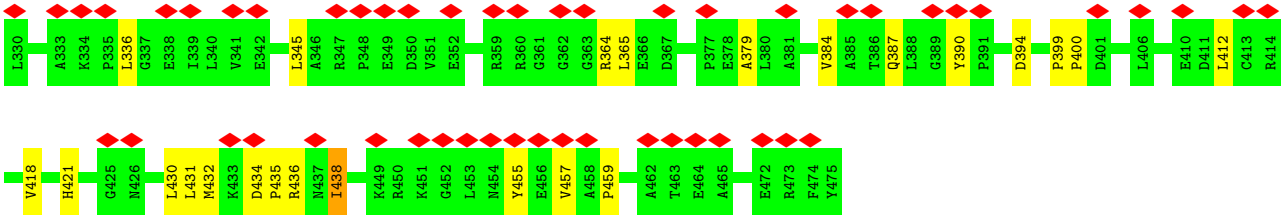
• Molecule 1: Type IV pilus assembly protein PilF

Chain H:



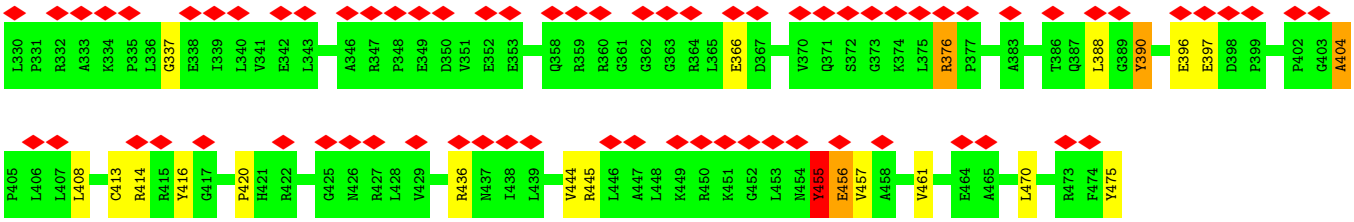
• Molecule 1: Type IV pilus assembly protein PilF

Chain I:



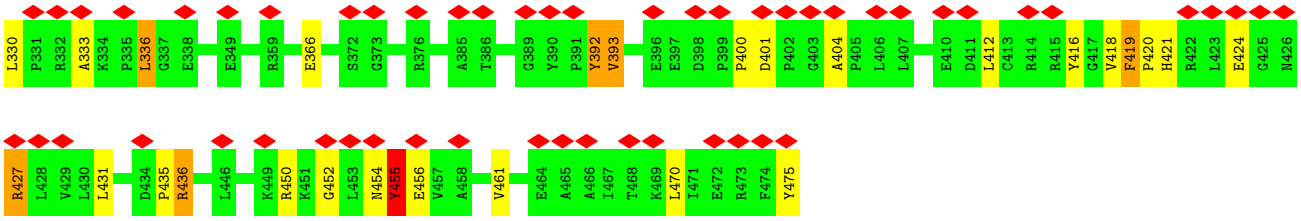
• Molecule 1: Type IV pilus assembly protein PilF

Chain M:



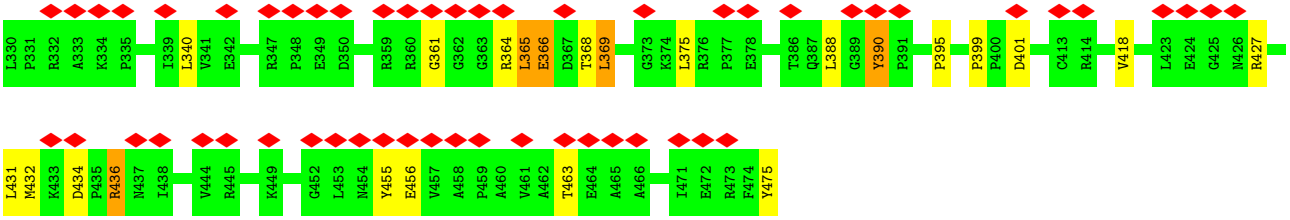
- Molecule 1: Type IV pilus assembly protein PilF

Chain Q:



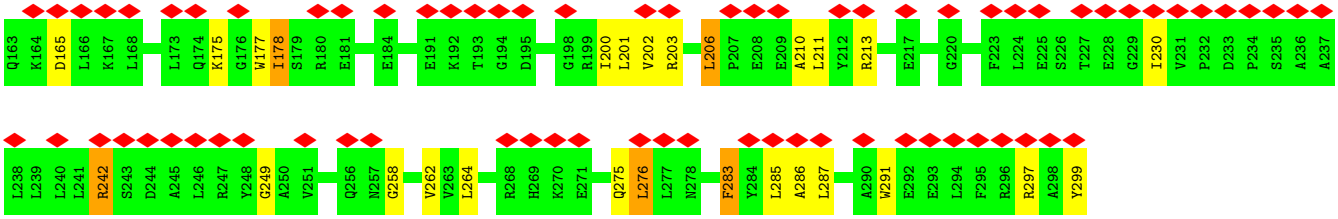
- Molecule 1: Type IV pilus assembly protein PilF

Chain R:



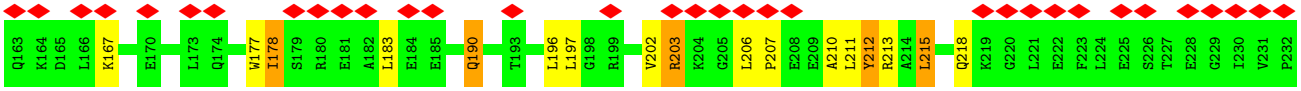
- Molecule 2: Type IV pilus assembly protein PilF

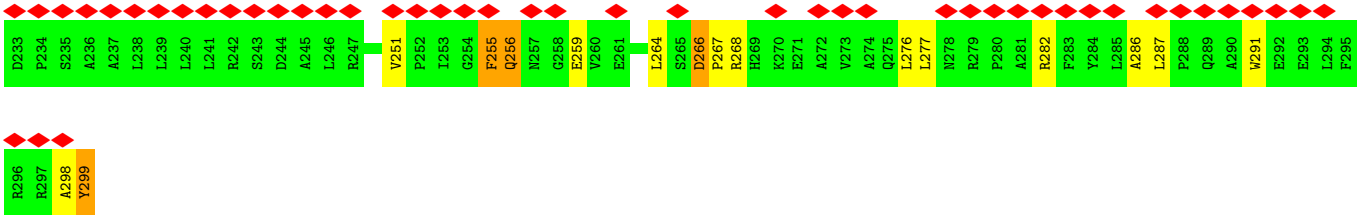
Chain J:



- Molecule 2: Type IV pilus assembly protein PilF

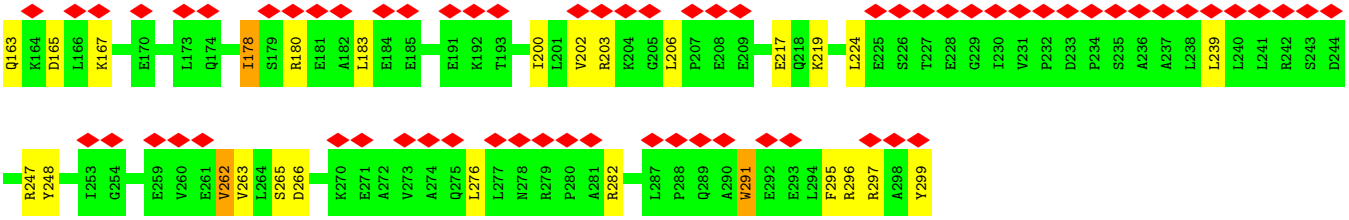
Chain K:





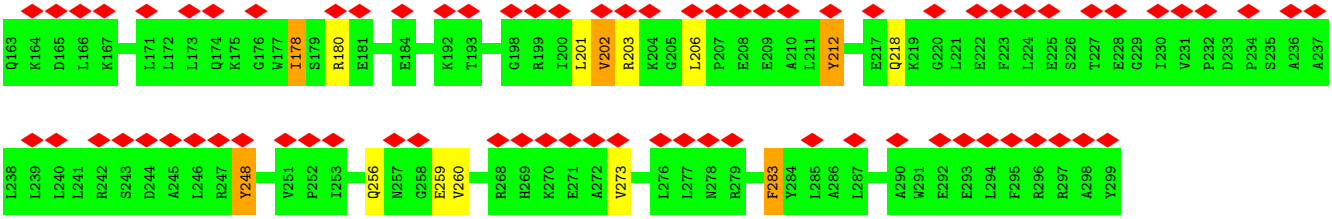
• Molecule 2: Type IV pilus assembly protein PilF

Chain L:



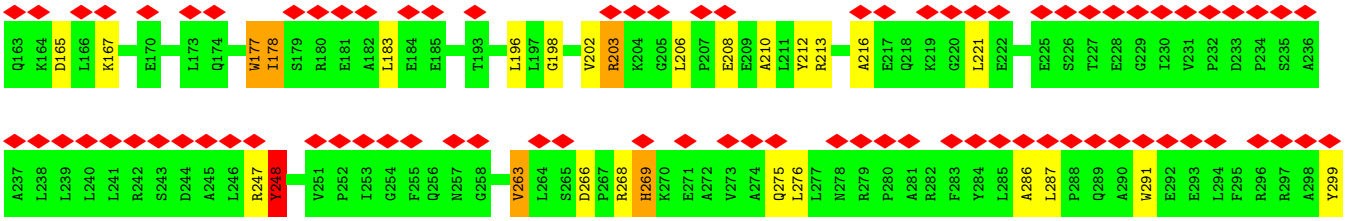
• Molecule 2: Type IV pilus assembly protein PilF

Chain N:



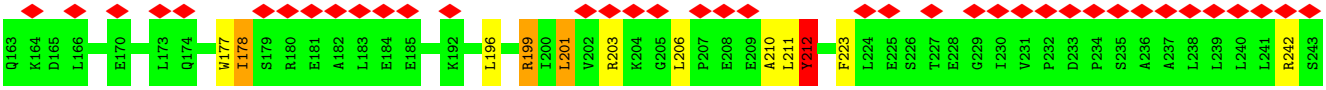
• Molecule 2: Type IV pilus assembly protein PilF

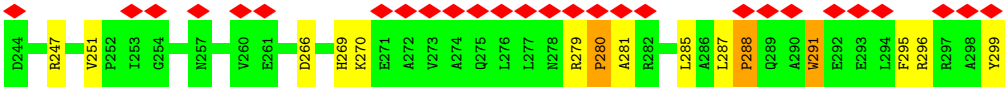
Chain O:



• Molecule 2: Type IV pilus assembly protein PilF

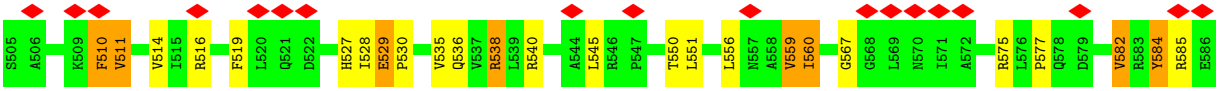
Chain P:

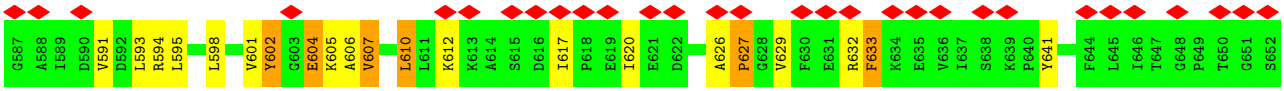


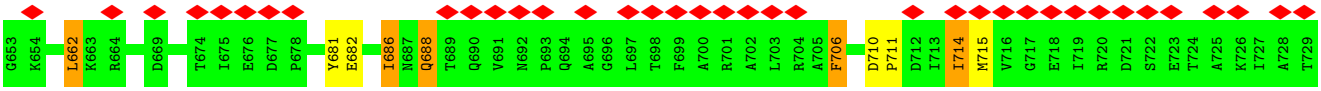


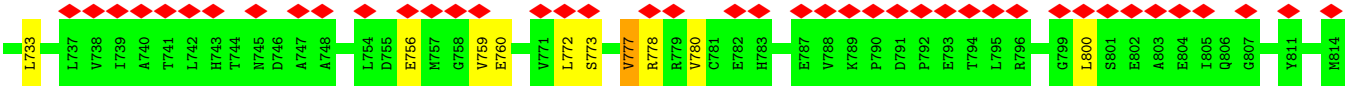
• Molecule 3: Type IV pilus assembly protein PilF

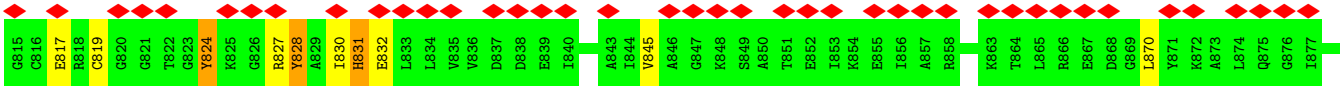
Chain A:

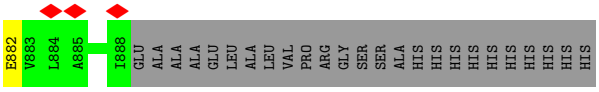






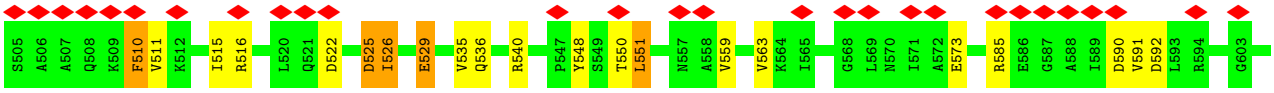


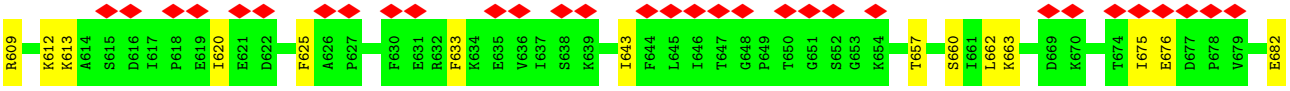


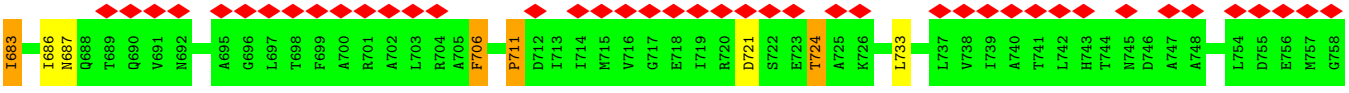


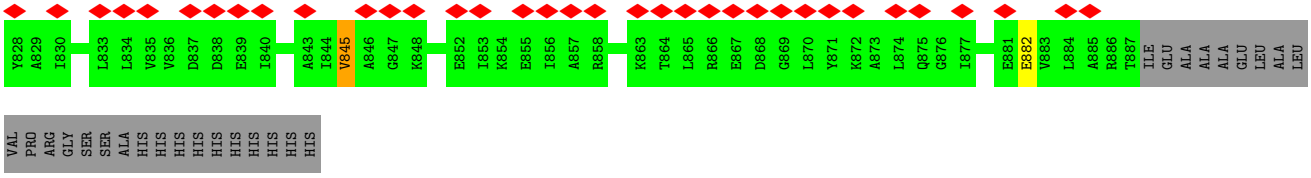
• Molecule 3: Type IV pilus assembly protein PilF

Chain B:



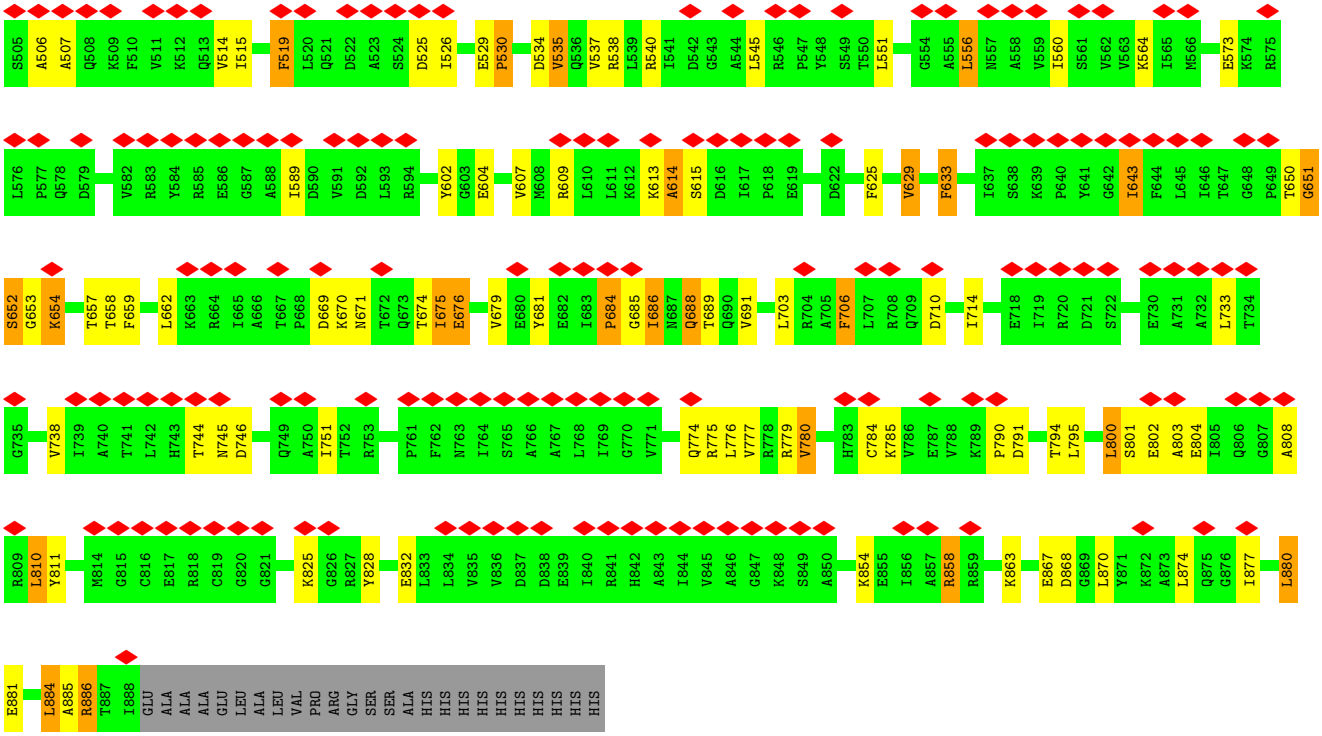






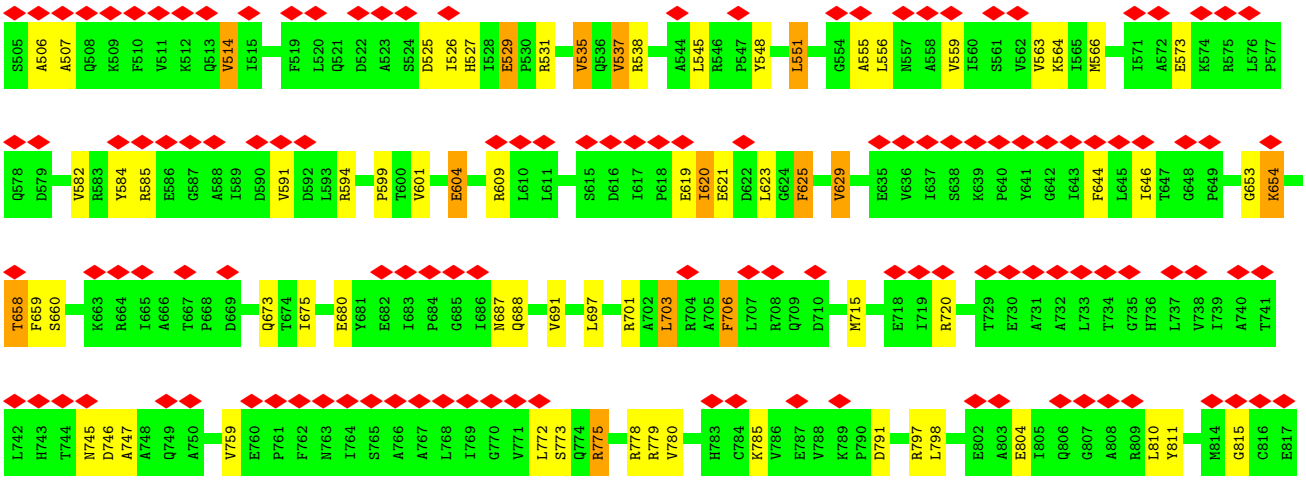
• Molecule 3: Type IV pilus assembly protein PilF

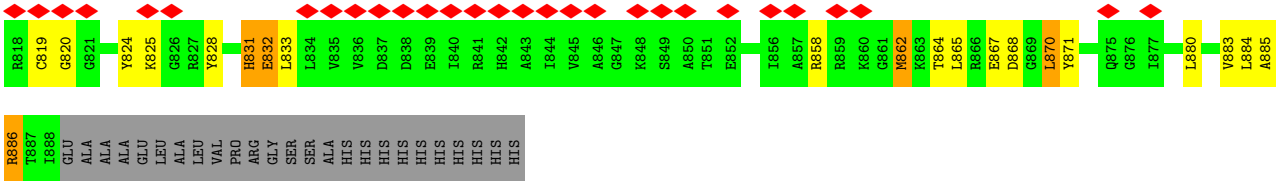
Chain C:



• Molecule 3: Type IV pilus assembly protein PilF

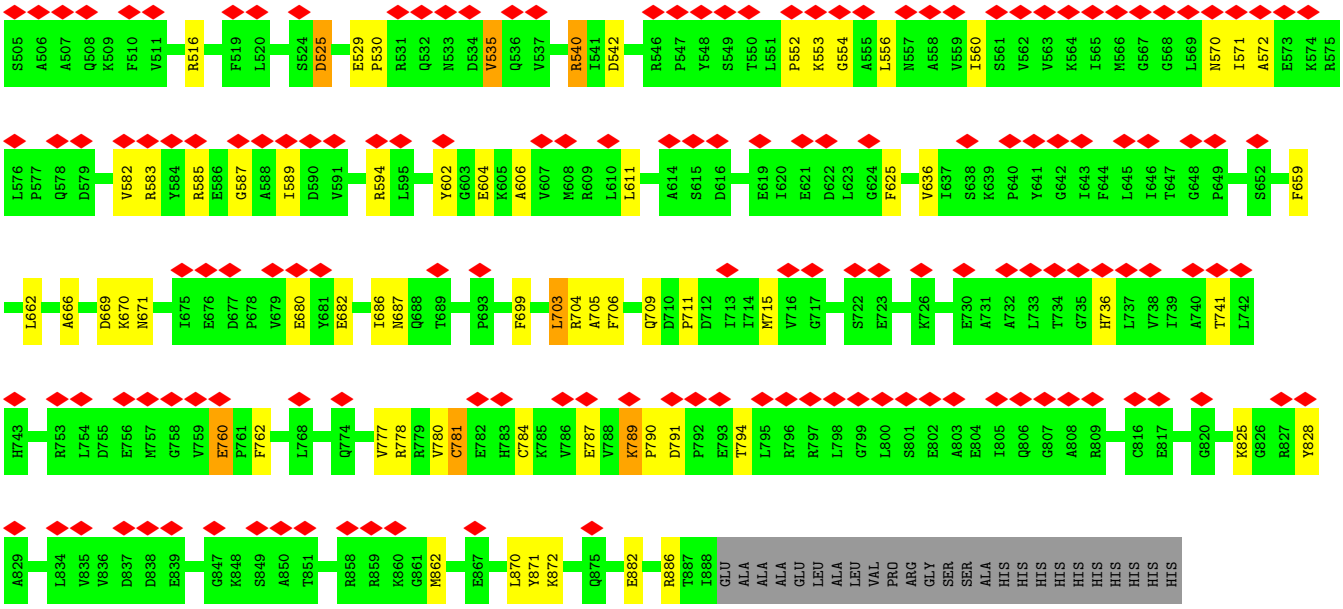
Chain D:





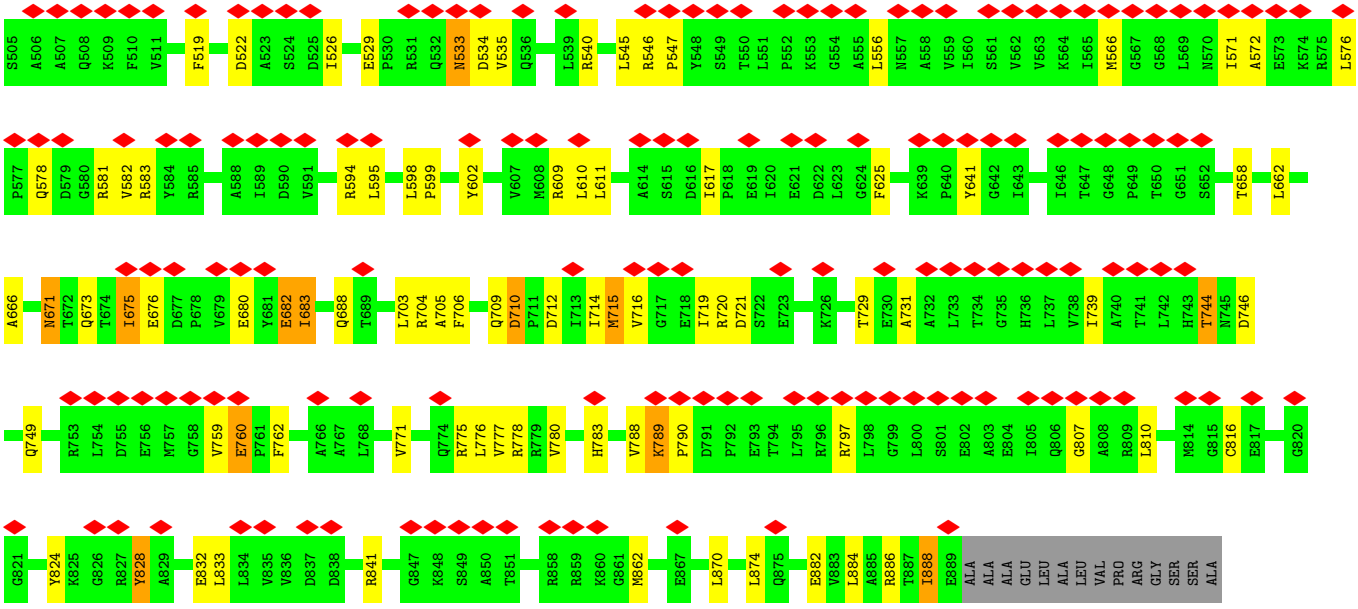
• Molecule 3: Type IV pilus assembly protein PilF

Chain E:



• Molecule 3: Type IV pilus assembly protein PilF

Chain F:



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4 Experimental information (i)

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 ($e^-/Å^2$)	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 (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	G	1.23	5/1165 (0.4%)	1.10	2/1580 (0.1%)
1	H	1.27	5/1165 (0.4%)	1.17	8/1580 (0.5%)
1	I	1.24	5/1165 (0.4%)	1.02	0/1580
1	M	1.31	11/1165 (0.9%)	1.03	3/1580 (0.2%)
1	Q	1.28	6/1165 (0.5%)	1.13	8/1580 (0.5%)
1	R	1.23	6/1165 (0.5%)	1.04	4/1580 (0.3%)
2	J	1.22	3/1110 (0.3%)	1.13	7/1499 (0.5%)
2	K	1.39	8/1110 (0.7%)	1.18	6/1499 (0.4%)
2	L	1.28	8/1110 (0.7%)	1.17	7/1499 (0.5%)
2	N	1.25	7/1110 (0.6%)	1.08	3/1499 (0.2%)
2	O	1.31	8/1110 (0.7%)	1.16	5/1499 (0.3%)
2	P	1.45	13/1110 (1.2%)	1.16	8/1499 (0.5%)
3	A	1.51	41/3017 (1.4%)	1.19	16/4073 (0.4%)
3	B	1.39	27/3008 (0.9%)	1.18	13/4061 (0.3%)
3	C	1.51	45/3017 (1.5%)	1.22	14/4073 (0.3%)
3	D	1.47	41/3017 (1.4%)	1.21	19/4073 (0.5%)
3	E	1.30	16/3017 (0.5%)	1.13	9/4073 (0.2%)
3	F	1.40	35/3026 (1.2%)	1.18	17/4085 (0.4%)
All	All	1.37	290/31752 (0.9%)	1.16	149/42912 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	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 (290) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	511	VAL	CB-CG2	-16.02	1.19	1.52
3	C	529	GLU	CG-CD	-13.24	1.32	1.51
1	M	413	CYS	CB-SG	-12.71	1.60	1.82
3	A	591	VAL	CB-CG1	-11.17	1.29	1.52
3	D	529	GLU	CG-CD	-10.26	1.36	1.51
2	P	212	TYR	CG-CD1	-10.24	1.25	1.39
2	P	212	TYR	CE1-CZ	-10.04	1.25	1.38
3	B	625	PHE	CB-CG	-9.95	1.34	1.51
2	J	178	ILE	CB-CG2	-9.68	1.22	1.52
3	A	584	TYR	CG-CD2	-9.68	1.26	1.39
3	A	582	VAL	CB-CG2	-9.64	1.32	1.52
1	Q	418	VAL	CB-CG1	-9.41	1.33	1.52
3	B	563	VAL	CB-CG2	-9.37	1.33	1.52
3	D	804	GLU	CG-CD	-9.14	1.38	1.51
3	C	556	LEU	CB-CG	-9.04	1.26	1.52
3	A	714	ILE	CB-CG2	-9.03	1.24	1.52
3	C	810	LEU	CB-CG	-9.01	1.26	1.52
3	F	832	GLU	CD-OE1	-8.90	1.15	1.25
3	F	529	GLU	CG-CD	-8.80	1.38	1.51
3	D	775	ARG	CD-NE	-8.74	1.31	1.46
2	P	285	LEU	CB-CG	-8.73	1.27	1.52
2	P	212	TYR	CB-CG	-8.71	1.38	1.51
3	D	775	ARG	NE-CZ	-8.46	1.22	1.33
3	A	582	VAL	CB-CG1	-8.31	1.35	1.52
3	C	629	VAL	CB-CG1	-8.28	1.35	1.52
3	A	604	GLU	CD-OE1	-8.22	1.16	1.25
2	J	262	VAL	CB-CG2	-8.17	1.35	1.52
2	P	291	TRP	CZ3-CH2	-8.14	1.27	1.40
3	D	791	ASP	CB-CG	-8.13	1.34	1.51
3	B	706	PHE	CB-CG	-8.12	1.37	1.51
3	F	760	GLU	CG-CD	-8.03	1.40	1.51
3	A	819	CYS	CB-SG	-8.01	1.68	1.82
3	A	584	TYR	CB-CG	-7.97	1.39	1.51
3	B	784	CYS	CB-SG	-7.93	1.68	1.82
2	K	251	VAL	CB-CG1	-7.92	1.36	1.52
3	C	681	TYR	CB-CG	-7.91	1.39	1.51
2	L	178	ILE	CB-CG2	-7.86	1.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	178	ILE	CB-CG2	-7.82	1.28	1.52
3	D	535	VAL	CB-CG2	-7.81	1.36	1.52
3	E	777	VAL	CB-CG2	-7.80	1.36	1.52
3	C	791	ASP	CB-CG	-7.80	1.35	1.51
3	A	514	VAL	CB-CG2	-7.79	1.36	1.52
3	D	604	GLU	CG-CD	-7.76	1.40	1.51
2	K	218	GLN	CG-CD	-7.74	1.33	1.51
3	F	882	GLU	CG-CD	-7.70	1.40	1.51
1	R	340	LEU	CG-CD2	-7.70	1.23	1.51
3	F	777	VAL	CB-CG2	-7.68	1.36	1.52
3	C	777	VAL	CB-CG2	-7.68	1.36	1.52
3	B	559	VAL	CB-CG1	-7.67	1.36	1.52
3	E	604	GLU	CG-CD	-7.66	1.40	1.51
3	A	584	TYR	CD2-CE2	-7.61	1.27	1.39
3	D	706	PHE	CG-CD1	-7.53	1.27	1.38
3	A	686	ILE	CB-CG1	-7.49	1.33	1.54
3	D	675	ILE	CB-CG1	-7.48	1.33	1.54
3	A	780	VAL	CB-CG2	-7.35	1.37	1.52
3	A	559	VAL	CB-CG1	-7.34	1.37	1.52
3	C	537	VAL	CB-CG1	-7.34	1.37	1.52
1	R	418	VAL	CB-CG1	-7.32	1.37	1.52
3	D	867	GLU	CG-CD	-7.31	1.41	1.51
3	D	775	ARG	CB-CG	-7.31	1.32	1.52
3	A	529	GLU	CG-CD	-7.28	1.41	1.51
2	P	178	ILE	CB-CG2	-7.26	1.30	1.52
3	D	538	ARG	CZ-NH1	-7.25	1.23	1.33
3	C	675	ILE	CB-CG1	-7.25	1.33	1.54
3	C	777	VAL	CB-CG1	-7.24	1.37	1.52
3	D	527	HIS	CB-CG	-7.15	1.37	1.50
3	F	522	ASP	CB-CG	7.09	1.66	1.51
2	O	263	VAL	CB-CG2	-7.08	1.38	1.52
2	N	218	GLN	CG-CD	-7.07	1.34	1.51
3	B	660	SER	CB-OG	-7.06	1.33	1.42
3	C	676	GLU	CD-OE2	-7.06	1.17	1.25
3	F	775	ARG	CG-CD	-7.03	1.34	1.51
1	R	375	LEU	CG-CD1	-6.98	1.26	1.51
3	A	662	LEU	CB-CG	-6.94	1.32	1.52
3	A	529	GLU	CD-OE1	-6.93	1.18	1.25
3	C	832	GLU	CD-OE1	-6.92	1.18	1.25
1	G	416	TYR	CB-CG	-6.89	1.41	1.51
3	C	780	VAL	CB-CG2	-6.86	1.38	1.52
3	E	706	PHE	CB-CG	-6.83	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	831	HIS	CB-CG	-6.82	1.37	1.50
2	O	212	TYR	CG-CD1	-6.81	1.30	1.39
3	D	629	VAL	CB-CG2	-6.77	1.38	1.52
2	P	212	TYR	CG-CD2	-6.74	1.30	1.39
3	C	675	ILE	CB-CG2	-6.74	1.31	1.52
1	M	397	GLU	CD-OE2	-6.73	1.18	1.25
3	C	688	GLN	CG-CD	-6.73	1.35	1.51
3	A	633	PHE	CB-CG	-6.73	1.40	1.51
1	M	461	VAL	CB-CG1	-6.72	1.38	1.52
3	E	525	ASP	CB-CG	-6.72	1.37	1.51
3	A	777	VAL	CB-CG1	-6.70	1.38	1.52
3	F	582	VAL	CB-CG1	-6.70	1.38	1.52
3	A	824	TYR	CB-CG	6.70	1.61	1.51
3	A	607	VAL	CB-CG2	-6.69	1.38	1.52
3	C	751	ILE	CB-CG2	-6.67	1.32	1.52
3	D	537	VAL	CB-CG2	-6.66	1.38	1.52
1	I	418	VAL	CB-CG1	-6.65	1.38	1.52
3	D	703	LEU	CB-CG	-6.62	1.33	1.52
3	C	625	PHE	CB-CG	-6.61	1.40	1.51
3	A	538	ARG	CD-NE	-6.61	1.35	1.46
3	D	828	TYR	CB-CG	-6.56	1.41	1.51
1	H	392	TYR	CB-CG	6.55	1.61	1.51
3	B	510	PHE	CB-CG	-6.55	1.40	1.51
3	D	858	ARG	CD-NE	-6.55	1.35	1.46
2	L	295	PHE	CB-CG	-6.54	1.40	1.51
3	C	654	LYS	CB-CG	-6.52	1.34	1.52
3	A	529	GLU	CD-OE2	-6.51	1.18	1.25
2	N	260	VAL	CB-CG1	-6.50	1.39	1.52
3	D	591	VAL	CB-CG1	-6.49	1.39	1.52
3	A	538	ARG	CG-CD	-6.49	1.35	1.51
3	A	560	ILE	CB-CG1	-6.48	1.35	1.54
2	O	178	ILE	CB-CG2	-6.48	1.32	1.52
1	Q	419	PHE	CB-CG	-6.45	1.40	1.51
3	D	746	ASP	CB-CG	-6.43	1.38	1.51
3	D	883	VAL	CB-CG1	-6.40	1.39	1.52
2	P	251	VAL	CB-CG2	-6.40	1.39	1.52
3	F	703	LEU	CB-CG	-6.39	1.34	1.52
1	H	375	LEU	CB-CG	-6.38	1.34	1.52
3	B	529	GLU	CD-OE2	-6.38	1.18	1.25
3	C	858	ARG	CD-NE	-6.38	1.35	1.46
3	C	832	GLU	CG-CD	-6.32	1.42	1.51
3	C	538	ARG	CD-NE	-6.32	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	461	VAL	CB-CG2	-6.31	1.39	1.52
3	F	760	GLU	CD-OE2	-6.31	1.18	1.25
1	I	384	VAL	CB-CG1	-6.29	1.39	1.52
3	F	759	VAL	CB-CG1	-6.29	1.39	1.52
2	N	283	PHE	CB-CG	-6.27	1.40	1.51
3	B	525	ASP	CB-CG	-6.27	1.38	1.51
3	C	832	GLU	CD-OE2	-6.25	1.18	1.25
3	C	800	LEU	CB-CG	-6.24	1.34	1.52
3	F	546	ARG	CG-CD	-6.24	1.36	1.51
3	B	591	VAL	CB-CG2	-6.23	1.39	1.52
3	D	582	VAL	CB-CG2	-6.20	1.39	1.52
3	F	526	ILE	CB-CG1	-6.19	1.36	1.54
3	C	686	ILE	CB-CG1	-6.17	1.36	1.54
3	D	759	VAL	CB-CG2	-6.17	1.39	1.52
3	D	870	LEU	CG-CD1	-6.17	1.29	1.51
3	D	529	GLU	CD-OE2	-6.15	1.18	1.25
3	E	636	VAL	CB-CG2	-6.15	1.40	1.52
1	I	421	HIS	CB-CG	-6.10	1.39	1.50
3	F	810	LEU	CB-CG	-6.09	1.34	1.52
3	F	703	LEU	CG-CD1	-6.08	1.29	1.51
3	C	858	ARG	CG-CD	-6.07	1.36	1.51
3	C	529	GLU	CD-OE2	-6.07	1.19	1.25
2	K	266	ASP	CB-CG	-6.06	1.39	1.51
3	F	874	LEU	CG-CD1	-6.05	1.29	1.51
3	A	559	VAL	CB-CG2	-6.05	1.40	1.52
3	C	880	LEU	CB-CG	-6.04	1.35	1.52
3	C	691	VAL	CB-CG2	-6.04	1.40	1.52
3	F	602	TYR	CG-CD1	-6.04	1.31	1.39
3	E	760	GLU	CG-CD	-6.04	1.42	1.51
3	D	832	GLU	CD-OE1	-6.03	1.19	1.25
1	R	390	TYR	CG-CD1	-6.02	1.31	1.39
3	D	706	PHE	CB-CG	-5.99	1.41	1.51
3	D	867	GLU	CD-OE1	-5.99	1.19	1.25
3	B	590	ASP	CB-CG	5.97	1.64	1.51
2	L	262	VAL	CB-CG1	-5.97	1.40	1.52
3	B	824	TYR	CB-CG	5.95	1.60	1.51
3	C	514	VAL	CB-CG2	-5.95	1.40	1.52
2	P	288	PRO	N-CD	-5.94	1.39	1.47
2	N	202	VAL	CB-CG1	-5.93	1.40	1.52
3	F	671	ASN	CB-CG	-5.91	1.37	1.51
3	B	529	GLU	CD-OE1	-5.90	1.19	1.25
3	B	511	VAL	CB-CG2	-5.89	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	212	TYR	CG-CD2	-5.89	1.31	1.39
3	C	529	GLU	CD-OE1	-5.88	1.19	1.25
3	F	675	ILE	CB-CG1	-5.87	1.37	1.54
2	K	215	LEU	CB-CG	-5.85	1.35	1.52
3	F	828	TYR	CB-CG	-5.84	1.42	1.51
1	M	366	GLU	CD-OE1	-5.84	1.19	1.25
3	C	529	GLU	CB-CG	-5.84	1.41	1.52
3	D	680	GLU	CB-CG	-5.83	1.41	1.52
1	M	397	GLU	CG-CD	-5.83	1.43	1.51
1	G	413	CYS	CB-SG	-5.81	1.72	1.81
3	A	686	ILE	CB-CG2	-5.81	1.34	1.52
2	O	212	TYR	CB-CG	-5.81	1.43	1.51
3	A	577	PRO	N-CD	-5.80	1.39	1.47
3	E	686	ILE	CB-CG1	-5.80	1.37	1.54
3	F	688	GLN	CG-CD	-5.80	1.37	1.51
1	M	397	GLU	CD-OE1	-5.78	1.19	1.25
3	D	810	LEU	CB-CG	-5.78	1.35	1.52
2	K	264	LEU	CB-CG	-5.77	1.35	1.52
3	E	535	VAL	CB-CG2	-5.77	1.40	1.52
3	E	781	CYS	CB-SG	-5.76	1.72	1.81
3	B	682	GLU	CG-CD	-5.75	1.43	1.51
3	D	780	VAL	CB-CG1	-5.73	1.40	1.52
3	F	715	MET	CG-SD	-5.72	1.66	1.81
3	C	625	PHE	CG-CD1	-5.72	1.30	1.38
2	K	218	GLN	CB-CG	-5.71	1.37	1.52
1	G	397	GLU	CD-OE2	-5.70	1.19	1.25
3	F	775	ARG	CD-NE	-5.68	1.36	1.46
3	F	716	VAL	CB-CG2	-5.68	1.41	1.52
3	C	652	SER	CB-OG	-5.66	1.34	1.42
2	P	291	TRP	CE2-CZ2	-5.65	1.30	1.39
3	D	604	GLU	CD-OE1	-5.65	1.19	1.25
3	A	882	GLU	CB-CG	-5.65	1.41	1.52
3	D	680	GLU	CD-OE1	-5.64	1.19	1.25
3	E	760	GLU	CD-OE2	-5.63	1.19	1.25
2	L	224	LEU	CB-CG	-5.62	1.36	1.52
3	B	675	ILE	CB-CG1	-5.61	1.38	1.54
3	A	528	ILE	CB-CG2	-5.60	1.35	1.52
3	A	527	HIS	CB-CG	-5.60	1.40	1.50
3	B	526	ILE	CB-CG1	-5.59	1.38	1.54
2	L	291	TRP	CB-CG	-5.59	1.40	1.50
2	J	206	LEU	CG-CD1	-5.57	1.31	1.51
1	M	390	TYR	CG-CD2	-5.57	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	662	LEU	CB-CG	-5.53	1.36	1.52
1	I	457	VAL	CB-CG2	-5.53	1.41	1.52
3	A	510	PHE	CB-CG	-5.53	1.42	1.51
3	D	673	GLN	CG-CD	-5.52	1.38	1.51
3	F	676	GLU	CD-OE1	-5.52	1.19	1.25
3	D	691	VAL	CB-CG2	-5.52	1.41	1.52
3	C	804	GLU	CD-OE1	-5.51	1.19	1.25
3	B	529	GLU	CG-CD	-5.51	1.43	1.51
3	C	530	PRO	N-CD	-5.50	1.40	1.47
3	E	703	LEU	CB-CG	-5.50	1.36	1.52
3	D	601	VAL	CB-CG1	-5.49	1.41	1.52
1	H	351	VAL	CB-CG2	-5.49	1.41	1.52
3	C	535	VAL	CB-CG1	-5.49	1.41	1.52
1	G	475	TYR	CD1-CE1	-5.47	1.31	1.39
3	B	777	VAL	CB-CG1	-5.46	1.41	1.52
1	M	416	TYR	CB-CG	-5.46	1.43	1.51
1	H	366	GLU	CD-OE2	-5.46	1.19	1.25
3	F	529	GLU	CD-OE2	-5.46	1.19	1.25
3	E	636	VAL	CB-CG1	-5.44	1.41	1.52
3	D	832	GLU	CD-OE2	-5.43	1.19	1.25
3	F	870	LEU	CG-CD2	-5.43	1.31	1.51
3	F	882	GLU	CD-OE2	-5.42	1.19	1.25
3	F	771	VAL	CB-CG2	-5.39	1.41	1.52
1	I	431	LEU	CB-CG	-5.37	1.36	1.52
2	O	196	LEU	CB-CG	-5.36	1.36	1.52
1	G	475	TYR	CG-CD1	-5.36	1.32	1.39
1	Q	392	TYR	CE1-CZ	-5.36	1.31	1.38
3	D	604	GLU	CD-OE2	-5.36	1.19	1.25
3	C	738	VAL	CB-CG2	-5.35	1.41	1.52
2	O	177	TRP	CZ3-CH2	-5.34	1.31	1.40
2	N	178	ILE	CB-CG2	-5.34	1.36	1.52
3	A	610	LEU	CG-CD1	-5.33	1.32	1.51
3	F	771	VAL	CB-CG1	-5.33	1.41	1.52
3	A	688	GLN	CG-CD	-5.33	1.38	1.51
3	C	886	ARG	CG-CD	-5.32	1.38	1.51
2	N	259	GLU	CD-OE1	-5.32	1.19	1.25
3	D	658	THR	CB-CG2	-5.31	1.34	1.52
2	P	212	TYR	CD1-CE1	-5.31	1.31	1.39
3	E	780	VAL	CB-CG1	-5.30	1.41	1.52
2	O	212	TYR	CG-CD2	-5.30	1.32	1.39
3	C	714	ILE	CB-CG1	-5.29	1.39	1.54
1	R	418	VAL	CB-CG2	-5.28	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	LEU	CB-CG	-5.27	1.37	1.52
3	B	882	GLU	CD-OE2	-5.26	1.19	1.25
3	B	551	LEU	CB-CG	-5.25	1.37	1.52
3	C	625	PHE	CE1-CZ	-5.23	1.27	1.37
3	A	830	ILE	CB-CG2	-5.22	1.36	1.52
2	L	217	GLU	CD-OE2	-5.22	1.20	1.25
3	B	711	PRO	N-CD	-5.22	1.40	1.47
3	D	883	VAL	CA-CB	-5.21	1.43	1.54
3	F	744	THR	CB-CG2	-5.20	1.35	1.52
3	A	756	GLU	CG-CD	5.19	1.59	1.51
3	B	676	GLU	CD-OE2	-5.19	1.20	1.25
3	B	780	VAL	CB-CG1	-5.19	1.42	1.52
1	M	416	TYR	CD2-CE2	-5.18	1.31	1.39
2	P	201	LEU	CB-CG	-5.18	1.37	1.52
3	F	780	VAL	CB-CG1	-5.17	1.42	1.52
3	A	617	ILE	CB-CG1	-5.17	1.39	1.54
3	E	682	GLU	CG-CD	-5.16	1.44	1.51
1	Q	431	LEU	CB-CG	-5.16	1.37	1.52
3	A	831	HIS	CB-CG	-5.16	1.40	1.50
2	O	177	TRP	CD2-CE3	-5.15	1.32	1.40
3	E	529	GLU	CD-OE2	-5.15	1.20	1.25
3	A	882	GLU	CD-OE2	-5.14	1.20	1.25
3	C	607	VAL	CB-CG2	-5.14	1.42	1.52
2	L	178	ILE	CB-CG1	-5.13	1.39	1.54
3	B	625	PHE	CG-CD1	-5.12	1.31	1.38
1	Q	421	HIS	CB-CG	-5.11	1.40	1.50
2	P	291	TRP	CD2-CE2	-5.10	1.35	1.41
1	M	396	GLU	CD-OE2	-5.10	1.20	1.25
3	A	780	VAL	CB-CG1	-5.10	1.42	1.52
3	B	810	LEU	CB-CG	-5.10	1.37	1.52
3	C	643	ILE	CB-CG2	-5.08	1.37	1.52
3	F	832	GLU	CG-CD	-5.08	1.44	1.51
1	M	475	TYR	CE1-CZ	-5.07	1.31	1.38
3	A	777	VAL	CB-CG2	-5.07	1.42	1.52
3	B	724	THR	CB-CG2	-5.06	1.35	1.52
3	E	870	LEU	CB-CG	-5.05	1.37	1.52
3	F	704	ARG	CB-CG	-5.04	1.39	1.52
3	C	884	LEU	CB-CG	-5.03	1.38	1.52
1	H	393	VAL	CB-CG2	-5.02	1.42	1.52
3	F	721	ASP	CB-CG	5.02	1.62	1.51
1	R	369	LEU	CG-CD1	-5.01	1.33	1.51
2	L	217	GLU	CD-OE1	-5.01	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	273	VAL	CB-CG2	-5.01	1.42	1.52

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	538	ARG	NE-CZ-NH2	-12.23	114.19	120.30
3	F	720	ARG	NE-CZ-NH2	-10.98	114.81	120.30
2	P	212	TYR	CB-CG-CD1	-10.61	114.63	121.00
3	E	540	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	H	455	TYR	CB-CG-CD2	-10.06	114.96	121.00
2	L	282	ARG	NE-CZ-NH1	9.38	124.99	120.30
3	E	583	ARG	NE-CZ-NH2	9.32	124.96	120.30
3	F	540	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	G	427	ARG	NE-CZ-NH2	-9.01	115.80	120.30
3	C	828	TYR	CB-CG-CD2	-8.86	115.68	121.00
3	F	715	MET	CG-SD-CE	-8.76	86.19	100.20
2	N	180	ARG	NE-CZ-NH2	-8.57	116.01	120.30
3	A	827	ARG	NE-CZ-NH2	-8.42	116.09	120.30
3	C	602	TYR	CB-CG-CD2	-8.38	115.97	121.00
3	D	886	ARG	NE-CZ-NH2	-8.38	116.11	120.30
3	A	602	TYR	CB-CG-CD2	-8.34	116.00	121.00
3	F	797	ARG	NE-CZ-NH2	-8.12	116.24	120.30
2	K	213	ARG	NE-CZ-NH1	8.07	124.33	120.30
2	K	282	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	Q	455	TYR	CB-CG-CD2	-7.88	116.27	121.00
1	H	376	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	M	414	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	M	416	TYR	CB-CG-CD2	-7.75	116.35	121.00
3	D	858	ARG	NE-CZ-NH2	7.65	124.12	120.30
3	A	594	ARG	NE-CZ-NH2	7.61	124.11	120.30
3	E	540	ARG	NE-CZ-NH1	7.61	124.10	120.30
2	P	212	TYR	CA-CB-CG	-7.57	99.02	113.40
3	B	548	TYR	CB-CG-CD2	-7.52	116.49	121.00
3	A	538	ARG	NE-CZ-NH1	7.50	124.05	120.30
3	B	778	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	H	455	TYR	CB-CG-CD1	7.40	125.44	121.00
3	A	516	ARG	NE-CZ-NH2	-7.38	116.61	120.30
3	C	681	TYR	CB-CG-CD1	-7.34	116.60	121.00
2	K	213	ARG	NE-CZ-NH2	-7.30	116.65	120.30
2	P	247	ARG	NE-CZ-NH2	-7.23	116.69	120.30
2	L	282	ARG	NE-CZ-NH2	-7.22	116.69	120.30
3	F	641	TYR	CB-CG-CD2	-7.22	116.67	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	516	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	Q	450	ARG	NE-CZ-NH2	-7.21	116.70	120.30
3	B	609	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	H	414	ARG	NE-CZ-NH2	-7.05	116.77	120.30
3	F	540	ARG	NE-CZ-NH1	7.05	123.83	120.30
2	N	178	ILE	CB-CA-C	-7.04	97.52	111.60
3	D	858	ARG	NE-CZ-NH1	-7.03	116.78	120.30
2	L	247	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	H	414	ARG	NE-CZ-NH1	6.88	123.74	120.30
3	E	778	ARG	NE-CZ-NH2	-6.88	116.86	120.30
3	C	886	ARG	NE-CZ-NH1	-6.83	116.88	120.30
2	L	297	ARG	NE-CZ-NH2	-6.83	116.89	120.30
3	D	775	ARG	NE-CZ-NH2	-6.79	116.91	120.30
3	B	778	ARG	NE-CZ-NH1	6.75	123.67	120.30
3	A	641	TYR	CB-CG-CD2	-6.74	116.95	121.00
3	A	632	ARG	NE-CZ-NH2	-6.74	116.93	120.30
2	J	213	ARG	NE-CZ-NH2	-6.72	116.94	120.30
3	D	715	MET	CG-SD-CE	-6.70	89.48	100.20
3	C	609	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	G	416	TYR	CB-CG-CD2	-6.64	117.01	121.00
2	L	296	ARG	NE-CZ-NH2	-6.61	116.99	120.30
2	O	248	TYR	CB-CG-CD2	-6.61	117.03	121.00
3	F	583	ARG	NE-CZ-NH2	-6.59	117.01	120.30
3	B	797	ARG	NE-CZ-NH2	-6.57	117.02	120.30
3	B	516	ARG	NE-CZ-NH1	6.54	123.57	120.30
3	F	712	ASP	CB-CG-OD1	6.49	124.14	118.30
3	E	789	LYS	C-N-CD	-6.47	106.37	120.60
2	P	296	ARG	NE-CZ-NH2	-6.46	117.07	120.30
3	C	602	TYR	CB-CG-CD1	6.45	124.87	121.00
1	R	364	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	P	199	ARG	NE-CZ-NH2	-6.42	117.09	120.30
2	K	299	TYR	CB-CG-CD2	-6.30	117.22	121.00
3	D	585	ARG	NE-CZ-NH2	-6.27	117.17	120.30
3	C	828	TYR	CB-CG-CD1	6.26	124.76	121.00
2	J	297	ARG	NE-CZ-NH1	6.20	123.40	120.30
3	E	602	TYR	CB-CG-CD2	-6.16	117.30	121.00
2	L	180	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	H	390	TYR	CB-CG-CD2	-6.12	117.33	121.00
2	O	247	ARG	NE-CZ-NH2	-6.11	117.24	120.30
2	J	178	ILE	CB-CA-C	-6.10	99.40	111.60
3	B	845	VAL	CA-CB-CG2	-5.91	102.04	110.90
3	A	510	PHE	CB-CG-CD1	-5.90	116.67	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	871	TYR	CA-CB-CG	5.89	124.60	113.40
3	C	651	GLY	N-CA-C	-5.89	98.37	113.10
3	F	841	ARG	NE-CZ-NH2	-5.89	117.35	120.30
3	E	791	ASP	CB-CG-OD2	-5.89	113.00	118.30
3	A	585	ARG	NE-CZ-NH2	-5.88	117.36	120.30
3	C	625	PHE	CB-CG-CD1	-5.87	116.69	120.80
1	Q	392	TYR	CB-CG-CD1	-5.82	117.51	121.00
3	A	828	TYR	CB-CG-CD2	-5.82	117.51	121.00
3	D	545	LEU	CB-CA-C	-5.81	99.16	110.20
3	F	828	TYR	CB-CG-CD1	-5.80	117.52	121.00
3	D	625	PHE	CA-CB-CG	5.79	127.80	113.90
3	C	775	ARG	NE-CZ-NH1	5.78	123.19	120.30
3	F	729	THR	CA-CB-CG2	-5.75	104.36	112.40
1	Q	427	ARG	NE-CZ-NH2	-5.73	117.44	120.30
3	F	566	MET	CG-SD-CE	5.72	109.36	100.20
2	O	212	TYR	CB-CG-CD1	-5.71	117.58	121.00
1	R	427	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	P	242	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	K	178	ILE	CB-CA-C	-5.59	100.43	111.60
2	O	196	LEU	CB-CG-CD2	-5.54	101.57	111.00
3	A	575	ARG	NE-CZ-NH2	-5.49	117.56	120.30
3	D	871	TYR	CB-CG-CD2	-5.48	117.71	121.00
3	A	706	PHE	CB-CG-CD2	-5.41	117.01	120.80
3	D	706	PHE	CB-CG-CD1	-5.41	117.01	120.80
3	F	884	LEU	CB-CA-C	-5.36	100.02	110.20
3	D	514	VAL	CA-CB-CG2	-5.36	102.87	110.90
3	C	633	PHE	CB-CG-CD1	-5.35	117.06	120.80
3	F	578	GLN	CG-CD-OE1	-5.32	110.95	121.60
3	D	654	LYS	CA-CB-CG	5.32	125.11	113.40
2	P	203	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	R	436	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	Q	392	TYR	CD1-CE1-CZ	5.29	124.56	119.80
3	A	715	MET	CG-SD-CE	5.28	108.65	100.20
3	A	602	TYR	CB-CG-CD1	5.27	124.17	121.00
3	D	584	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	M	404	ALA	CB-CA-C	5.24	117.96	110.10
3	D	862	MET	CG-SD-CE	5.24	108.58	100.20
3	B	763	ASN	N-CA-C	-5.22	96.90	111.00
3	C	858	ARG	NE-CZ-NH1	-5.22	117.69	120.30
3	A	602	TYR	CA-CB-CG	5.19	123.27	113.40
3	D	556	LEU	CB-CA-C	-5.19	100.33	110.20
2	K	196	LEU	CB-CG-CD1	-5.19	102.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	641	TYR	CB-CG-CD1	5.18	124.11	121.00
2	J	297	ARG	NE-CZ-NH2	-5.15	117.72	120.30
3	C	884	LEU	CB-CG-CD2	-5.15	102.25	111.00
2	P	212	TYR	CB-CG-CD2	5.14	124.09	121.00
3	F	797	ARG	NE-CZ-NH1	5.14	122.87	120.30
3	B	609	ARG	NE-CZ-NH2	-5.13	117.73	120.30
3	D	625	PHE	CB-CA-C	-5.13	100.13	110.40
3	E	704	ARG	NE-CZ-NH1	-5.13	117.73	120.30
3	B	687	ASN	CA-CB-CG	-5.12	102.14	113.40
2	O	213	ARG	NE-CZ-NH2	5.11	122.86	120.30
3	D	548	TYR	CB-CG-CD1	-5.11	117.94	121.00
3	C	625	PHE	CB-CG-CD2	5.08	124.36	120.80
2	N	212	TYR	CB-CG-CD1	-5.08	117.95	121.00
3	F	546	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	H	432	MET	CG-SD-CE	-5.08	92.07	100.20
1	Q	431	LEU	N-CA-C	-5.08	97.29	111.00
3	E	659	PHE	CB-CG-CD1	-5.05	117.26	120.80
2	J	242	ARG	NE-CZ-NH2	-5.05	117.78	120.30
3	B	657	THR	CA-CB-CG2	-5.05	105.33	112.40
1	Q	455	TYR	CB-CG-CD1	5.04	124.03	121.00
1	Q	392	TYR	CB-CG-CD2	5.04	124.02	121.00
3	B	585	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	J	283	PHE	CB-CG-CD2	5.02	124.31	120.80
3	D	772	LEU	CB-CA-C	-5.02	100.67	110.20
1	R	475	TYR	CB-CG-CD2	-5.01	117.99	121.00
1	H	416	TYR	CB-CG-CD1	-5.01	118.00	121.00
2	L	263	VAL	CB-CA-C	-5.01	101.89	111.40
2	J	262	VAL	CB-CA-C	-5.00	101.89	111.40

There are no chirality outliers.

All (23) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
3	F	888	ILE	Peptide,Mainchain
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	15	0
1	I	1144	0	1182	16	0
1	M	1144	0	1182	10	0
1	Q	1144	0	1182	23	0
1	R	1144	0	1182	11	0
2	J	1091	0	1117	22	0
2	K	1091	0	1117	27	0
2	L	1091	0	1117	21	0
2	N	1091	0	1117	11	0
2	O	1091	0	1117	29	0
2	P	1091	0	1117	19	0
3	A	2975	0	3080	53	0
3	B	2966	0	3066	40	0
3	C	2975	0	3080	69	0
3	D	2975	0	3080	49	0
3	E	2975	0	3080	38	0
3	F	2984	0	3084	38	0
All	All	31260	0	32264	493	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 (493) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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	1.85	0.76
3:F:710:ASP:O	3:F:710:ASP:CG	2.22	0.75
2:K:190:GLN:HE21	2:K:190:GLN:C	1.88	0.74
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
2:O:276:LEU:C	2:O:276:LEU:HD23	2.09	0.73
3:D:720:ARG:O	3:D:720:ARG:HG2	1.88	0.73
2:J:276:LEU:HD23	2:J:276:LEU:C	2.10	0.72
3:D:697:LEU:HD23	3:D:697:LEU:C	2.09	0.72
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
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
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
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
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
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:I:412:LEU:HD23	1:I:412:LEU:C	2.17	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:Q:412:LEU:HD23	1:Q:412:LEU:C	2.18	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:Q:366:GLU:H	1:Q:366:GLU:CD	1.98	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
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
2:L:165:ASP:OD1	2:L:165:ASP:C	2.36	0.62
3:D:747:ALA:N	3:D:773:SER:OG	2.32	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
1:H:336:LEU:HD22	1:H:336:LEU:C	2.21	0.61
2:K:291:TRP:HA	2:K:291:TRP:HE3	1.65	0.61
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:D:697:LEU:C	3:D:697:LEU:CD2	2.68	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
1:I:438:ILE:HD13	1:I:438:ILE:C	2.23	0.59
3:C:790:PRO:O	3:C:790:PRO:CG	2.51	0.59
2:O:165:ASP:OD1	2:O:165:ASP:C	2.40	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
2:L:163:GLN:O	2:L:163:GLN:HG2	2.03	0.58
2:P:266:ASP:OD1	2:P:266:ASP:C	2.41	0.58
3:D:535:VAL:HB	3:D:551:LEU:HB2	1.85	0.58
3:C:774:GLN:HG3	3:C:774:GLN:O	2.03	0.58
2:L:299:TYR:CG	2:L:299:TYR:OXT	2.56	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: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:F:595:LEU:N	3:F:595:LEU:HD12	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:365:LEU:O	1:R:366:GLU:C	2.43	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
3:C:564:LYS:NZ	3:C:573:GLU:O	2.38	0.56
2:K:190:GLN:C	2:K:190:GLN:NE2	2.58	0.56
2:O:276:LEU:C	2:O:276:LEU:CD2	2.74	0.56
3:C:733:LEU:HD23	3:C:733:LEU:C	2.25	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
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: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
3:F:576:LEU:C	3:F:576:LEU:HD12	2.26	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
2:O:183:LEU:C	2:O:183:LEU:HD23	2.28	0.54
1:G:330:LEU:C	1:G:330:LEU:HD12	2.27	0.53
2:J:276:LEU:C	2:J:276:LEU:CD2	2.76	0.53
2:K:183:LEU:HD22	2:K:183:LEU:C	2.28	0.53
2:L:183:LEU:HD23	2:L:183:LEU:C	2.29	0.53
3:A:582:VAL:CG2	3:A:595:LEU:HB2	2.37	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
3:C:525:ASP:OD1	3:C:525:ASP:C	2.45	0.53
1:H:475:TYR:CD2	1:H:475:TYR:O	2.62	0.53
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
2:L:202:VAL:O	2:L:203:ARG:HB2	2.08	0.52
3:C:613:LYS:O	3:C:614:ALA:C	2.46	0.52
3:D:619:GLU:O	3:D:621:GLU:N	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:299:TYR:CD2	2:J:299:TYR:OXT	2.63	0.52
3:D:779:ARG:O	3:D:825:LYS:N	2.42	0.52
3:D:862:MET:SD	3:D:862:MET:C	2.88	0.52
3:D:551:LEU:HB3	3:D:555:ALA:HB3	1.89	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
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:455:TYR:O	1:Q:456:GLU:C	2.48	0.52
3:C:800:LEU:N	3:C:800:LEU:HD12	2.25	0.52
3:E:662:LEU:HD12	3:E:662:LEU:C	2.26	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
3:D:706:PHE:HD1	3:D:706:PHE:H	1.59	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
2:O:268:ARG:O	2:O:269:HIS:C	2.49	0.51
3:C:551:LEU:N	3:C:551:LEU:HD12	2.26	0.50
3:E:784:CYS:O	3:E:784:CYS:SG	2.67	0.50
2:O:202:VAL:O	2:O:203:ARG:CB	2.59	0.50
1:Q:392:TYR:CD1	1:Q:392:TYR:C	2.85	0.50
1:R:463:THR:HG23	1:R:463:THR:O	2.11	0.50
3:C:651:GLY:O	3:C:653:GLY:N	2.44	0.50
1:Q:330:LEU:N	1:Q:330:LEU:CD2	2.74	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
2:N:248:TYR:CD1	2:N:248:TYR:C	2.85	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
2:K:286:ALA:H	2:K:291:TRP:HE1	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:787:GLU:OE2	3:E:789:LYS:NZ	2.45	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
3:F:862:MET:HG2	3:F:862:MET:O	2.12	0.49
1:I:412:LEU:HD23	1:I:412:LEU:O	2.13	0.49
2:P:196:LEU:CD2	2:P:270:LYS:H	2.26	0.49
3:A:510:PHE:CD1	3:A:510:PHE:C	2.86	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: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
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:H:408:LEU:C	1:H:408:LEU:HD23	2.34	0.48
2:O:248:TYR:CD1	2:O:248:TYR:C	2.87	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
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
1:H:462:ALA:O	1:H:463:THR:C	2.51	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:721:ASP:OD1	3:B:721:ASP:C	2.52	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:R:432:MET:HG2	1:R:434:ASP:H	1.77	0.47
2:K:266:ASP:OD1	2:K:266:ASP:C	2.46	0.47
3:A:778:ARG:HB3	3:A:824:TYR:CB	2.44	0.47
3:C:657:THR:O	3:C:657:THR:HG22	2.14	0.47
3:E:705:ALA:O	3:E:709:GLN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:165:ASP:OD1	2:J:165:ASP:C	2.53	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
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
1:Q:412:LEU:C	1:Q:412:LEU:CD2	2.83	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
3:B:525:ASP:OD1	3:B:525:ASP:C	2.51	0.47
1:G:330:LEU:HD12	1:G:330:LEU:O	2.15	0.46
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: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
1:H:394:ASP:C	1:H:394:ASP:OD1	2.54	0.46
1:I:434:ASP:OD1	1:I:434:ASP:C	2.53	0.46
2:O:286:ALA:HB3	2:O:291:TRP:CZ2	2.50	0.46
3:C:884:LEU:HD23	3:C:884:LEU:HA	1.30	0.46
3:F:788:VAL:O	3:F:788:VAL:HG23	2.16	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
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
3:C:650:THR:O	3:C:651:GLY:C	2.53	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: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:E:715:MET:SD	3:E:715:MET:C	2.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:620:ILE:H	3:D:660:SER:HG	1.63	0.46
3:A:828:TYR:CD2	3:A:828:TYR:C	2.90	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
1:G:419:PHE:CD1	1:G:419:PHE:C	2.89	0.45
2:K:215:LEU:HA	2:K:215:LEU:HD23	1.73	0.45
3:A:686:ILE:O	3:A:686:ILE:HG23	2.16	0.45
3:A:540:ARG:O	3:A:540:ARG:HG2	2.16	0.45
3:B:759:VAL:O	3:B:760:GLU:C	2.53	0.45
3:D:833:LEU:O	3:D:833:LEU:HG	2.16	0.45
3:E:828:TYR:C	3:E:828:TYR:CD1	2.90	0.45
3:F:598:LEU:HD12	3:F:599:PRO:HD2	1.98	0.45
1:I:364:ARG:O	1:I:365:LEU:C	2.54	0.45
3:A:817:GLU:H	3:A:817:GLU:CD	2.18	0.45
3:C:540:ARG:O	3:C:540:ARG:HG2	2.17	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
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
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
1:I:394:ASP:OD1	1:I:394:ASP:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:248:TYR:HD1	2:N:248:TYR:C	2.19	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
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
1:Q:400:PRO:O	1:Q:401:ASP:C	2.56	0.44
3:C:800:LEU:N	3:C:800:LEU:CD1	2.81	0.44
3:E:525:ASP:OD1	3:E:525:ASP:C	2.56	0.44
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:H:434:ASP:OD1	1:H:434:ASP:C	2.53	0.44
1:M:470:LEU:HD12	1:M:470:LEU:HA	1.80	0.44
2:N:248:TYR:O	2:N:248:TYR:CD1	2.64	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
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
2:J:201:LEU:HB3	2:J:206:LEU:CD2	2.48	0.43
2:P:199:ARG:HD3	2:P:199:ARG:C	2.38	0.43
3:C:710:ASP:O	3:C:710:ASP:CG	2.57	0.43
2:K:215:LEU:HD22	2:K:267:PRO:HD2	1.99	0.43
3:B:573:GLU:HG3	3:B:573:GLU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:384:VAL:O	1:G:384:VAL:HG12	2.18	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:845:VAL:O	3:B:845:VAL:CG2	2.64	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
3:F:658:THR:O	3:F:715:MET:HE1	2.18	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:B:662:LEU:O	3:B:663:LYS:C	2.55	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:E:582:VAL:O	3:E:582:VAL:HG13	2.17	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:559:VAL:O	3:D:559:VAL:HG12	2.18	0.43
3:D:720:ARG:O	3:D:720:ARG:CG	2.58	0.43
3:F:776:LEU:O	3:F:886:ARG:NE	2.52	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:759:VAL:O	3:A:760:GLU:C	2.57	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:A:598:LEU:C	3:A:604:GLU:HG3	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:582:VAL:HB	3:A:593:LEU:HB2	2.00	0.42
3:A:714:ILE:O	3:A:714:ILE:CG2	2.61	0.42
3:B:733:LEU:HD13	3:C:881:GLU:O	2.20	0.42
2:K:256:GLN:N	2:K:256:GLN:OE1	2.52	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: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:A:605:LYS:HZ3	3:A:607:VAL:CG2	2.33	0.42
3:B:510:PHE:CD1	3:B:510:PHE:C	2.93	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
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: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
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: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
1:I:336:LEU:HD22	1:I:336:LEU:C	2.40	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:D:864:THR:O	3:D:865:LEU:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:R:455:TYR:O	1:R:456:GLU:C	2.58	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: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
3:F:671:ASN:C	3:F:671:ASN:OD1	2.56	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
2:L:178:ILE:CG2	2:L:206:LEU:HD13	2.50	0.41
2:O:266:ASP:C	2:O:266:ASP:OD1	2.59	0.41
3:D:785:LYS:HB2	3:D:811:TYR:HB3	2.01	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: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:F:611:LEU:HB3	3:F:680:GLU:HB3	2.02	0.41
1:G:400:PRO:O	1:G:401:ASP:C	2.58	0.41
2:K:206:LEU:HA	2:K:207:PRO:HD2	1.96	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:K:276:LEU:HD23	2:K:276:LEU:C	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:434:ASP:OD1	1:G:434:ASP:C	2.58	0.40
1:I:399:PRO:HA	1:I:400:PRO:HD2	1.91	0.40
1:M:444:VAL:O	1:M:445:ARG:C	2.59	0.40
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:F:617:ILE:HD13	3:F:617:ILE:HG21	1.83	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:626:ALA:O	3:A:627:PRO:C	2.60	0.40
3:A:772:LEU:HD11	3:A:831:HIS:HD1	1.86	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
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:F:828:TYR:C	3:F:828:TYR:CD1	2.84	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:Q:435:PRO:O	1:Q:436:ARG:C	2.59	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	144/146 (99%)	135 (94%)	8 (6%)	1 (1%)	22	63
1	H	144/146 (99%)	132 (92%)	8 (6%)	4 (3%)	5	30
1	I	144/146 (99%)	131 (91%)	12 (8%)	1 (1%)	22	63
1	M	144/146 (99%)	132 (92%)	9 (6%)	3 (2%)	7	36
1	Q	144/146 (99%)	130 (90%)	8 (6%)	6 (4%)	3	22
1	R	144/146 (99%)	126 (88%)	13 (9%)	5 (4%)	3	25
2	J	135/137 (98%)	124 (92%)	9 (7%)	2 (2%)	10	46
2	K	135/137 (98%)	123 (91%)	9 (7%)	3 (2%)	6	35
2	L	135/137 (98%)	118 (87%)	15 (11%)	2 (2%)	10	46
2	N	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
2	O	135/137 (98%)	124 (92%)	8 (6%)	3 (2%)	6	35
2	P	135/137 (98%)	122 (90%)	11 (8%)	2 (2%)	10	46
3	A	382/409 (93%)	365 (96%)	16 (4%)	1 (0%)	41	77
3	B	381/409 (93%)	363 (95%)	16 (4%)	2 (0%)	29	69
3	C	382/409 (93%)	363 (95%)	15 (4%)	4 (1%)	15	55
3	D	382/409 (93%)	361 (94%)	17 (4%)	4 (1%)	15	55
3	E	382/409 (93%)	363 (95%)	16 (4%)	3 (1%)	19	60
3	F	383/409 (94%)	362 (94%)	15 (4%)	6 (2%)	9	44
All	All	3966/4152 (96%)	3700 (93%)	214 (5%)	52 (1%)	16	48

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	456	GLU

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

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Mol	Chain	Res	Type
1	Q	333	ALA
1	Q	455	TYR
3	F	683	ILE
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	120/120 (100%)	120 (100%)	0	100	100
1	H	120/120 (100%)	118 (98%)	2 (2%)	60	78
1	I	120/120 (100%)	119 (99%)	1 (1%)	81	89
1	M	120/120 (100%)	119 (99%)	1 (1%)	81	89
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%)	111 (99%)	1 (1%)	78	87
2	K	112/112 (100%)	110 (98%)	2 (2%)	59	77
2	L	112/112 (100%)	111 (99%)	1 (1%)	78	87
2	N	112/112 (100%)	111 (99%)	1 (1%)	78	87
2	O	112/112 (100%)	111 (99%)	1 (1%)	78	87
2	P	112/112 (100%)	111 (99%)	1 (1%)	78	87
3	A	317/336 (94%)	317 (100%)	0	100	100
3	B	315/336 (94%)	315 (100%)	0	100	100
3	C	317/336 (94%)	315 (99%)	2 (1%)	86	92
3	D	317/336 (94%)	314 (99%)	3 (1%)	78	87
3	E	317/336 (94%)	316 (100%)	1 (0%)	92	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	318/336 (95%)	317 (100%)	1 (0%)	92	95
All	All	3293/3408 (97%)	3275 (100%)	18 (0%)	89	93

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	242	ARG
2	K	190	GLN
2	K	256	GLN
2	L	248	TYR
1	H	392	TYR
1	H	436	ARG
1	I	438	ILE
1	M	376	ARG
2	N	248	TYR
2	O	248	TYR
2	P	223	PHE
3	C	519	PHE
3	C	706	PHE
3	D	551	LEU
3	D	644	PHE
3	D	797	ARG
3	E	585	ARG
3	F	581	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	673	GLN
3	B	527	HIS
3	E	774	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

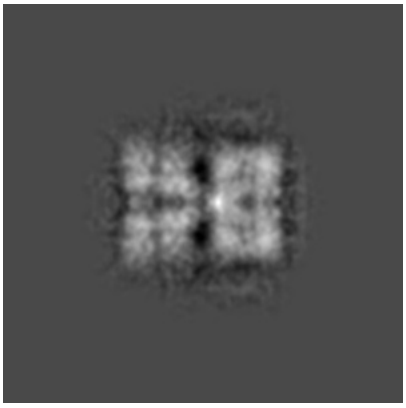
This section contains visualisations of the EMDB entry EMD-3882. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

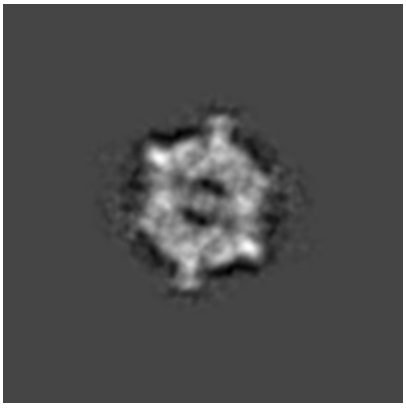
6.1 Orthogonal projections (i)

6.1.1 Primary map

X



Y

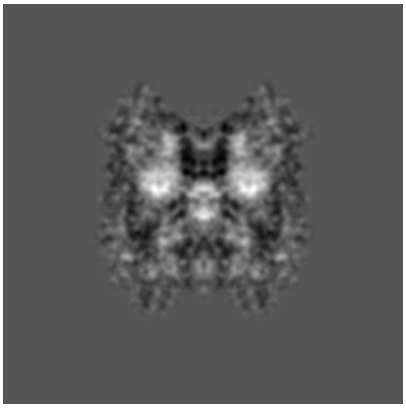


Z

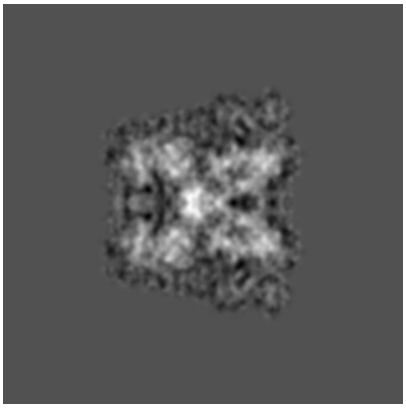
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

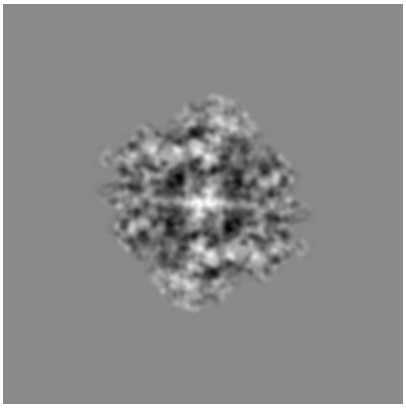
6.2.1 Primary map



X Index: 96



Y Index: 96

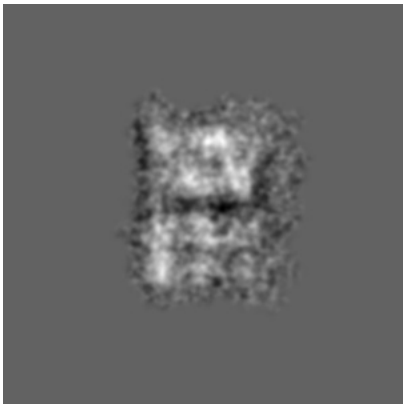


Z Index: 96

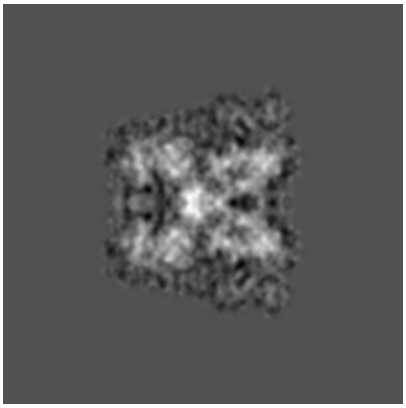
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

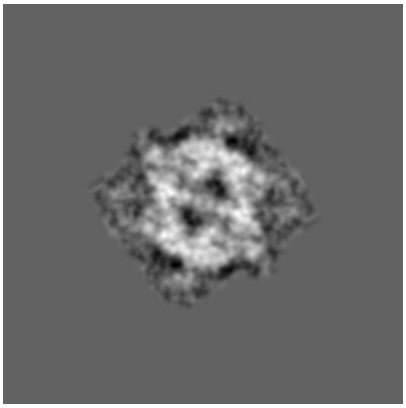
6.3.1 Primary map



X Index: 114



Y Index: 96

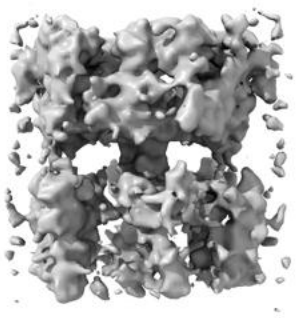


Z Index: 106

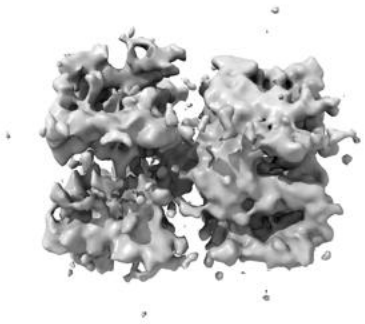
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

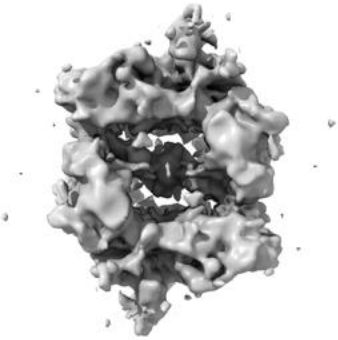
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

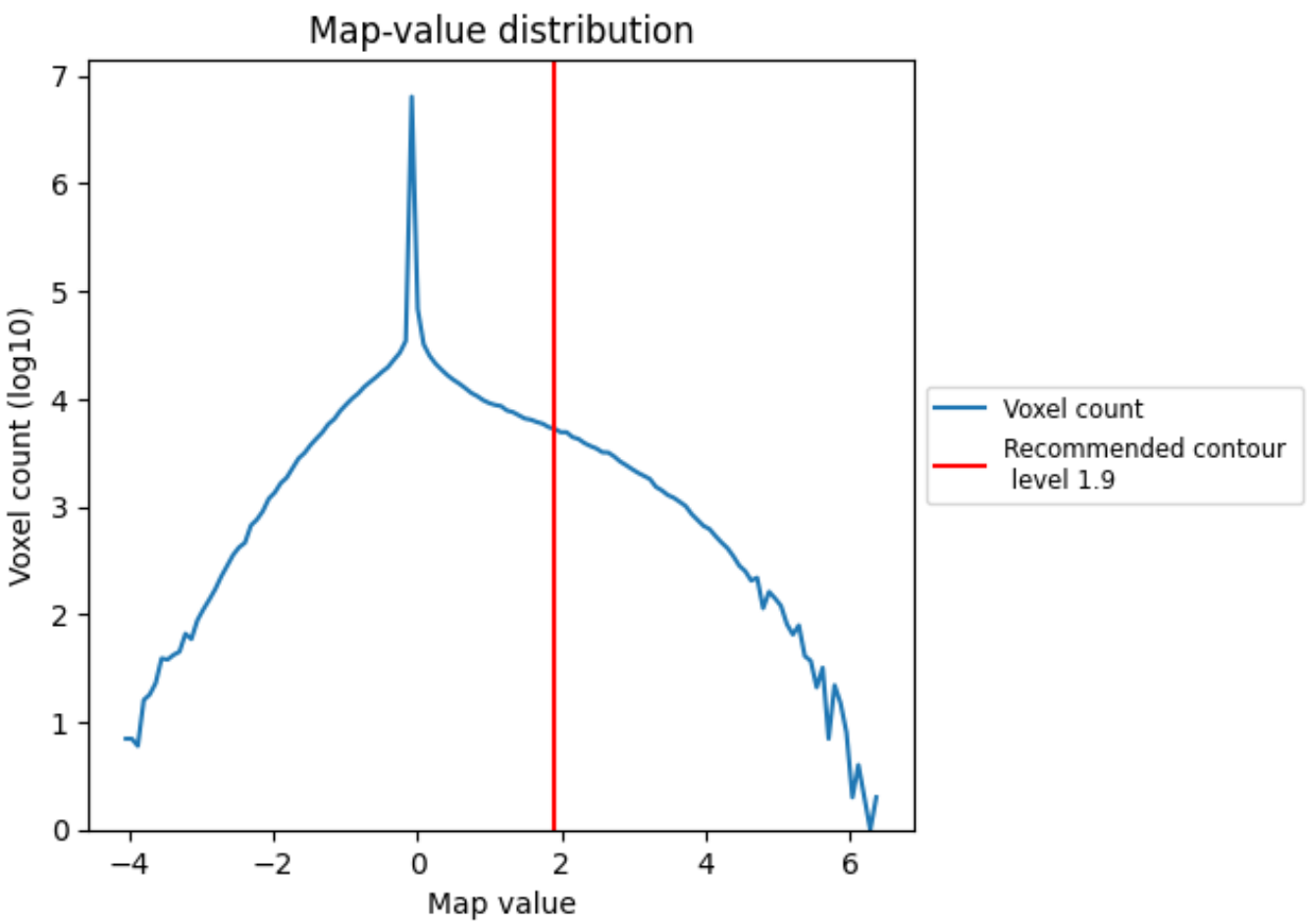
6.5 Mask visualisation (i)

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

7 Map analysis (i)

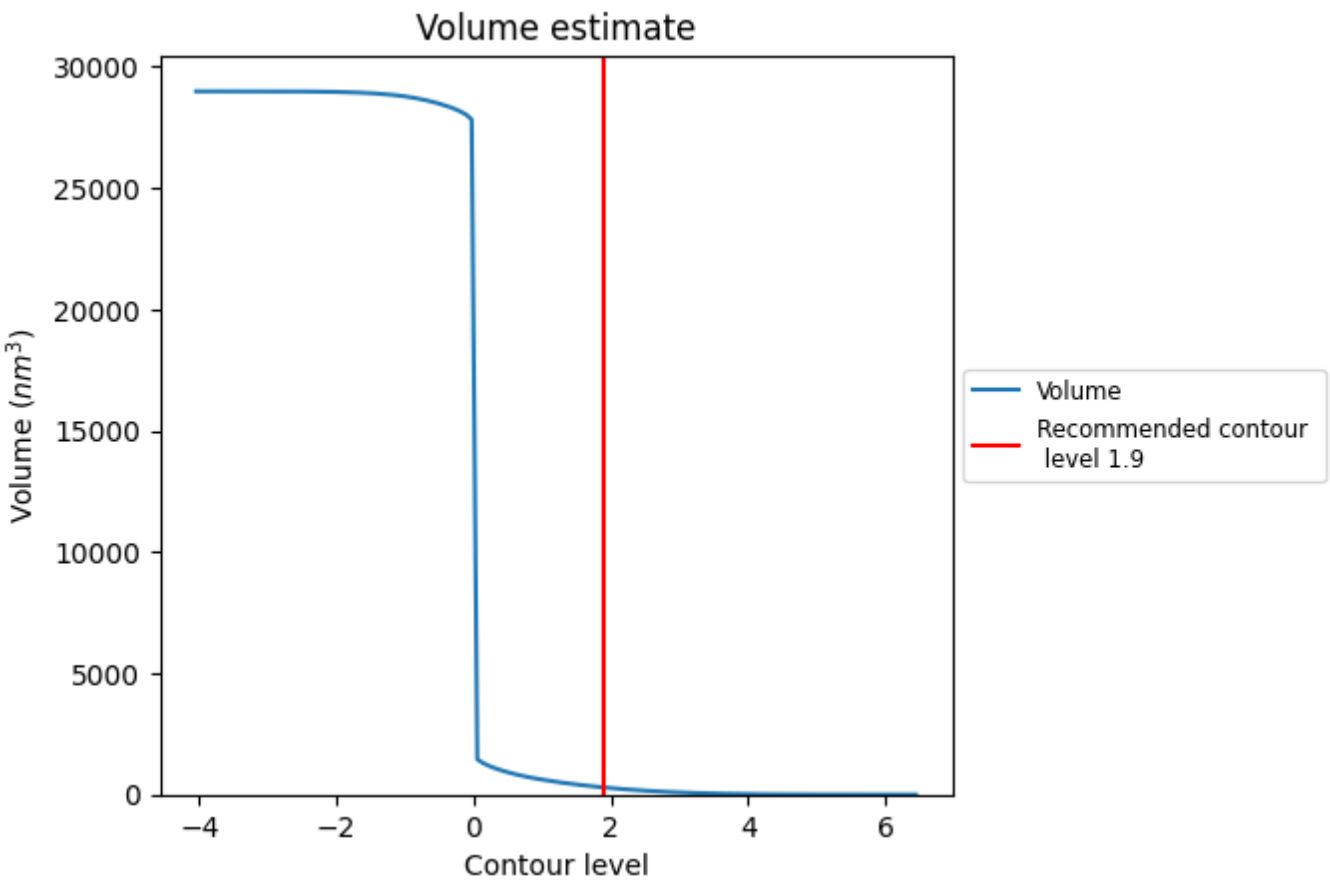
This section contains the results of statistical analysis of the map.

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.

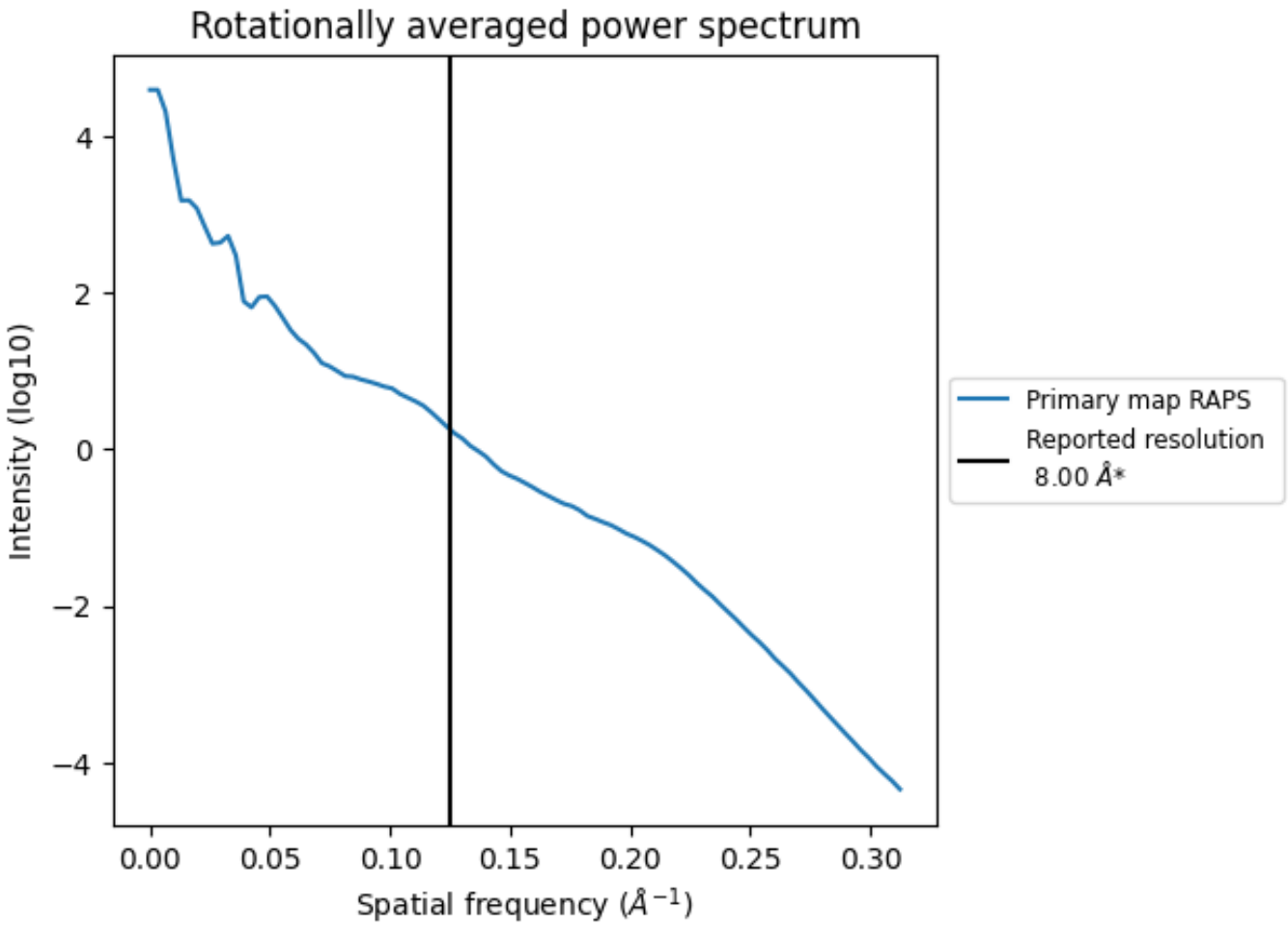
7.2 Volume estimate (i)



The volume at the recommended contour level is 294 nm^3; 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 (i)



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

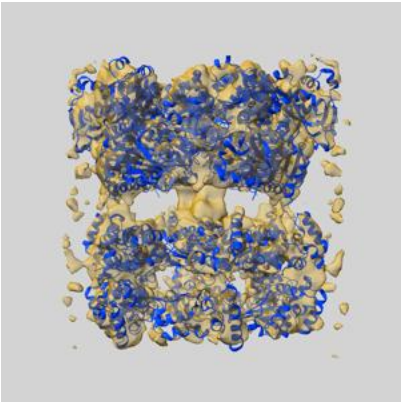
8 Fourier-Shell correlation (i)

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

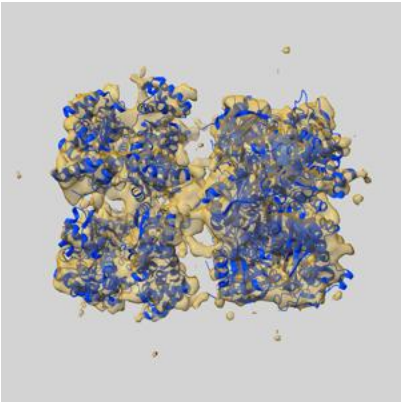
9 Map-model fit (i)

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.

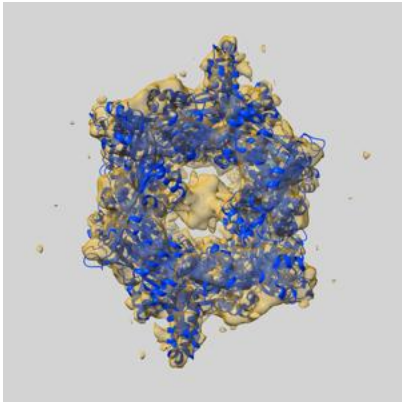
9.1 Map-model overlay (i)



X



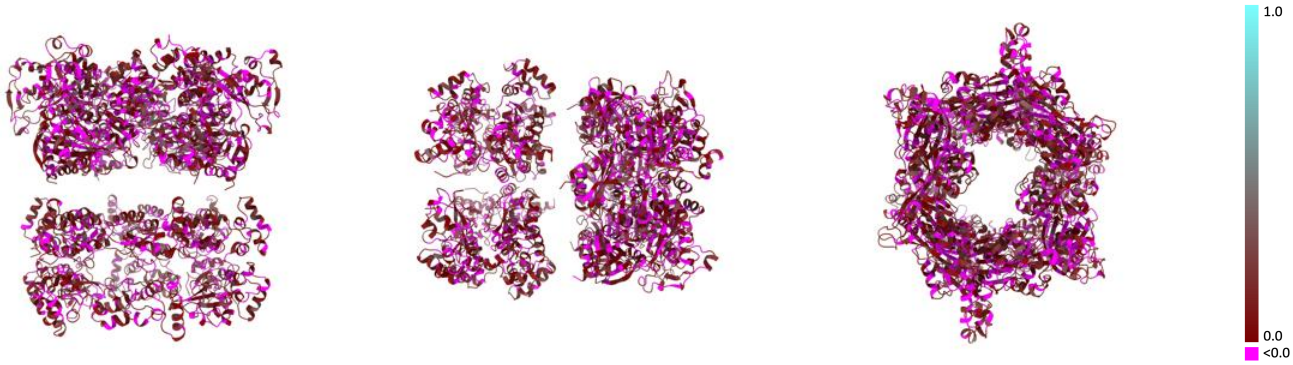
Y



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.

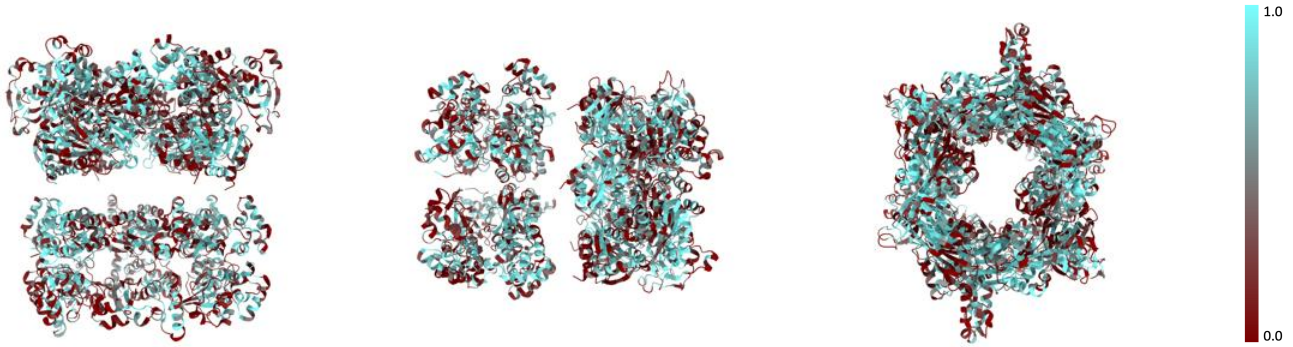
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

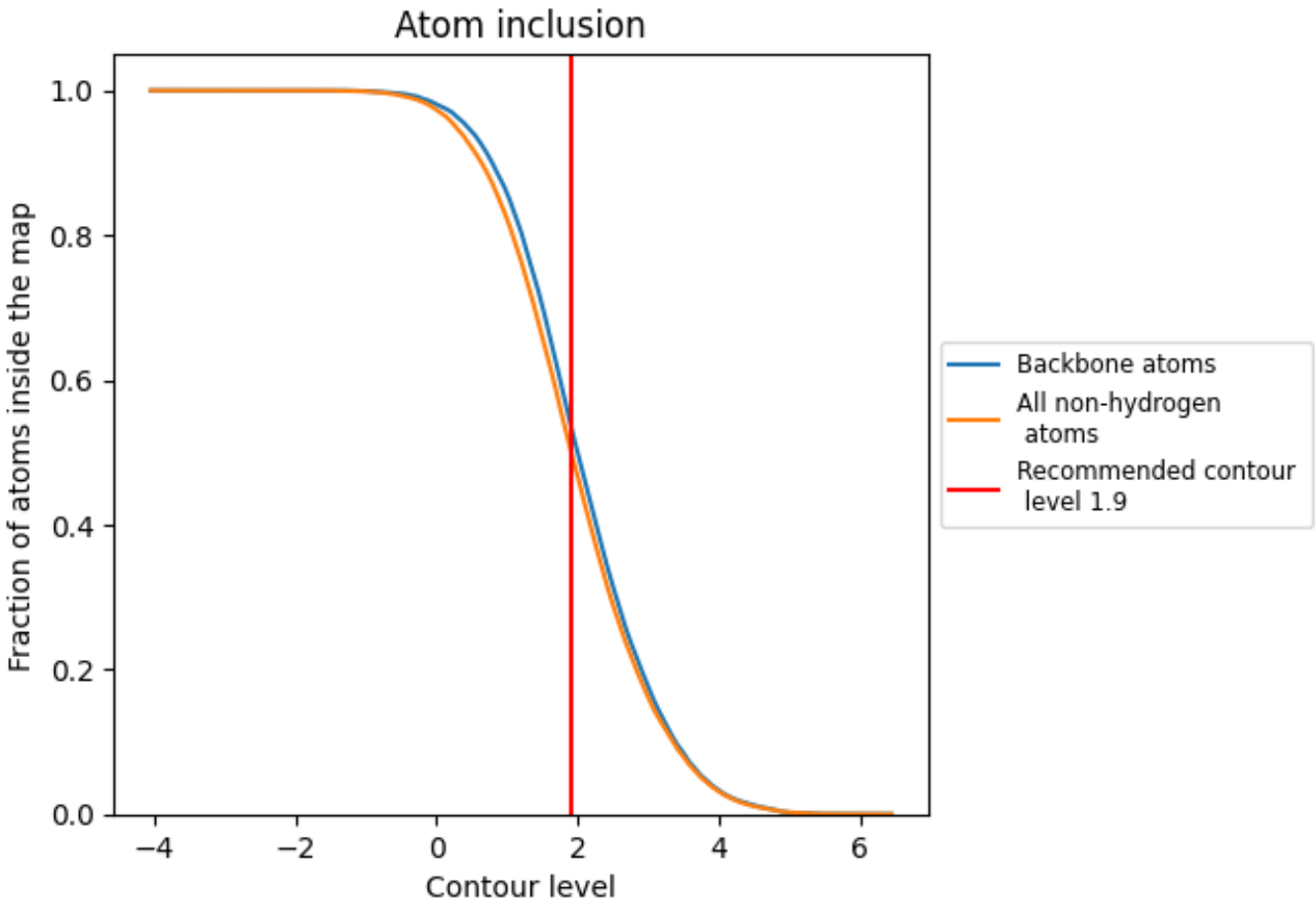
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)

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	0.5047	0.0690
A	0.5148	0.0660
B	0.5071	0.0510
C	0.5393	0.0640
D	0.5486	0.0700
E	0.5203	0.0570
F	0.5314	0.0580
G	0.4437	0.0870
H	0.5644	0.0760
I	0.5644	0.0800
J	0.3979	0.0840
K	0.3791	0.0730
L	0.4741	0.0730
M	0.4536	0.0830
N	0.4111	0.0920
O	0.3810	0.0740
P	0.4948	0.0690
Q	0.5590	0.0800
R	0.5626	0.0730