



Full wwPDB EM Validation Report ⓘ

May 7, 2026 – 03:22 PM JST

PDB ID : 8Z5U / pdb_00008z5u
EMDB ID : EMD-39782
Title : Cryo-EM structure of the rod-export apparatus with partial hook within the polar flagellar motor
Authors : Zhang, L.; Tan, J.X.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2024-04-18
Resolution : 3.04 Å(reported)
Based on initial model : .

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 EMD 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

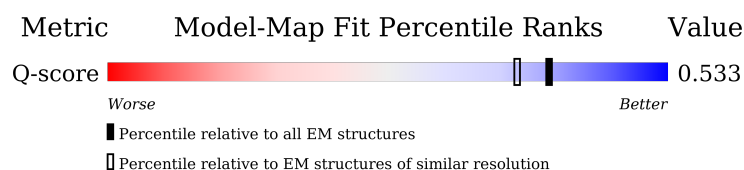
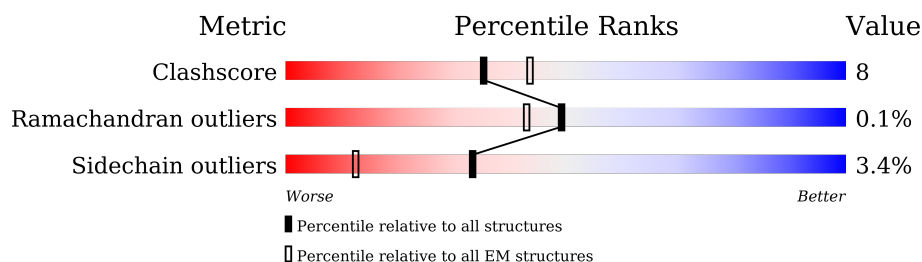
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 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.



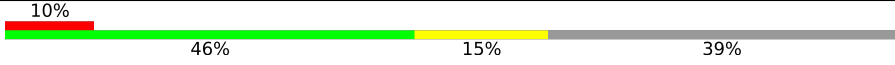
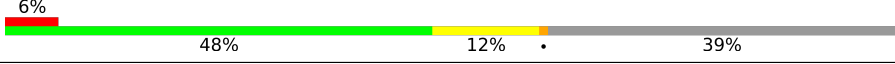
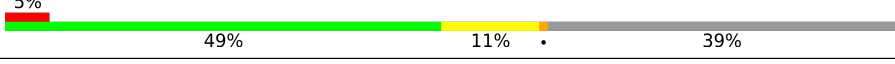
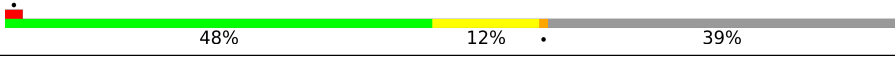
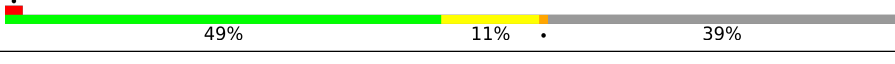
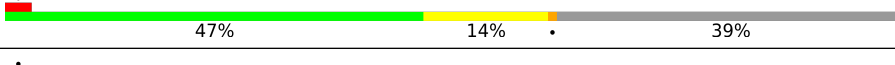
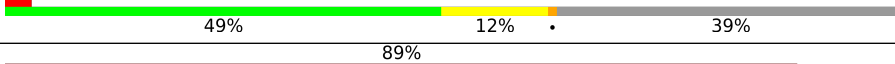
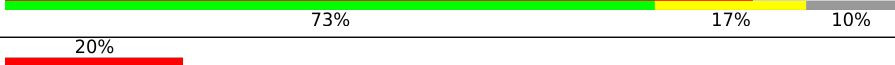
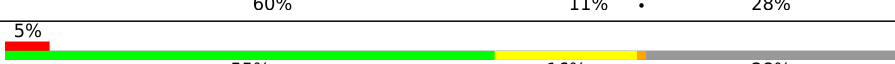
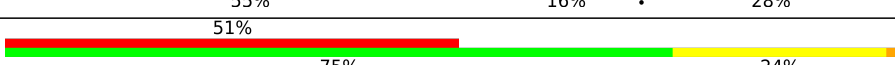
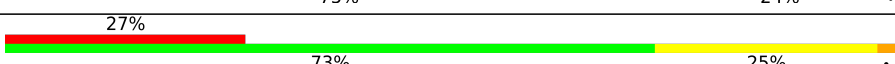
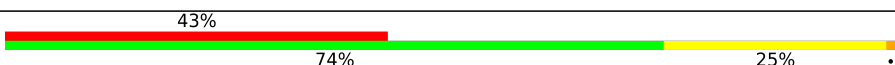
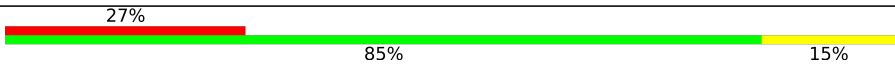
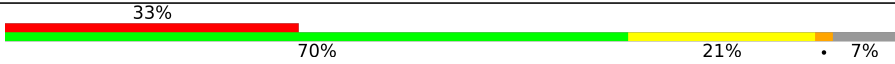
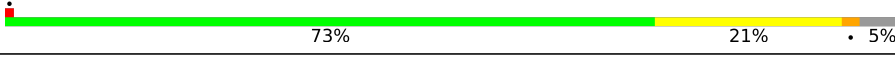
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13952 (2.54 - 3.54)

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	D	437	32% 50% 11% 39%
1	E	437	27% 51% 9% 39%
1	F	437	21% 49% 11% 39%
1	G	437	15% 46% 14% 39%

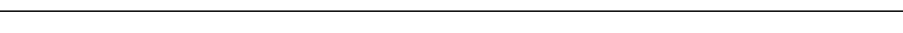
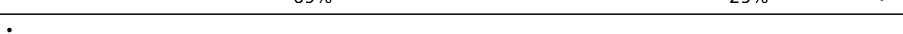
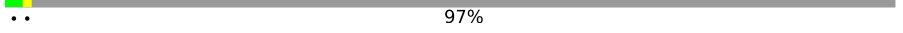
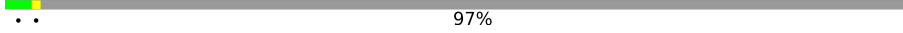
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Mol	Chain	Length	Quality of chain
1	H	437	
1	I	437	
1	J	437	
1	K	437	
1	L	437	
1	M	437	
1	N	437	
1	O	437	
2	0	199	
2	9	199	
3	1	289	
3	2	289	
3	3	289	
3	y	289	
3	z	289	
4	4	89	
4	5	89	
4	6	89	
4	7	89	
5	8	260	
6	A	262	
6	AP	262	
6	AQ	262	
6	AR	262	
6	AS	262	

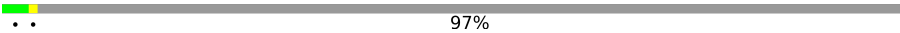
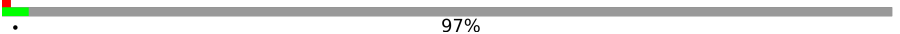
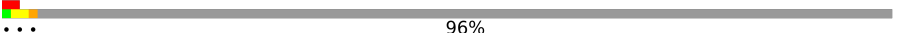
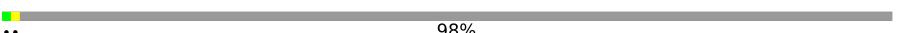
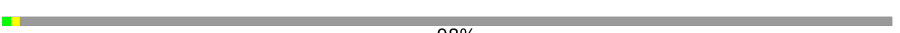
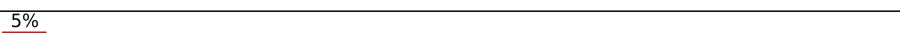
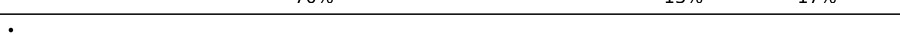
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Mol	Chain	Length	Quality of chain
6	AT	262	 77% 16% 5%
6	AU	262	 74% 20% 5%
6	AV	262	 77% 16% 5%
6	AW	262	 82% 17% .
6	AX	262	 79% 19% .
6	AY	262	 81% 18% .
6	AZ	262	 78% 21% .
6	Aa	262	 79% 20% .
6	B	262	 77% 22% .
6	C	262	 78% 20% .
6	P	262	 77% 21% .
6	Q	262	 82% 16% .
6	R	262	 81% 18% .
6	S	262	 75% 24% .
6	T	262	 69% 29% .
6	U	262	 79% 20% .
6	V	262	 79% 20% .
6	W	262	 74% 25% .
6	X	262	 81% 18% .
6	Y	262	 81% 17% .
6	Z	262	 83% 15% .
6	a	262	 80% 19% .
7	AA	580	 97%
7	AB	580	 97%
7	AC	580	 97%

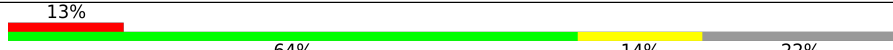
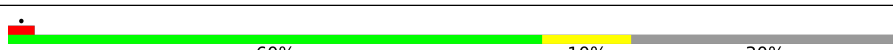
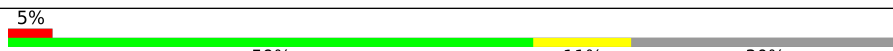
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Mol	Chain	Length	Quality of chain
7	AD	580	 97%
7	AE	580	 97%
7	AF	580	 96%
7	AG	580	 98%
7	AH	580	 98%
7	AI	580	 98%
7	AJ	580	 96%
7	AK	580	 96%
7	AL	580	 5% 94%
7	AM	580	 5% 94%
7	AN	580	 5% 94%
7	AO	580	 5% 94%
8	b	131	 69% 14% 17%
8	c	131	 8% 66% 15% 18%
8	d	131	 5% 70% 13% 17%
8	e	131	 66% 15% 18%
8	f	131	 69% 13% 18%
9	g	137	 5% 79% 16% 5%
9	h	137	 72% 23% 5%
9	i	137	 64% 27% 5%
9	j	137	 81% 13% 5%
9	k	137	 75% 20% 5%
9	l	137	 74% 20% 5%
10	m	249	 77% 22%
10	n	249	 70% 29%

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Mol	Chain	Length	Quality of chain
10	o	249	
10	p	249	
10	q	249	
11	r	103	
11	s	103	
11	t	103	
11	u	103	
11	v	103	
11	w	103	
12	x	376	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 118072 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 Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	E	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	F	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	G	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	H	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	I	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	J	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	K	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	L	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	M	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	N	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		
1	O	268	Total	C	N	O	S	0	0
			2057	1270	356	426	5		

- Molecule 2 is a protein called Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	180	Total	C	N	O	S	0	0
			1361	876	231	253	1		
2	9	180	Total	C	N	O	S	0	0
			1361	876	231	253	1		

- Molecule 3 is a protein called Flagellar biosynthetic protein FlpP.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	207	Total	C	N	O	S	0	0
			1599	1055	243	282	19		
3	2	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		
3	3	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		
3	y	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		
3	z	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		

- Molecule 4 is a protein called Flagellar biosynthetic protein FliQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	89	Total	C	N	O	S	0	0
			722	489	107	117	9		
4	5	89	Total	C	N	O	S	0	0
			722	489	107	117	9		
4	6	89	Total	C	N	O	S	0	0
			722	489	107	117	9		
4	7	89	Total	C	N	O	S	0	0
			722	489	107	117	9		

- Molecule 5 is a protein called Flagellar biosynthetic protein FliR.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	242	Total	C	N	O	S	0	0
			1896	1265	295	315	21		

- Molecule 6 is a protein called Flagellar basal-body rod protein FlgG.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	B	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	C	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	AP	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	AQ	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	AR	248	Total	C	N	O	S	0	0
			1858	1151	317	382	8		
6	AS	248	Total	C	N	O	S	0	0
			1858	1151	317	382	8		
6	AT	249	Total	C	N	O	S	0	0
			1866	1156	318	383	9		
6	AU	248	Total	C	N	O	S	0	0
			1858	1151	317	382	8		
6	AV	248	Total	C	N	O	S	0	0
			1858	1151	317	382	8		
6	AW	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	AX	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	AY	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	AZ	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	Aa	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	P	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	Q	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	R	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	S	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	T	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	U	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	V	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	W	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	X	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	Y	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
6	Z	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		

- Molecule 7 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AA	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AB	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AC	20	Total	C	N	O	S	0	0
			139	84	24	30	1		
7	AD	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AE	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AF	23	Total	C	N	O	S	0	0
			158	97	27	33	1		
7	AG	11	Total	C	N	O		0	0
			73	46	13	14			
7	AH	11	Total	C	N	O		0	0
			73	46	13	14			
7	AI	11	Total	C	N	O		0	0
			73	46	13	14			
7	AJ	24	Total	C	N	O	S	0	0
			163	100	28	34	1		
7	AK	25	Total	C	N	O	S	0	0
			169	104	29	35	1		
7	AL	32	Total	C	N	O	S	0	0
			220	134	38	46	2		
7	AM	33	Total	C	N	O	S	0	0
			224	136	39	47	2		
7	AN	33	Total	C	N	O	S	0	0
			224	136	39	47	2		
7	AO	32	Total	C	N	O	S	0	0
			220	134	38	46	2		

- Molecule 8 is a protein called Flagellar basal body rod protein FlgB.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	109	Total	C	N	O	S	0	0
			845	523	155	166	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	107	Total	C	N	O	S	0	0
			835	518	153	163	1		
8	d	109	Total	C	N	O	S	0	0
			845	523	155	166	1		
8	e	108	Total	C	N	O	S	0	0
			837	519	154	163	1		
8	f	108	Total	C	N	O	S	0	0
			837	519	154	163	1		

- Molecule 9 is a protein called Flagellar basal-body rod protein FlgC.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	h	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	i	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	j	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	k	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	l	130	Total	C	N	O	S	0	0
			983	605	168	203	7		

- Molecule 10 is a protein called Flagellar basal-body rod protein FlgF.

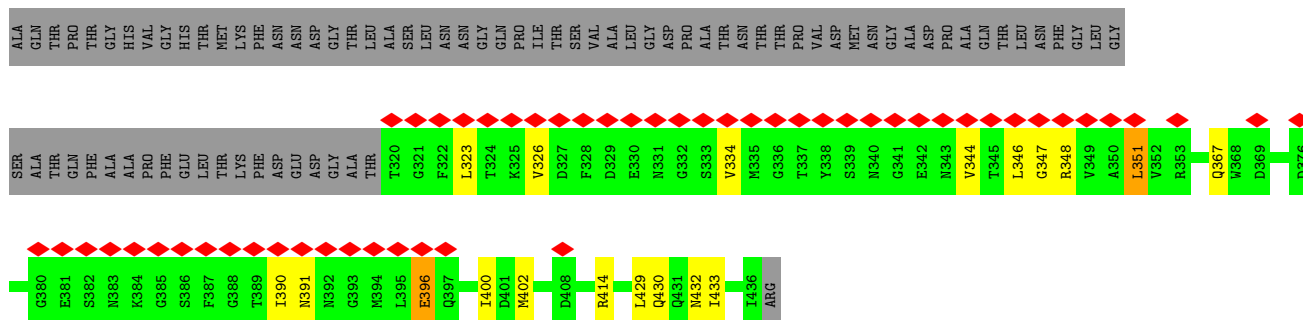
Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
10	n	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
10	o	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
10	p	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
10	q	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		

- Molecule 11 is a protein called Flagellar hook-basal body complex protein FliE.

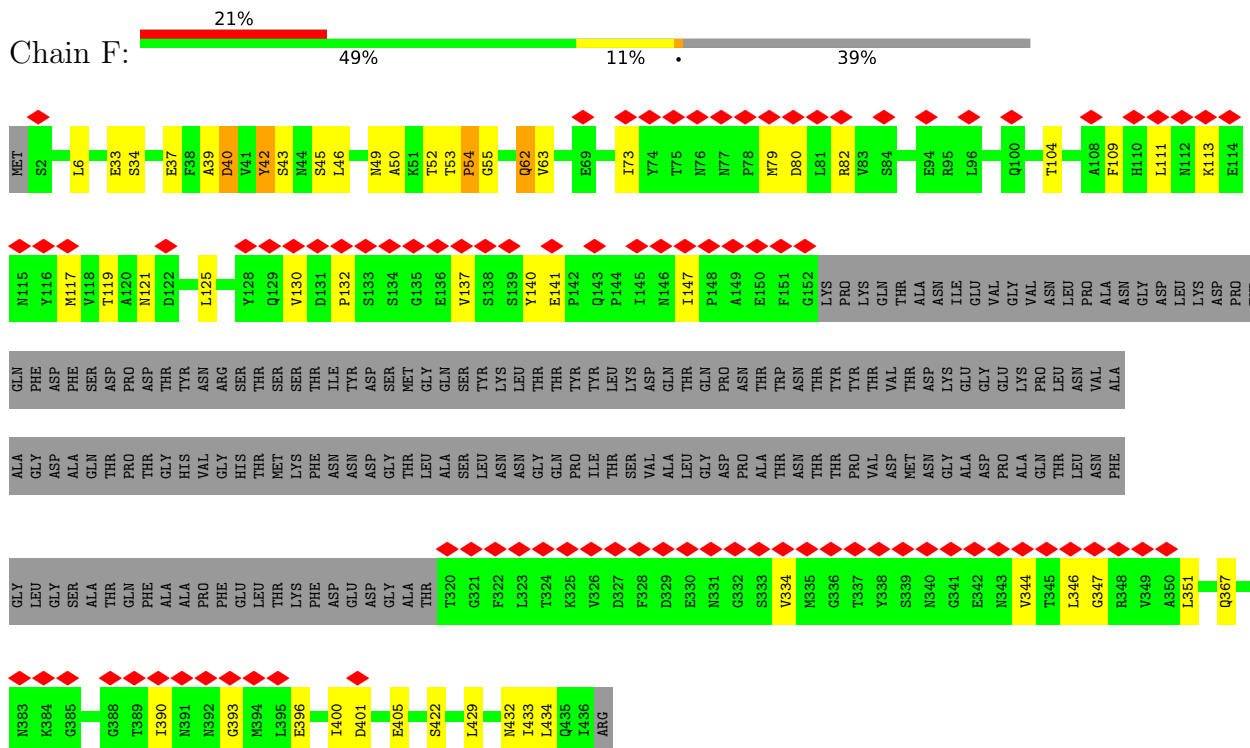
Mol	Chain	Residues	Atoms					AltConf	Trace
11	r	72	Total	C	N	O	S	0	0
			560	345	99	113	3		
11	s	80	Total	C	N	O	S	0	0
			605	372	108	122	3		
11	t	80	Total	C	N	O	S	0	0
			605	372	108	122	3		
11	u	72	Total	C	N	O	S	0	0
			560	345	99	113	3		
11	v	72	Total	C	N	O	S	0	0
			560	345	99	113	3		
11	w	40	Total	C	N	O	S	0	0
			311	194	53	61	3		

- Molecule 12 is a protein called Flagellar biosynthetic protein FlhB.

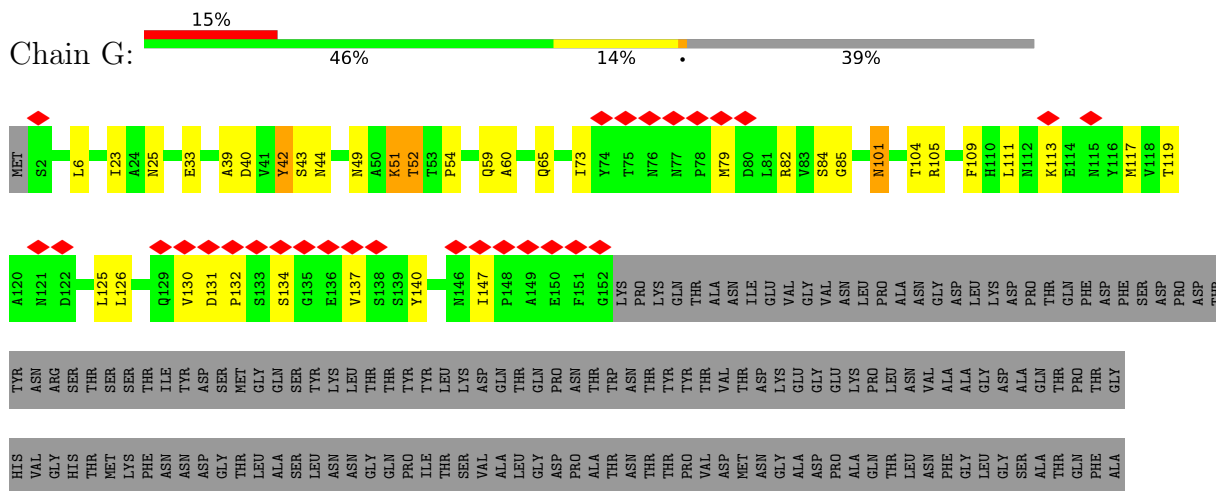
Mol	Chain	Residues	Atoms					AltConf	Trace
12	x	71	Total	C	N	O	S	0	0
			552	370	83	95	4		

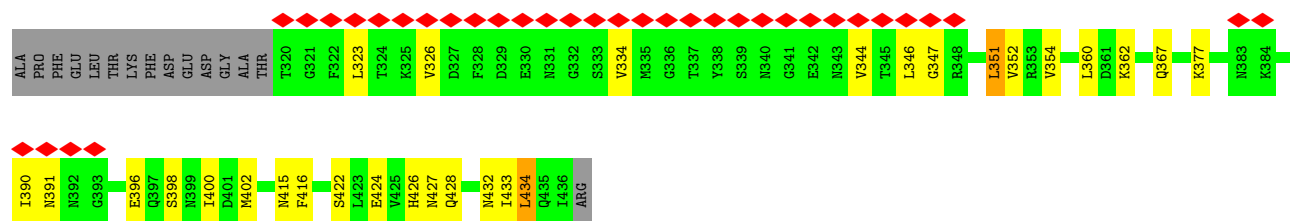


- Molecule 1: Flagellar hook protein FlgE

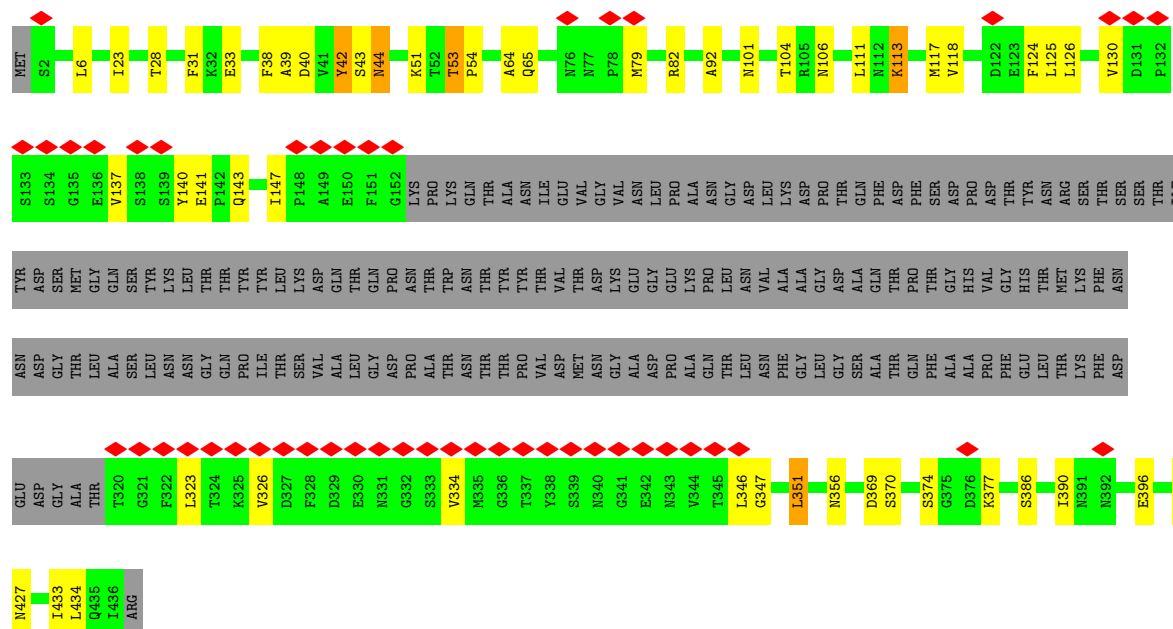


- Molecule 1: Flagellar hook protein FlgE

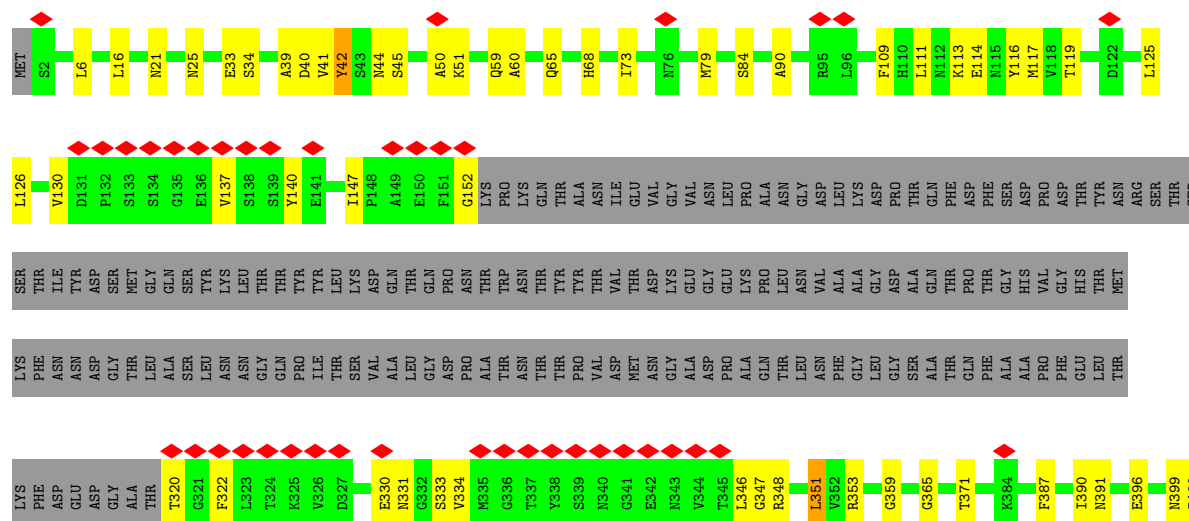




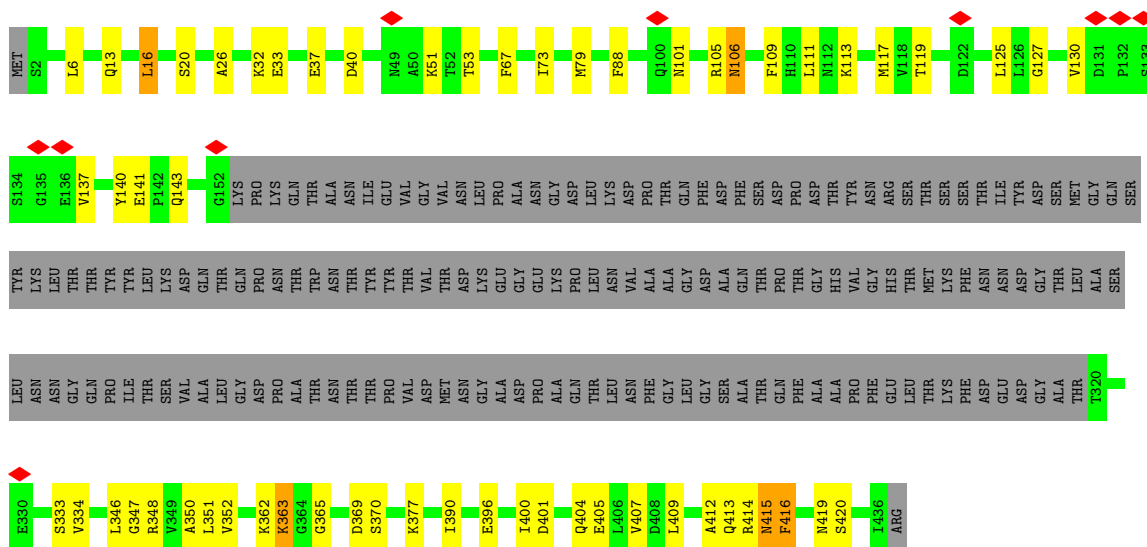
• Molecule 1: Flagellar hook protein FlgE



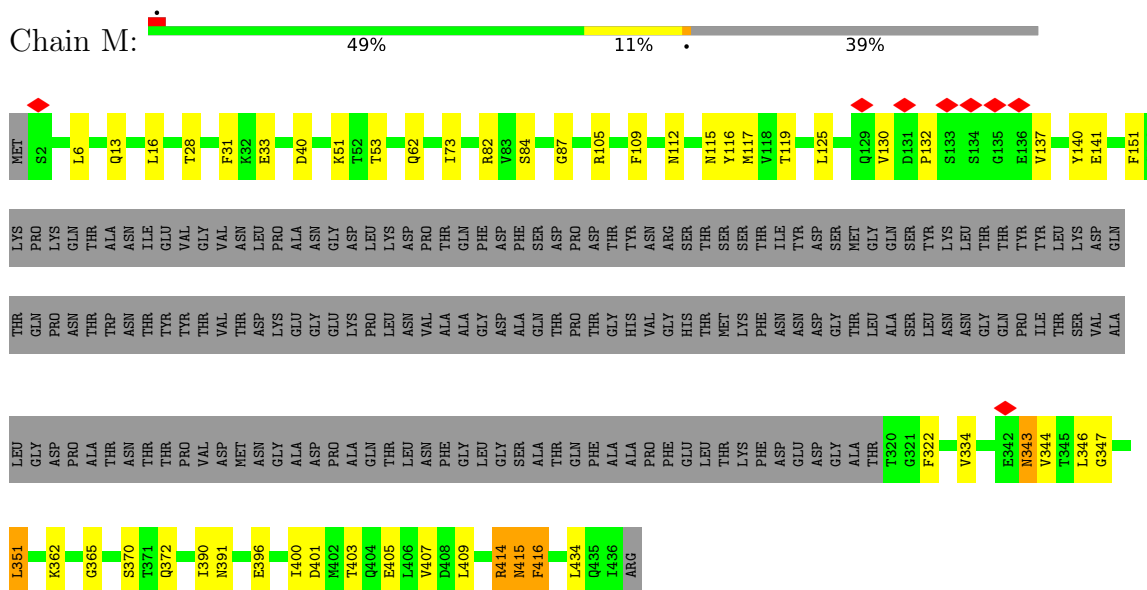
• Molecule 1: Flagellar hook protein FlgE



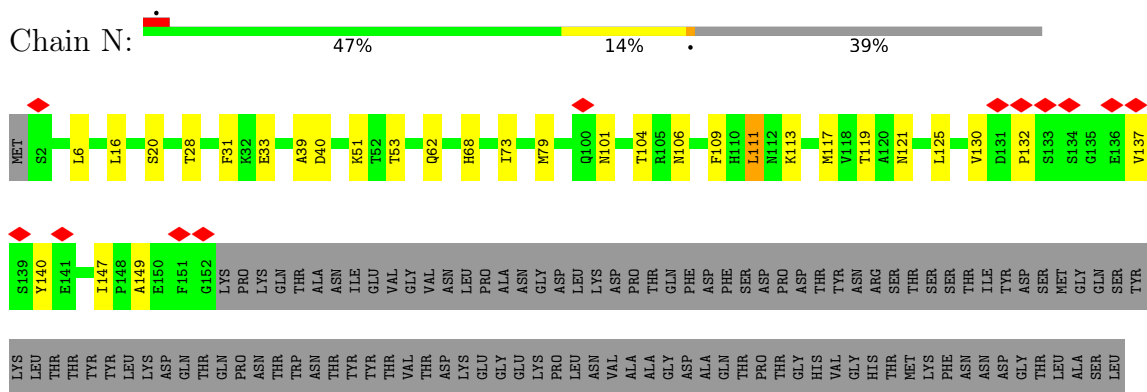


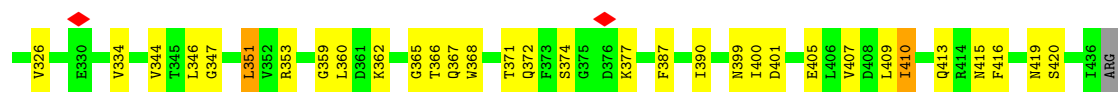


- Molecule 1: Flagellar hook protein FlgE

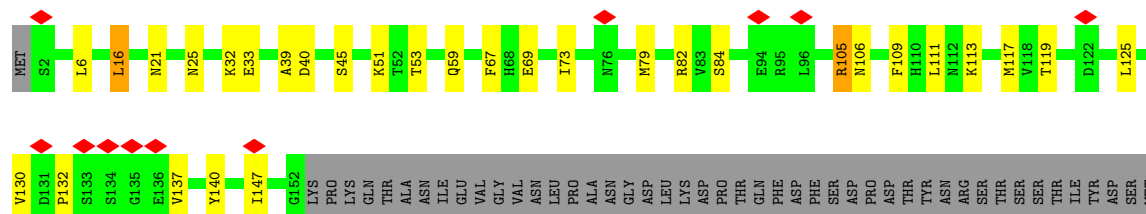


- Molecule 1: Flagellar hook protein FlgE

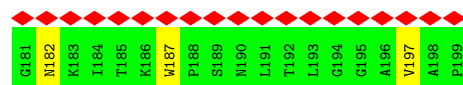
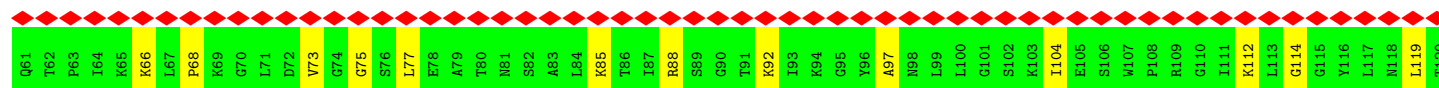




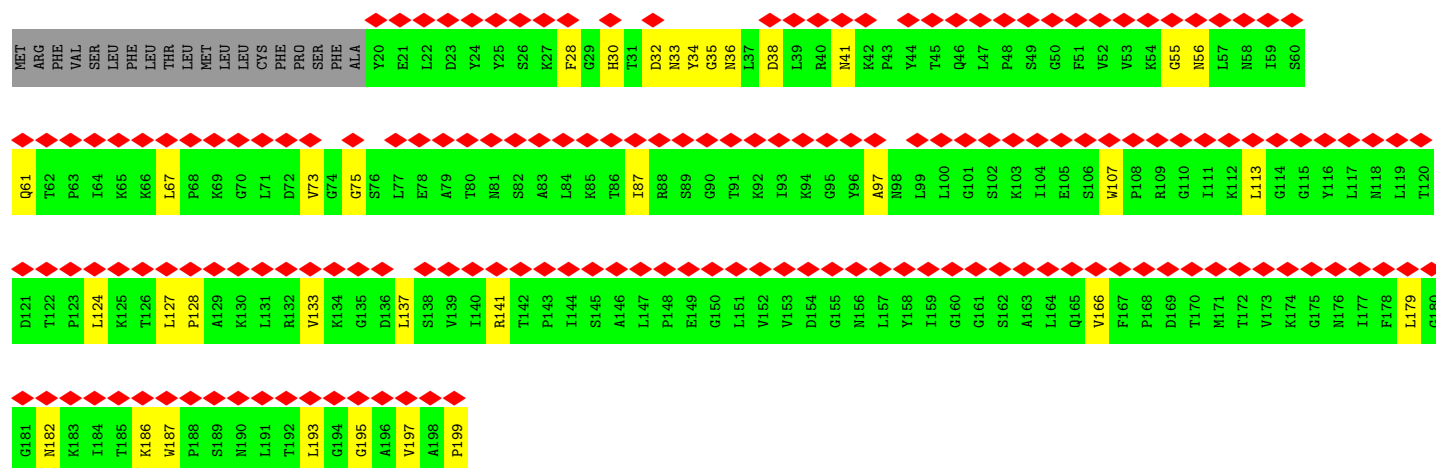
Chain 0: 49% 12% 39%



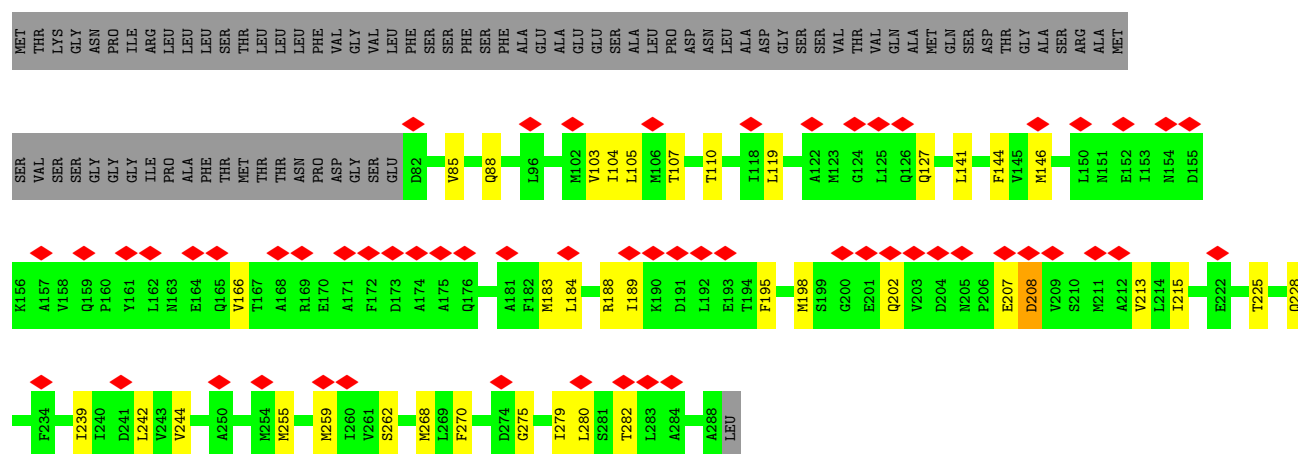
Chain 0: 89% 67% 22% 10%



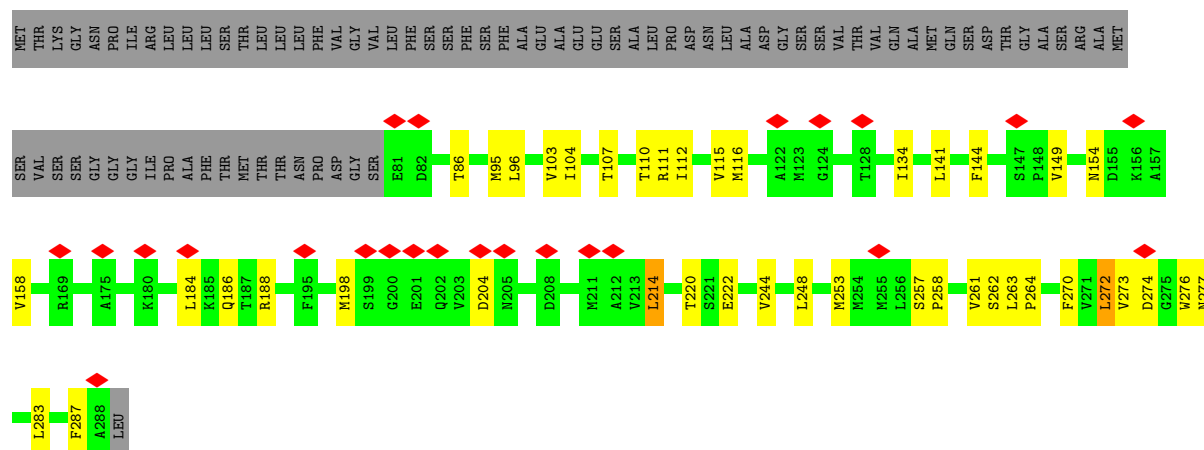
Chain 9: 84% 17% 10%



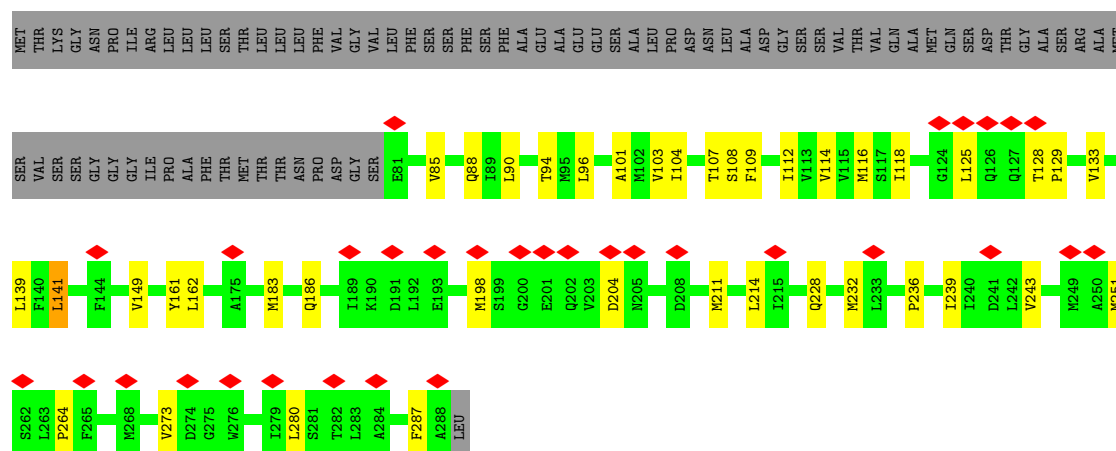
• Molecule 3: Flagellar biosynthetic protein FlpP



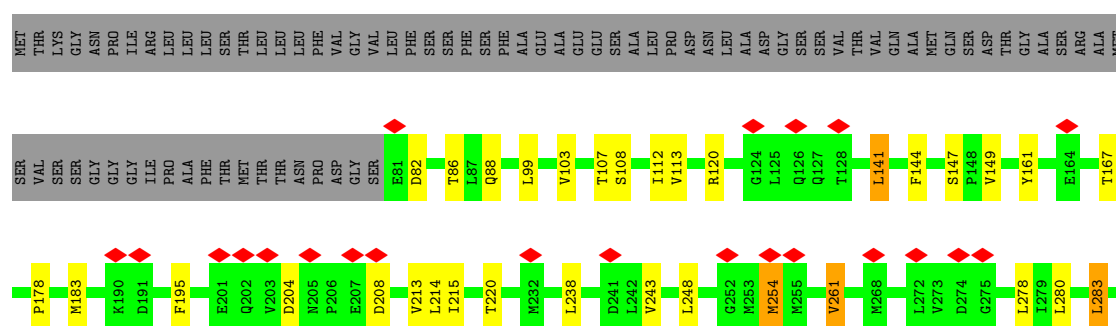
• Molecule 3: Flagellar biosynthetic protein FlpP



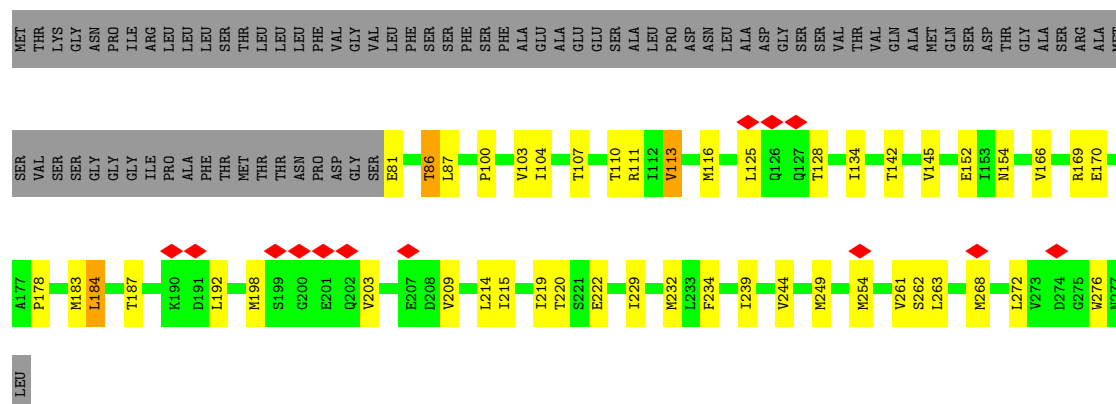
• Molecule 3: Flagellar biosynthetic protein FlpP



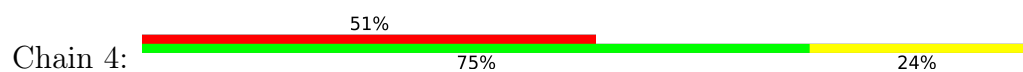
• Molecule 3: Flagellar biosynthetic protein FliP

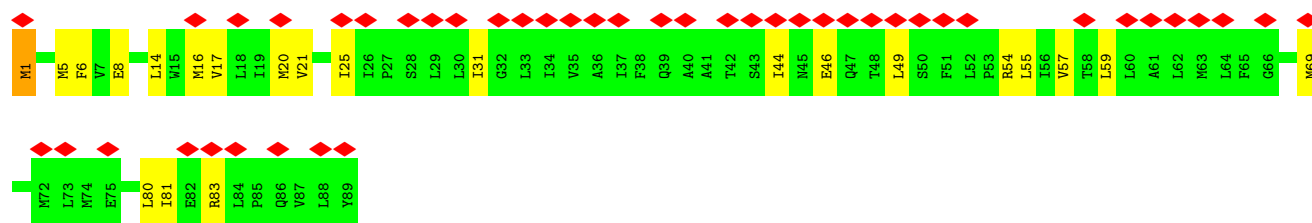


• Molecule 3: Flagellar biosynthetic protein FliP

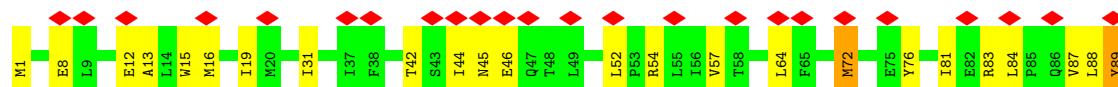
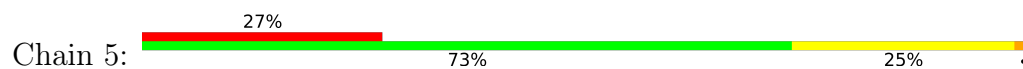


• Molecule 4: Flagellar biosynthetic protein FliQ

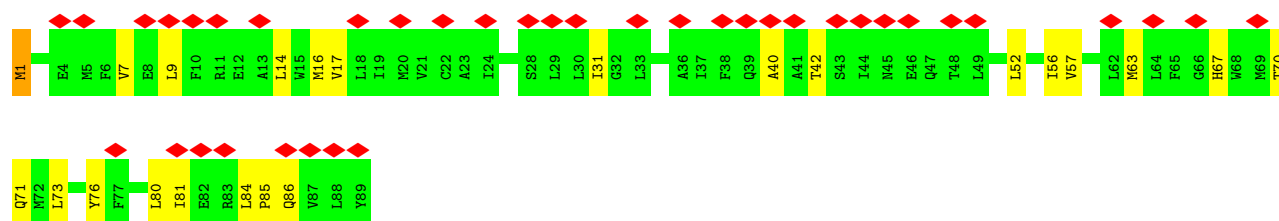
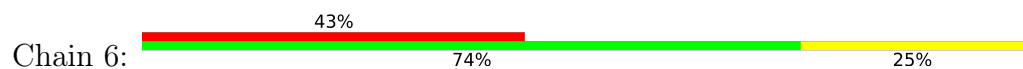




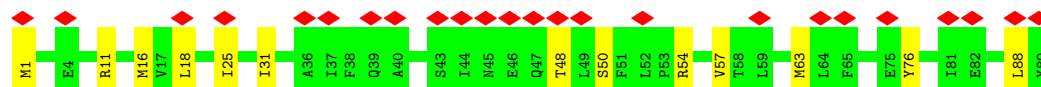
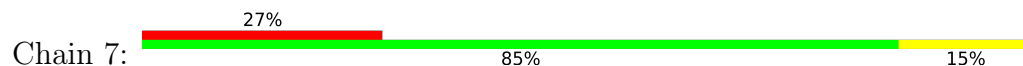
• Molecule 4: Flagellar biosynthetic protein FliQ



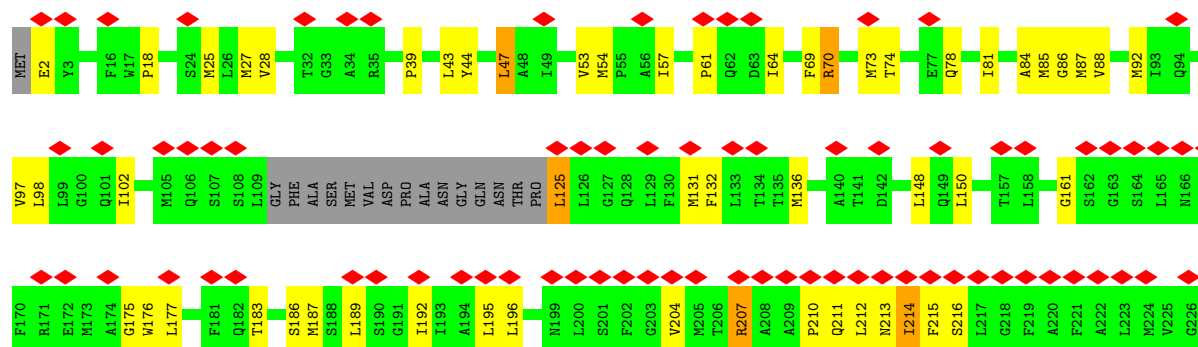
• Molecule 4: Flagellar biosynthetic protein FliQ

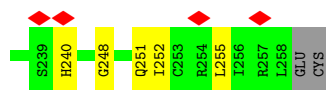


• Molecule 4: Flagellar biosynthetic protein FliQ



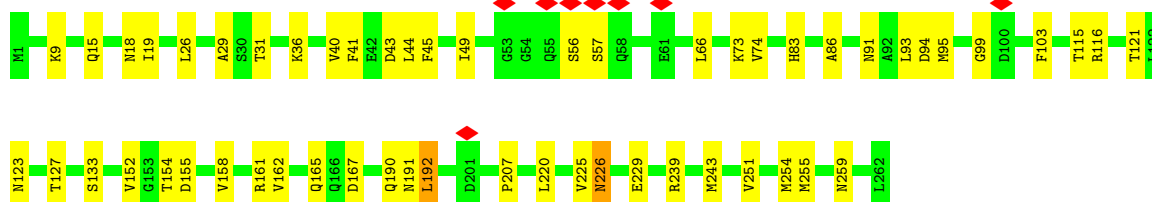
• Molecule 5: Flagellar biosynthetic protein FliR





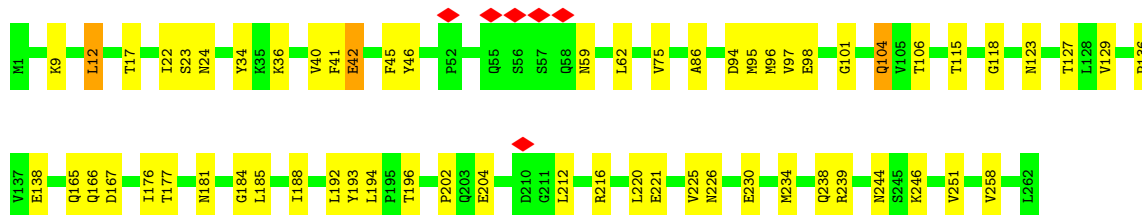
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain A: 79% 20%



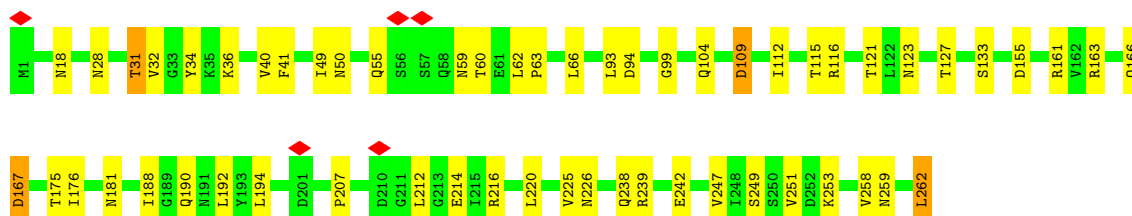
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain B: 77% 22%



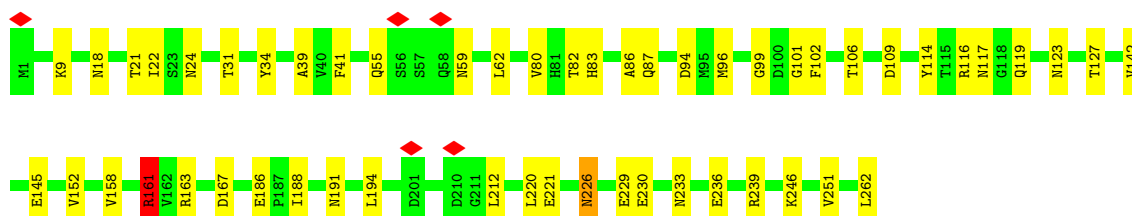
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain C: 78% 20%



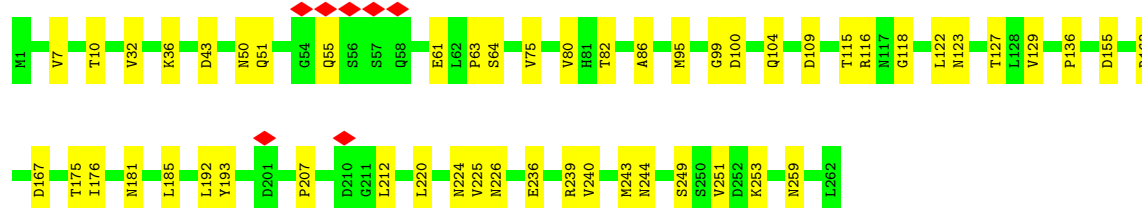
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain AP: 80% 19%



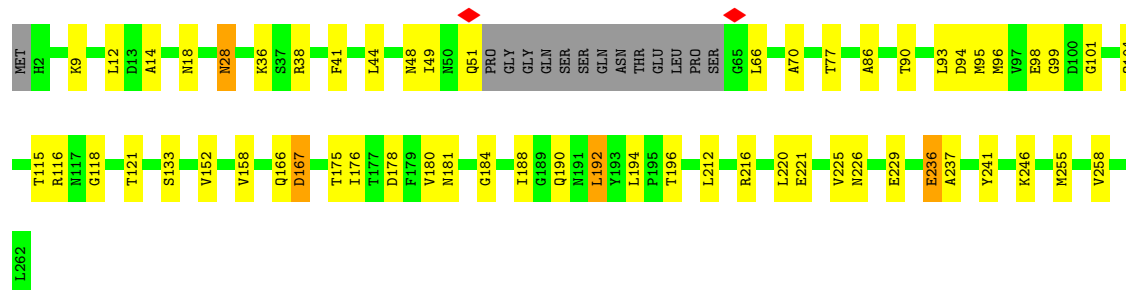
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain AQ:  80% 20%



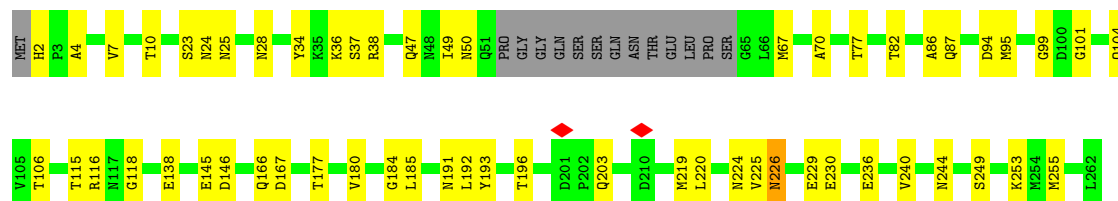
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain AR:  73% 21% 5%



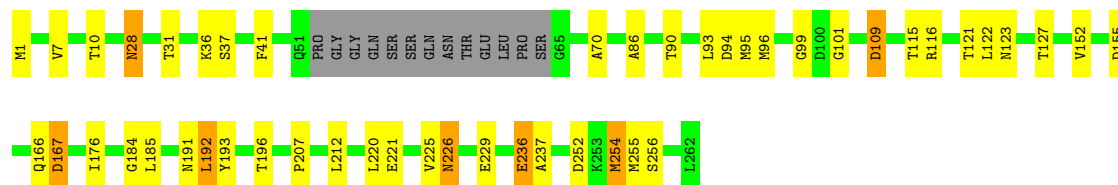
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain AS:  73% 21% 5%



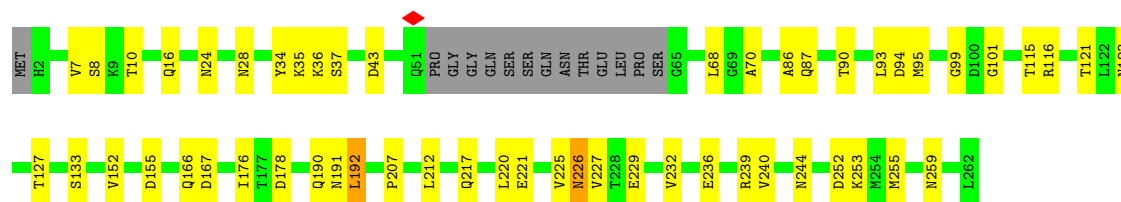
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain AT:  77% 16% 5%

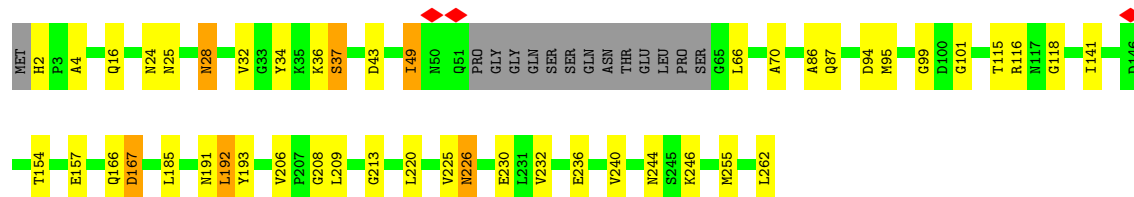
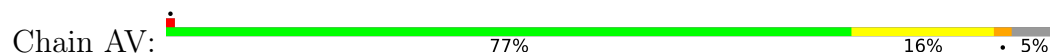


- Molecule 6: Flagellar basal-body rod protein FlgG

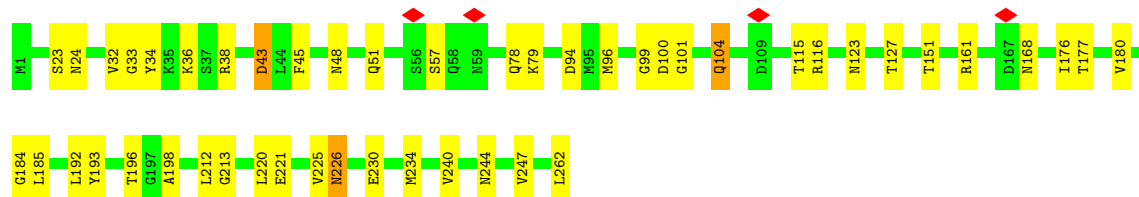
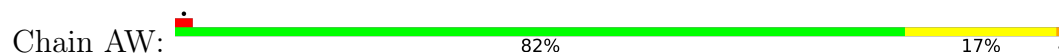
Chain AU:  74% 20% 5%



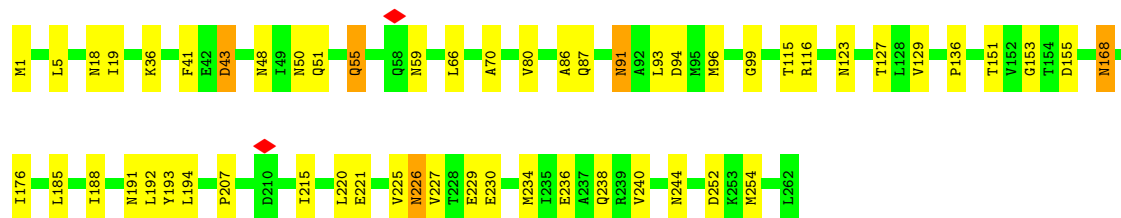
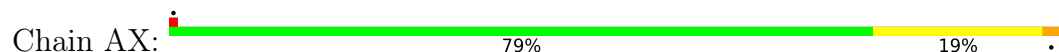
• Molecule 6: Flagellar basal-body rod protein FlgG



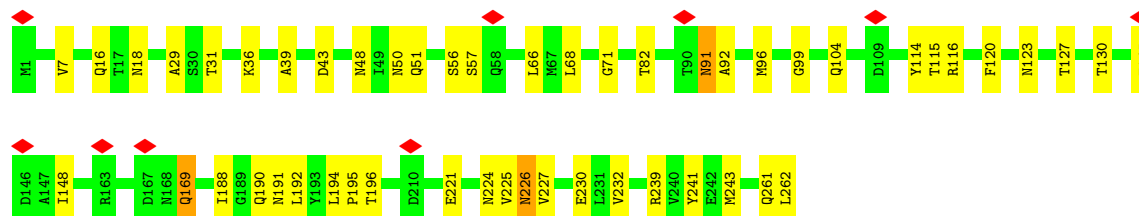
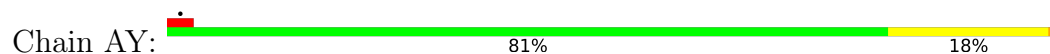
• Molecule 6: Flagellar basal-body rod protein FlgG



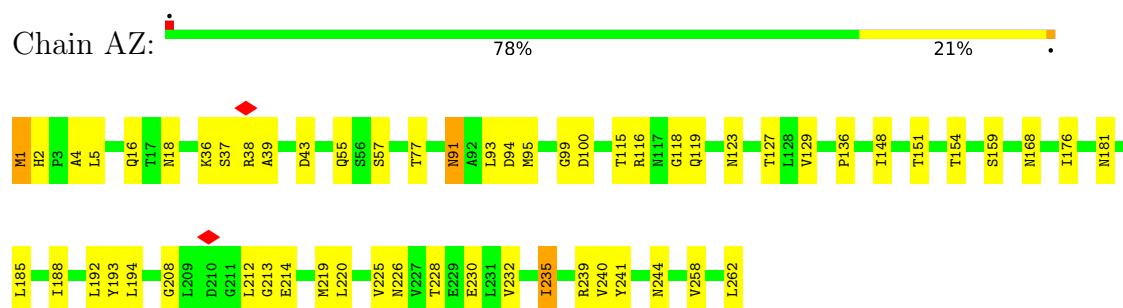
• Molecule 6: Flagellar basal-body rod protein FlgG



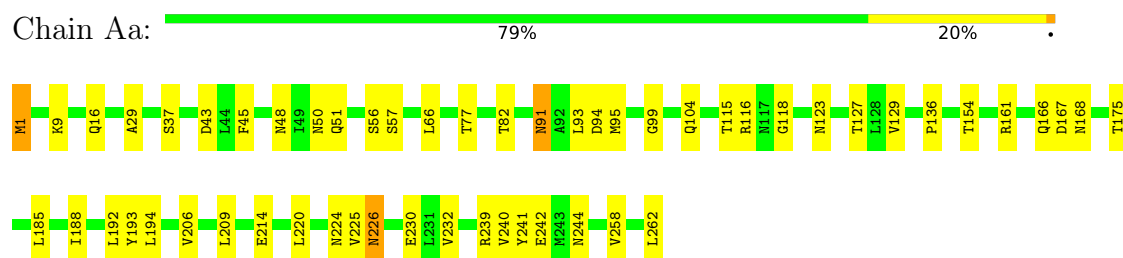
• Molecule 6: Flagellar basal-body rod protein FlgG



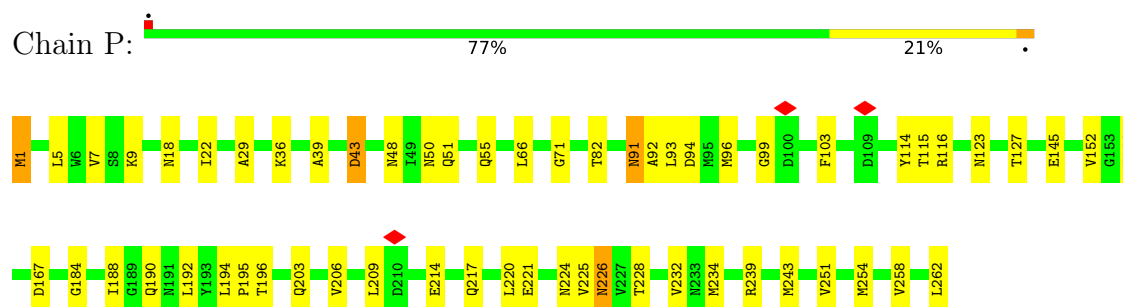
- Molecule 6: Flagellar basal-body rod protein FlgG



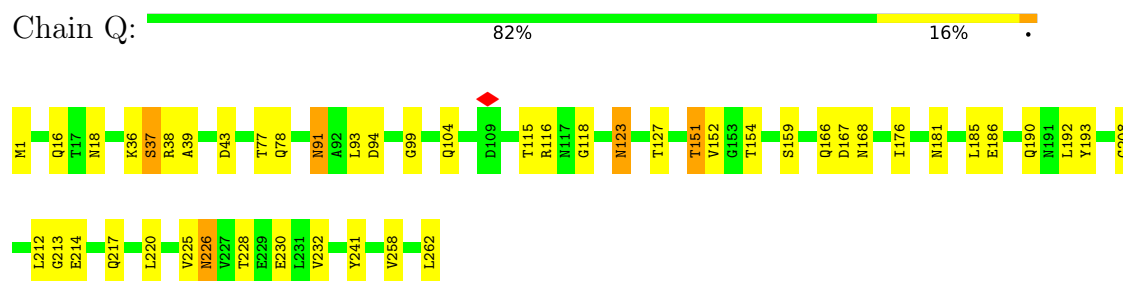
- Molecule 6: Flagellar basal-body rod protein FlgG



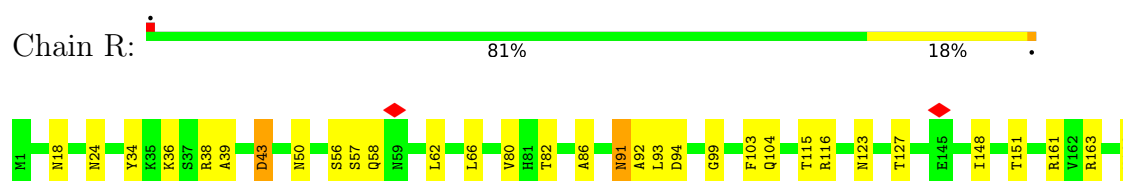
- Molecule 6: Flagellar basal-body rod protein FlgG

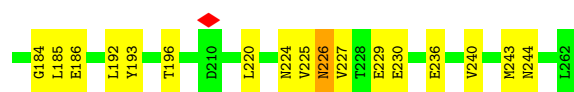


- Molecule 6: Flagellar basal-body rod protein FlgG

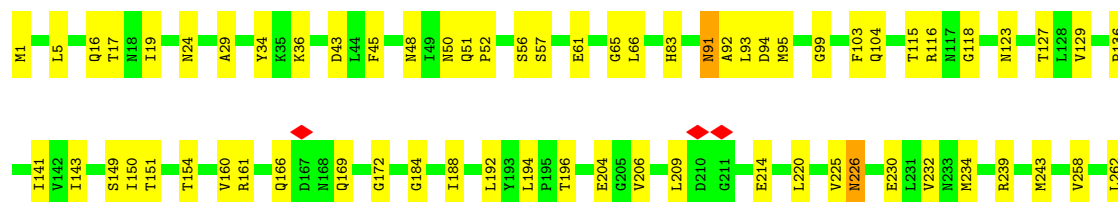
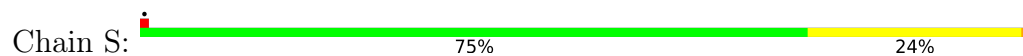


- Molecule 6: Flagellar basal-body rod protein FlgG

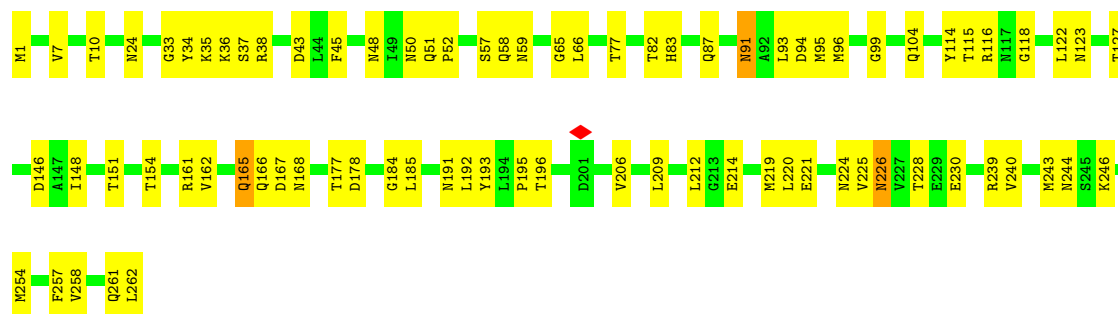




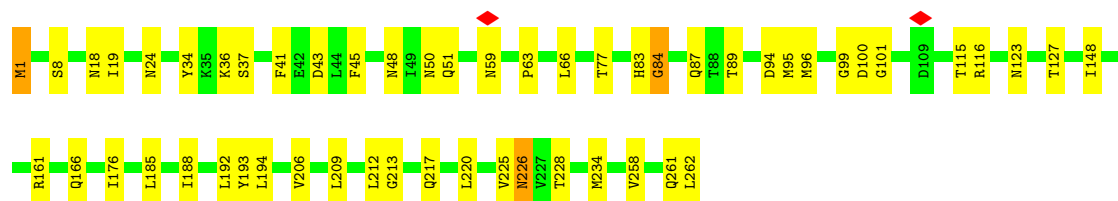
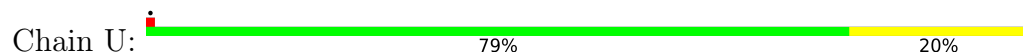
- Molecule 6: Flagellar basal-body rod protein FlgG



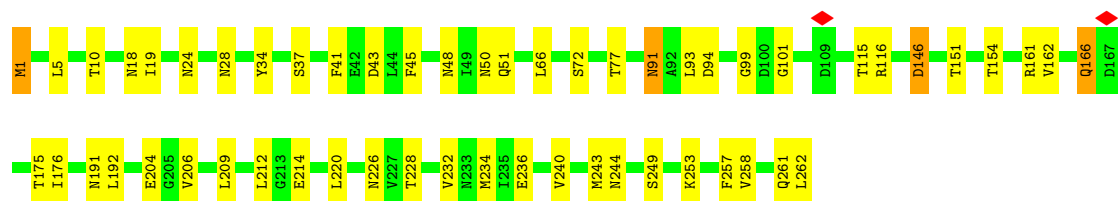
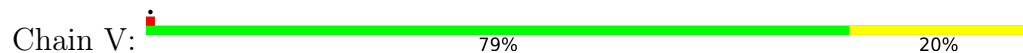
- Molecule 6: Flagellar basal-body rod protein FlgG



- Molecule 6: Flagellar basal-body rod protein FlgG

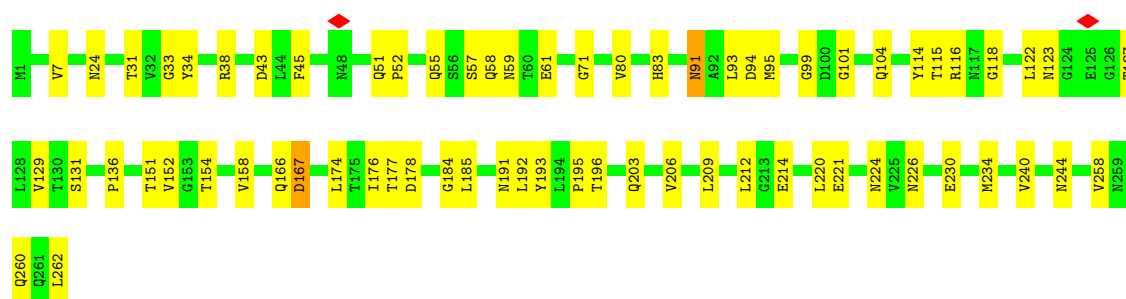


- Molecule 6: Flagellar basal-body rod protein FlgG



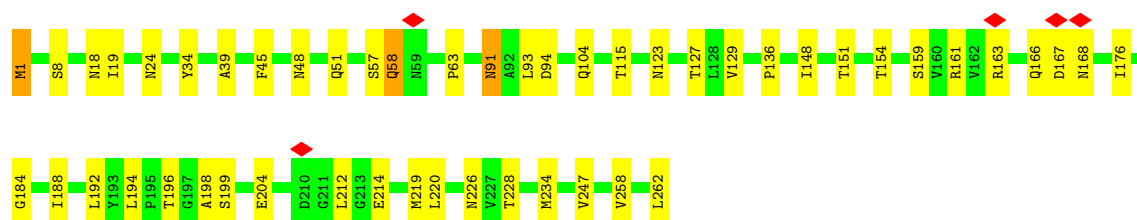
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain W:  74% 25%



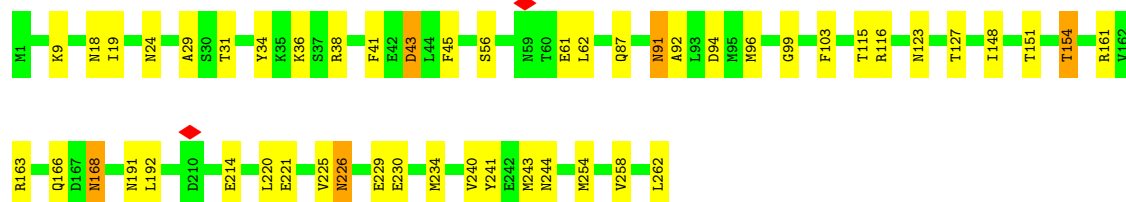
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain X:  81% 18%



- Molecule 6: Flagellar basal-body rod protein FlgG

Chain Y:  81% 17%



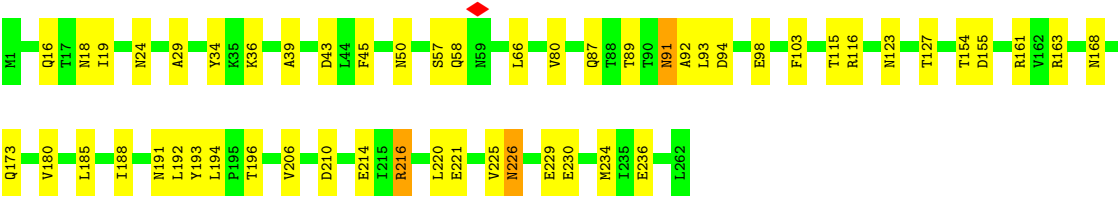
- Molecule 6: Flagellar basal-body rod protein FlgG

Chain Z:  83% 15%

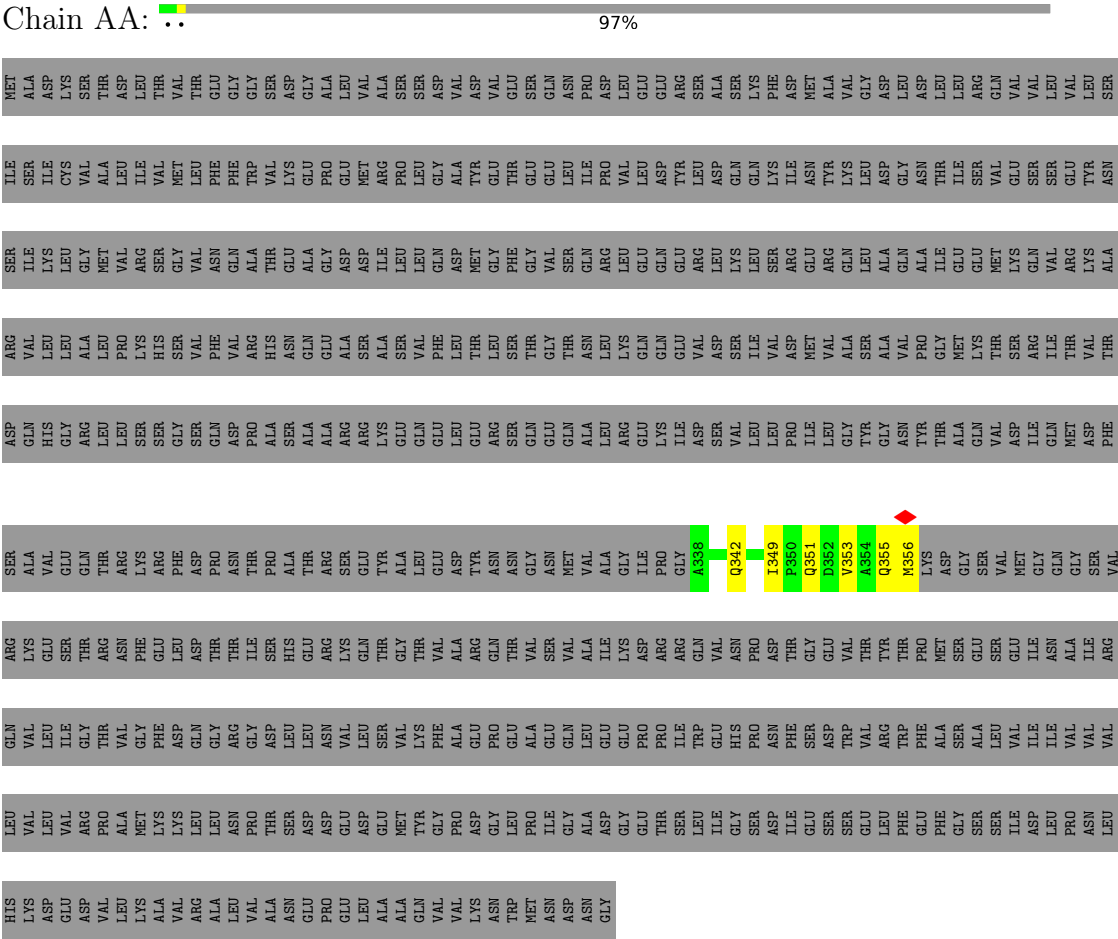


- Molecule 6: Flagellar basal-body rod protein FlgG

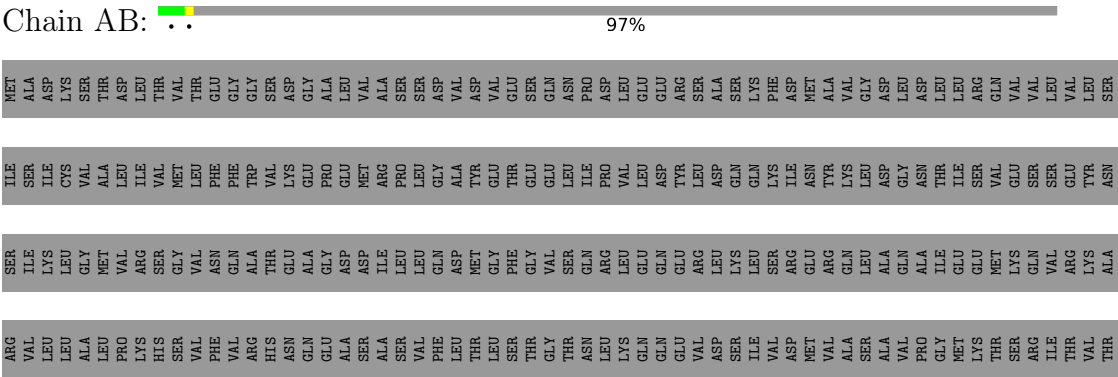
Chain a:  80% 19%



• Molecule 7: Flagellar M-ring protein



• Molecule 7: Flagellar M-ring protein







Chain AK: 96%



[illegible]

- Molecule 7: Flagellar M-ring protein

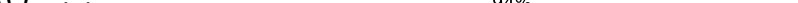
[illegible]

- Molecule 7: Flagellar M-ring protein

[illegible]

[illegible]

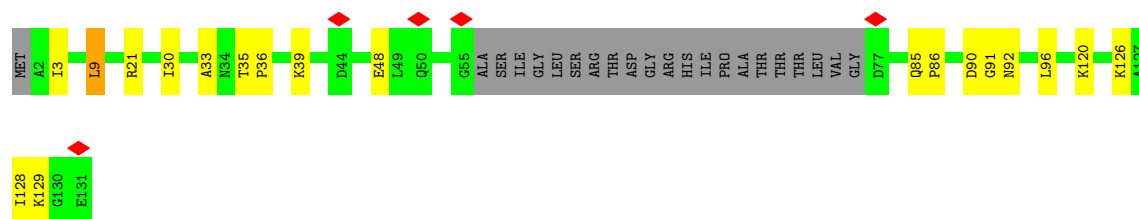
- Molecule 7: Flagellar M-ring protein

Chain AO:  94%

[illegible]

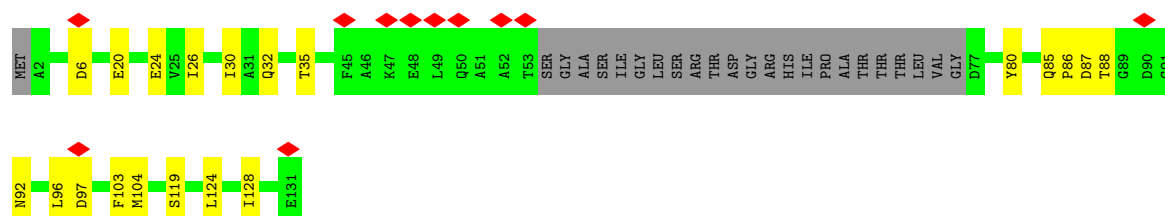
- Molecule 8: Flagellar basal body rod protein FlgB

Chain b: 



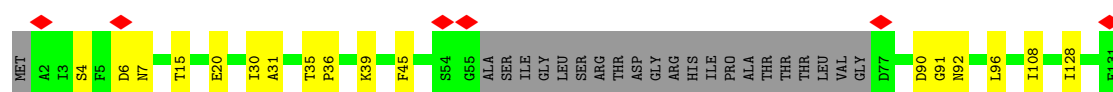
- Molecule 8: Flagellar basal body rod protein FlgB

Chain c: 



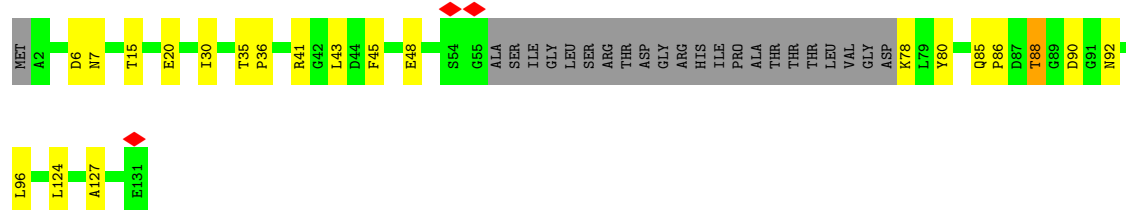
- Molecule 8: Flagellar basal body rod protein FlgB

Chain d: 



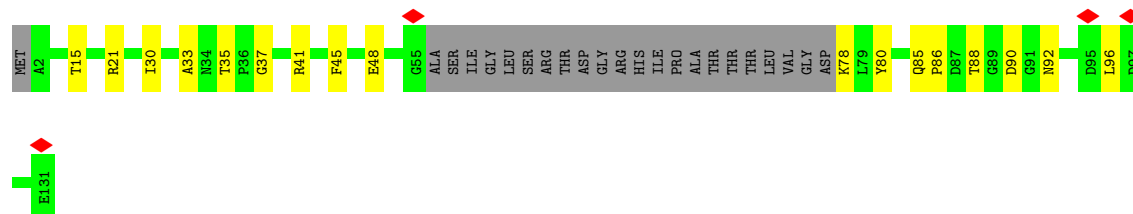
- Molecule 8: Flagellar basal body rod protein FlgB

Chain e: 

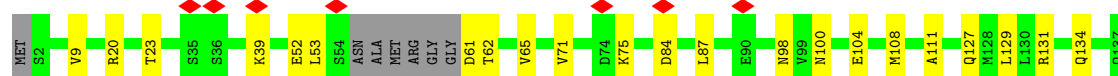
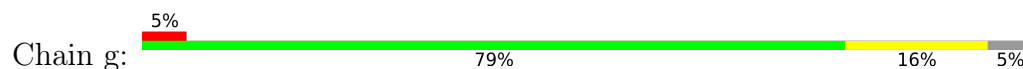


- Molecule 8: Flagellar basal body rod protein FlgB

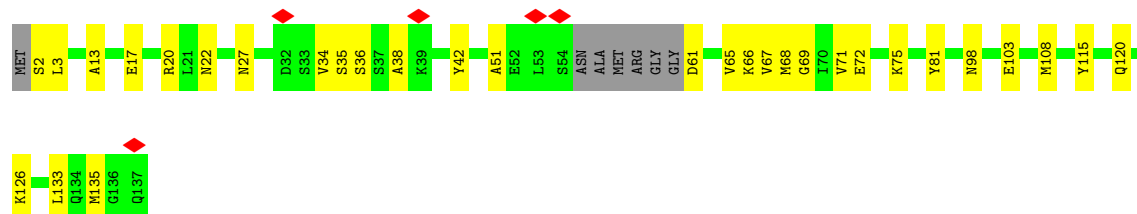
Chain f: 



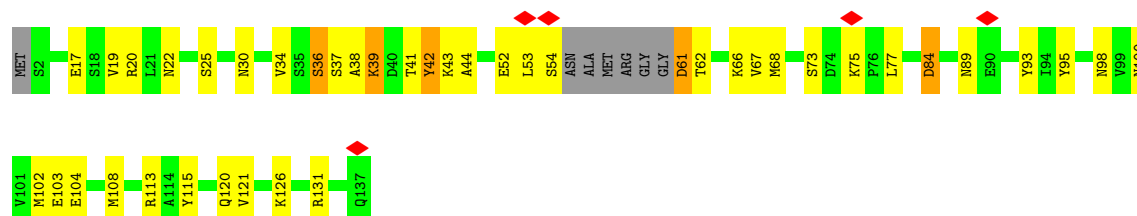
- Molecule 9: Flagellar basal-body rod protein FlgC



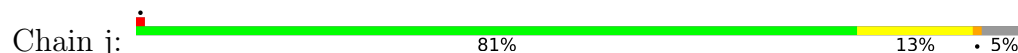
- Molecule 9: Flagellar basal-body rod protein FlgC



- Molecule 9: Flagellar basal-body rod protein FlgC



- Molecule 9: Flagellar basal-body rod protein FlgC

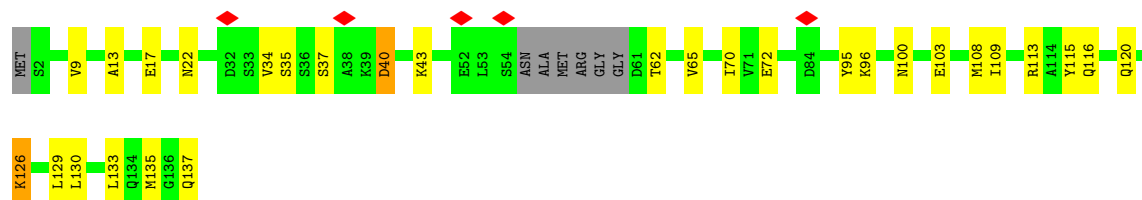


- Molecule 9: Flagellar basal-body rod protein FlgC

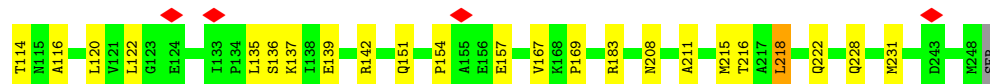
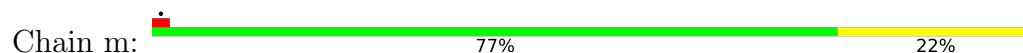


- Molecule 9: Flagellar basal-body rod protein FlgC

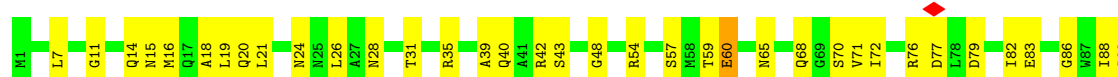




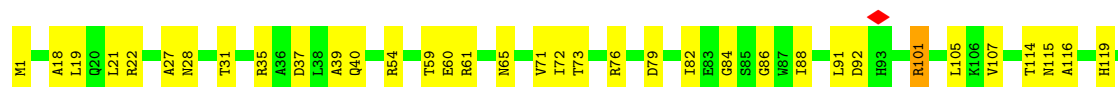
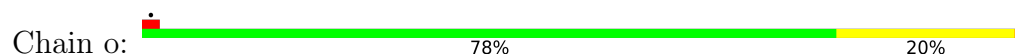
- Molecule 10: Flagellar basal-body rod protein FlgF



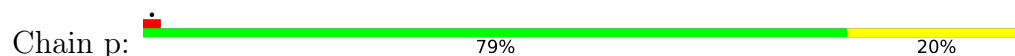
- Molecule 10: Flagellar basal-body rod protein FlgF

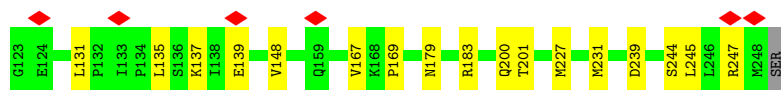


- Molecule 10: Flagellar basal-body rod protein FlgF

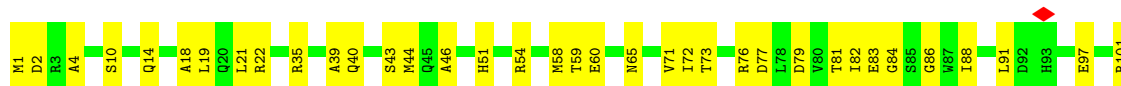
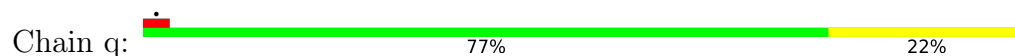


- Molecule 10: Flagellar basal-body rod protein FlgF

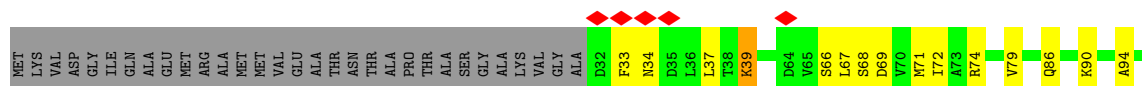




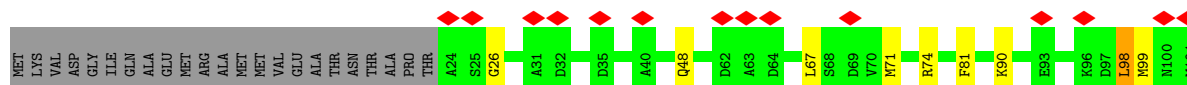
- Molecule 10: Flagellar basal-body rod protein FlgF



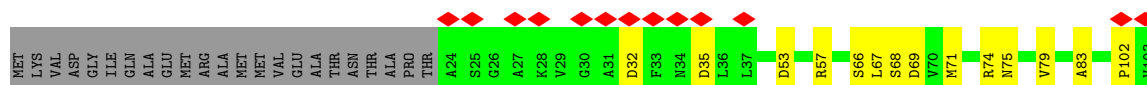
- Molecule 11: Flagellar hook-basal body complex protein FliE



- Molecule 11: Flagellar hook-basal body complex protein FliE



- Molecule 11: Flagellar hook-basal body complex protein FliE



- Molecule 11: Flagellar hook-basal body complex protein FliE



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.745	Depositor
Minimum map value	-1.973	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.42	Depositor
Map size (Å)	744.0, 744.0, 744.0	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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	D	0.35	0/2092	0.57	4/2833 (0.1%)
1	E	0.31	0/2092	0.52	0/2833
1	F	0.35	0/2092	0.58	4/2833 (0.1%)
1	G	0.39	0/2092	0.61	1/2833 (0.0%)
1	H	0.32	0/2092	0.53	2/2833 (0.1%)
1	I	0.31	0/2092	0.50	2/2833 (0.1%)
1	J	0.32	0/2092	0.55	3/2833 (0.1%)
1	K	0.25	0/2092	0.43	1/2833 (0.0%)
1	L	0.15	0/2092	0.36	2/2833 (0.1%)
1	M	0.20	0/2092	0.42	2/2833 (0.1%)
1	N	0.14	0/2092	0.33	0/2833
1	O	0.10	0/2092	0.25	0/2833
2	0	0.09	0/1389	0.25	0/1884
2	9	0.09	0/1389	0.28	0/1884
3	1	0.13	0/1628	0.29	0/2209
3	2	0.16	0/1637	0.33	0/2221
3	3	0.09	0/1637	0.26	0/2221
3	y	0.10	0/1637	0.27	0/2221
3	z	0.11	0/1637	0.28	0/2221
4	4	0.12	0/739	0.31	0/1005
4	5	0.16	0/739	0.34	0/1005
4	6	0.28	0/739	0.49	0/1005
4	7	0.15	0/739	0.33	0/1005
5	8	0.08	0/1941	0.25	0/2631
6	A	0.16	0/1985	0.33	0/2697
6	AP	0.15	0/1985	0.34	1/2697 (0.0%)
6	AQ	0.09	0/1985	0.24	0/2697
6	AR	0.14	0/1884	0.28	0/2558
6	AS	0.13	0/1884	0.29	0/2558
6	AT	0.12	0/1892	0.25	0/2568
6	AU	0.11	0/1884	0.24	0/2558
6	AV	0.10	0/1884	0.24	0/2558
6	AW	0.10	0/1985	0.25	0/2697
6	AX	0.11	0/1985	0.26	0/2697

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	AY	0.10	0/1985	0.25	0/2697
6	AZ	0.10	0/1985	0.23	0/2697
6	Aa	0.10	0/1985	0.25	0/2697
6	B	0.14	0/1985	0.32	0/2697
6	C	0.10	0/1985	0.24	0/2697
6	P	0.11	0/1985	0.25	0/2697
6	Q	0.21	1/1985 (0.1%)	0.28	0/2697
6	R	0.11	0/1985	0.25	0/2697
6	S	0.10	0/1985	0.24	0/2697
6	T	0.11	0/1985	0.24	0/2697
6	U	0.22	0/1985	0.37	3/2697 (0.1%)
6	V	0.10	0/1985	0.25	0/2697
6	W	0.24	1/1985 (0.1%)	0.39	0/2697
6	X	0.11	0/1985	0.25	0/2697
6	Y	0.10	0/1985	0.25	0/2697
6	Z	0.10	0/1985	0.24	0/2697
6	a	0.10	0/1985	0.24	0/2697
7	AA	0.35	0/137	0.45	0/188
7	AB	0.28	0/137	0.43	0/188
7	AC	0.14	0/141	0.31	0/193
7	AD	0.30	0/137	0.46	0/188
7	AE	0.12	0/137	0.28	0/188
7	AF	0.92	0/161	1.23	0/221
7	AG	0.16	0/75	0.32	0/103
7	AH	0.20	0/75	0.42	0/103
7	AI	0.94	0/75	1.34	0/103
7	AJ	0.37	0/166	0.57	0/228
7	AK	0.31	0/172	0.69	0/237
7	AL	0.39	0/223	0.61	0/304
7	AM	0.19	0/227	0.44	0/309
7	AN	0.23	0/227	0.49	0/309
7	AO	0.16	0/223	0.40	0/304
8	b	0.22	0/856	0.36	0/1151
8	c	0.21	0/846	0.30	0/1138
8	d	0.24	0/856	0.31	0/1151
8	e	0.19	0/848	0.31	0/1140
8	f	0.22	0/848	0.35	0/1140
9	g	0.10	0/996	0.26	0/1348
9	h	0.10	0/996	0.26	0/1348
9	i	0.30	0/996	0.46	0/1348
9	j	0.09	0/996	0.24	0/1348
9	k	0.10	0/996	0.28	0/1348
9	l	0.13	0/996	0.30	0/1348

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	m	0.10	0/1905	0.26	0/2572
10	n	0.13	0/1905	0.26	0/2572
10	o	0.10	0/1905	0.26	0/2572
10	p	0.17	0/1905	0.36	1/2572 (0.0%)
10	q	0.09	0/1905	0.25	0/2572
11	r	0.31	0/564	0.43	0/759
11	s	0.07	0/609	0.20	0/819
11	t	0.07	0/609	0.17	0/819
11	u	0.07	0/564	0.16	0/759
11	v	0.06	0/564	0.18	0/759
11	w	0.09	0/313	0.19	0/420
12	x	0.07	0/562	0.19	0/760
All	All	0.18	2/119906 (0.0%)	0.34	26/162571 (0.0%)

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	E	0	1
1	I	0	1
1	J	0	2
1	K	0	1
1	M	0	1
3	2	0	1
6	AP	0	2
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	52	PRO	C-O	-5.55	1.17	1.23
6	Q	37	SER	CA-CB	-5.44	1.45	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	46	LEU	N-CA-C	-8.64	102.51	113.23
1	J	54	PRO	N-CA-CB	-8.45	93.30	102.76
10	p	227	MET	N-CA-C	-8.15	103.46	113.41
6	AP	161	ARG	CB-CA-C	-7.50	97.38	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	54	PRO	N-CA-CB	-6.69	96.22	103.25
1	F	55	GLY	CA-C-O	-6.45	115.17	122.33
1	J	54	PRO	N-CA-C	6.17	125.23	114.75
1	L	415	ASN	N-CA-C	-6.14	105.95	113.50
1	G	51	LYS	CB-CA-C	-5.96	103.48	111.88
1	D	416	PHE	N-CA-C	-5.90	106.21	113.41
1	L	416	PHE	N-CA-C	-5.87	105.21	112.90
1	I	427	ASN	N-CA-C	-5.82	104.94	111.28
1	I	41	VAL	N-CA-C	-5.79	99.84	108.46
1	F	52	THR	CB-CA-C	-5.71	104.14	111.50
1	M	416	PHE	N-CA-C	-5.71	105.04	112.23
1	D	54	PRO	N-CA-CB	-5.68	97.28	103.25
1	H	40	ASP	CB-CA-C	-5.67	98.66	111.30
1	D	48	THR	CB-CA-C	5.60	118.89	109.48
6	U	84	GLY	CA-C-N	-5.42	113.12	123.32
6	U	84	GLY	C-N-CA	-5.42	113.12	123.32
1	M	415	ASN	N-CA-C	-5.37	106.90	113.50
1	H	54	PRO	N-CA-CB	-5.36	97.62	103.25
6	U	84	GLY	N-CA-C	-5.36	103.12	112.55
1	J	53	THR	CB-CA-C	5.26	117.92	110.02
1	K	403	THR	CB-CA-C	5.04	119.42	110.85
1	D	424	GLU	CA-C-O	-5.02	115.53	120.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	188	ARG	Sidechain
6	AP	161	ARG	Sidechain
6	AP	163	ARG	Sidechain
1	E	414	ARG	Sidechain
1	I	50	ALA	Mainchain
1	J	414	ARG	Sidechain
1	J	50	ALA	Mainchain
1	K	414	ARG	Sidechain
1	M	414	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2057	0	1944	28	0
1	E	2057	0	1944	37	0
1	F	2057	0	1944	39	0
1	G	2057	0	1944	48	0
1	H	2057	0	1944	38	0
1	I	2057	0	1944	44	0
1	J	2057	0	1944	33	0
1	K	2057	0	1944	38	0
1	L	2057	0	1944	39	0
1	M	2057	0	1944	38	0
1	N	2057	0	1944	41	0
1	O	2057	0	1944	31	0
2	0	1361	0	1418	28	0
2	9	1361	0	1418	23	0
3	1	1599	0	1685	23	0
3	2	1608	0	1691	27	0
3	3	1608	0	1691	33	0
3	y	1608	0	1691	24	0
3	z	1608	0	1691	34	0
4	4	722	0	768	16	0
4	5	722	0	768	19	0
4	6	722	0	768	15	0
4	7	722	0	768	10	0
5	8	1896	0	1968	44	0
6	A	1956	0	1907	39	0
6	AP	1956	0	1907	39	0
6	AQ	1956	0	1907	30	0
6	AR	1858	0	1813	43	0
6	AS	1858	0	1813	36	0
6	AT	1866	0	1825	33	0
6	AU	1858	0	1813	42	0
6	AV	1858	0	1813	34	0
6	AW	1956	0	1907	36	0
6	AX	1956	0	1907	38	0
6	AY	1956	0	1907	36	0
6	AZ	1956	0	1907	39	0
6	Aa	1956	0	1907	37	0
6	B	1956	0	1907	41	0
6	C	1956	0	1907	38	0
6	P	1956	0	1907	37	0
6	Q	1956	0	1907	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	1956	0	1907	34	0
6	S	1956	0	1907	44	0
6	T	1956	0	1907	50	0
6	U	1956	0	1907	36	0
6	V	1956	0	1907	37	0
6	W	1956	0	1907	39	0
6	X	1956	0	1907	33	0
6	Y	1956	0	1907	36	0
6	Z	1956	0	1907	30	0
6	a	1956	0	1907	37	0
7	AA	135	0	128	4	0
7	AB	135	0	128	2	0
7	AC	139	0	131	0	0
7	AD	135	0	128	2	0
7	AE	135	0	128	2	0
7	AF	158	0	152	16	0
7	AG	73	0	72	4	0
7	AH	73	0	72	4	0
7	AI	73	0	72	8	0
7	AJ	163	0	157	5	0
7	AK	169	0	164	5	0
7	AL	220	0	215	3	0
7	AM	224	0	218	5	0
7	AN	224	0	218	2	0
7	AO	220	0	215	3	0
8	b	845	0	833	12	0
8	c	835	0	825	18	0
8	d	845	0	833	10	0
8	e	837	0	829	14	0
8	f	837	0	829	11	0
9	g	983	0	958	12	0
9	h	983	0	958	24	0
9	i	983	0	958	37	0
9	j	983	0	958	12	0
9	k	983	0	958	20	0
9	l	983	0	958	25	0
10	m	1879	0	1864	37	0
10	n	1879	0	1864	55	0
10	o	1879	0	1864	36	0
10	p	1879	0	1864	33	0
10	q	1879	0	1864	41	0
11	r	560	0	561	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	s	605	0	609	9	0
11	t	605	0	609	9	0
11	u	560	0	561	7	0
11	v	560	0	561	10	0
11	w	311	0	320	8	0
12	x	552	0	577	13	0
All	All	118072	0	115897	1850	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 (1850) 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)
9:i:52:GLU:HG3	9:i:52:GLU:O	1.47	1.06
9:i:52:GLU:O	9:i:52:GLU:CG	2.15	0.94
1:H:42:TYR:CD1	1:M:362:LYS:HB2	2.06	0.91
6:AP:161:ARG:NH1	6:a:196:THR:HG22	1.89	0.88
1:H:42:TYR:HE2	1:H:44:ASN:HB2	1.39	0.87
1:F:42:TYR:CD2	1:K:362:LYS:HB2	2.12	0.83
3:y:82:ASP:HB3	3:y:167:THR:HG23	1.62	0.80
6:AP:161:ARG:HH12	6:a:196:THR:HG22	1.47	0.79
1:I:433:ILE:HD11	1:N:416:PHE:HZ	1.48	0.78
6:Aa:123:ASN:HD21	6:Aa:127:THR:HB	1.50	0.77
1:J:39:ALA:HB1	1:O:365:GLY:HA2	1.68	0.75
1:G:39:ALA:HB1	1:L:365:GLY:HA2	1.68	0.74
1:I:39:ALA:HB1	1:N:365:GLY:HA2	1.69	0.74
6:S:50:ASN:HB2	6:S:66:LEU:H	1.52	0.74
2:9:34:TYR:HD2	9:i:39:LYS:HA	1.51	0.74
1:I:40:ASP:HB2	1:N:366:THR:H	1.53	0.73
2:0:138:SER:OG	7:AF:356:MET:HE1	1.88	0.73
1:D:39:ALA:HB1	1:I:365:GLY:HA2	1.69	0.73
1:E:33:GLU:HB3	1:E:400:ILE:HG22	1.71	0.72
10:n:102:ASN:HD21	10:n:116:ALA:HB3	1.55	0.72
1:M:33:GLU:HB3	1:M:400:ILE:HG22	1.72	0.72
6:AX:87:GLN:HE22	6:Y:38:ARG:HH22	1.38	0.72
1:H:33:GLU:HB3	1:H:400:ILE:HG22	1.72	0.72
2:0:119:LEU:HD13	2:0:124:LEU:HD22	1.71	0.71
2:9:34:TYR:CD2	9:i:39:LYS:HA	2.24	0.71
2:9:179:LEU:O	2:9:182:ASN:ND2	2.22	0.71
1:H:39:ALA:HB1	1:M:365:GLY:HA2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:TYR:CE2	1:K:362:LYS:HB2	2.25	0.71
4:4:25:ILE:HG13	4:5:52:LEU:HD12	1.73	0.71
8:c:86:PRO:O	10:n:54:ARG:NH1	2.24	0.71
1:E:50:ALA:O	1:E:51:LYS:C	2.34	0.71
6:Q:91:ASN:HD22	6:Q:93:LEU:H	1.39	0.70
1:N:33:GLU:HB3	1:N:400:ILE:HG22	1.73	0.70
1:F:39:ALA:HB1	1:K:365:GLY:HA2	1.73	0.70
1:H:42:TYR:HD1	1:M:362:LYS:HB2	1.56	0.70
6:AR:98:GLU:HG3	6:AR:216:ARG:HG3	1.74	0.69
5:8:47:LEU:HD21	11:s:98:LEU:HD21	1.72	0.69
6:R:161:ARG:HH11	6:R:168:ASN:HD21	1.39	0.69
11:v:103:VAL:O	3:y:120:ARG:NH2	2.25	0.69
1:F:33:GLU:HB3	1:F:400:ILE:HG22	1.73	0.69
6:AX:123:ASN:HD21	6:AX:127:THR:HB	1.56	0.69
10:m:22:ARG:HE	10:m:39:ALA:HB3	1.58	0.69
1:I:42:TYR:CE2	1:N:362:LYS:HB2	2.28	0.68
1:K:33:GLU:HB3	1:K:400:ILE:HG22	1.75	0.68
6:AP:239:ARG:NH1	6:AT:252:ASP:OD1	2.26	0.68
6:AR:133:SER:OG	6:AR:190:GLN:NE2	2.25	0.68
1:G:130:VAL:HG12	1:G:137:VAL:HA	1.76	0.68
7:AL:341:ASN:ND2	8:c:88:THR:OG1	2.27	0.68
9:l:40:ASP:OD1	9:l:40:ASP:N	2.27	0.68
1:G:42:TYR:CE2	1:L:362:LYS:HD2	2.29	0.68
1:G:433:ILE:HD11	1:L:416:PHE:HZ	1.57	0.68
7:AF:335:ILE:HG13	7:AF:338:ALA:HB2	1.74	0.68
11:r:103:VAL:HG23	3:z:113:VAL:HG13	1.76	0.68
5:8:92:MET:HE2	5:8:248:GLY:HA3	1.77	0.67
6:AP:117:ASN:HD21	6:AP:119:GLN:HE21	1.42	0.67
6:A:154:THR:HG22	6:T:57:SER:HB3	1.75	0.67
6:A:99:GLY:O	6:A:116:ARG:NH2	2.27	0.67
6:AQ:99:GLY:O	6:AQ:116:ARG:NH2	2.28	0.67
9:i:36:SER:HB2	10:n:43:SER:HB2	1.77	0.67
10:q:86:GLY:O	10:q:101:ARG:NH1	2.28	0.67
3:2:244:VAL:HG11	3:2:262:SER:HB2	1.77	0.66
4:5:54:ARG:NH1	4:7:48:THR:OG1	2.28	0.66
10:n:24:ASN:O	10:n:28:ASN:ND2	2.24	0.66
6:Aa:50:ASN:HB2	6:Aa:66:LEU:H	1.59	0.66
10:o:65:ASN:O	10:o:208:ASN:ND2	2.29	0.66
3:2:141:LEU:HG	3:z:198:MET:HE1	1.78	0.66
7:AA:355:GLN:O	7:AA:356:MET:HB3	1.94	0.66
1:E:39:ALA:HB1	1:J:365:GLY:HA2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AV:87:GLN:HE22	6:Z:38:ARG:HH22	1.43	0.66
1:M:82:ARG:HH11	1:M:396:GLU:HB3	1.61	0.65
6:AY:123:ASN:HD21	6:AY:127:THR:HB	1.61	0.65
6:Q:99:GLY:O	6:Q:116:ARG:NH2	2.29	0.65
9:j:75:LYS:O	9:j:98:ASN:ND2	2.29	0.65
9:i:53:LEU:O	9:i:54:SER:C	2.38	0.65
1:F:37:GLU:OE1	1:F:62:GLN:NE2	2.29	0.65
6:AS:191:ASN:ND2	6:AW:43:ASP:OD1	2.29	0.65
6:Y:99:GLY:O	6:Y:116:ARG:NH2	2.30	0.65
3:y:103:VAL:O	3:y:107:THR:OG1	2.15	0.65
6:AP:87:GLN:HE22	6:AS:38:ARG:HH22	1.44	0.65
6:U:176:ILE:HG13	6:U:212:LEU:HD22	1.78	0.65
9:h:22:ASN:HD22	10:o:54:ARG:HE	1.45	0.65
3:y:88:GLN:OE1	3:y:161:TYR:OH	2.14	0.65
1:I:429:LEU:HD21	1:N:413:GLN:HG3	1.78	0.65
6:AU:101:GLY:O	6:AU:116:ARG:NH1	2.30	0.65
10:o:135:LEU:HD13	10:o:138:ILE:HD11	1.78	0.65
6:B:42:GLU:HG2	6:B:75:VAL:HB	1.78	0.64
6:AW:99:GLY:O	6:AW:116:ARG:NH2	2.30	0.64
6:AZ:91:ASN:HD22	6:AZ:93:LEU:H	1.45	0.64
3:1:239:ILE:HG23	4:6:17:VAL:HG12	1.79	0.64
4:6:9:LEU:HD21	4:6:80:LEU:HD21	1.80	0.64
3:3:198:MET:HE2	3:y:144:PHE:HB2	1.80	0.64
6:Y:94:ASP:HB2	6:Y:220:LEU:HD21	1.80	0.64
1:N:6:LEU:HD13	6:Q:232:VAL:HG11	1.79	0.64
6:AV:191:ASN:ND2	6:Z:43:ASP:OD1	2.30	0.64
10:n:83:GLU:OE2	10:n:142:ARG:NH1	2.30	0.64
3:z:244:VAL:HG11	3:z:262:SER:HB3	1.80	0.64
6:C:239:ARG:NH1	6:AU:252:ASP:OD1	2.31	0.64
1:G:42:TYR:CD2	1:L:362:LYS:HB2	2.33	0.64
1:O:79:MET:HE3	1:O:111:LEU:HD21	1.80	0.64
6:X:91:ASN:HD22	6:X:93:LEU:H	1.46	0.64
6:AS:94:ASP:HB2	6:AS:220:LEU:HD21	1.80	0.64
6:AQ:176:ILE:HD11	6:AQ:212:LEU:HB3	1.79	0.63
3:2:184:LEU:HG	3:2:214:LEU:HD11	1.81	0.63
4:7:50:SER:O	4:7:54:ARG:NH1	2.31	0.63
5:8:186:SER:HA	5:8:189:LEU:HD23	1.80	0.63
7:AI:335:ILE:HG13	7:AI:338:ALA:HB2	1.79	0.63
6:AV:246:LYS:NZ	6:Y:262:LEU:OXT	2.30	0.63
8:c:85:GLN:OE1	10:n:54:ARG:NH2	2.31	0.63
9:i:108:MET:HE2	10:n:231:MET:HE2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:82:ARG:HH11	1:O:396:GLU:HG2	1.64	0.63
3:1:183:MET:HE1	3:1:215:ILE:HG12	1.80	0.63
6:Aa:91:ASN:HD22	6:Aa:93:LEU:H	1.45	0.63
3:1:85:VAL:HA	3:1:88:GLN:HE21	1.63	0.63
6:a:24:ASN:ND2	6:a:34:TYR:OH	2.31	0.63
6:V:91:ASN:HD22	6:V:93:LEU:H	1.45	0.63
9:i:43:LYS:HG2	9:i:77:LEU:HD21	1.80	0.63
6:AT:94:ASP:HB2	6:AT:220:LEU:HD21	1.81	0.62
6:Z:99:GLY:O	6:Z:116:ARG:NH2	2.32	0.62
10:m:91:LEU:HD23	10:m:122:LEU:HD21	1.80	0.62
1:K:130:VAL:HG12	1:K:137:VAL:HA	1.80	0.62
6:Aa:161:ARG:HG2	6:Aa:168:ASN:HB3	1.80	0.62
6:W:99:GLY:O	6:W:116:ARG:NH2	2.33	0.62
6:W:104:GLN:NE2	6:W:177:THR:OG1	2.32	0.62
10:p:137:LYS:NZ	10:p:139:GLU:OE2	2.33	0.62
1:N:130:VAL:HG12	1:N:137:VAL:HA	1.81	0.62
1:H:422:SER:HA	1:M:409:LEU:HD21	1.81	0.62
8:f:30:ILE:HG23	8:f:96:LEU:HD11	1.80	0.62
1:D:82:ARG:HH11	1:D:396:GLU:HG2	1.63	0.62
1:G:109:PHE:HE1	1:G:119:THR:HG22	1.65	0.62
7:AI:334:GLY:O	7:AI:335:ILE:C	2.40	0.62
3:2:103:VAL:O	3:2:107:THR:OG1	2.18	0.62
6:Aa:115:THR:HB	6:Aa:192:LEU:HD23	1.81	0.62
9:i:61:ASP:OD1	9:i:61:ASP:N	2.33	0.62
10:m:11:GLY:O	10:m:15:ASN:ND2	2.31	0.62
6:AY:115:THR:HB	6:AY:192:LEU:HD23	1.81	0.61
3:z:103:VAL:O	3:z:107:THR:OG1	2.17	0.61
1:F:42:TYR:CD1	1:F:42:TYR:C	2.78	0.61
6:A:133:SER:OG	6:A:190:GLN:NE2	2.33	0.61
6:AU:133:SER:OG	6:AU:190:GLN:NE2	2.30	0.61
8:d:35:THR:O	8:d:92:ASN:ND2	2.33	0.61
1:O:130:VAL:HG12	1:O:137:VAL:HA	1.82	0.61
6:AX:43:ASP:OD1	6:AX:43:ASP:N	2.32	0.61
6:AZ:99:GLY:O	6:AZ:116:ARG:NH2	2.33	0.61
6:P:123:ASN:HD21	6:P:127:THR:HB	1.65	0.61
11:w:71:MET:O	11:w:75:ASN:ND2	2.30	0.61
1:G:426:HIS:HE1	1:L:20:SER:OG	1.83	0.61
2:O:136:ASP:HB2	7:AF:356:MET:HE3	1.82	0.61
6:AU:24:ASN:ND2	6:AU:34:TYR:OH	2.33	0.61
1:L:130:VAL:HG12	1:L:137:VAL:HA	1.82	0.61
3:1:141:LEU:HD11	3:1:280:LEU:HD22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AH:335:ILE:HB	7:AH:338:ALA:HB2	1.82	0.61
6:AZ:115:THR:HB	6:AZ:192:LEU:HD23	1.82	0.61
1:G:49:ASN:HB3	1:G:52:THR:HG22	1.83	0.61
1:O:33:GLU:HB3	1:O:400:ILE:HG22	1.82	0.61
3:1:104:ILE:O	3:1:110:THR:OG1	2.19	0.61
6:AW:123:ASN:HD21	6:AW:127:THR:HB	1.65	0.61
6:AX:50:ASN:HB2	6:AX:66:LEU:H	1.66	0.61
9:k:108:MET:HE2	10:p:231:MET:HE2	1.83	0.61
4:4:59:LEU:HD13	12:x:90:LEU:HD22	1.82	0.61
9:h:17:GLU:OE1	9:h:20:ARG:NH2	2.32	0.61
3:1:244:VAL:HG11	3:1:262:SER:HB3	1.81	0.61
4:4:1:MET:N	4:4:1:MET:SD	2.73	0.61
6:B:246:LYS:HE3	10:o:215:MET:HE2	1.82	0.61
6:AP:239:ARG:HG3	6:AT:255:MET:HE3	1.82	0.61
1:M:130:VAL:HG12	1:M:137:VAL:HA	1.82	0.60
6:AS:104:GLN:NE2	6:AS:177:THR:OG1	2.34	0.60
6:R:43:ASP:OD1	6:R:43:ASP:N	2.32	0.60
1:E:49:ASN:HD21	1:E:51:LYS:HD3	1.66	0.60
6:C:249:SER:OG	6:C:253:LYS:NZ	2.33	0.60
6:AT:99:GLY:O	6:AT:116:ARG:NH2	2.33	0.60
1:L:6:LEU:HD13	6:Aa:232:VAL:HG11	1.81	0.60
6:B:123:ASN:HD21	6:B:127:THR:HB	1.66	0.60
6:U:123:ASN:HD21	6:U:127:THR:HB	1.66	0.60
10:n:76:ARG:NH1	10:n:79:ASP:OD1	2.34	0.60
10:p:84:GLY:O	10:p:101:ARG:NH2	2.32	0.60
1:K:6:LEU:HD13	6:AZ:232:VAL:HG11	1.82	0.60
4:7:31:ILE:HG13	4:7:57:VAL:HG11	1.81	0.60
6:T:36:LYS:HB3	6:T:225:VAL:HG12	1.82	0.60
6:AU:191:ASN:ND2	6:R:43:ASP:OD1	2.35	0.60
9:l:35:SER:OG	10:q:40:GLN:NE2	2.35	0.60
10:p:11:GLY:O	10:p:15:ASN:ND2	2.30	0.60
7:AI:335:ILE:HD12	9:h:71:VAL:HG23	1.83	0.60
6:AV:101:GLY:O	6:AV:116:ARG:NH1	2.35	0.60
6:S:99:GLY:O	6:S:116:ARG:NH2	2.34	0.60
6:AS:2:HIS:HD2	6:AS:4:ALA:H	1.48	0.60
9:k:75:LYS:O	9:k:98:ASN:ND2	2.34	0.60
1:E:432:ASN:ND2	1:J:420:SER:OG	2.34	0.60
1:H:117:MET:HE3	1:H:125:LEU:HD23	1.83	0.60
6:AX:226:ASN:HB3	6:AX:229:GLU:HB2	1.84	0.60
6:AZ:176:ILE:HG13	6:AZ:212:LEU:HD22	1.83	0.60
8:e:15:THR:HG23	8:e:45:PHE:HZ	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:22:ASN:HD22	10:n:54:ARG:HE	1.49	0.60
3:y:112:ILE:HG23	3:y:283:LEU:HD23	1.84	0.60
1:G:42:TYR:HE2	1:L:362:LYS:HD2	1.66	0.60
6:P:50:ASN:HB2	6:P:66:LEU:H	1.67	0.60
9:h:135:MET:HE2	11:t:75:ASN:HD22	1.66	0.60
9:i:100:ASN:HD22	9:i:103:GLU:H	1.49	0.60
9:k:22:ASN:HD22	10:p:54:ARG:HE	1.49	0.60
1:E:130:VAL:HG12	1:E:137:VAL:HA	1.82	0.60
1:I:42:TYR:HE2	1:N:362:LYS:HD2	1.66	0.60
1:O:130:VAL:HG22	1:O:347:GLY:HA2	1.84	0.60
2:0:22:LEU:HB3	2:0:48:PRO:HD3	1.84	0.60
6:Aa:99:GLY:O	6:Aa:116:ARG:NH2	2.34	0.60
1:G:416:PHE:HZ	1:M:403:THR:HG21	1.67	0.59
6:AR:36:LYS:HB3	6:AR:225:VAL:HG12	1.84	0.59
6:AS:86:ALA:HB2	6:W:45:PHE:HE1	1.67	0.59
6:AZ:43:ASP:OD1	6:T:191:ASN:ND2	2.35	0.59
6:Aa:1:MET:HG2	6:V:236:GLU:HG3	1.84	0.59
9:l:37:SER:HB3	10:q:44:MET:HA	1.84	0.59
1:F:130:VAL:HG12	1:F:137:VAL:HA	1.84	0.59
1:G:433:ILE:HD11	1:L:416:PHE:CZ	2.37	0.59
6:W:185:LEU:HB3	6:W:193:TYR:HB3	1.85	0.59
10:q:65:ASN:O	10:q:208:ASN:ND2	2.34	0.59
6:AU:94:ASP:HB2	6:AU:220:LEU:HD21	1.83	0.59
6:AX:1:MET:HE2	6:AX:5:LEU:HD22	1.84	0.59
6:AZ:123:ASN:HD21	6:AZ:127:THR:HB	1.66	0.59
9:j:133:LEU:HD23	11:u:71:MET:HE3	1.83	0.59
10:m:86:GLY:O	10:m:101:ARG:NH1	2.35	0.59
1:N:79:MET:HE3	1:N:111:LEU:HD21	1.84	0.59
6:W:24:ASN:ND2	6:W:34:TYR:OH	2.35	0.59
8:f:86:PRO:O	10:p:54:ARG:NH1	2.36	0.59
6:AS:24:ASN:ND2	6:AS:34:TYR:OH	2.36	0.59
9:l:113:ARG:NH2	9:l:116:GLN:OE1	2.36	0.59
1:F:42:TYR:CE2	1:K:362:LYS:HD2	2.38	0.59
1:H:42:TYR:C	1:H:42:TYR:CD2	2.80	0.59
1:N:117:MET:HE3	1:N:125:LEU:HD23	1.84	0.59
7:AF:350:PRO:HA	7:AF:353:VAL:HG22	1.83	0.59
1:E:46:LEU:HD11	6:S:150:ILE:HG13	1.85	0.59
6:AP:127:THR:HG22	6:AP:142:VAL:HG22	1.84	0.59
6:Aa:16:GLN:HG3	6:Aa:241:TYR:HE2	1.68	0.59
8:d:108:ILE:HD11	9:h:126:LYS:HG3	1.85	0.59
10:o:91:LEU:HD23	10:o:122:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:q:102:ASN:HD21	10:q:116:ALA:HB3	1.66	0.59
1:J:33:GLU:HB3	1:J:400:ILE:HG22	1.85	0.58
9:j:22:ASN:HD22	10:m:54:ARG:HE	1.51	0.58
1:H:130:VAL:HG12	1:H:137:VAL:HA	1.84	0.58
6:AP:86:ALA:HB2	6:a:45:PHE:HE1	1.68	0.58
6:AR:176:ILE:HG13	6:AR:212:LEU:HD22	1.83	0.58
4:4:31:ILE:HG13	4:4:57:VAL:HG21	1.85	0.58
7:AH:341:ASN:ND2	10:m:50:GLY:O	2.36	0.58
8:f:35:THR:O	8:f:92:ASN:ND2	2.37	0.58
6:C:28:ASN:HD22	6:C:31:THR:HG21	1.68	0.58
9:j:61:ASP:N	9:j:61:ASP:OD1	2.35	0.58
1:E:132:PRO:HB3	1:E:344:VAL:HG13	1.86	0.58
1:I:130:VAL:HG22	1:I:347:GLY:HA2	1.86	0.58
6:AV:86:ALA:HB2	6:T:45:PHE:HE1	1.68	0.58
6:C:109:ASP:OD1	6:C:109:ASP:N	2.36	0.58
6:AX:91:ASN:HD22	6:AX:93:LEU:H	1.52	0.58
1:G:424:GLU:O	1:G:428:GLN:HG3	2.02	0.58
1:K:109:PHE:HE1	1:K:119:THR:HG22	1.69	0.58
6:AR:86:ALA:HB2	6:X:45:PHE:HE1	1.68	0.58
6:AX:115:THR:HB	6:AX:192:LEU:HD23	1.86	0.58
6:AU:86:ALA:HB2	6:U:45:PHE:HE1	1.68	0.58
11:s:90:LYS:HE3	11:w:74:ARG:HH21	1.68	0.58
1:I:130:VAL:HG12	1:I:137:VAL:HA	1.86	0.58
6:A:94:ASP:HB2	6:A:220:LEU:HD21	1.84	0.58
1:D:386:SER:HB3	1:I:322:PHE:HB3	1.86	0.58
6:A:86:ALA:HB2	6:Y:45:PHE:HE1	1.68	0.58
10:o:22:ARG:HE	10:o:39:ALA:HB3	1.69	0.58
3:z:183:MET:HE1	3:z:215:ILE:HG12	1.86	0.58
1:J:6:LEU:HD13	6:AY:232:VAL:HG11	1.86	0.57
6:AP:161:ARG:HG2	6:W:51:GLN:NE2	2.19	0.57
6:AR:101:GLY:O	6:AR:116:ARG:NH1	2.37	0.57
6:T:35:LYS:NZ	6:T:221:GLU:OE2	2.34	0.57
8:f:41:ARG:HG2	8:f:78:LYS:HE2	1.86	0.57
4:4:54:ARG:NH1	4:5:46:GLU:OE2	2.38	0.57
3:y:248:LEU:HD11	3:y:261:VAL:HG11	1.86	0.57
1:H:42:TYR:CE2	1:H:44:ASN:HB2	2.30	0.57
1:L:117:MET:HE3	1:L:125:LEU:HD23	1.86	0.57
5:8:70:ARG:HA	5:8:73:MET:HE2	1.85	0.57
7:AG:335:ILE:HB	7:AG:338:ALA:HB2	1.86	0.57
6:Aa:104:GLN:NE2	6:Aa:175:THR:OG1	2.38	0.57
6:P:18:ASN:HD22	6:P:39:ALA:HB3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:29:ALA:HA	6:P:225:VAL:HG21	1.86	0.57
6:Q:176:ILE:HD11	6:Q:212:LEU:HB3	1.86	0.57
6:Q:185:LEU:HB3	6:Q:193:TYR:HB3	1.86	0.57
6:T:99:GLY:O	6:T:116:ARG:NH2	2.38	0.57
8:e:86:PRO:O	10:m:54:ARG:NH1	2.35	0.57
7:AO:335:ILE:O	7:AO:340:SER:OG	2.14	0.57
6:T:91:ASN:HD22	6:T:93:LEU:H	1.50	0.57
6:T:178:ASP:HB2	6:T:212:LEU:HD21	1.86	0.57
10:q:22:ARG:HE	10:q:39:ALA:HB3	1.68	0.57
7:AJ:341:ASN:ND2	10:n:48:GLY:O	2.38	0.57
6:C:99:GLY:O	6:C:116:ARG:NH2	2.37	0.57
6:AU:176:ILE:HD11	6:AU:212:LEU:HB3	1.87	0.57
6:AW:115:THR:HB	6:AW:192:LEU:HD23	1.86	0.57
6:AZ:36:LYS:HB3	6:AZ:225:VAL:HG12	1.86	0.57
8:b:86:PRO:O	10:q:54:ARG:NH1	2.38	0.57
10:n:104:ASN:HB3	10:n:116:ALA:HB2	1.87	0.57
10:o:86:GLY:O	10:o:101:ARG:NH1	2.37	0.57
11:v:66:SER:OG	11:v:69:ASP:OD1	2.23	0.57
5:8:187:MET:HE2	5:8:240:HIS:HB3	1.85	0.57
6:C:251:VAL:HG22	10:m:19:LEU:HD21	1.87	0.57
6:Q:18:ASN:HD22	6:Q:39:ALA:HB3	1.70	0.57
6:S:115:THR:HB	6:S:192:LEU:HD23	1.86	0.57
8:d:20:GLU:OE2	11:u:68:SER:OG	2.20	0.57
9:h:35:SER:OG	10:o:40:GLN:NE2	2.38	0.57
9:k:61:ASP:N	9:k:61:ASP:OD1	2.38	0.57
10:o:40:GLN:NE2	10:o:60:GLU:OE2	2.35	0.57
2:9:166:VAL:HG13	2:9:186:LYS:HB3	1.86	0.57
6:A:152:VAL:HG22	6:A:158:VAL:HG22	1.86	0.57
9:g:75:LYS:O	9:g:98:ASN:ND2	2.33	0.57
7:AK:331:MET:HE3	9:g:52:GLU:HB2	1.87	0.57
7:AN:352:ASP:OD1	7:AN:352:ASP:N	2.38	0.57
9:l:34:VAL:HG12	9:l:96:LYS:HG2	1.87	0.57
3:3:239:ILE:HG23	12:x:89:LEU:HD22	1.87	0.56
6:AQ:239:ARG:HG3	6:AS:255:MET:HE3	1.86	0.56
6:AT:101:GLY:O	6:AT:116:ARG:NH1	2.38	0.56
6:Aa:45:PHE:HE1	6:R:86:ALA:HB2	1.70	0.56
6:Z:24:ASN:ND2	6:Z:34:TYR:OH	2.37	0.56
10:p:82:ILE:HD11	10:p:88:ILE:HG13	1.87	0.56
1:E:52:THR:HA	1:J:63:VAL:HG23	1.87	0.56
1:H:104:THR:OG1	1:H:106:ASN:ND2	2.37	0.56
3:1:228:GLN:HA	5:8:136:MET:HE1	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AP:188:ILE:HD13	6:AP:194:LEU:HG	1.88	0.56
6:P:43:ASP:OD1	6:V:191:ASN:ND2	2.37	0.56
6:P:94:ASP:HB2	6:P:220:LEU:HD21	1.87	0.56
9:h:61:ASP:N	9:h:61:ASP:OD1	2.36	0.56
1:D:117:MET:HE3	1:D:125:LEU:HD23	1.88	0.56
1:K:353:ARG:NH2	6:AY:145:GLU:O	2.38	0.56
3:3:136:GLY:HA3	5:8:87:MET:HE2	1.87	0.56
7:AI:335:ILE:HD11	9:h:69:GLY:HA3	1.86	0.56
6:S:123:ASN:OD1	6:S:127:THR:N	2.38	0.56
6:Z:91:ASN:HD22	6:Z:93:LEU:H	1.51	0.56
6:Z:115:THR:HB	6:Z:192:LEU:HD23	1.87	0.56
6:a:57:SER:OG	6:a:58:GLN:N	2.39	0.56
9:j:108:MET:HE2	10:m:231:MET:HE2	1.87	0.56
10:m:83:GLU:OE2	10:m:142:ARG:NH2	2.39	0.56
4:5:31:ILE:HG13	4:5:57:VAL:HG21	1.88	0.56
6:Q:36:LYS:HB3	6:Q:225:VAL:HG12	1.88	0.56
9:i:17:GLU:OE1	9:i:20:ARG:NH2	2.34	0.56
6:W:94:ASP:HB2	6:W:220:LEU:HD21	1.88	0.56
1:E:104:THR:OG1	1:E:106:ASN:ND2	2.38	0.56
1:E:130:VAL:HG22	1:E:347:GLY:HA2	1.87	0.56
6:AP:94:ASP:HB2	6:AP:220:LEU:HD21	1.88	0.56
6:AT:86:ALA:HB2	6:V:45:PHE:HE1	1.70	0.56
9:h:108:MET:HE2	10:o:231:MET:HE2	1.87	0.56
3:2:144:PHE:HB2	3:z:198:MET:HE2	1.86	0.56
6:AP:251:VAL:HG22	10:p:19:LEU:HD21	1.88	0.56
6:R:99:GLY:O	6:R:116:ARG:NH2	2.39	0.56
6:R:123:ASN:HD21	6:R:127:THR:HB	1.70	0.56
6:U:50:ASN:HB2	6:U:66:LEU:H	1.71	0.56
9:l:22:ASN:HD22	10:q:54:ARG:HE	1.53	0.56
1:D:130:VAL:HG22	1:D:347:GLY:HA2	1.88	0.56
1:M:6:LEU:HD13	6:P:232:VAL:HG11	1.87	0.56
6:B:166:GLN:HG2	6:B:167:ASP:OD1	2.06	0.56
10:p:86:GLY:O	10:p:101:ARG:NH1	2.39	0.56
1:J:101:ASN:OD1	1:J:377:LYS:NZ	2.37	0.56
6:AX:168:ASN:OD1	6:AX:168:ASN:N	2.35	0.56
6:X:184:GLY:O	6:X:196:THR:OG1	2.24	0.56
6:Z:185:LEU:HB3	6:Z:193:TYR:HB3	1.88	0.56
7:AH:335:ILE:HD12	7:AN:356:MET:HE1	1.87	0.55
10:n:126:ASP:OD1	10:n:165:LYS:NZ	2.31	0.55
6:AY:50:ASN:HB2	6:AY:66:LEU:H	1.71	0.55
6:Aa:16:GLN:NE2	6:V:228:THR:OG1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:240:VAL:O	6:T:244:ASN:ND2	2.39	0.55
6:U:99:GLY:O	6:U:116:ARG:NH2	2.39	0.55
8:c:20:GLU:OE2	11:t:68:SER:OG	2.24	0.55
3:y:220:THR:HG23	3:z:276:TRP:HB3	1.88	0.55
1:E:109:PHE:HE1	1:E:119:THR:HG22	1.71	0.55
1:I:42:TYR:CE2	1:N:362:LYS:HD2	2.41	0.55
6:S:48:ASN:HD21	6:S:51:GLN:HE21	1.54	0.55
6:V:146:ASP:OD1	6:V:146:ASP:N	2.39	0.55
6:X:115:THR:HB	6:X:192:LEU:HD23	1.88	0.55
1:F:117:MET:HE3	1:F:125:LEU:HD23	1.87	0.55
1:K:401:ASP:O	1:K:405:GLU:HG2	2.06	0.55
1:L:130:VAL:HG22	1:L:347:GLY:HA2	1.89	0.55
7:AF:350:PRO:O	7:AF:351:GLN:C	2.50	0.55
10:p:76:ARG:NH1	10:p:79:ASP:OD1	2.39	0.55
6:AQ:259:ASN:O	9:i:120:GLN:NE2	2.39	0.55
9:g:20:ARG:HH21	9:g:111:ALA:HA	1.71	0.55
1:J:13:GLN:HE22	6:AY:226:ASN:HD21	1.53	0.55
3:1:103:VAL:O	3:1:107:THR:HG22	2.06	0.55
6:AP:101:GLY:O	6:AP:116:ARG:NH1	2.35	0.55
6:Z:240:VAL:O	6:Z:244:ASN:ND2	2.33	0.55
1:F:433:ILE:HD11	1:K:416:PHE:HZ	1.70	0.55
1:L:13:GLN:HE22	6:Aa:226:ASN:HD21	1.55	0.55
4:6:40:ALA:HA	5:8:211:GLN:HG3	1.87	0.55
6:AW:96:MET:HE3	6:AW:221:GLU:HG3	1.87	0.55
6:R:50:ASN:HB2	6:R:66:LEU:H	1.71	0.55
6:V:146:ASP:HB2	6:V:162:VAL:HG13	1.89	0.55
3:2:115:VAL:HG11	3:2:283:LEU:HD11	1.87	0.55
4:5:13:ALA:HB1	3:z:239:ILE:HD11	1.89	0.55
6:AT:123:ASN:OD1	6:AT:127:THR:N	2.38	0.55
6:AW:116:ARG:NH1	6:AW:221:GLU:OE2	2.40	0.55
6:AZ:16:GLN:HG3	6:AZ:241:TYR:HE2	1.70	0.55
6:V:176:ILE:HG13	6:V:212:LEU:HD22	1.88	0.55
9:g:129:LEU:HD22	11:w:67:LEU:HD12	1.88	0.55
1:G:422:SER:HA	1:L:409:LEU:HD21	1.88	0.55
1:L:370:SER:O	6:U:161:ARG:NH2	2.40	0.55
6:A:36:LYS:HB3	6:A:225:VAL:HG12	1.89	0.55
6:AZ:185:LEU:HB3	6:AZ:193:TYR:HB3	1.89	0.55
6:Q:43:ASP:OD1	6:W:191:ASN:ND2	2.39	0.55
6:W:258:VAL:HG13	6:W:262:LEU:HD22	1.89	0.55
9:k:135:MET:HE1	11:r:72:ILE:HG12	1.89	0.55
10:p:244:SER:HA	10:p:247:ARG:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:LEU:HD23	1:D:387:PHE:HB3	1.88	0.55
1:F:130:VAL:HG22	1:F:347:GLY:HA2	1.89	0.55
1:O:351:LEU:HD23	1:O:387:PHE:HB3	1.88	0.55
3:1:268:MET:HE1	4:7:1:MET:HG3	1.88	0.55
6:A:162:VAL:HG23	6:A:165:GLN:HB3	1.88	0.55
6:C:161:ARG:NH1	6:R:186:GLU:OE1	2.40	0.55
6:AS:49:ILE:HG22	6:AS:50:ASN:H	1.72	0.55
6:AS:226:ASN:HB3	6:AS:229:GLU:HB2	1.87	0.55
6:AU:99:GLY:O	6:AU:116:ARG:NH2	2.38	0.55
6:S:43:ASP:OD1	6:S:43:ASP:N	2.40	0.55
6:Y:154:THR:HG23	6:Y:214:GLU:HB3	1.89	0.55
9:k:3:LEU:HD21	9:k:128:MET:HE3	1.89	0.55
3:z:104:ILE:O	3:z:110:THR:OG1	2.24	0.55
1:F:433:ILE:HD11	1:K:416:PHE:CZ	2.41	0.54
1:G:427:ASN:OD1	1:M:414:ARG:NH2	2.40	0.54
1:H:42:TYR:C	1:H:42:TYR:HD2	2.15	0.54
1:I:422:SER:HA	1:N:409:LEU:HD21	1.89	0.54
3:3:103:VAL:O	3:3:107:THR:OG1	2.23	0.54
4:6:84:LEU:N	4:6:85:PRO:HD2	2.21	0.54
6:AX:96:MET:HG3	6:AX:221:GLU:HB2	1.89	0.54
6:T:258:VAL:HG13	6:T:262:LEU:HD22	1.89	0.54
10:p:91:LEU:HD23	10:p:122:LEU:HD21	1.89	0.54
1:D:429:LEU:HD21	1:I:413:GLN:HG3	1.88	0.54
1:F:42:TYR:HD1	1:F:42:TYR:O	1.90	0.54
6:AW:43:ASP:OD1	6:AW:43:ASP:N	2.28	0.54
6:Aa:239:ARG:NH1	6:Aa:242:GLU:OE1	2.39	0.54
6:P:188:ILE:HD13	6:P:194:LEU:HG	1.89	0.54
6:Q:123:ASN:HD21	6:Q:127:THR:HB	1.72	0.54
6:S:91:ASN:HD22	6:S:93:LEU:H	1.55	0.54
6:U:48:ASN:HD21	6:U:51:GLN:HE21	1.54	0.54
6:X:48:ASN:HD21	6:X:51:GLN:HE21	1.56	0.54
3:3:112:ILE:HD13	3:3:141:LEU:HB3	1.89	0.54
9:g:108:MET:HE2	9:i:121:VAL:HG22	1.89	0.54
1:H:42:TYR:HD2	1:H:43:SER:N	2.05	0.54
1:K:117:MET:HE3	1:K:125:LEU:HD23	1.89	0.54
7:AD:348:SER:HB2	7:AD:356:MET:HE3	1.89	0.54
6:AR:246:LYS:NZ	6:AW:262:LEU:OXT	2.40	0.54
6:AY:16:GLN:HG3	6:AY:241:TYR:HE2	1.71	0.54
1:D:130:VAL:HG12	1:D:137:VAL:HA	1.88	0.54
6:AR:28:ASN:HD21	6:AX:43:ASP:HB3	1.72	0.54
6:AV:94:ASP:HB2	6:AV:220:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AW:24:ASN:ND2	6:AW:34:TYR:OH	2.40	0.54
10:m:154:PRO:HG2	10:m:157:GLU:HG3	1.89	0.54
11:u:66:SER:OG	11:u:69:ASP:OD1	2.25	0.54
1:G:25:ASN:O	1:G:398:SER:OG	2.26	0.54
7:AF:352:ASP:O	7:AF:353:VAL:C	2.51	0.54
6:B:36:LYS:HB3	6:B:225:VAL:HG12	1.89	0.54
6:AQ:249:SER:OG	6:AQ:253:LYS:NZ	2.40	0.54
6:X:196:THR:H	6:X:199:SER:HB3	1.72	0.54
9:k:3:LEU:HB3	9:k:129:LEU:HD21	1.89	0.54
9:k:43:LYS:HG2	9:k:77:LEU:HD21	1.90	0.54
1:D:401:ASP:HB3	1:D:404:GLN:HB3	1.90	0.54
4:4:6:PHE:HB2	3:z:268:MET:HE2	1.89	0.54
6:A:43:ASP:OD1	6:A:43:ASP:N	2.41	0.54
6:Q:176:ILE:HG13	6:Q:212:LEU:HD22	1.90	0.54
6:R:185:LEU:HB3	6:R:193:TYR:HB3	1.89	0.54
6:AQ:123:ASN:HD21	6:AQ:127:THR:HB	1.71	0.54
6:AX:99:GLY:O	6:AX:116:ARG:NH2	2.40	0.54
6:R:91:ASN:HD22	6:R:93:LEU:H	1.55	0.54
10:p:18:ALA:HB2	10:p:59:THR:HG21	1.90	0.54
1:D:33:GLU:HB3	1:D:400:ILE:HG22	1.89	0.54
1:H:130:VAL:HG22	1:H:347:GLY:HA2	1.90	0.54
1:I:42:TYR:CD2	1:N:362:LYS:HB2	2.43	0.54
1:K:130:VAL:HG22	1:K:347:GLY:HA2	1.89	0.54
1:N:130:VAL:HG22	1:N:347:GLY:HA2	1.89	0.54
6:AQ:115:THR:HB	6:AQ:192:LEU:HD12	1.90	0.54
6:AS:240:VAL:O	6:AS:244:ASN:ND2	2.36	0.54
6:U:36:LYS:HB3	6:U:225:VAL:HG12	1.89	0.54
6:Y:56:SER:HB2	6:Y:62:LEU:HD12	1.89	0.54
8:c:30:ILE:HG23	8:c:96:LEU:HD11	1.89	0.54
1:I:6:LEU:HD13	1:O:407:VAL:HG11	1.89	0.54
1:J:117:MET:HE3	1:J:125:LEU:HD23	1.89	0.54
1:M:13:GLN:HE22	6:P:226:ASN:HD21	1.56	0.54
3:3:198:MET:HE1	3:y:141:LEU:HD22	1.90	0.54
3:3:239:ILE:HD12	12:x:89:LEU:HD22	1.90	0.54
6:AR:184:GLY:O	6:AR:196:THR:OG1	2.24	0.54
6:P:1:MET:HE2	6:P:5:LEU:HD22	1.88	0.54
6:T:185:LEU:HB3	6:T:193:TYR:HB3	1.90	0.54
6:U:115:THR:HB	6:U:192:LEU:HD23	1.90	0.54
9:g:9:VAL:HG21	9:g:62:THR:HB	1.90	0.54
9:l:126:LYS:HD3	10:q:248:MET:HG2	1.91	0.54
1:F:42:TYR:C	1:F:42:TYR:HD1	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:TYR:CD1	1:G:42:TYR:C	2.86	0.53
6:AR:99:GLY:O	6:AR:116:ARG:NH2	2.38	0.53
6:a:50:ASN:HB2	6:a:66:LEU:H	1.73	0.53
9:g:84:ASP:OD1	9:i:73:SER:OG	2.23	0.53
9:l:108:MET:HE2	10:q:231:MET:HE2	1.89	0.53
6:C:242:GLU:OE1	6:AU:259:ASN:ND2	2.39	0.53
1:O:132:PRO:HB3	1:O:344:VAL:HG13	1.91	0.53
2:9:97:ALA:HB2	2:9:113:LEU:HD11	1.90	0.53
6:C:214:GLU:OE1	6:C:216:ARG:NH1	2.32	0.53
1:J:23:ILE:HG23	1:J:402:MET:HE1	1.91	0.53
6:AQ:36:LYS:HB3	6:AQ:225:VAL:HG12	1.89	0.53
6:AU:240:VAL:O	6:AU:244:ASN:ND2	2.38	0.53
6:T:43:ASP:OD1	6:T:43:ASP:N	2.41	0.53
10:m:65:ASN:O	10:m:208:ASN:ND2	2.36	0.53
10:o:76:ARG:NH1	10:o:79:ASP:OD1	2.39	0.53
11:r:94:ALA:HA	3:z:100:PRO:HG3	1.90	0.53
5:8:54:MET:HE2	11:s:26:GLY:HA3	1.90	0.53
7:AI:339:LEU:HD11	9:h:72:GLU:HG3	1.91	0.53
6:AP:9:LYS:HD2	10:q:216:THR:HG21	1.90	0.53
6:AS:115:THR:HB	6:AS:192:LEU:HD12	1.89	0.53
6:AZ:100:ASP:O	6:AZ:213:GLY:N	2.41	0.53
6:P:206:VAL:HG23	6:P:209:LEU:HB2	1.91	0.53
9:h:133:LEU:HA	11:t:71:MET:HE3	1.89	0.53
11:t:66:SER:OG	11:t:69:ASP:OD1	2.26	0.53
6:A:41:PHE:HB2	10:n:31:THR:HA	1.89	0.53
6:B:24:ASN:ND2	6:B:34:TYR:OH	2.41	0.53
6:AT:36:LYS:HB3	6:AT:225:VAL:HG12	1.89	0.53
6:AU:226:ASN:HD22	6:AU:229:GLU:H	1.55	0.53
6:AW:123:ASN:ND2	6:AW:127:THR:O	2.42	0.53
6:S:239:ARG:O	6:S:243:MET:HG2	2.09	0.53
1:G:49:ASN:HB3	1:G:52:THR:CG2	2.38	0.53
1:N:359:GLY:O	1:N:371:THR:OG1	2.26	0.53
7:AJ:335:ILE:HG22	9:g:87:LEU:HD11	1.89	0.53
6:AS:184:GLY:O	6:AS:196:THR:OG1	2.23	0.53
6:AU:176:ILE:HG13	6:AU:212:LEU:HD22	1.90	0.53
6:AX:55:GLN:HG3	6:AX:59:ASN:HA	1.90	0.53
6:AZ:176:ILE:HD11	6:AZ:212:LEU:HB3	1.90	0.53
6:Q:37:SER:HB3	6:Q:77:THR:HG22	1.89	0.53
6:AV:28:ASN:ND2	6:Z:43:ASP:HB3	2.24	0.53
6:P:184:GLY:O	6:P:196:THR:OG1	2.23	0.53
8:d:31:ALA:HA	9:j:118:ASN:HD21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:433:ILE:HD11	1:M:416:PHE:HZ	1.73	0.53
6:A:74:VAL:HG12	6:AV:66:LEU:HD11	1.91	0.53
6:AY:188:ILE:HD13	6:AY:194:LEU:HG	1.91	0.53
6:Aa:43:ASP:OD1	6:Aa:43:ASP:N	2.38	0.53
6:P:99:GLY:O	6:P:116:ARG:NH2	2.41	0.53
3:3:85:VAL:HG13	8:b:3:ILE:HA	1.90	0.53
4:5:81:ILE:HG13	3:z:278:LEU:HD21	1.91	0.53
2:9:179:LEU:HB2	2:9:199:PRO:HA	1.91	0.53
6:B:239:ARG:HG3	6:AV:255:MET:HE3	1.91	0.53
6:AP:83:HIS:HE1	6:AP:96:MET:HE2	1.74	0.53
8:c:85:GLN:HE21	9:i:19:VAL:HG22	1.73	0.53
8:e:36:PRO:HB3	8:e:90:ASP:HB2	1.91	0.53
8:f:37:GLY:N	8:f:90:ASP:O	2.42	0.53
9:l:133:LEU:HD23	11:v:71:MET:HE3	1.91	0.53
1:D:430:GLN:HE21	1:O:402:MET:HB2	1.74	0.52
5:8:64:ILE:HG22	5:8:70:ARG:HG2	1.92	0.52
5:8:97:VAL:HG22	5:8:131:MET:HB2	1.90	0.52
6:Aa:94:ASP:HB2	6:Aa:220:LEU:HD21	1.90	0.52
6:W:91:ASN:HD22	6:W:93:LEU:H	1.56	0.52
1:I:51:LYS:HB3	1:N:62:GLN:HG3	1.91	0.52
1:J:130:VAL:HG12	1:J:137:VAL:HA	1.90	0.52
1:K:79:MET:HE3	1:K:111:LEU:HD21	1.91	0.52
3:3:125:LEU:HB3	3:3:128:THR:HB	1.91	0.52
7:AM:340:SER:HA	7:AM:349:ILE:HD11	1.90	0.52
6:AS:185:LEU:HB3	6:AS:193:TYR:HB3	1.91	0.52
6:AW:240:VAL:O	6:AW:244:ASN:ND2	2.36	0.52
6:P:96:MET:HG3	6:P:221:GLU:HB2	1.90	0.52
1:J:109:PHE:HE1	1:J:119:THR:HG22	1.73	0.52
1:L:333:SER:HA	1:L:348:ARG:HA	1.90	0.52
2:0:152:VAL:HG13	2:0:172:THR:HB	1.90	0.52
6:AQ:185:LEU:HB3	6:AQ:193:TYR:HB3	1.92	0.52
6:AS:99:GLY:O	6:AS:116:ARG:NH2	2.35	0.52
6:U:24:ASN:ND2	6:U:34:TYR:OH	2.43	0.52
6:Y:19:ILE:HG23	6:Y:234:MET:HE1	1.90	0.52
8:b:128:ILE:HG13	8:b:129:LYS:HG3	1.91	0.52
6:AU:93:LEU:HD13	6:AU:121:THR:HA	1.91	0.52
6:P:91:ASN:HD22	6:P:93:LEU:H	1.55	0.52
8:e:41:ARG:NH2	8:e:80:TYR:OH	2.38	0.52
10:m:18:ALA:HB2	10:m:59:THR:HG21	1.90	0.52
10:n:82:ILE:HD11	10:n:88:ILE:HG13	1.92	0.52
10:q:77:ASP:N	10:q:77:ASP:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AY:16:GLN:NE2	6:T:228:THR:OG1	2.43	0.52
1:D:425:VAL:O	1:D:429:LEU:HG	2.09	0.52
1:G:130:VAL:HG22	1:G:347:GLY:HA2	1.91	0.52
2:9:67:LEU:HD12	2:9:87:ILE:HG12	1.91	0.52
7:AE:351:GLN:O	10:n:42:ARG:NH1	2.38	0.52
6:AW:234:MET:HE3	6:X:247:VAL:HG22	1.92	0.52
6:AY:18:ASN:HD22	6:AY:39:ALA:HB3	1.72	0.52
6:Q:159:SER:HB3	6:Q:168:ASN:HB3	1.90	0.52
6:S:61:GLU:HG3	6:X:198:ALA:HB2	1.91	0.52
6:U:83:HIS:HE1	6:U:99:GLY:H	1.58	0.52
3:y:208:ASP:OD1	3:y:208:ASP:N	2.42	0.52
1:F:109:PHE:HE1	1:F:119:THR:HG22	1.74	0.52
1:H:23:ILE:HG23	1:H:402:MET:HE1	1.92	0.52
5:8:150:LEU:HD13	5:8:252:ILE:HG21	1.92	0.52
6:C:226:ASN:HD21	6:AU:16:GLN:HE22	1.58	0.52
6:P:251:VAL:HA	6:P:254:MET:HE2	1.92	0.52
1:F:147:ILE:HA	1:F:346:LEU:HD23	1.92	0.52
4:5:81:ILE:HG21	3:z:278:LEU:HD11	1.91	0.52
6:AS:249:SER:OG	6:AS:253:LYS:NZ	2.43	0.52
6:AT:166:GLN:O	6:AT:167:ASP:HB2	2.08	0.52
6:P:22:ILE:HG21	6:P:234:MET:HB2	1.92	0.52
6:R:161:ARG:HH11	6:R:168:ASN:ND2	2.06	0.52
6:W:115:THR:HB	6:W:192:LEU:HD23	1.92	0.52
6:X:104:GLN:NE2	6:X:204:GLU:OE2	2.39	0.52
1:I:152:GLY:HA3	1:I:320:THR:HA	1.91	0.52
5:8:28:VAL:HB	5:8:86:GLY:HA3	1.91	0.52
6:AQ:240:VAL:HA	6:AQ:243:MET:HE2	1.92	0.52
6:U:43:ASP:OD1	6:Z:191:ASN:ND2	2.42	0.52
6:W:43:ASP:OD1	6:W:43:ASP:N	2.36	0.52
1:D:422:SER:HA	1:I:409:LEU:HD21	1.92	0.52
1:I:33:GLU:HB3	1:I:400:ILE:HG22	1.91	0.52
1:K:141:GLU:OE1	1:K:143:GLN:NE2	2.31	0.52
1:L:33:GLU:HB3	1:L:400:ILE:HG22	1.91	0.52
2:0:73:VAL:HG12	2:0:75:GLY:H	1.74	0.52
3:2:248:LEU:HD11	3:2:261:VAL:HG11	1.92	0.52
6:A:93:LEU:HD13	6:A:121:THR:HA	1.92	0.52
6:C:181:ASN:ND2	10:m:107:VAL:O	2.42	0.52
6:X:123:ASN:HD21	6:X:127:THR:HB	1.75	0.52
1:I:147:ILE:HA	1:I:346:LEU:HD23	1.93	0.51
1:L:109:PHE:HE1	1:L:119:THR:HG22	1.74	0.51
6:C:41:PHE:HB2	10:m:31:THR:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:94:ASP:HB2	6:C:220:LEU:HD21	1.90	0.51
6:C:123:ASN:HD21	6:C:127:THR:HB	1.75	0.51
6:AP:152:VAL:HG22	6:AP:158:VAL:HG22	1.91	0.51
6:AT:176:ILE:HG13	6:AT:212:LEU:HD22	1.90	0.51
6:AU:28:ASN:ND2	6:R:43:ASP:HB3	2.25	0.51
6:AU:36:LYS:HB3	6:AU:225:VAL:HG12	1.92	0.51
6:AV:87:GLN:NE2	6:Z:38:ARG:HH22	2.08	0.51
6:Q:43:ASP:OD1	6:Q:43:ASP:N	2.40	0.51
6:S:83:HIS:CE1	6:S:99:GLY:H	2.28	0.51
6:a:161:ARG:HH11	6:a:168:ASN:HD21	1.58	0.51
10:o:18:ALA:HB2	10:o:59:THR:HG21	1.91	0.51
1:G:432:ASN:ND2	1:L:420:SER:OG	2.43	0.51
3:2:112:ILE:HD13	3:2:141:LEU:HB3	1.92	0.51
6:AZ:240:VAL:O	6:AZ:244:ASN:ND2	2.38	0.51
6:Y:24:ASN:ND2	6:Y:34:TYR:OH	2.43	0.51
10:n:86:GLY:O	10:n:101:ARG:NH1	2.44	0.51
10:o:82:ILE:HD11	10:o:88:ILE:HG13	1.92	0.51
1:F:79:MET:HE3	1:F:111:LEU:HD21	1.92	0.51
6:A:95:MET:HE2	6:A:152:VAL:HG21	1.92	0.51
6:AQ:181:ASN:ND2	10:q:107:VAL:O	2.44	0.51
6:AR:115:THR:HB	6:AR:192:LEU:HD12	1.92	0.51
9:l:9:VAL:HG21	9:l:62:THR:HB	1.92	0.51
6:R:56:SER:HB2	6:R:62:LEU:HD12	1.93	0.51
6:a:226:ASN:HB3	6:a:229:GLU:HB2	1.93	0.51
1:H:101:ASN:OD1	1:H:377:LYS:NZ	2.43	0.51
3:1:198:MET:HE2	5:8:53:VAL:HG11	1.92	0.51
3:3:139:LEU:HD21	11:w:98:LEU:HD13	1.93	0.51
3:3:255:MET:HB2	5:8:214:ILE:HG12	1.93	0.51
6:B:98:GLU:OE1	6:B:216:ARG:NH1	2.40	0.51
6:W:38:ARG:HH22	6:a:87:GLN:HE22	1.58	0.51
10:n:70:SER:O	10:n:206:GLY:N	2.30	0.51
1:G:65:GLN:HE22	1:G:362:LYS:HG2	1.75	0.51
1:I:42:TYR:CD1	1:I:42:TYR:C	2.88	0.51
1:I:117:MET:HE3	1:I:125:LEU:HD23	1.92	0.51
7:AF:347:ALA:O	7:AF:353:VAL:HG13	2.10	0.51
6:AU:28:ASN:HD21	6:R:43:ASP:HB3	1.74	0.51
6:Aa:240:VAL:O	6:Aa:244:ASN:ND2	2.43	0.51
6:R:115:THR:HB	6:R:192:LEU:HD23	1.93	0.51
6:Y:96:MET:HE3	6:Y:221:GLU:HG3	1.93	0.51
10:o:84:GLY:O	10:o:101:ARG:NH2	2.43	0.51
10:q:84:GLY:O	10:q:101:ARG:NH2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AI:339:LEU:HD11	9:h:72:GLU:CG	2.41	0.51
6:AP:41:PHE:HB2	10:p:31:THR:HA	1.91	0.51
6:AP:226:ASN:HB3	6:AP:229:GLU:HB2	1.93	0.51
6:P:239:ARG:O	6:P:243:MET:HG2	2.11	0.51
6:Q:208:GLY:N	6:Q:213:GLY:O	2.42	0.51
8:c:119:SER:OG	11:s:74:ARG:NH2	2.44	0.51
3:1:282:THR:HG21	4:6:81:ILE:HG23	1.93	0.51
3:2:112:ILE:HG22	3:2:116:MET:HE2	1.93	0.51
6:AS:47:GLN:HG3	6:AS:49:ILE:HD11	1.92	0.51
6:AU:232:VAL:HG11	6:Z:9:LYS:HG3	1.93	0.51
1:H:82:ARG:HH11	1:H:396:GLU:HG2	1.76	0.51
2:9:141:ARG:HH22	7:AJ:356:MET:HB3	1.76	0.51
6:A:44:LEU:HD21	6:A:73:LYS:HD3	1.92	0.51
6:AR:98:GLU:CD	6:X:45:PHE:HB3	2.36	0.51
10:q:14:GLN:HG3	10:q:58:MET:HA	1.92	0.51
1:G:42:TYR:C	1:G:42:TYR:HD1	2.19	0.51
6:AS:82:THR:HB	6:AS:224:ASN:HD22	1.76	0.51
6:AX:94:ASP:HB2	6:AX:220:LEU:HD21	1.93	0.51
4:6:52:LEU:HB2	4:7:25:ILE:HG21	1.93	0.50
6:C:31:THR:HG22	6:AT:41:PHE:HB3	1.93	0.50
6:C:59:ASN:HB3	6:C:62:LEU:HB2	1.93	0.50
6:AR:49:ILE:HD11	6:AR:66:LEU:HD13	1.93	0.50
6:AT:7:VAL:O	6:AT:10:THR:OG1	2.29	0.50
6:S:104:GLN:NE2	6:S:204:GLU:OE2	2.43	0.50
8:b:35:THR:O	8:b:92:ASN:ND2	2.44	0.50
8:e:88:THR:HG22	10:m:56:PHE:HZ	1.74	0.50
10:o:1:MET:HG3	10:o:239:ASP:HB2	1.93	0.50
1:G:82:ARG:HH11	1:G:396:GLU:HG2	1.76	0.50
1:H:351:LEU:HD13	1:H:390:ILE:HD11	1.93	0.50
5:8:81:ILE:HG22	5:8:85:MET:HE1	1.93	0.50
5:8:204:VAL:HG23	12:x:39:LEU:HD22	1.93	0.50
7:AH:342:GLN:HG3	7:AH:343:PRO:HD2	1.92	0.50
6:AR:28:ASN:ND2	6:AX:43:ASP:HB3	2.27	0.50
1:H:38:PHE:HB2	1:M:28:THR:HG22	1.92	0.50
1:H:427:ASN:HD21	1:N:410:ILE:HG23	1.74	0.50
1:L:141:GLU:OE1	1:L:143:GLN:NE2	2.35	0.50
7:AG:336:PRO:HG2	7:AO:352:ASP:HB3	1.92	0.50
6:AQ:122:LEU:O	6:AR:181:ASN:ND2	2.44	0.50
6:AZ:154:THR:HG23	6:AZ:214:GLU:HB3	1.94	0.50
6:P:154:THR:HG23	6:P:214:GLU:HB3	1.91	0.50
1:K:82:ARG:HH11	1:K:396:GLU:HG2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:82:ARG:NH1	1:M:396:GLU:HB3	2.25	0.50
6:B:184:GLY:O	6:B:196:THR:OG1	2.30	0.50
6:AS:28:ASN:ND2	6:AW:43:ASP:HB3	2.26	0.50
6:AV:28:ASN:OD1	6:AV:28:ASN:N	2.43	0.50
6:AW:185:LEU:HB3	6:AW:193:TYR:HB3	1.93	0.50
6:T:154:THR:HG23	6:T:214:GLU:HB3	1.93	0.50
6:Z:123:ASN:HD21	6:Z:127:THR:HB	1.74	0.50
8:c:104:MET:SD	9:i:126:LYS:NZ	2.80	0.50
9:l:70:ILE:HD13	10:q:51:HIS:HB3	1.93	0.50
1:M:112:ASN:OD1	1:M:115:ASN:N	2.45	0.50
1:N:132:PRO:HB3	1:N:344:VAL:HG13	1.93	0.50
1:O:84:SER:OG	1:O:391:ASN:ND2	2.44	0.50
2:9:32:ASP:OD1	2:9:36:ASN:N	2.30	0.50
2:9:33:ASN:ND2	9:i:95:TYR:O	2.40	0.50
2:9:193:LEU:HG	2:9:195:GLY:H	1.76	0.50
6:A:56:SER:OG	6:A:57:SER:N	2.42	0.50
6:B:94:ASP:HB2	6:B:220:LEU:HD21	1.94	0.50
6:B:104:GLN:HE22	6:B:204:GLU:HG3	1.76	0.50
6:C:133:SER:OG	6:C:190:GLN:NE2	2.45	0.50
6:AR:94:ASP:HB2	6:AR:220:LEU:HD21	1.92	0.50
6:U:18:ASN:HB2	6:U:41:PHE:HZ	1.76	0.50
6:a:155:ASP:O	6:a:173:GLN:NE2	2.43	0.50
1:E:79:MET:HE3	1:E:111:LEU:HD21	1.94	0.50
7:AK:330:ASN:HD22	7:AK:330:ASN:N	2.10	0.50
6:B:246:LYS:NZ	6:AV:262:LEU:O	2.45	0.50
6:C:238:GLN:HG3	6:AT:254:MET:HG3	1.93	0.50
6:AV:208:GLY:N	6:AV:213:GLY:O	2.44	0.50
6:V:154:THR:HG23	6:V:214:GLU:HB3	1.93	0.50
6:Y:226:ASN:HB3	6:Y:229:GLU:HB2	1.94	0.50
6:a:94:ASP:HB2	6:a:220:LEU:HD21	1.93	0.50
10:n:21:LEU:HD23	10:n:39:ALA:HB2	1.94	0.50
1:E:429:LEU:HD21	1:J:413:GLN:CG	2.41	0.50
1:H:433:ILE:HD11	1:M:416:PHE:CZ	2.47	0.50
1:N:353:ARG:NH2	6:P:145:GLU:O	2.45	0.50
7:AK:353:VAL:HG21	9:g:71:VAL:HG11	1.94	0.50
3:2:276:TRP:HB3	3:z:220:THR:HG23	1.93	0.50
3:3:183:MET:HE1	3:3:211:MET:HG3	1.92	0.50
7:AF:347:ALA:HA	7:AF:353:VAL:CG1	2.42	0.50
6:C:188:ILE:HD13	6:C:194:LEU:HG	1.94	0.50
6:AR:90:THR:HG23	6:AX:80:VAL:HG11	1.94	0.50
6:AR:255:MET:HE3	10:n:223:ARG:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AR:258:VAL:HG11	9:i:102:MET:HE1	1.93	0.50
9:i:37:SER:O	9:i:38:ALA:HB3	2.11	0.50
1:F:351:LEU:HD13	1:F:390:ILE:HD11	1.94	0.50
1:J:351:LEU:HD13	1:J:390:ILE:HD11	1.92	0.50
1:J:415:ASN:O	1:J:419:ASN:ND2	2.45	0.50
3:1:104:ILE:HD12	5:8:44:TYR:HE2	1.77	0.50
2:9:33:ASN:ND2	9:i:34:VAL:O	2.45	0.50
6:AQ:43:ASP:N	6:AQ:43:ASP:OD1	2.45	0.50
6:AR:166:GLN:O	6:AR:167:ASP:HB2	2.12	0.50
6:R:240:VAL:O	6:R:244:ASN:ND2	2.45	0.50
6:W:178:ASP:HB2	6:W:212:LEU:HD21	1.93	0.50
6:X:188:ILE:HD13	6:X:194:LEU:HG	1.94	0.50
6:a:103:PHE:HB2	6:a:115:THR:HG23	1.94	0.50
11:u:60:ARG:NH1	11:u:62:ASP:OD1	2.45	0.50
3:z:142:THR:HA	3:z:145:VAL:HG22	1.93	0.50
1:E:323:LEU:HD11	1:E:326:VAL:HG23	1.94	0.49
5:8:43:LEU:HD21	11:s:99:MET:HA	1.94	0.49
6:AQ:82:THR:OG1	6:AQ:224:ASN:ND2	2.37	0.49
6:AU:115:THR:HB	6:AU:192:LEU:HD12	1.94	0.49
6:AW:101:GLY:HA3	6:AW:176:ILE:HD12	1.93	0.49
6:AX:176:ILE:HG21	6:AX:215:ILE:HD11	1.93	0.49
6:T:83:HIS:CE1	6:T:99:GLY:H	2.30	0.49
6:U:87:GLN:HB2	6:U:220:LEU:HB2	1.94	0.49
8:d:128:ILE:HD13	11:u:83:ALA:HB2	1.94	0.49
2:0:153:VAL:HG12	2:0:155:GLY:H	1.77	0.49
6:AQ:129:VAL:HG12	6:AQ:136:PRO:HA	1.94	0.49
6:AY:36:LYS:HB3	6:AY:225:VAL:HG12	1.94	0.49
8:e:85:GLN:NE2	10:m:53:SER:OG	2.34	0.49
9:l:120:GLN:HE22	10:p:247:ARG:HG2	1.77	0.49
1:G:428:GLN:NE2	1:L:413:GLN:HE22	2.11	0.49
1:I:426:HIS:HE1	1:N:20:SER:OG	1.95	0.49
1:J:79:MET:HE3	1:J:111:LEU:HD21	1.94	0.49
4:4:5:MET:SD	4:4:83:ARG:NH2	2.85	0.49
6:T:50:ASN:HB2	6:T:66:LEU:H	1.78	0.49
6:U:188:ILE:HD13	6:U:194:LEU:HG	1.94	0.49
3:2:112:ILE:HG23	3:2:283:LEU:HD23	1.94	0.49
6:B:46:TYR:HB2	10:o:178:THR:HA	1.94	0.49
6:AY:262:LEU:OXT	6:T:246:LYS:NZ	2.40	0.49
10:q:35:ARG:NH1	10:q:101:ARG:HD3	2.27	0.49
3:y:144:PHE:O	3:y:147:SER:OG	2.27	0.49
2:9:41:ASN:ND2	2:9:61:GLN:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:154:THR:HG23	6:a:214:GLU:HB3	1.94	0.49
2:9:32:ASP:HB2	9:i:41:THR:HB	1.94	0.49
6:C:31:THR:OG1	6:C:34:TYR:HB2	2.12	0.49
6:AY:91:ASN:HD22	6:AY:92:ALA:N	2.11	0.49
1:F:40:ASP:HB2	1:K:366:THR:H	1.78	0.49
1:N:104:THR:HB	1:N:367:GLN:HG2	1.94	0.49
1:O:6:LEU:HD13	6:S:232:VAL:HG11	1.93	0.49
3:1:195:PHE:HB3	3:1:213:VAL:HG22	1.95	0.49
3:2:116:MET:HE3	3:2:134:ILE:HG23	1.94	0.49
6:AY:48:ASN:HD21	6:AY:51:GLN:HE21	1.60	0.49
6:S:258:VAL:HG13	6:S:262:LEU:HD22	1.93	0.49
1:E:50:ALA:O	1:E:52:THR:N	2.46	0.49
1:E:351:LEU:HD13	1:E:390:ILE:HD11	1.93	0.49
1:H:42:TYR:CE1	1:M:362:LYS:HB2	2.46	0.49
1:H:44:ASN:OD1	1:H:53:THR:HG21	2.12	0.49
1:K:109:PHE:CE1	1:K:119:THR:HG22	2.48	0.49
6:AV:232:VAL:HG11	6:Y:9:LYS:HG3	1.95	0.49
6:AY:196:THR:O	6:Y:166:GLN:NE2	2.46	0.49
6:Aa:29:ALA:HA	6:Aa:225:VAL:HG21	1.94	0.49
6:S:188:ILE:HD13	6:S:194:LEU:HG	1.95	0.49
9:k:133:LEU:HD23	11:r:71:MET:HE3	1.95	0.49
1:J:422:SER:HA	1:O:409:LEU:HD21	1.95	0.49
6:A:226:ASN:HB3	6:A:229:GLU:HB3	1.95	0.49
6:P:258:VAL:HG13	6:P:262:LEU:HD22	1.94	0.49
6:Q:166:GLN:HG2	6:Q:167:ASP:H	1.77	0.49
6:S:103:PHE:HB2	6:S:115:THR:HG23	1.94	0.49
8:f:33:ALA:O	8:f:92:ASN:ND2	2.45	0.49
9:h:75:LYS:O	9:h:98:ASN:ND2	2.43	0.49
1:E:429:LEU:HD21	1:J:413:GLN:HG2	1.94	0.49
6:B:96:MET:HG3	6:B:221:GLU:HB2	1.95	0.49
6:C:239:ARG:HG3	6:AU:255:MET:HE3	1.94	0.49
6:P:91:ASN:HD22	6:P:92:ALA:N	2.11	0.49
6:Q:123:ASN:H	6:Q:123:ASN:HD22	1.59	0.49
1:E:104:THR:HB	1:E:367:GLN:HG2	1.95	0.48
1:H:141:GLU:OE1	1:H:143:GLN:NE2	2.34	0.48
1:K:147:ILE:HA	1:K:346:LEU:HD23	1.95	0.48
1:M:151:PHE:CD2	1:M:344:VAL:HG21	2.48	0.48
6:V:115:THR:HB	6:V:192:LEU:HD23	1.95	0.48
1:E:82:ARG:HH11	1:E:396:GLU:HB3	1.77	0.48
1:G:59:GLN:NE2	1:G:60:ALA:O	2.44	0.48
1:J:356:ASN:HB3	1:J:374:SER:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:226:ASN:HD21	6:AV:16:GLN:HE22	1.60	0.48
6:AP:123:ASN:ND2	6:AP:127:THR:OG1	2.46	0.48
6:AT:109:ASP:OD1	6:AT:109:ASP:N	2.45	0.48
6:AU:35:LYS:NZ	6:AU:221:GLU:OE2	2.37	0.48
6:AX:191:ASN:ND2	6:Y:43:ASP:OD1	2.46	0.48
6:R:236:GLU:HG3	6:U:1:MET:HG2	1.95	0.48
6:Z:1:MET:HE2	6:Z:5:LEU:HD22	1.94	0.48
10:p:200:GLN:NE2	10:p:201:THR:O	2.45	0.48
2:0:66:LYS:HD3	2:0:88:ARG:HE	1.78	0.48
3:2:253:MET:HA	3:z:249:MET:HE3	1.96	0.48
6:A:251:VAL:HG22	10:n:19:LEU:HD21	1.96	0.48
7:AL:353:VAL:HG21	9:h:71:VAL:HG11	1.94	0.48
6:AQ:240:VAL:O	6:AQ:244:ASN:ND2	2.41	0.48
6:AW:33:GLY:N	6:AW:221:GLU:O	2.40	0.48
6:AX:185:LEU:HB3	6:AX:193:TYR:HB3	1.95	0.48
6:Aa:258:VAL:HG13	6:Aa:262:LEU:HD22	1.94	0.48
6:Q:16:GLN:NE2	6:X:228:THR:OG1	2.47	0.48
6:R:36:LYS:HB3	6:R:225:VAL:HG12	1.94	0.48
6:Z:33:GLY:N	6:Z:221:GLU:O	2.45	0.48
1:I:425:VAL:O	1:I:429:LEU:HG	2.13	0.48
2:0:41:ASN:ND2	7:AM:352:ASP:OD1	2.46	0.48
3:1:184:LEU:HD11	3:1:207:GLU:HA	1.95	0.48
6:A:239:ARG:NH1	6:AX:252:ASP:OD1	2.45	0.48
6:A:255:MET:HE3	10:o:223:ARG:HG3	1.94	0.48
6:AQ:104:GLN:NE2	6:AQ:175:THR:OG1	2.47	0.48
6:AS:101:GLY:O	6:AS:116:ARG:NH1	2.46	0.48
6:AX:86:ALA:HB2	6:S:45:PHE:HE1	1.77	0.48
6:S:36:LYS:HB3	6:S:225:VAL:HG12	1.96	0.48
6:V:99:GLY:O	6:V:116:ARG:NH2	2.47	0.48
6:V:206:VAL:HG23	6:V:209:LEU:HB2	1.95	0.48
8:c:97:ASP:OD1	9:i:115:TYR:OH	2.32	0.48
12:x:49:PHE:HB3	12:x:96:VAL:HG22	1.95	0.48
6:AR:12:LEU:HD13	10:n:212:VAL:HG11	1.96	0.48
6:Aa:188:ILE:HD13	6:Aa:194:LEU:HG	1.95	0.48
6:V:50:ASN:HB2	6:V:66:LEU:H	1.78	0.48
10:m:35:ARG:NH1	10:m:101:ARG:HD3	2.29	0.48
10:q:40:GLN:NE2	10:q:60:GLU:OE2	2.40	0.48
1:M:343:ASN:HD22	1:M:343:ASN:N	2.11	0.48
1:O:363:LYS:HD3	1:O:369:ASP:HB2	1.95	0.48
2:0:114:GLY:HA2	2:0:134:LYS:HD2	1.95	0.48
2:9:187:TRP:HH2	2:9:197:VAL:HG11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:176:ILE:HD11	6:B:212:LEU:HB3	1.96	0.48
6:Aa:154:THR:HG23	6:Aa:214:GLU:HB3	1.95	0.48
6:T:115:THR:HB	6:T:192:LEU:HD23	1.95	0.48
10:n:89:SER:HB3	10:n:122:LEU:HD12	1.95	0.48
10:p:22:ARG:HE	10:p:39:ALA:HB3	1.78	0.48
1:I:109:PHE:CE1	1:I:119:THR:HG22	2.48	0.48
1:J:425:VAL:O	1:J:429:LEU:HG	2.14	0.48
1:M:112:ASN:ND2	1:M:116:TYR:HB2	2.28	0.48
5:8:183:THR:HG22	5:8:187:MET:HE3	1.95	0.48
6:A:18:ASN:HB2	6:A:41:PHE:HZ	1.79	0.48
6:AS:25:ASN:HD21	6:AS:37:SER:H	1.62	0.48
6:AZ:258:VAL:HG13	6:AZ:262:LEU:HD22	1.96	0.48
6:R:226:ASN:HB3	6:R:229:GLU:HB2	1.96	0.48
6:X:129:VAL:HG12	6:X:136:PRO:HA	1.96	0.48
9:g:61:ASP:N	9:g:61:ASP:OD1	2.45	0.48
3:y:82:ASP:OD1	3:y:82:ASP:N	2.45	0.48
3:y:183:MET:HE1	3:y:215:ILE:HG12	1.95	0.48
1:D:109:PHE:HE1	1:D:119:THR:HG22	1.78	0.48
1:F:62:GLN:O	1:F:62:GLN:HG2	2.11	0.48
1:F:109:PHE:CE1	1:F:119:THR:HG22	2.48	0.48
1:M:130:VAL:HG22	1:M:347:GLY:HA2	1.95	0.48
6:AP:24:ASN:ND2	6:AP:34:TYR:OH	2.47	0.48
6:AP:186:GLU:HG3	6:AS:67:MET:HE3	1.95	0.48
6:AR:176:ILE:HD11	6:AR:212:LEU:HB3	1.95	0.48
6:AY:114:TYR:HE2	6:AY:195:PRO:HD3	1.77	0.48
6:AY:239:ARG:O	6:AY:243:MET:HG2	2.13	0.48
3:3:236:PRO:HB2	12:x:61:MET:HG2	1.95	0.48
6:A:243:MET:HE3	10:n:26:LEU:HD22	1.96	0.48
6:B:9:LYS:HG3	10:m:216:THR:HG21	1.94	0.48
6:B:101:GLY:HA3	6:B:176:ILE:HD12	1.95	0.48
6:AV:24:ASN:ND2	6:AV:34:TYR:OH	2.47	0.48
6:T:104:GLN:NE2	6:T:177:THR:OG1	2.47	0.48
3:z:111:ARG:NE	3:z:222:GLU:OE1	2.44	0.48
1:G:42:TYR:CE2	1:L:362:LYS:HB2	2.48	0.48
1:L:109:PHE:CE1	1:L:119:THR:HG22	2.49	0.48
1:N:360:LEU:HB3	1:N:368:TRP:HB3	1.96	0.48
6:Q:258:VAL:HG13	6:Q:262:LEU:HD22	1.96	0.48
6:W:123:ASN:HD21	6:W:127:THR:HB	1.78	0.48
6:a:91:ASN:HD22	6:a:92:ALA:N	2.12	0.48
8:d:39:LYS:NZ	8:d:91:GLY:O	2.40	0.48
1:D:109:PHE:CE1	1:D:119:THR:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:187:TRP:HH2	2:0:197:VAL:HG11	1.79	0.47
3:1:119:LEU:HD21	3:1:270:PHE:CE1	2.49	0.47
4:5:8:GLU:HG2	4:5:83:ARG:NH2	2.29	0.47
6:AT:28:ASN:OD1	6:AT:28:ASN:N	2.45	0.47
6:AX:19:ILE:HG23	6:AX:234:MET:HE1	1.96	0.47
6:AX:238:GLN:HG3	6:Y:254:MET:HG3	1.95	0.47
6:Q:16:GLN:HG3	6:Q:241:TYR:HE2	1.78	0.47
6:U:185:LEU:HB3	6:U:193:TYR:HB3	1.96	0.47
6:W:154:THR:HG23	6:W:214:GLU:HB3	1.94	0.47
6:W:166:GLN:O	6:W:167:ASP:HB2	2.14	0.47
9:h:13:ALA:O	9:h:17:GLU:HG2	2.14	0.47
10:n:40:GLN:NE2	10:n:60:GLU:OE2	2.39	0.47
1:G:79:MET:HE3	1:G:111:LEU:HD21	1.95	0.47
1:H:92:ALA:HB2	1:H:126:LEU:HD11	1.95	0.47
1:O:147:ILE:HA	1:O:346:LEU:HD23	1.96	0.47
2:0:31:THR:HG23	2:0:35:GLY:HA2	1.96	0.47
6:A:259:ASN:ND2	10:o:226:GLU:OE1	2.47	0.47
6:AU:7:VAL:O	6:AU:10:THR:OG1	2.28	0.47
1:G:84:SER:OG	1:G:391:ASN:ND2	2.47	0.47
1:N:415:ASN:O	1:N:419:ASN:ND2	2.47	0.47
4:5:42:THR:HG23	4:5:44:ILE:HG12	1.96	0.47
6:A:40:VAL:HG11	10:n:116:ALA:HB1	1.95	0.47
6:B:177:THR:HG21	6:B:202:PRO:HB3	1.96	0.47
6:AP:236:GLU:HG3	6:AT:1:MET:HG2	1.96	0.47
6:AV:95:MET:O	6:AV:118:GLY:HA3	2.15	0.47
6:P:7:VAL:HG13	6:P:71:GLY:HA2	1.96	0.47
6:T:94:ASP:HB2	6:T:220:LEU:HD21	1.95	0.47
10:m:76:ARG:NH1	10:m:79:ASP:OD1	2.44	0.47
10:n:14:GLN:HB3	10:n:59:THR:HG23	1.95	0.47
3:y:149:VAL:HG23	3:y:178:PRO:HB2	1.96	0.47
1:M:372:GLN:NE2	6:V:168:ASN:OD1	2.48	0.47
5:8:27:MET:HE1	11:w:92:VAL:HG13	1.96	0.47
6:P:36:LYS:HB3	6:P:225:VAL:HG12	1.95	0.47
6:S:24:ASN:ND2	6:S:34:TYR:OH	2.47	0.47
11:u:71:MET:O	11:u:75:ASN:ND2	2.28	0.47
1:D:44:ASN:HD21	1:D:53:THR:HG21	1.79	0.47
6:AV:157:GLU:HG2	6:AZ:55:GLN:HG2	1.96	0.47
6:AW:176:ILE:HD11	6:AW:212:LEU:HB3	1.96	0.47
6:R:24:ASN:ND2	6:R:34:TYR:OH	2.47	0.47
6:a:214:GLU:OE1	6:a:216:ARG:NH1	2.47	0.47
8:b:9:LEU:HD12	8:b:120:LYS:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d:30:ILE:HG23	8:d:96:LEU:HD11	1.97	0.47
8:f:85:GLN:OE1	9:k:22:ASN:ND2	2.47	0.47
11:s:71:MET:SD	11:s:74:ARG:NH1	2.85	0.47
11:w:88:ARG:HH11	11:w:92:VAL:HG21	1.80	0.47
1:H:28:THR:OG1	1:H:31:PHE:HB2	2.14	0.47
3:2:154:ASN:HA	3:2:158:VAL:HB	1.95	0.47
6:AT:226:ASN:HB3	6:AT:229:GLU:HB2	1.97	0.47
6:AV:36:LYS:HB3	6:AV:225:VAL:HG12	1.97	0.47
6:AW:226:ASN:O	6:AW:230:GLU:HG2	2.15	0.47
6:AX:48:ASN:HD21	6:AX:51:GLN:NE2	2.11	0.47
6:T:184:GLY:O	6:T:196:THR:OG1	2.30	0.47
8:c:24:GLU:OE2	9:h:2:SER:N	2.47	0.47
1:E:46:LEU:CD1	6:S:150:ILE:HG13	2.44	0.47
1:E:50:ALA:C	1:E:52:THR:N	2.71	0.47
1:G:351:LEU:HD13	1:G:390:ILE:HD11	1.96	0.47
1:H:147:ILE:HA	1:H:346:LEU:HD23	1.96	0.47
1:M:84:SER:OG	1:M:391:ASN:ND2	2.48	0.47
1:M:112:ASN:HD21	1:M:116:TYR:HB2	1.79	0.47
1:M:351:LEU:HD13	1:M:390:ILE:HD11	1.97	0.47
2:0:119:LEU:O	2:0:122:THR:OG1	2.28	0.47
3:2:264:PRO:HG3	3:z:234:PHE:CG	2.49	0.47
6:A:49:ILE:HD11	6:A:66:LEU:HD23	1.96	0.47
6:B:17:THR:HG23	6:AU:68:LEU:HD11	1.97	0.47
6:AS:87:GLN:HE22	6:AW:38:ARG:HH22	1.63	0.47
6:AW:23:SER:HG	6:X:8:SER:HG	1.57	0.47
6:AW:104:GLN:NE2	6:AW:177:THR:OG1	2.47	0.47
6:AX:36:LYS:HB3	6:AX:225:VAL:HG12	1.97	0.47
6:V:24:ASN:ND2	6:V:34:TYR:OH	2.48	0.47
6:a:36:LYS:HB3	6:a:225:VAL:HG12	1.96	0.47
8:b:30:ILE:HG23	8:b:96:LEU:HD11	1.96	0.47
9:i:126:LYS:HD3	10:n:248:MET:HA	1.96	0.47
10:m:114:THR:HG22	10:m:120:LEU:HD13	1.96	0.47
10:o:35:ARG:NH1	10:o:101:ARG:HD3	2.30	0.47
2:0:39:LEU:HD12	2:0:59:ILE:HG22	1.97	0.47
6:AQ:251:VAL:HG22	10:q:19:LEU:HD21	1.97	0.47
6:AS:7:VAL:O	6:AS:10:THR:OG1	2.29	0.47
6:AS:87:GLN:NE2	6:AW:38:ARG:HH22	2.13	0.47
6:AY:120:PHE:HD1	6:AY:130:THR:HA	1.80	0.47
6:P:48:ASN:HD21	6:P:51:GLN:HE21	1.63	0.47
6:a:98:GLU:OE1	6:a:216:ARG:NH1	2.48	0.47
1:F:422:SER:HA	1:K:409:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:426:HIS:CE1	1:L:20:SER:OG	2.66	0.47
1:L:37:GLU:HG2	6:AZ:119:GLN:HE22	1.78	0.47
1:M:370:SER:O	6:V:161:ARG:NH2	2.48	0.47
3:1:105:LEU:HD23	5:8:44:TYR:HB3	1.97	0.47
6:A:83:HIS:CD2	6:A:99:GLY:H	2.33	0.47
6:AR:18:ASN:HB2	6:AR:41:PHE:HZ	1.80	0.47
6:AS:36:LYS:HB3	6:AS:225:VAL:HG12	1.96	0.47
6:AY:68:LEU:HD11	6:S:17:THR:HG23	1.97	0.47
6:Aa:16:GLN:HG3	6:Aa:241:TYR:CE2	2.50	0.47
6:R:227:VAL:HB	6:V:243:MET:SD	2.54	0.47
6:U:19:ILE:HG23	6:U:234:MET:HE1	1.97	0.47
6:Y:240:VAL:O	6:Y:244:ASN:ND2	2.47	0.47
1:K:73:ILE:HG23	1:K:395:LEU:HB2	1.97	0.47
2:9:107:TRP:HD1	2:9:128:PRO:HG3	1.79	0.47
6:AQ:86:ALA:HB2	6:AW:45:PHE:HE1	1.79	0.47
6:AT:115:THR:HB	6:AT:192:LEU:HD12	1.96	0.47
6:AV:70:ALA:HB1	10:o:71:VAL:HG21	1.97	0.47
6:AW:36:LYS:HB3	6:AW:225:VAL:HG12	1.96	0.47
6:W:38:ARG:HH22	6:a:87:GLN:NE2	2.13	0.47
6:W:206:VAL:HG23	6:W:209:LEU:HB2	1.97	0.47
8:f:21:ARG:NH1	8:f:48:GLU:OE1	2.48	0.47
9:i:84:ASP:OD1	9:i:84:ASP:N	2.32	0.47
1:G:101:ASN:O	1:G:377:LYS:NZ	2.48	0.46
1:N:109:PHE:HE1	1:N:119:THR:HG22	1.81	0.46
7:AF:349:ILE:O	7:AF:350:PRO:C	2.58	0.46
6:AU:226:ASN:HB3	6:AU:229:GLU:HB2	1.96	0.46
6:R:94:ASP:HB2	6:R:220:LEU:HD21	1.97	0.46
6:T:24:ASN:ND2	6:T:34:TYR:OH	2.48	0.46
6:T:206:VAL:HG23	6:T:209:LEU:HB2	1.96	0.46
6:V:249:SER:OG	6:V:253:LYS:NZ	2.48	0.46
6:X:19:ILE:HG23	6:X:234:MET:HE1	1.97	0.46
6:Y:103:PHE:HB2	6:Y:115:THR:HG23	1.96	0.46
1:D:79:MET:HE3	1:D:111:LEU:HD21	1.95	0.46
1:D:433:ILE:HD11	1:I:416:PHE:HZ	1.80	0.46
1:G:33:GLU:HB3	1:G:400:ILE:HG22	1.98	0.46
1:H:51:LYS:NZ	1:M:62:GLN:HE21	2.13	0.46
1:L:415:ASN:O	1:L:419:ASN:ND2	2.48	0.46
3:2:258:PRO:HA	3:2:261:VAL:HG12	1.98	0.46
4:5:87:VAL:C	4:5:89:TYR:H	2.23	0.46
7:AM:341:ASN:ND2	8:f:88:THR:OG1	2.48	0.46
6:AV:115:THR:HB	6:AV:192:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:80:VAL:O	6:W:224:ASN:ND2	2.48	0.46
8:e:43:LEU:HG	8:e:48:GLU:HG3	1.96	0.46
1:G:147:ILE:HA	1:G:346:LEU:HD23	1.98	0.46
7:AK:340:SER:HA	7:AK:349:ILE:HD11	1.97	0.46
6:AR:44:LEU:HB2	6:AR:70:ALA:HB3	1.98	0.46
6:AV:99:GLY:O	6:AV:116:ARG:NH2	2.47	0.46
6:Aa:129:VAL:HG12	6:Aa:136:PRO:HA	1.96	0.46
6:P:103:PHE:HB2	6:P:115:THR:HG23	1.97	0.46
6:S:16:GLN:HE22	6:Y:226:ASN:HD21	1.63	0.46
6:Z:94:ASP:HB2	6:Z:220:LEU:HD21	1.97	0.46
6:Z:154:THR:HG23	6:Z:214:GLU:HB3	1.97	0.46
9:j:20:ARG:HH21	9:j:111:ALA:HA	1.79	0.46
10:o:21:LEU:HD23	10:o:39:ALA:HB2	1.97	0.46
3:z:81:GLU:O	3:z:169:ARG:NH2	2.49	0.46
5:8:43:LEU:HB2	11:s:103:VAL:HG11	1.98	0.46
6:AZ:159:SER:HB3	6:AZ:168:ASN:HB3	1.96	0.46
6:Aa:166:GLN:HG2	6:Aa:167:ASP:H	1.81	0.46
6:W:184:GLY:O	6:W:196:THR:OG1	2.25	0.46
8:c:35:THR:O	8:c:92:ASN:ND2	2.48	0.46
9:j:100:ASN:O	9:j:104:GLU:HG2	2.16	0.46
1:G:23:ILE:HG23	1:G:402:MET:HE1	1.98	0.46
1:J:82:ARG:HH11	1:J:396:GLU:HG2	1.79	0.46
6:AX:153:GLY:HA2	6:AY:56:SER:HA	1.98	0.46
6:S:94:ASP:HB2	6:S:220:LEU:HD21	1.96	0.46
6:W:55:GLN:NE2	6:W:57:SER:O	2.48	0.46
6:a:89:THR:OG1	6:a:94:ASP:OD2	2.25	0.46
8:d:15:THR:HG23	8:d:45:PHE:HZ	1.81	0.46
9:h:66:LYS:HE3	9:h:68:MET:SD	2.56	0.46
9:j:100:ASN:HB3	9:j:103:GLU:HG2	1.97	0.46
11:s:90:LYS:HG3	11:w:74:ARG:HE	1.80	0.46
1:F:34:SER:HB3	1:F:63:VAL:HG12	1.98	0.46
3:3:264:PRO:HG2	5:8:196:LEU:HD11	1.98	0.46
5:8:85:MET:HG3	5:8:252:ILE:HG23	1.98	0.46
6:A:161:ARG:HD2	6:T:51:GLN:NE2	2.30	0.46
6:B:185:LEU:HB3	6:B:193:TYR:HB3	1.97	0.46
6:R:123:ASN:ND2	6:R:127:THR:HB	2.30	0.46
3:y:141:LEU:HD11	3:y:280:LEU:HD22	1.98	0.46
2:0:179:LEU:O	2:0:182:ASN:ND2	2.48	0.46
3:1:208:ASP:N	3:1:208:ASP:OD1	2.49	0.46
6:P:82:THR:HG22	6:P:224:ASN:HD22	1.79	0.46
9:k:70:ILE:HD13	10:p:51:HIS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:LEU:HD12	6:S:149:SER:CA	2.45	0.46
6:B:40:VAL:HG11	10:o:116:ALA:HB1	1.98	0.46
6:AY:43:ASP:OD1	6:AY:43:ASP:N	2.48	0.46
6:AZ:181:ASN:ND2	6:T:122:LEU:O	2.49	0.46
6:Aa:9:LYS:HG3	6:V:232:VAL:HG11	1.96	0.46
6:P:114:TYR:HE2	6:P:195:PRO:HD3	1.81	0.46
6:S:29:ALA:HA	6:S:225:VAL:HG21	1.98	0.46
9:h:36:SER:OG	9:h:38:ALA:O	2.27	0.46
10:o:28:ASN:O	10:o:31:THR:OG1	2.34	0.46
10:p:28:ASN:O	10:p:31:THR:OG1	2.32	0.46
11:r:39:LYS:HE2	11:r:39:LYS:HB3	1.56	0.46
1:J:432:ASN:ND2	1:O:420:SER:OG	2.48	0.46
3:2:186:GLN:NE2	3:2:287:PHE:O	2.49	0.46
4:6:16:MET:HE1	4:6:76:TYR:HB2	1.97	0.46
6:A:44:LEU:HD13	9:h:81:TYR:HB2	1.98	0.46
7:AI:342:GLN:O	7:AI:343:PRO:C	2.59	0.46
6:AS:95:MET:O	6:AS:118:GLY:HA3	2.16	0.46
6:AZ:43:ASP:OD1	6:AZ:43:ASP:N	2.37	0.46
6:S:19:ILE:HG23	6:S:234:MET:HE1	1.97	0.46
6:S:48:ASN:HD21	6:S:51:GLN:NE2	2.13	0.46
6:S:154:THR:HG23	6:S:214:GLU:HB3	1.97	0.46
6:U:83:HIS:CE1	6:U:99:GLY:H	2.34	0.46
6:X:166:GLN:HG2	6:X:167:ASP:H	1.81	0.46
6:Y:96:MET:HG3	6:Y:221:GLU:HB2	1.98	0.46
10:p:9:MET:HE3	10:p:9:MET:HB3	1.82	0.46
1:D:351:LEU:HD13	1:D:390:ILE:HD11	1.96	0.46
2:0:129:ALA:HA	2:0:148:PRO:HB2	1.97	0.46
3:3:128:THR:HG22	5:8:98:LEU:HG	1.98	0.46
6:AR:36:LYS:HD3	6:AR:225:VAL:HA	1.98	0.46
6:AV:154:THR:HG22	6:AZ:57:SER:HB3	1.98	0.46
6:AX:70:ALA:HB1	10:n:71:VAL:HG21	1.97	0.46
6:AZ:226:ASN:O	6:AZ:230:GLU:HG2	2.16	0.46
6:Q:94:ASP:HB2	6:Q:220:LEU:HD21	1.98	0.46
6:Q:151:THR:HG23	6:Q:159:SER:HB2	1.98	0.46
6:Q:154:THR:HG23	6:Q:214:GLU:HB3	1.97	0.46
1:E:82:ARG:NH1	1:E:396:GLU:HB3	2.32	0.45
1:I:84:SER:OG	1:I:391:ASN:ND2	2.49	0.45
1:M:117:MET:HE3	1:M:125:LEU:HD23	1.97	0.45
6:AT:93:LEU:HD13	6:AT:121:THR:HA	1.97	0.45
6:AW:32:VAL:HG11	6:AW:220:LEU:HD22	1.98	0.45
6:AY:99:GLY:O	6:AY:116:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AZ:2:HIS:HD1	6:AZ:4:ALA:H	1.63	0.45
6:U:94:ASP:HB2	6:U:220:LEU:HD21	1.96	0.45
10:n:91:LEU:HD21	10:n:128:PRO:HG3	1.97	0.45
10:p:131:LEU:HD23	10:p:148:VAL:HG11	1.97	0.45
1:N:101:ASN:OD1	1:N:377:LYS:NZ	2.50	0.45
2:0:92:LYS:HG2	2:0:112:LYS:HD2	1.97	0.45
5:8:25:MET:HE1	5:8:148:LEU:HD23	1.98	0.45
6:B:123:ASN:ND2	6:B:127:THR:HB	2.31	0.45
6:B:181:ASN:ND2	10:o:107:VAL:O	2.49	0.45
6:AR:188:ILE:HD13	6:AR:194:LEU:HG	1.97	0.45
1:G:117:MET:HE3	1:G:125:LEU:HD23	1.99	0.45
1:M:415:ASN:OD1	6:Aa:29:ALA:HB3	2.15	0.45
7:AF:344:PRO:O	7:AF:345:ALA:C	2.57	0.45
6:AW:94:ASP:HB2	6:AW:220:LEU:HD21	1.97	0.45
6:Aa:206:VAL:HG23	6:Aa:209:LEU:HB2	1.98	0.45
6:R:103:PHE:HB2	6:R:115:THR:HG23	1.99	0.45
6:U:43:ASP:OD1	6:U:43:ASP:N	2.43	0.45
6:X:176:ILE:HG13	6:X:212:LEU:HD22	1.97	0.45
6:a:161:ARG:HH11	6:a:168:ASN:ND2	2.14	0.45
1:D:432:ASN:ND2	1:I:420:SER:OG	2.50	0.45
1:E:48:THR:O	1:E:49:ASN:C	2.58	0.45
1:F:42:TYR:CD2	1:K:362:LYS:HD2	2.52	0.45
1:F:42:TYR:CD1	1:F:42:TYR:O	2.69	0.45
3:2:263:LEU:HD23	3:z:234:PHE:HE2	1.80	0.45
4:5:19:ILE:HG21	4:5:72:MET:HE1	1.98	0.45
6:AP:83:HIS:CD2	6:AP:99:GLY:H	2.35	0.45
6:AV:49:ILE:HG23	6:AV:66:LEU:HB3	1.97	0.45
6:AZ:18:ASN:HD22	6:AZ:39:ALA:HB3	1.80	0.45
6:T:166:GLN:HG2	6:T:167:ASP:H	1.81	0.45
6:W:240:VAL:O	6:W:244:ASN:ND2	2.47	0.45
8:b:39:LYS:NZ	8:b:91:GLY:O	2.42	0.45
8:b:126:LYS:HE2	11:v:82:ASP:OD1	2.16	0.45
8:e:30:ILE:HG23	8:e:96:LEU:HD11	1.98	0.45
10:n:91:LEU:HD23	10:n:122:LEU:HD21	1.98	0.45
11:t:53:ASP:OD2	11:t:57:ARG:NH1	2.50	0.45
3:y:183:MET:HE2	3:y:214:LEU:HG	1.98	0.45
1:I:109:PHE:HE1	1:I:119:THR:HG22	1.81	0.45
1:L:106:ASN:H	1:L:106:ASN:HD22	1.64	0.45
1:N:351:LEU:HD13	1:N:390:ILE:HD11	1.98	0.45
1:O:117:MET:HE3	1:O:125:LEU:HD23	1.98	0.45
6:B:251:VAL:HG22	10:o:19:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:56:SER:O	6:S:57:SER:HB3	2.16	0.45
6:S:206:VAL:HG23	6:S:209:LEU:HB2	1.99	0.45
6:T:146:ASP:HB3	6:T:162:VAL:HG13	1.99	0.45
1:H:106:ASN:HD22	1:H:106:ASN:H	1.65	0.45
1:I:433:ILE:HD11	1:N:416:PHE:CZ	2.39	0.45
1:N:147:ILE:HA	1:N:346:LEU:HD23	1.98	0.45
4:6:1:MET:SD	4:6:1:MET:N	2.70	0.45
5:8:74:THR:O	5:8:78:GLN:HG2	2.17	0.45
7:AF:336:PRO:HG2	7:AM:352:ASP:HB3	1.98	0.45
6:C:115:THR:HB	6:C:192:LEU:HD12	1.98	0.45
6:AP:87:GLN:NE2	6:AS:38:ARG:HH22	2.12	0.45
6:AV:185:LEU:HB3	6:AV:193:TYR:HB3	1.97	0.45
6:AX:240:VAL:O	6:AX:244:ASN:ND2	2.49	0.45
6:Aa:185:LEU:HB3	6:Aa:193:TYR:HB3	1.97	0.45
6:W:33:GLY:N	6:W:221:GLU:O	2.46	0.45
6:a:123:ASN:OD1	6:a:127:THR:N	2.49	0.45
9:i:30:ASN:OD1	10:n:57:SER:HB3	2.17	0.45
10:q:18:ALA:HB2	10:q:59:THR:HG21	1.99	0.45
1:F:132:PRO:HB3	1:F:344:VAL:HG13	1.98	0.45
1:L:127:GLY:HA2	1:L:350:ALA:H	1.81	0.45
1:M:109:PHE:HE1	1:M:119:THR:HG22	1.81	0.45
1:O:109:PHE:CE1	1:O:119:THR:HG22	2.52	0.45
6:AR:48:ASN:HB3	6:AR:51:GLN:HG3	1.98	0.45
6:AT:28:ASN:ND2	6:a:43:ASP:HB3	2.32	0.45
6:AV:240:VAL:O	6:AV:244:ASN:ND2	2.45	0.45
6:AX:87:GLN:NE2	6:Y:38:ARG:HH22	2.11	0.45
6:Aa:56:SER:O	6:Aa:57:SER:HB3	2.16	0.45
6:V:258:VAL:HG13	6:V:262:LEU:HD22	1.99	0.45
6:Z:129:VAL:HG12	6:Z:136:PRO:HA	1.99	0.45
9:i:52:GLU:O	9:i:53:LEU:C	2.59	0.45
1:I:330:GLU:OE2	1:I:331:ASN:ND2	2.50	0.45
3:3:90:LEU:O	3:3:94:THR:OG1	2.34	0.45
3:3:116:MET:HE3	5:8:177:LEU:HD22	1.98	0.45
6:C:49:ILE:HD11	6:C:66:LEU:HD23	1.99	0.45
6:AZ:95:MET:O	6:AZ:118:GLY:HA3	2.17	0.45
6:S:52:PRO:HB3	6:S:65:GLY:H	1.82	0.45
6:T:239:ARG:O	6:T:243:MET:HG2	2.17	0.45
6:W:31:THR:HG21	6:W:191:ASN:HD21	1.81	0.45
1:F:104:THR:HB	1:F:367:GLN:HG2	1.99	0.45
1:N:39:ALA:HB1	6:P:190:GLN:HA	1.99	0.45
3:1:144:PHE:HD2	3:2:198:MET:HE3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:204:ASP:OD1	3:2:204:ASP:N	2.49	0.45
6:AV:2:HIS:HD2	6:AV:4:ALA:H	1.64	0.45
6:AZ:188:ILE:HD13	6:AZ:194:LEU:HG	1.99	0.45
6:Aa:95:MET:O	6:Aa:118:GLY:HA3	2.16	0.45
6:P:91:ASN:ND2	6:P:93:LEU:H	2.14	0.45
6:R:184:GLY:O	6:R:196:THR:OG1	2.30	0.45
6:U:206:VAL:HG23	6:U:209:LEU:HB2	1.98	0.45
10:p:114:THR:HG22	10:p:120:LEU:HD13	1.99	0.45
10:q:244:SER:HA	10:q:247:ARG:HB2	1.98	0.45
1:I:351:LEU:HD13	1:I:390:ILE:HD11	1.98	0.45
4:6:31:ILE:HG13	4:6:57:VAL:HG11	1.99	0.45
7:AJ:341:ASN:HD21	8:c:86:PRO:HG3	1.82	0.45
6:AQ:7:VAL:O	6:AQ:10:THR:OG1	2.34	0.45
6:AW:176:ILE:HG13	6:AW:212:LEU:HD22	1.97	0.45
6:P:123:ASN:ND2	6:P:127:THR:HB	2.32	0.45
6:S:143:ILE:HG23	6:S:160:VAL:HG11	1.99	0.45
6:U:37:SER:HB3	6:U:77:THR:HG23	1.97	0.45
8:e:20:GLU:OE2	11:r:68:SER:OG	2.34	0.45
9:h:27:ASN:OD1	9:h:42:TYR:OH	2.27	0.45
10:n:167:VAL:HG12	10:n:169:PRO:HD3	1.98	0.45
11:r:86:GLN:O	11:r:90:LYS:HG2	2.17	0.45
3:z:116:MET:SD	3:z:134:ILE:HG23	2.57	0.45
1:F:80:ASP:O	1:F:393:GLY:N	2.51	0.44
3:3:108:SER:HB2	3:3:287:PHE:CZ	2.51	0.44
4:5:1:MET:HE2	4:5:87:VAL:HG11	1.98	0.44
6:B:86:ALA:HB2	6:Z:45:PHE:HE1	1.82	0.44
6:AS:145:GLU:HG2	6:AW:180:VAL:HG22	1.99	0.44
6:AU:123:ASN:OD1	6:AU:127:THR:N	2.51	0.44
6:AX:227:VAL:HB	6:Y:243:MET:SD	2.57	0.44
6:Aa:82:THR:HG22	6:Aa:224:ASN:HD22	1.81	0.44
6:S:91:ASN:HD22	6:S:92:ALA:N	2.15	0.44
6:S:143:ILE:HG21	6:S:150:ILE:HD11	1.99	0.44
6:U:148:ILE:HD11	6:U:161:ARG:HG2	1.99	0.44
6:W:7:VAL:HG13	6:W:71:GLY:HA2	1.99	0.44
6:W:114:TYR:HE2	6:W:195:PRO:HD3	1.82	0.44
8:c:26:ILE:HG21	8:c:103:PHE:HB2	1.99	0.44
1:F:50:ALA:HA	1:F:53:THR:HG22	1.98	0.44
1:G:101:ASN:HD22	1:G:126:LEU:CD1	2.30	0.44
1:K:51:LYS:HE3	1:K:51:LYS:HB2	1.84	0.44
7:AF:339:LEU:HD11	9:l:72:GLU:HG3	1.99	0.44
6:AP:18:ASN:HB2	6:AP:41:PHE:HZ	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AR:152:VAL:HG22	6:AR:158:VAL:HG22	1.99	0.44
6:AU:227:VAL:HB	6:R:243:MET:SD	2.57	0.44
6:T:95:MET:O	6:T:118:GLY:HA3	2.17	0.44
6:U:100:ASP:O	6:U:213:GLY:N	2.46	0.44
6:W:226:ASN:O	6:W:230:GLU:HG2	2.16	0.44
10:n:18:ALA:HB2	10:n:59:THR:HG21	1.98	0.44
3:z:125:LEU:HD22	3:z:263:LEU:HD11	1.98	0.44
1:J:21:ASN:O	1:J:25:ASN:ND2	2.45	0.44
3:3:251:MET:HE2	12:x:39:LEU:HD23	1.99	0.44
4:5:87:VAL:C	4:5:89:TYR:N	2.74	0.44
5:8:18:PRO:HB3	5:8:57:ILE:HD13	2.00	0.44
5:8:215:PHE:HD2	5:8:216:SER:H	1.66	0.44
7:AM:331:MET:HE2	7:AM:331:MET:HB3	1.87	0.44
6:AR:104:GLN:NE2	6:AR:175:THR:OG1	2.49	0.44
6:AY:48:ASN:HD21	6:AY:51:GLN:NE2	2.15	0.44
10:m:137:LYS:NZ	10:m:139:GLU:OE2	2.48	0.44
10:p:21:LEU:HD23	10:p:39:ALA:HB2	1.98	0.44
1:H:79:MET:HE3	1:H:111:LEU:HD21	1.99	0.44
1:J:109:PHE:CE1	1:J:119:THR:HG22	2.52	0.44
1:L:351:LEU:HD13	1:L:390:ILE:HD11	1.98	0.44
2:0:176:ASN:N	2:0:176:ASN:OD1	2.49	0.44
6:AP:80:VAL:HG12	6:AP:82:THR:HG23	2.00	0.44
6:AR:178:ASP:HB2	6:AR:212:LEU:HD23	1.99	0.44
6:V:94:ASP:HB2	6:V:220:LEU:HD21	1.98	0.44
6:Z:226:ASN:O	6:Z:230:GLU:HG2	2.17	0.44
6:a:18:ASN:HD22	6:a:39:ALA:HB3	1.82	0.44
9:i:22:ASN:ND2	10:n:54:ARG:HE	2.16	0.44
10:n:131:LEU:HD23	10:n:148:VAL:HG11	1.99	0.44
1:E:52:THR:O	1:E:52:THR:OG1	2.33	0.44
1:G:85:GLY:O	1:G:105:ARG:NH2	2.51	0.44
1:I:59:GLN:NE2	1:I:60:ALA:O	2.51	0.44
1:K:16:LEU:HD22	1:K:412:ALA:HB1	2.00	0.44
2:0:154:ASP:HA	2:0:174:LYS:HB2	1.99	0.44
6:A:29:ALA:HA	6:A:225:VAL:HG21	1.99	0.44
6:AZ:239:ARG:HD3	6:AZ:239:ARG:HA	1.79	0.44
6:T:38:ARG:HH22	6:Y:87:GLN:NE2	2.16	0.44
6:W:43:ASP:OD1	6:a:191:ASN:ND2	2.51	0.44
6:X:161:ARG:HH11	6:X:168:ASN:HD21	1.64	0.44
8:b:85:GLN:OE1	9:l:22:ASN:ND2	2.51	0.44
10:q:82:ILE:HD11	10:q:88:ILE:HG13	2.00	0.44
1:I:68:HIS:CD2	1:I:399:ASN:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:115:THR:HB	6:B:192:LEU:HD12	1.99	0.44
6:AU:239:ARG:HA	6:AU:239:ARG:HD3	1.82	0.44
6:Aa:37:SER:HB3	6:Aa:77:THR:HG22	1.99	0.44
9:l:129:LEU:HD22	11:v:67:LEU:HD12	1.99	0.44
11:s:48:GLN:HE21	11:s:81:PHE:HB2	1.81	0.44
11:w:96:LYS:O	11:w:100:ASN:ND2	2.45	0.44
1:L:363:LYS:HD3	1:L:369:ASP:HB2	2.00	0.44
1:O:32:LYS:HG3	1:O:67:PHE:CE1	2.53	0.44
2:0:47:LEU:HB2	2:0:68:PRO:HG3	1.99	0.44
6:A:115:THR:HB	6:A:192:LEU:HD12	2.00	0.44
6:C:93:LEU:HD23	6:C:121:THR:HA	1.99	0.44
6:AR:93:LEU:HD13	6:AR:121:THR:HA	1.99	0.44
6:AR:226:ASN:HB3	6:AR:229:GLU:HB2	2.00	0.44
6:AV:166:GLN:O	6:AV:167:ASP:HB2	2.16	0.44
6:Y:258:VAL:HG13	6:Y:262:LEU:HD22	1.99	0.44
1:D:147:ILE:HA	1:D:346:LEU:HD23	2.00	0.44
1:J:105:ARG:HD3	1:J:105:ARG:HA	1.88	0.44
2:0:136:ASP:CB	7:AF:356:MET:HE3	2.47	0.44
4:6:63:MET:HG2	4:7:11:ARG:HA	1.99	0.44
7:AA:349:ILE:HG12	10:q:46:ALA:HA	1.99	0.44
7:AF:348:SER:O	7:AF:349:ILE:HB	2.17	0.44
6:AU:70:ALA:HB1	10:m:71:VAL:HG21	1.99	0.44
6:AZ:151:THR:HG23	6:AZ:159:SER:HB2	1.99	0.44
6:P:115:THR:HB	6:P:192:LEU:HD23	2.00	0.44
6:Q:226:ASN:O	6:Q:230:GLU:HG2	2.17	0.44
6:S:1:MET:HE2	6:S:5:LEU:HD22	2.00	0.44
6:T:226:ASN:O	6:T:230:GLU:HG2	2.18	0.44
10:p:40:GLN:HG2	10:p:62:PRO:HD3	1.99	0.44
12:x:71:GLU:HA	12:x:77:LYS:HD2	1.99	0.44
1:I:114:GLU:HB2	1:I:116:TYR:HD2	1.83	0.44
2:0:92:LYS:HA	2:0:112:LYS:HB2	1.99	0.44
4:6:67:HIS:HD2	4:7:11:ARG:HH22	1.65	0.44
7:AA:353:VAL:O	7:AA:356:MET:HG2	2.18	0.44
6:B:129:VAL:HG12	6:B:136:PRO:HA	2.00	0.44
6:AR:9:LYS:HG3	10:n:216:THR:HG21	1.99	0.44
6:Aa:239:ARG:HA	6:Aa:239:ARG:HD3	1.82	0.44
6:Q:38:ARG:HH11	6:Q:78:GLN:NE2	2.16	0.44
9:i:66:LYS:HE3	9:i:68:MET:HG2	1.99	0.44
10:m:211:ALA:O	10:m:215:MET:HG2	2.18	0.44
10:o:105:LEU:HA	10:o:115:ASN:HA	2.00	0.44
10:q:91:LEU:HD21	10:q:128:PRO:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:SER:OG	1:E:391:ASN:ND2	2.50	0.43
1:I:79:MET:HE3	1:I:111:LEU:HD21	1.98	0.43
6:B:12:LEU:HD13	6:B:244:ASN:HB2	2.00	0.43
6:AP:262:LEU:HG	9:l:109:ILE:HD11	1.99	0.43
6:AS:70:ALA:HB1	10:q:71:VAL:HG21	1.99	0.43
9:k:39:LYS:HD2	9:k:39:LYS:HA	1.85	0.43
10:q:21:LEU:HD23	10:q:39:ALA:HB2	2.00	0.43
11:v:64:ASP:OD1	11:v:64:ASP:N	2.48	0.43
1:F:432:ASN:ND2	1:K:420:SER:OG	2.51	0.43
1:H:118:VAL:HG12	1:H:124:PHE:HA	2.01	0.43
1:J:16:LEU:HD22	1:J:412:ALA:HB1	2.00	0.43
1:L:401:ASP:HB3	1:L:404:GLN:HB3	2.00	0.43
1:N:109:PHE:CE1	1:N:119:THR:HG22	2.53	0.43
4:4:20:MET:HE1	4:4:69:MET:HB3	2.00	0.43
4:5:12:GLU:OE1	4:5:83:ARG:NH1	2.50	0.43
6:B:96:MET:HG2	6:B:97:VAL:N	2.33	0.43
6:AT:155:ASP:C	6:AT:207:PRO:HG2	2.42	0.43
6:AT:191:ASN:ND2	6:a:43:ASP:OD1	2.51	0.43
6:AV:32:VAL:HG11	6:AV:220:LEU:HD22	2.00	0.43
6:AW:78:GLN:NE2	6:AW:79:LYS:O	2.51	0.43
8:b:21:ARG:NH1	8:b:48:GLU:OE1	2.51	0.43
9:j:70:ILE:HD13	10:m:51:HIS:HB3	1.99	0.43
1:F:429:LEU:HD11	1:K:16:LEU:HG	2.00	0.43
1:K:114:GLU:HB2	1:K:116:TYR:HD2	1.83	0.43
1:L:16:LEU:HD22	1:L:412:ALA:HB1	1.99	0.43
1:N:401:ASP:O	1:N:405:GLU:HG2	2.18	0.43
4:5:8:GLU:HG2	4:5:83:ARG:HH22	1.82	0.43
6:AS:166:GLN:O	6:AS:167:ASP:HB2	2.18	0.43
6:Au:155:ASP:OD1	6:Aa:57:SER:HA	2.19	0.43
6:Aa:48:ASN:HD21	6:Aa:51:GLN:HE22	1.65	0.43
6:Q:78:GLN:NE2	6:W:131:SER:OG	2.51	0.43
6:T:83:HIS:NE2	6:T:96:MET:HE3	2.32	0.43
6:U:95:MET:HG3	6:U:217:GLN:HA	2.00	0.43
6:Y:43:ASP:OD1	6:Y:43:ASP:N	2.41	0.43
6:Z:123:ASN:ND2	6:Z:127:THR:HB	2.33	0.43
6:a:29:ALA:HA	6:a:225:VAL:HG21	1.99	0.43
6:a:226:ASN:O	6:a:230:GLU:HG2	2.18	0.43
10:n:15:ASN:ND2	10:n:228:GLN:HE22	2.16	0.43
3:y:238:LEU:HD11	3:z:261:VAL:HG13	2.00	0.43
1:O:372:GLN:HB2	6:X:167:ASP:HA	2.00	0.43
6:C:166:GLN:O	6:C:167:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Aa:226:ASN:O	6:Aa:230:GLU:HG2	2.18	0.43
6:V:19:ILE:HG23	6:V:234:MET:HE1	1.99	0.43
6:a:91:ASN:HD22	6:a:93:LEU:H	1.66	0.43
9:g:100:ASN:O	9:g:104:GLU:HG2	2.18	0.43
9:j:22:ASN:ND2	10:m:54:ARG:HE	2.14	0.43
10:o:92:ASP:OD1	10:o:92:ASP:N	2.46	0.43
1:G:109:PHE:CE1	1:G:119:THR:HG22	2.48	0.43
1:I:21:ASN:O	1:I:25:ASN:ND2	2.51	0.43
2:0:33:ASN:ND2	9:l:95:TYR:O	2.34	0.43
6:A:103:PHE:HB2	6:A:115:THR:HG23	2.00	0.43
6:B:106:THR:OG1	6:B:138:GLU:OE2	2.36	0.43
6:AZ:94:ASP:HB2	6:AZ:220:LEU:HD21	2.00	0.43
6:AZ:219:MET:HE3	6:AZ:219:MET:HB2	1.96	0.43
10:o:154:PRO:HG2	10:o:157:GLU:HG3	1.99	0.43
3:y:108:SER:HB2	3:y:287:PHE:CZ	2.53	0.43
3:y:204:ASP:OD1	3:y:204:ASP:N	2.46	0.43
1:D:88:PHE:N	1:D:352:VAL:O	2.48	0.43
1:G:6:LEU:HD13	1:M:407:VAL:HG11	1.99	0.43
1:G:51:LYS:O	1:G:52:THR:HB	2.18	0.43
1:I:432:ASN:ND2	1:N:420:SER:OG	2.51	0.43
1:J:25:ASN:O	1:J:398:SER:OG	2.34	0.43
1:N:372:GLN:HB2	6:W:167:ASP:HA	2.00	0.43
1:O:16:LEU:HD12	1:O:409:LEU:HD12	2.00	0.43
6:AU:94:ASP:OD1	6:AU:94:ASP:N	2.52	0.43
6:AU:95:MET:HE1	6:AU:152:VAL:HG21	2.01	0.43
6:AY:31:THR:HG21	6:AY:191:ASN:HD21	1.83	0.43
6:AY:226:ASN:O	6:AY:230:GLU:HG2	2.18	0.43
6:V:37:SER:HB3	6:V:77:THR:HG23	2.01	0.43
6:X:258:VAL:HG13	6:X:262:LEU:HD22	1.99	0.43
6:Y:29:ALA:HA	6:Y:225:VAL:HG21	2.01	0.43
6:Y:115:THR:HB	6:Y:192:LEU:HD23	2.00	0.43
6:a:19:ILE:HG23	6:a:234:MET:HE1	1.99	0.43
8:b:33:ALA:O	8:b:92:ASN:ND2	2.51	0.43
8:e:35:THR:O	8:e:92:ASN:ND2	2.52	0.43
8:e:41:ARG:HD3	8:e:78:LYS:HD2	2.00	0.43
9:k:100:ASN:HB3	9:k:103:GLU:HG2	1.99	0.43
10:m:97:GLU:O	10:m:183:ARG:NH1	2.52	0.43
10:m:218:LEU:O	10:m:222:GLN:HG3	2.18	0.43
10:q:91:LEU:HD23	10:q:122:LEU:HD21	2.01	0.43
11:v:55:GLN:NE2	11:v:74:ARG:HE	2.16	0.43
1:E:23:ILE:HG23	1:E:402:MET:HE1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:ILE:HA	1:E:346:LEU:HD23	2.01	0.43
1:H:6:LEU:HD13	1:N:407:VAL:HG11	1.99	0.43
1:H:369:ASP:OD1	1:H:370:SER:N	2.52	0.43
1:O:351:LEU:HD13	1:O:390:ILE:HD11	2.01	0.43
2:9:133:VAL:HG21	2:9:137:LEU:HD13	2.01	0.43
6:B:95:MET:O	6:B:118:GLY:HA3	2.18	0.43
6:AR:28:ASN:N	6:AR:28:ASN:OD1	2.51	0.43
6:Q:152:VAL:H	6:Q:217:GLN:NE2	2.16	0.43
6:Y:148:ILE:HD13	6:Y:163:ARG:HG2	1.99	0.43
1:I:90:ALA:HB3	1:I:126:LEU:HB2	2.01	0.43
6:AP:116:ARG:NH2	6:AP:221:GLU:OE2	2.42	0.43
6:AP:145:GLU:HG3	6:AS:180:VAL:HG22	2.00	0.43
6:AY:96:MET:HG3	6:AY:221:GLU:HB2	2.01	0.43
6:T:48:ASN:HD21	6:T:51:GLN:HE21	1.65	0.43
6:U:8:SER:OG	6:Z:23:SER:OG	2.31	0.43
6:V:101:GLY:HA3	6:V:176:ILE:HD12	2.00	0.43
6:Y:36:LYS:HB3	6:Y:225:VAL:HG12	2.00	0.43
8:b:36:PRO:HB3	8:b:90:ASP:HB2	2.01	0.43
8:f:15:THR:HG23	8:f:45:PHE:HZ	1.84	0.43
3:z:203:VAL:HG11	3:z:209:VAL:HG12	1.99	0.43
1:G:415:ASN:OD1	1:L:26:ALA:HB3	2.18	0.43
3:1:255:MET:HG2	3:2:257:SER:HA	2.01	0.43
3:3:114:VAL:O	3:3:118:ILE:HG12	2.17	0.43
4:5:84:LEU:HD11	3:z:229:ILE:HG12	2.00	0.43
5:8:132:PHE:O	5:8:136:MET:HG2	2.19	0.43
7:AE:343:PRO:HG3	8:c:80:TYR:CZ	2.54	0.43
6:AQ:50:ASN:ND2	6:AQ:63:PRO:O	2.36	0.43
6:AY:82:THR:HG22	6:AY:224:ASN:HD22	1.84	0.43
6:U:226:ASN:HD22	6:U:228:THR:H	1.65	0.43
6:V:175:THR:OG1	6:V:204:GLU:OE2	2.27	0.43
6:W:152:VAL:HG22	6:W:158:VAL:HG13	2.00	0.43
6:X:94:ASP:HB2	6:X:220:LEU:HD21	2.00	0.43
6:a:116:ARG:NH1	6:a:221:GLU:OE2	2.51	0.43
9:l:37:SER:N	10:q:43:SER:O	2.52	0.43
9:l:115:TYR:CG	10:q:238:MET:HE3	2.53	0.43
10:m:136:SER:HB2	10:m:151:GLN:HA	2.00	0.43
10:n:77:ASP:N	10:n:77:ASP:OD1	2.51	0.43
10:q:1:MET:SD	10:q:1:MET:N	2.79	0.43
1:D:68:HIS:CD2	1:D:399:ASN:HB2	2.54	0.43
1:F:6:LEU:HD13	1:L:407:VAL:HG11	1.99	0.43
1:G:132:PRO:HB3	1:G:344:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:323:LEU:HD11	1:H:326:VAL:HG23	2.01	0.43
1:I:333:SER:HA	1:I:348:ARG:HA	2.00	0.43
1:O:21:ASN:O	1:O:25:ASN:ND2	2.50	0.43
4:4:81:ILE:HG13	3:y:278:LEU:HD21	2.01	0.43
4:7:16:MET:HE1	4:7:76:TYR:HB2	2.01	0.43
2:9:30:HIS:HB3	2:9:38:ASP:O	2.19	0.43
6:AQ:80:VAL:HG12	6:AQ:82:THR:HG23	2.01	0.43
6:AT:90:THR:HG23	6:a:80:VAL:HG11	2.00	0.43
6:AT:96:MET:HG3	6:AT:221:GLU:HB2	2.01	0.43
6:Q:115:THR:HB	6:Q:192:LEU:HD23	2.01	0.43
6:W:129:VAL:HG12	6:W:136:PRO:HA	2.01	0.43
8:d:36:PRO:HB3	8:d:90:ASP:HB2	2.01	0.43
9:i:75:LYS:HB2	9:i:98:ASN:HD22	1.84	0.43
9:l:13:ALA:O	9:l:17:GLU:HG2	2.19	0.43
3:y:195:PHE:HB3	3:y:213:VAL:HG13	2.01	0.43
1:D:51:LYS:HG3	1:D:52:THR:HG23	2.01	0.42
1:G:104:THR:HB	1:G:367:GLN:HG2	2.01	0.42
1:K:427:ASN:HD21	6:AZ:235:ILE:HG23	1.84	0.42
1:O:59:GLN:HG3	6:X:219:MET:HE1	2.01	0.42
3:1:275:GLY:O	3:1:279:ILE:HG12	2.19	0.42
3:3:204:ASP:OD1	3:3:204:ASP:N	2.52	0.42
5:8:207:ARG:HH12	5:8:210:PRO:HA	1.84	0.42
2:9:32:ASP:CG	2:9:36:ASN:HD22	2.26	0.42
6:C:176:ILE:HD11	6:C:212:LEU:HB3	2.01	0.42
6:C:247:VAL:O	6:C:251:VAL:HG23	2.19	0.42
6:AQ:95:MET:O	6:AQ:118:GLY:HA3	2.19	0.42
6:AV:43:ASP:OD1	6:AV:43:ASP:N	2.51	0.42
6:AV:226:ASN:O	6:AV:230:GLU:HG2	2.19	0.42
6:AW:48:ASN:HD21	6:AW:51:GLN:HE21	1.65	0.42
6:Q:226:ASN:ND2	6:Q:228:THR:HB	2.34	0.42
6:T:123:ASN:HD21	6:T:127:THR:HB	1.82	0.42
6:U:258:VAL:HG13	6:U:262:LEU:HD22	2.00	0.42
6:X:57:SER:O	6:X:58:GLN:HB2	2.18	0.42
3:3:243:VAL:HG21	12:x:89:LEU:HD11	2.01	0.42
2:9:73:VAL:HG12	2:9:75:GLY:H	1.83	0.42
6:AV:206:VAL:HB	6:AV:209:LEU:HD12	2.00	0.42
6:AW:161:ARG:NE	6:Q:186:GLU:OE1	2.51	0.42
6:AY:114:TYR:CE2	6:AY:195:PRO:HD3	2.54	0.42
6:S:129:VAL:HG12	6:S:136:PRO:HA	2.01	0.42
6:S:141:ILE:HD12	6:S:172:GLY:HA3	2.01	0.42
6:V:48:ASN:HD21	6:V:51:GLN:HE21	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:PHE:CE1	1:E:119:THR:HG22	2.51	0.42
1:K:80:ASP:O	1:K:393:GLY:N	2.52	0.42
1:L:32:LYS:HG3	1:L:67:PHE:CE1	2.55	0.42
1:L:88:PHE:N	1:L:352:VAL:O	2.52	0.42
3:3:228:GLN:O	3:3:232:MET:HG2	2.18	0.42
4:4:49:LEU:H	4:4:49:LEU:HD23	1.84	0.42
6:A:31:THR:HG21	6:A:191:ASN:HD21	1.85	0.42
6:A:254:MET:SD	10:n:222:GLN:HG2	2.59	0.42
6:B:238:GLN:HE22	6:AU:253:LYS:HE2	1.84	0.42
6:AQ:109:ASP:OD1	6:AQ:109:ASP:N	2.49	0.42
6:AT:70:ALA:HB1	10:p:71:VAL:HG21	2.01	0.42
6:AZ:1:MET:HE2	6:AZ:5:LEU:HD22	2.01	0.42
9:h:115:TYR:CG	10:o:238:MET:HE3	2.54	0.42
9:i:100:ASN:O	9:i:104:GLU:HG2	2.19	0.42
9:k:126:LYS:HE2	9:k:126:LYS:HB3	1.86	0.42
9:l:22:ASN:ND2	10:q:54:ARG:HE	2.17	0.42
1:G:131:ASP:HB2	1:G:134:SER:HB3	2.01	0.42
2:0:138:SER:HA	2:0:158:TYR:HB2	2.02	0.42
5:8:176:TRP:HE1	5:8:251:GLN:HG2	1.83	0.42
7:AL:338:ALA:HB1	9:h:103:GLU:HB2	2.01	0.42
6:B:22:ILE:HG21	6:B:234:MET:HG2	2.01	0.42
6:B:23:SER:OG	6:AU:8:SER:OG	2.35	0.42
6:C:50:ASN:ND2	6:C:63:PRO:O	2.40	0.42
6:AP:21:THR:HG21	6:AP:39:ALA:HB2	2.01	0.42
6:AU:166:GLN:O	6:AU:167:ASP:HB2	2.18	0.42
6:AZ:16:GLN:HE22	6:U:226:ASN:HD21	1.67	0.42
6:T:33:GLY:N	6:T:221:GLU:O	2.50	0.42
6:T:257:PHE:CE2	6:T:261:GLN:HG3	2.54	0.42
6:W:83:HIS:CE1	6:W:99:GLY:H	2.37	0.42
9:i:44:ALA:O	9:i:73:SER:N	2.46	0.42
9:k:119:VAL:HG13	10:p:245:LEU:HG	2.00	0.42
1:F:141:GLU:H	1:F:141:GLU:HG3	1.63	0.42
1:G:101:ASN:HD22	1:G:126:LEU:HD12	1.84	0.42
1:G:416:PHE:CZ	1:M:403:THR:HG21	2.51	0.42
4:5:15:TRP:HE3	4:7:63:MET:HE1	1.85	0.42
6:AQ:32:VAL:HG11	6:AQ:220:LEU:HD22	2.00	0.42
6:AU:90:THR:HG23	6:R:80:VAL:HG11	2.01	0.42
6:AZ:208:GLY:N	6:AZ:213:GLY:O	2.53	0.42
6:T:7:VAL:O	6:T:10:THR:OG1	2.31	0.42
6:Z:161:ARG:HH11	6:Z:168:ASN:ND2	2.17	0.42
6:a:94:ASP:OD1	6:a:94:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:n:200:GLN:NE2	10:n:201:THR:O	2.53	0.42
1:D:333:SER:HA	1:D:348:ARG:HA	2.02	0.42
1:E:430:GLN:HE21	6:AY:227:VAL:HG21	1.83	0.42
1:I:359:GLY:O	1:I:371:THR:OG1	2.37	0.42
1:K:16:LEU:HD13	1:K:16:LEU:HA	1.91	0.42
1:K:39:ALA:HB1	6:AY:190:GLN:HA	2.02	0.42
1:N:28:THR:OG1	1:N:31:PHE:HB2	2.19	0.42
3:3:101:ALA:HB2	11:v:95:TYR:OH	2.19	0.42
4:6:70:THR:O	4:6:71:GLN:C	2.63	0.42
5:8:84:ALA:HB1	5:8:255:LEU:HD13	2.01	0.42
6:AS:23:SER:HB3	6:AW:247:VAL:HG11	2.02	0.42
6:AX:155:ASP:C	6:AX:207:PRO:HG2	2.45	0.42
6:AY:169:GLN:HE21	6:AY:169:GLN:HB3	1.50	0.42
6:AZ:16:GLN:HG3	6:AZ:241:TYR:CE2	2.51	0.42
6:AZ:123:ASN:H	6:AZ:123:ASN:HD22	1.66	0.42
6:R:57:SER:OG	6:R:58:GLN:N	2.52	0.42
6:R:148:ILE:HG21	6:R:163:ARG:HG2	2.02	0.42
6:Z:91:ASN:HD22	6:Z:92:ALA:N	2.17	0.42
9:i:41:THR:O	9:i:42:TYR:C	2.62	0.42
9:k:133:LEU:HA	11:r:71:MET:HE3	2.01	0.42
1:F:42:TYR:HE2	1:K:362:LYS:HD2	1.81	0.42
1:J:65:GLN:HE22	1:J:362:LYS:HD3	1.85	0.42
7:AF:342:GLN:O	7:AF:343:PRO:C	2.61	0.42
7:AO:333:ALA:HB3	7:AO:356:MET:HB3	2.02	0.42
6:C:155:ASP:C	6:C:207:PRO:HG2	2.44	0.42
6:AQ:123:ASN:ND2	6:AQ:127:THR:HB	2.34	0.42
6:AR:14:ALA:HB1	6:AR:41:PHE:HE1	1.84	0.42
6:AY:7:VAL:HG13	6:AY:71:GLY:HA2	2.01	0.42
6:T:52:PRO:HB3	6:T:65:GLY:H	1.84	0.42
6:a:115:THR:HB	6:a:192:LEU:HD23	2.00	0.42
8:e:85:GLN:HE21	10:m:53:SER:HG	1.61	0.42
9:g:127:GLN:O	9:g:131:ARG:HG2	2.20	0.42
1:D:23:ILE:HG23	1:D:402:MET:HE1	2.01	0.42
1:I:42:TYR:C	1:I:42:TYR:HD1	2.28	0.42
1:L:101:ASN:OD1	1:L:377:LYS:NZ	2.53	0.42
1:M:87:GLY:O	1:M:105:ARG:NE	2.51	0.42
2:0:85:LYS:HA	2:0:104:ILE:HA	2.00	0.42
4:4:17:VAL:HG23	3:y:243:VAL:HG23	2.01	0.42
7:AK:337:GLY:O	7:AK:341:ASN:ND2	2.53	0.42
6:AQ:51:GLN:NE2	6:AQ:64:SER:OG	2.52	0.42
6:AX:226:ASN:O	6:AX:230:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AZ:129:VAL:HG12	6:AZ:136:PRO:HA	2.02	0.42
6:X:148:ILE:HG21	6:X:163:ARG:HG2	2.02	0.42
9:k:22:ASN:ND2	10:p:54:ARG:HE	2.14	0.42
10:n:35:ARG:NH1	10:n:101:ARG:HD3	2.34	0.42
10:n:40:GLN:HE21	10:n:60:GLU:CD	2.27	0.42
10:q:210:ASN:O	10:q:214:GLU:HG2	2.20	0.42
11:r:33:PHE:HE1	3:z:154:ASN:HB2	1.84	0.42
11:r:66:SER:OG	11:r:69:ASP:OD1	2.38	0.42
3:z:110:THR:HG21	3:z:219:ILE:HD11	2.01	0.42
3:z:166:VAL:HB	3:z:170:GLU:HB2	2.00	0.42
1:D:434:LEU:HD12	1:D:434:LEU:HA	1.87	0.42
1:E:106:ASN:H	1:E:106:ASN:HD22	1.66	0.42
1:K:407:VAL:O	1:K:410:ILE:HB	2.20	0.42
1:M:132:PRO:HB3	1:M:344:VAL:HG13	2.00	0.42
3:2:272:LEU:HD12	3:2:273:VAL:HG23	2.02	0.42
3:3:280:LEU:HD11	5:8:175:GLY:HA2	2.02	0.42
4:4:21:VAL:O	4:4:25:ILE:HG12	2.20	0.42
4:4:80:LEU:HA	4:4:83:ARG:HG2	2.01	0.42
4:5:16:MET:HE2	4:5:76:TYR:HB2	2.02	0.42
2:9:36:ASN:OD1	2:9:56:ASN:N	2.41	0.42
6:B:41:PHE:HB2	10:o:31:THR:HA	2.02	0.42
6:C:18:ASN:HB2	6:C:41:PHE:HZ	1.84	0.42
6:AV:25:ASN:HD21	6:AV:37:SER:H	1.66	0.42
6:R:82:THR:HG22	6:R:224:ASN:HD22	1.85	0.42
6:U:83:HIS:NE2	6:U:96:MET:HE3	2.35	0.42
6:a:185:LEU:HB3	6:a:193:TYR:HB3	2.01	0.42
10:q:76:ARG:NH1	10:q:79:ASP:OD1	2.47	0.42
11:r:71:MET:HA	11:r:74:ARG:HG2	2.02	0.42
3:y:167:THR:HG22	3:y:169:ARG:H	1.84	0.42
1:L:16:LEU:HD13	1:L:16:LEU:HA	1.88	0.42
3:3:162:LEU:HD21	5:8:69:PHE:HB3	2.02	0.42
6:B:258:VAL:HG22	10:o:229:VAL:HG21	2.00	0.42
6:AR:98:GLU:OE1	6:X:45:PHE:HB3	2.20	0.42
6:AX:96:MET:HE3	6:AX:221:GLU:HG3	2.02	0.42
6:P:152:VAL:H	6:P:217:GLN:NE2	2.17	0.42
6:R:226:ASN:O	6:R:230:GLU:HG2	2.19	0.42
6:Y:91:ASN:HD22	6:Y:92:ALA:N	2.17	0.42
10:o:37:ASP:HB3	10:o:61:ARG:HD2	2.02	0.42
10:p:87:TRP:HB3	10:p:99:LEU:HB3	2.01	0.42
10:q:97:GLU:O	10:q:183:ARG:NH1	2.53	0.42
12:x:105:MET:HE2	12:x:105:MET:HB3	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:15:GLN:O	6:A:19:ILE:HG12	2.20	0.41
7:AB:343:PRO:HG3	8:f:80:TYR:CZ	2.55	0.41
7:AD:346:ASP:OD1	8:d:39:LYS:NZ	2.44	0.41
6:AP:31:THR:HG21	6:AP:191:ASN:HD21	1.85	0.41
6:AR:94:ASP:OD1	6:AR:94:ASP:N	2.53	0.41
6:AX:18:ASN:HB2	6:AX:41:PHE:HZ	1.85	0.41
6:Q:18:ASN:HD22	6:Q:39:ALA:CB	2.32	0.41
6:T:254:MET:HE3	6:Y:241:TYR:CD1	2.55	0.41
6:V:1:MET:HE2	6:V:5:LEU:HD22	2.01	0.41
6:Z:239:ARG:HA	6:Z:239:ARG:HD3	1.89	0.41
9:l:100:ASN:HB3	9:l:103:GLU:HG2	2.01	0.41
10:m:84:GLY:O	10:m:101:ARG:NH2	2.31	0.41
10:n:123:GLY:N	10:n:127:ALA:O	2.53	0.41
10:n:218:LEU:O	10:n:222:GLN:HG3	2.20	0.41
3:z:183:MET:HB2	3:z:214:LEU:HD21	2.02	0.41
6:A:123:ASN:OD1	6:A:127:THR:N	2.53	0.41
6:AQ:155:ASP:C	6:AQ:207:PRO:HG2	2.45	0.41
6:AU:152:VAL:H	6:AU:217:GLN:NE2	2.18	0.41
6:AV:94:ASP:OD1	6:AV:94:ASP:N	2.52	0.41
6:AX:129:VAL:HG12	6:AX:136:PRO:HA	2.02	0.41
6:AY:261:GLN:HE21	6:AY:261:GLN:HB3	1.71	0.41
6:P:226:ASN:ND2	6:P:228:THR:HB	2.34	0.41
6:S:184:GLY:O	6:S:196:THR:OG1	2.32	0.41
6:Y:161:ARG:HH11	6:Y:168:ASN:ND2	2.18	0.41
6:Y:226:ASN:O	6:Y:230:GLU:HG2	2.20	0.41
6:Z:43:ASP:OD1	6:Z:43:ASP:N	2.28	0.41
8:c:128:ILE:HD13	11:t:83:ALA:HB2	2.02	0.41
10:m:167:VAL:HG12	10:m:169:PRO:HD3	2.03	0.41
1:G:434:LEU:HD12	1:G:434:LEU:HA	1.85	0.41
1:J:84:SER:OG	1:J:391:ASN:ND2	2.53	0.41
1:L:401:ASP:O	1:L:405:GLU:HG2	2.21	0.41
1:O:105:ARG:HD3	1:O:105:ARG:HA	1.90	0.41
3:2:274:ASP:OD2	3:2:277:ASN:ND2	2.52	0.41
3:3:255:MET:HE3	5:8:214:ILE:HG12	2.02	0.41
4:4:8:GLU:OE1	4:4:83:ARG:NH2	2.53	0.41
5:8:207:ARG:O	5:8:207:ARG:HD3	2.20	0.41
6:A:155:ASP:C	6:A:207:PRO:HG2	2.46	0.41
7:AB:353:VAL:HG21	9:k:38:ALA:HB2	2.01	0.41
7:AF:346:ASP:HB3	7:AF:347:ALA:H	1.61	0.41
6:C:31:THR:HA	6:AT:41:PHE:HB2	2.02	0.41
6:AR:181:ASN:OD1	6:AR:184:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AS:106:THR:OG1	6:AS:138:GLU:OE2	2.38	0.41
6:Aa:1:MET:SD	6:V:236:GLU:HA	2.60	0.41
6:X:18:ASN:HD22	6:X:39:ALA:HB3	1.85	0.41
6:a:188:ILE:HD13	6:a:194:LEU:HG	2.03	0.41
9:k:96:LYS:HE3	9:k:96:LYS:HB3	1.89	0.41
10:m:28:ASN:O	10:m:31:THR:OG1	2.37	0.41
10:m:82:ILE:HD11	10:m:88:ILE:HG13	2.02	0.41
10:n:65:ASN:O	10:n:208:ASN:ND2	2.51	0.41
10:q:81:THR:HG23	10:q:200:GLN:HB3	2.03	0.41
1:G:354:VAL:HG11	1:G:360:LEU:HD21	2.02	0.41
1:I:34:SER:OG	1:I:65:GLN:NE2	2.53	0.41
1:L:79:MET:HE3	1:L:111:LEU:HD21	2.02	0.41
3:3:253:MET:H	3:3:253:MET:HG2	1.69	0.41
6:AS:2:HIS:CD2	6:AS:4:ALA:H	2.34	0.41
6:AT:184:GLY:O	6:AT:196:THR:OG1	2.33	0.41
6:AW:198:ALA:HB1	6:X:63:PRO:HA	2.02	0.41
6:AX:236:GLU:HG3	6:X:1:MET:HG2	2.02	0.41
6:W:101:GLY:HA3	6:W:176:ILE:HD12	2.01	0.41
6:a:163:ARG:HD3	6:a:163:ARG:HA	1.91	0.41
10:n:11:GLY:O	10:n:15:ASN:ND2	2.45	0.41
10:n:142:ARG:HH12	10:n:200:GLN:HG2	1.86	0.41
12:x:77:LYS:HE3	12:x:77:LYS:HB2	1.89	0.41
1:D:113:LYS:H	1:D:113:LYS:HD3	1.86	0.41
1:I:353:ARG:HB2	1:I:387:PHE:CE1	2.56	0.41
3:3:273:VAL:HG22	12:x:58:PHE:CE2	2.55	0.41
5:8:88:VAL:HG12	5:8:92:MET:HE3	2.03	0.41
2:9:124:LEU:HD21	2:9:127:LEU:HD21	2.02	0.41
6:C:104:GLN:NE2	6:C:175:THR:OG1	2.54	0.41
6:AP:22:ILE:HD11	6:AP:233:ASN:HB2	2.03	0.41
6:AR:241:TYR:CD1	6:AX:254:MET:HE3	2.55	0.41
6:AW:184:GLY:O	6:AW:196:THR:OG1	2.33	0.41
6:T:148:ILE:HG12	6:T:161:ARG:O	2.21	0.41
6:U:261:GLN:HE21	6:U:261:GLN:HB3	1.71	0.41
6:Z:184:GLY:O	6:Z:196:THR:OG1	2.30	0.41
8:c:32:GLN:NE2	9:h:51:ALA:HB2	2.35	0.41
10:n:16:MET:O	10:n:20:GLN:HG3	2.20	0.41
10:n:68:GLN:OE1	10:n:101:ARG:NH2	2.53	0.41
1:E:46:LEU:HD12	6:S:149:SER:HA	2.02	0.41
1:E:128:TYR:HB2	1:E:348:ARG:HG3	2.03	0.41
1:K:2:SER:HB3	1:K:426:HIS:ND1	2.35	0.41
1:O:359:GLY:C	1:O:374:SER:HB3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:188:ARG:NH1	3:1:225:THR:OG1	2.46	0.41
3:3:88:GLN:OE1	3:3:161:TYR:OH	2.29	0.41
3:3:104:ILE:HG22	3:3:109:PHE:CD2	2.56	0.41
5:8:39:PRO:HD2	11:t:102:PRO:HG2	2.01	0.41
5:8:61:PRO:HG3	5:8:161:GLY:HA3	2.03	0.41
2:9:35:GLY:O	2:9:55:GLY:N	2.53	0.41
7:AA:351:GLN:OE1	6:AQ:64:SER:N	2.49	0.41
6:C:36:LYS:HB3	6:C:225:VAL:HG12	2.03	0.41
6:AR:95:MET:O	6:AR:118:GLY:HA3	2.20	0.41
6:AU:178:ASP:HB2	6:AU:212:LEU:HD23	2.03	0.41
6:Q:94:ASP:HA	6:Q:118:GLY:O	2.21	0.41
6:S:83:HIS:HE1	6:S:99:GLY:H	1.66	0.41
6:U:83:HIS:HD2	6:U:84:GLY:O	2.03	0.41
6:V:43:ASP:OD1	6:V:43:ASP:N	2.42	0.41
6:V:240:VAL:O	6:V:244:ASN:ND2	2.50	0.41
6:W:174:LEU:HD23	6:W:174:LEU:HA	1.93	0.41
6:Y:18:ASN:HB2	6:Y:41:PHE:HZ	1.86	0.41
6:Y:123:ASN:HD21	6:Y:127:THR:HB	1.86	0.41
9:j:43:LYS:HG2	9:j:77:LEU:HD21	2.02	0.41
10:q:14:GLN:HB3	10:q:59:THR:HG23	2.02	0.41
1:J:147:ILE:HA	1:J:346:LEU:HD23	2.03	0.41
1:N:68:HIS:CD2	1:N:399:ASN:HB2	2.56	0.41
1:N:359:GLY:C	1:N:374:SER:HB3	2.46	0.41
2:0:147:LEU:HB2	2:0:168:PRO:HD3	2.03	0.41
6:AT:121:THR:OG1	6:AT:122:LEU:N	2.54	0.41
6:AT:185:LEU:HB3	6:AT:193:TYR:HB3	2.02	0.41
6:AU:43:ASP:N	6:AU:43:ASP:OD1	2.53	0.41
6:AX:188:ILE:HD13	6:AX:194:LEU:HG	2.02	0.41
6:P:48:ASN:HD21	6:P:51:GLN:NE2	2.19	0.41
6:Q:181:ASN:ND2	6:W:122:LEU:O	2.54	0.41
6:R:18:ASN:HD22	6:R:39:ALA:HB3	1.85	0.41
6:U:63:PRO:HA	6:Z:198:ALA:HB1	2.02	0.41
6:W:95:MET:O	6:W:118:GLY:HA3	2.20	0.41
10:p:1:MET:HG3	10:p:239:ASP:HB2	2.03	0.41
3:z:184:LEU:O	3:z:187:THR:HG22	2.21	0.41
1:F:50:ALA:HA	1:F:53:THR:CG2	2.51	0.41
1:J:130:VAL:HG22	1:J:347:GLY:HA2	2.03	0.41
1:O:109:PHE:HE1	1:O:119:THR:HG22	1.84	0.41
4:4:44:ILE:HG22	4:4:46:GLU:H	1.86	0.41
4:6:73:LEU:HD13	4:6:73:LEU:HA	1.97	0.41
5:8:213:ASN:HB2	5:8:215:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AP:96:MET:HE3	6:AP:221:GLU:HA	2.02	0.41
6:AP:246:LYS:HE2	6:AP:246:LYS:HB3	1.93	0.41
6:AU:87:GLN:NE2	6:R:38:ARG:HH22	2.19	0.41
6:AW:100:ASP:O	6:AW:213:GLY:N	2.48	0.41
6:AY:29:ALA:HA	6:AY:225:VAL:HG21	2.03	0.41
6:S:226:ASN:O	6:S:230:GLU:HG2	2.21	0.41
8:c:124:LEU:HD23	11:t:79:VAL:HG11	2.03	0.41
9:i:89:ASN:OD1	9:i:93:TYR:N	2.51	0.41
9:l:130:LEU:HD11	10:q:248:MET:HE3	2.03	0.41
1:F:62:GLN:HE22	1:K:120:ALA:HB1	1.86	0.41
1:G:323:LEU:HD11	1:G:326:VAL:HG23	2.01	0.41
1:H:113:LYS:HD3	1:H:113:LYS:H	1.85	0.41
1:M:141:GLU:H	1:M:141:GLU:HG3	1.72	0.41
2:O:159:ILE:HG13	2:O:182:ASN:HD21	1.86	0.41
4:6:81:ILE:HA	4:6:84:LEU:HD13	2.02	0.41
6:A:9:LYS:HG3	10:o:216:THR:HG21	2.01	0.41
7:AI:335:ILE:O	7:AI:336:PRO:C	2.61	0.41
7:AJ:341:ASN:ND2	8:c:86:PRO:HG3	2.36	0.41
6:B:22:ILE:HG23	6:B:230:GLU:HB3	2.01	0.41
6:B:188:ILE:HD13	6:B:194:LEU:HG	2.03	0.41
6:B:244:ASN:HD21	10:o:27:ALA:HA	1.84	0.41
6:C:40:VAL:HG11	10:m:116:ALA:HB1	2.02	0.41
6:C:163:ARG:HD2	6:C:163:ARG:HA	1.97	0.41
6:AP:59:ASN:HB3	6:AP:62:LEU:HB2	2.02	0.41
6:AP:212:LEU:HD23	6:AP:212:LEU:HA	1.94	0.41
6:AR:95:MET:HE2	6:AR:95:MET:HB3	2.00	0.41
6:AU:28:ASN:OD1	6:AU:28:ASN:N	2.53	0.41
6:AU:155:ASP:C	6:AU:207:PRO:HG2	2.45	0.41
6:T:114:TYR:HE2	6:T:195:PRO:HD3	1.85	0.41
6:U:18:ASN:HB2	6:U:41:PHE:CZ	2.55	0.41
6:V:257:PHE:CE2	6:V:261:GLN:HG3	2.56	0.41
6:X:151:THR:HG23	6:X:159:SER:HB2	2.02	0.41
9:i:39:LYS:HA	9:i:39:LYS:HD3	1.74	0.41
9:l:135:MET:HE2	11:v:75:ASN:HD22	1.85	0.41
10:p:77:ASP:OD1	10:p:77:ASP:N	2.53	0.41
10:p:179:ASN:HD21	10:p:183:ARG:HH21	1.69	0.41
10:q:83:GLU:OE1	10:q:142:ARG:NH2	2.54	0.41
1:H:386:SER:HB3	1:M:322:PHE:HB3	2.03	0.41
1:N:149:ALA:O	1:N:323:LEU:N	2.51	0.41
3:2:104:ILE:O	3:2:110:THR:OG1	2.38	0.41
3:3:128:THR:HB	3:3:129:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:343:PRO:HA	7:AG:344:PRO:HD3	1.92	0.41
6:AR:236:GLU:HG3	6:AR:237:ALA:N	2.36	0.41
6:AY:120:PHE:HE1	6:AY:130:THR:HG22	1.86	0.41
6:S:95:MET:O	6:S:118:GLY:HA3	2.21	0.41
6:T:38:ARG:HH22	6:Y:87:GLN:HE22	1.67	0.41
6:V:161:ARG:HH12	6:V:166:GLN:HA	1.86	0.41
6:X:154:THR:HG23	6:X:214:GLU:HB3	2.02	0.41
10:n:108:ASP:OD1	10:n:112:MET:N	2.54	0.41
10:n:231:MET:HA	10:n:234:THR:HG22	2.04	0.41
10:p:108:ASP:OD1	10:p:112:MET:N	2.54	0.41
11:v:71:MET:SD	11:v:74:ARG:HD3	2.61	0.41
1:O:39:ALA:HB1	6:Q:190:GLN:HA	2.02	0.40
3:1:189:ILE:H	3:1:189:ILE:HD12	1.85	0.40
3:2:270:PHE:HE2	3:2:276:TRP:CD1	2.38	0.40
3:3:186:GLN:HE22	3:3:287:PHE:HA	1.85	0.40
7:AG:339:LEU:HD11	9:k:72:GLU:HG3	2.03	0.40
6:AQ:155:ASP:HA	6:AQ:207:PRO:O	2.21	0.40
6:AW:96:MET:HG3	6:AW:221:GLU:HB2	2.03	0.40
6:P:239:ARG:HA	6:P:239:ARG:HD3	1.74	0.40
6:T:219:MET:HE3	6:T:219:MET:HB2	1.97	0.40
6:W:58:GLN:HG2	6:W:59:ASN:ND2	2.36	0.40
6:X:24:ASN:ND2	6:X:34:TYR:OH	2.54	0.40
8:e:124:LEU:HD23	11:r:79:VAL:HG11	2.04	0.40
9:i:53:LEU:N	9:i:53:LEU:HD23	2.36	0.40
9:l:126:LYS:NZ	10:q:245:LEU:O	2.53	0.40
10:o:167:VAL:HG12	10:o:169:PRO:HD3	2.04	0.40
12:x:69:ARG:H	12:x:69:ARG:CZ	2.34	0.40
1:E:433:ILE:HD11	1:J:416:PHE:HZ	1.85	0.40
1:F:82:ARG:HH11	1:F:396:GLU:HG2	1.86	0.40
1:H:356:ASN:HB3	1:H:374:SER:HA	2.02	0.40
1:N:323:LEU:HD11	1:N:326:VAL:HG23	2.04	0.40
6:B:59:ASN:HB3	6:B:62:LEU:HB2	2.03	0.40
6:AR:96:MET:HG3	6:AR:221:GLU:HB2	2.03	0.40
6:AY:56:SER:O	6:AY:57:SER:HB3	2.22	0.40
6:AZ:38:ARG:HH22	6:T:87:GLN:HE22	1.69	0.40
6:Q:94:ASP:OD1	6:Q:94:ASP:N	2.49	0.40
6:V:1:MET:SD	6:a:236:GLU:HA	2.62	0.40
10:m:40:GLN:HG2	10:m:62:PRO:HD3	2.01	0.40
10:n:144:GLY:HA2	10:n:199:LEU:HD12	2.03	0.40
10:o:115:ASN:OD1	10:o:119:HIS:N	2.54	0.40
10:q:2:ASP:C	10:q:4:ALA:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:z:152:GLU:CD	3:z:178:PRO:HB3	2.46	0.40
1:E:136:GLU:OE1	1:E:348:ARG:NH1	2.52	0.40
1:F:54:PRO:HG2	1:K:17:ASN:HB2	2.02	0.40
1:K:68:HIS:CD2	1:K:399:ASN:HB2	2.56	0.40
1:O:328:PHE:CE2	1:O:334:VAL:HB	2.57	0.40
3:1:242:LEU:HD13	5:8:125:LEU:HD12	2.01	0.40
3:2:96:LEU:HB3	11:u:90:LYS:HB3	2.03	0.40
3:2:111:ARG:NE	3:2:222:GLU:OE1	2.50	0.40
4:5:84:LEU:HD13	3:z:232:MET:HG3	2.04	0.40
4:6:56:ILE:HG12	4:7:18:LEU:HD11	2.04	0.40
6:A:91:ASN:HB3	6:A:94:ASP:OD2	2.21	0.40
6:C:32:VAL:HG21	6:C:220:LEU:HD13	2.03	0.40
6:C:123:ASN:ND2	6:C:127:THR:HB	2.34	0.40
6:AP:102:PHE:HB3	6:AP:114:TYR:HB3	2.03	0.40
6:AP:239:ARG:NH1	6:AT:256:SER:HB2	2.36	0.40
6:T:58:GLN:HG2	6:T:59:ASN:ND2	2.37	0.40
6:U:101:GLY:HA3	6:U:176:ILE:HD12	2.03	0.40
6:Y:31:THR:HG21	6:Y:191:ASN:HD21	1.87	0.40
9:h:120:GLN:HE22	10:n:247:ARG:NE	2.18	0.40
9:i:25:SER:HB2	10:n:7:LEU:HD23	2.04	0.40
10:n:76:ARG:O	10:n:202:GLY:HA2	2.20	0.40
10:q:10:SER:O	10:q:14:GLN:HG2	2.22	0.40
11:t:71:MET:SD	11:t:74:ARG:HD3	2.61	0.40
3:y:254:MET:HB2	3:z:254:MET:SD	2.61	0.40
1:F:401:ASP:O	1:F:405:GLU:HG2	2.22	0.40
1:J:361:ASP:HB3	6:S:161:ARG:HH12	1.86	0.40
1:M:401:ASP:O	1:M:405:GLU:HG2	2.21	0.40
1:N:353:ARG:HB2	1:N:387:PHE:CE1	2.56	0.40
1:O:69:GLU:OE2	1:O:105:ARG:NH1	2.46	0.40
1:O:356:ASN:HB3	1:O:374:SER:HA	2.03	0.40
2:0:77:LEU:HB3	2:0:97:ALA:HA	2.04	0.40
4:4:14:LEU:HA	4:4:17:VAL:HG12	2.03	0.40
6:C:258:VAL:O	6:C:262:LEU:HB2	2.21	0.40
6:AP:226:ASN:O	6:AP:230:GLU:HG2	2.21	0.40
6:AS:226:ASN:O	6:AS:230:GLU:HG2	2.22	0.40
6:R:91:ASN:HD22	6:R:92:ALA:N	2.20	0.40
6:S:239:ARG:HA	6:S:239:ARG:HD3	1.75	0.40
6:T:82:THR:HG23	6:T:224:ASN:HD22	1.86	0.40
6:V:18:ASN:HB2	6:V:41:PHE:HZ	1.86	0.40
6:X:123:ASN:ND2	6:X:127:THR:HB	2.36	0.40
6:Z:151:THR:HG23	6:Z:159:SER:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:206:VAL:HG23	6:Z:209:LEU:HB2	2.03	0.40
1:E:113:LYS:HD3	1:E:113:LYS:H	1.86	0.40
1:M:28:THR:OG1	1:M:31:PHE:HB2	2.22	0.40
6:A:26:LEU:HD23	6:A:26:LEU:HA	1.93	0.40
6:A:155:ASP:OD1	6:T:57:SER:HA	2.21	0.40
6:AT:31:THR:HG21	6:AT:191:ASN:HD21	1.87	0.40
6:AT:95:MET:HE1	6:AT:152:VAL:HG21	2.04	0.40
6:AT:236:GLU:HG3	6:AT:237:ALA:N	2.35	0.40
6:AZ:37:SER:HB3	6:AZ:77:THR:HG22	2.04	0.40
6:P:43:ASP:HB3	6:V:28:ASN:HD21	1.86	0.40
6:Q:91:ASN:ND2	6:Q:93:LEU:H	2.12	0.40
6:T:37:SER:HB3	6:T:77:THR:HG23	2.02	0.40
6:T:162:VAL:HB	6:T:165:GLN:HE21	1.86	0.40
6:T:239:ARG:HA	6:T:239:ARG:HD3	1.81	0.40
6:V:10:THR:HB	6:V:72:SER:O	2.22	0.40
6:V:91:ASN:ND2	6:V:93:LEU:H	2.15	0.40
8:e:127:ALA:HB2	3:z:86:THR:HG22	2.02	0.40
10:m:15:ASN:ND2	10:m:228:GLN:HE22	2.18	0.40
10:p:167:VAL:HG12	10:p:169:PRO:HD3	2.04	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	D	264/437 (60%)	257 (97%)	7 (3%)	0	100	100
1	E	264/437 (60%)	256 (97%)	8 (3%)	0	100	100
1	F	264/437 (60%)	257 (97%)	7 (3%)	0	100	100
1	G	264/437 (60%)	259 (98%)	3 (1%)	2 (1%)	16	46
1	H	264/437 (60%)	256 (97%)	6 (2%)	2 (1%)	16	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	264/437 (60%)	256 (97%)	8 (3%)	0	100	100
1	J	264/437 (60%)	256 (97%)	8 (3%)	0	100	100
1	K	264/437 (60%)	258 (98%)	6 (2%)	0	100	100
1	L	264/437 (60%)	260 (98%)	4 (2%)	0	100	100
1	M	264/437 (60%)	257 (97%)	7 (3%)	0	100	100
1	N	264/437 (60%)	259 (98%)	5 (2%)	0	100	100
1	O	264/437 (60%)	259 (98%)	5 (2%)	0	100	100
2	0	178/199 (89%)	173 (97%)	5 (3%)	0	100	100
2	9	178/199 (89%)	174 (98%)	4 (2%)	0	100	100
3	1	205/289 (71%)	202 (98%)	3 (2%)	0	100	100
3	2	206/289 (71%)	203 (98%)	3 (2%)	0	100	100
3	3	206/289 (71%)	204 (99%)	2 (1%)	0	100	100
3	y	206/289 (71%)	202 (98%)	4 (2%)	0	100	100
3	z	206/289 (71%)	202 (98%)	4 (2%)	0	100	100
4	4	87/89 (98%)	87 (100%)	0	0	100	100
4	5	87/89 (98%)	86 (99%)	0	1 (1%)	11	39
4	6	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
4	7	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
5	8	238/260 (92%)	232 (98%)	6 (2%)	0	100	100
6	A	260/262 (99%)	251 (96%)	9 (4%)	0	100	100
6	AP	260/262 (99%)	253 (97%)	6 (2%)	1 (0%)	30	61
6	AQ	260/262 (99%)	248 (95%)	11 (4%)	1 (0%)	30	61
6	AR	244/262 (93%)	240 (98%)	3 (1%)	1 (0%)	30	61
6	AS	244/262 (93%)	235 (96%)	9 (4%)	0	100	100
6	AT	245/262 (94%)	239 (98%)	5 (2%)	1 (0%)	30	61
6	AU	244/262 (93%)	240 (98%)	4 (2%)	0	100	100
6	AV	244/262 (93%)	242 (99%)	1 (0%)	1 (0%)	30	61
6	AW	260/262 (99%)	254 (98%)	5 (2%)	1 (0%)	30	61
6	AX	260/262 (99%)	254 (98%)	6 (2%)	0	100	100
6	AY	260/262 (99%)	254 (98%)	6 (2%)	0	100	100
6	AZ	260/262 (99%)	255 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Aa	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
6	B	260/262 (99%)	250 (96%)	10 (4%)	0	100	100
6	C	260/262 (99%)	252 (97%)	7 (3%)	1 (0%)	30	61
6	P	260/262 (99%)	253 (97%)	6 (2%)	1 (0%)	30	61
6	Q	260/262 (99%)	257 (99%)	3 (1%)	0	100	100
6	R	260/262 (99%)	254 (98%)	6 (2%)	0	100	100
6	S	260/262 (99%)	253 (97%)	7 (3%)	0	100	100
6	T	260/262 (99%)	253 (97%)	7 (3%)	0	100	100
6	U	260/262 (99%)	255 (98%)	5 (2%)	0	100	100
6	V	260/262 (99%)	251 (96%)	9 (4%)	0	100	100
6	W	260/262 (99%)	253 (97%)	6 (2%)	1 (0%)	30	61
6	X	260/262 (99%)	250 (96%)	9 (4%)	1 (0%)	30	61
6	Y	260/262 (99%)	253 (97%)	7 (3%)	0	100	100
6	Z	260/262 (99%)	253 (97%)	7 (3%)	0	100	100
6	a	260/262 (99%)	253 (97%)	7 (3%)	0	100	100
7	AA	17/580 (3%)	17 (100%)	0	0	100	100
7	AB	17/580 (3%)	15 (88%)	2 (12%)	0	100	100
7	AC	18/580 (3%)	18 (100%)	0	0	100	100
7	AD	17/580 (3%)	17 (100%)	0	0	100	100
7	AE	17/580 (3%)	17 (100%)	0	0	100	100
7	AF	21/580 (4%)	14 (67%)	6 (29%)	1 (5%)	2	9
7	AG	9/580 (2%)	7 (78%)	2 (22%)	0	100	100
7	AH	9/580 (2%)	9 (100%)	0	0	100	100
7	AI	9/580 (2%)	8 (89%)	1 (11%)	0	100	100
7	AJ	22/580 (4%)	18 (82%)	4 (18%)	0	100	100
7	AK	23/580 (4%)	23 (100%)	0	0	100	100
7	AL	30/580 (5%)	26 (87%)	4 (13%)	0	100	100
7	AM	31/580 (5%)	31 (100%)	0	0	100	100
7	AN	31/580 (5%)	31 (100%)	0	0	100	100
7	AO	30/580 (5%)	30 (100%)	0	0	100	100
8	b	105/131 (80%)	104 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	c	103/131 (79%)	102 (99%)	1 (1%)	0	100	100
8	d	105/131 (80%)	103 (98%)	2 (2%)	0	100	100
8	e	104/131 (79%)	104 (100%)	0	0	100	100
8	f	104/131 (79%)	103 (99%)	1 (1%)	0	100	100
9	g	126/137 (92%)	122 (97%)	4 (3%)	0	100	100
9	h	126/137 (92%)	123 (98%)	3 (2%)	0	100	100
9	i	126/137 (92%)	122 (97%)	3 (2%)	1 (1%)	16	46
9	j	126/137 (92%)	125 (99%)	1 (1%)	0	100	100
9	k	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
9	l	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
10	m	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
10	n	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
10	o	246/249 (99%)	241 (98%)	5 (2%)	0	100	100
10	p	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
10	q	246/249 (99%)	240 (98%)	6 (2%)	0	100	100
11	r	70/103 (68%)	70 (100%)	0	0	100	100
11	s	78/103 (76%)	78 (100%)	0	0	100	100
11	t	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
11	u	70/103 (68%)	69 (99%)	1 (1%)	0	100	100
11	v	70/103 (68%)	69 (99%)	1 (1%)	0	100	100
11	w	38/103 (37%)	38 (100%)	0	0	100	100
12	x	69/376 (18%)	69 (100%)	0	0	100	100
All	All	15361/27193 (56%)	14986 (98%)	358 (2%)	17 (0%)	49	78

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	52	THR
1	G	54	PRO
1	H	64	ALA
6	X	58	GLN
1	H	65	GLN
4	5	88	LEU
6	AT	167	ASP

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Mol	Chain	Res	Type
6	AV	167	ASP
9	i	42	TYR
6	C	167	ASP
6	AR	167	ASP
6	P	167	ASP
6	W	167	ASP
6	AP	167	ASP
6	AQ	167	ASP
6	AW	57	SER
7	AF	349	ILE

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	D	225/366 (62%)	216 (96%)	9 (4%)	28	59
1	E	225/366 (62%)	215 (96%)	10 (4%)	25	56
1	F	225/366 (62%)	213 (95%)	12 (5%)	20	51
1	G	225/366 (62%)	213 (95%)	12 (5%)	20	51
1	H	225/366 (62%)	217 (96%)	8 (4%)	31	62
1	I	225/366 (62%)	214 (95%)	11 (5%)	22	53
1	J	225/366 (62%)	211 (94%)	14 (6%)	16	45
1	K	225/366 (62%)	213 (95%)	12 (5%)	20	51
1	L	225/366 (62%)	211 (94%)	14 (6%)	16	45
1	M	225/366 (62%)	214 (95%)	11 (5%)	22	53
1	N	225/366 (62%)	212 (94%)	13 (6%)	18	48
1	O	225/366 (62%)	211 (94%)	14 (6%)	16	45
2	0	149/167 (89%)	145 (97%)	4 (3%)	39	68
2	9	149/167 (89%)	148 (99%)	1 (1%)	76	84
3	1	181/247 (73%)	175 (97%)	6 (3%)	33	64
3	2	182/247 (74%)	176 (97%)	6 (3%)	33	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	182/247 (74%)	177 (97%)	5 (3%)	39	68
3	y	182/247 (74%)	175 (96%)	7 (4%)	29	60
3	z	182/247 (74%)	175 (96%)	7 (4%)	29	60
4	4	80/80 (100%)	77 (96%)	3 (4%)	29	60
4	5	80/80 (100%)	76 (95%)	4 (5%)	22	53
4	6	80/80 (100%)	75 (94%)	5 (6%)	16	45
4	7	80/80 (100%)	79 (99%)	1 (1%)	61	79
5	8	204/218 (94%)	194 (95%)	10 (5%)	22	53
6	A	218/218 (100%)	214 (98%)	4 (2%)	51	74
6	AP	218/218 (100%)	214 (98%)	4 (2%)	51	74
6	AQ	218/218 (100%)	211 (97%)	7 (3%)	34	64
6	AR	206/218 (94%)	200 (97%)	6 (3%)	37	67
6	AS	206/218 (94%)	200 (97%)	6 (3%)	37	67
6	AT	207/218 (95%)	200 (97%)	7 (3%)	32	63
6	AU	206/218 (94%)	202 (98%)	4 (2%)	50	73
6	AV	206/218 (94%)	199 (97%)	7 (3%)	32	63
6	AW	218/218 (100%)	213 (98%)	5 (2%)	44	70
6	AX	218/218 (100%)	212 (97%)	6 (3%)	38	67
6	AY	218/218 (100%)	213 (98%)	5 (2%)	44	70
6	AZ	218/218 (100%)	213 (98%)	5 (2%)	44	70
6	Aa	218/218 (100%)	215 (99%)	3 (1%)	59	78
6	B	218/218 (100%)	213 (98%)	5 (2%)	44	70
6	C	218/218 (100%)	211 (97%)	7 (3%)	34	64
6	P	218/218 (100%)	211 (97%)	7 (3%)	34	64
6	Q	218/218 (100%)	212 (97%)	6 (3%)	38	67
6	R	218/218 (100%)	213 (98%)	5 (2%)	44	70
6	S	218/218 (100%)	213 (98%)	5 (2%)	44	70
6	T	218/218 (100%)	212 (97%)	6 (3%)	38	67
6	U	218/218 (100%)	212 (97%)	6 (3%)	38	67
6	V	218/218 (100%)	212 (97%)	6 (3%)	38	67
6	W	218/218 (100%)	212 (97%)	6 (3%)	38	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	X	218/218 (100%)	215 (99%)	3 (1%)	59	78
6	Y	218/218 (100%)	211 (97%)	7 (3%)	34	64
6	Z	218/218 (100%)	212 (97%)	6 (3%)	38	67
6	a	218/218 (100%)	211 (97%)	7 (3%)	34	64
7	AA	15/500 (3%)	14 (93%)	1 (7%)	15	43
7	AB	15/500 (3%)	14 (93%)	1 (7%)	15	43
7	AC	15/500 (3%)	15 (100%)	0	100	100
7	AD	15/500 (3%)	14 (93%)	1 (7%)	15	43
7	AE	15/500 (3%)	15 (100%)	0	100	100
7	AF	17/500 (3%)	13 (76%)	4 (24%)	1	4
7	AG	8/500 (2%)	8 (100%)	0	100	100
7	AH	8/500 (2%)	7 (88%)	1 (12%)	4	18
7	AI	8/500 (2%)	8 (100%)	0	100	100
7	AJ	17/500 (3%)	16 (94%)	1 (6%)	18	47
7	AK	18/500 (4%)	15 (83%)	3 (17%)	2	10
7	AL	24/500 (5%)	23 (96%)	1 (4%)	26	58
7	AM	24/500 (5%)	24 (100%)	0	100	100
7	AN	24/500 (5%)	22 (92%)	2 (8%)	10	34
7	AO	24/500 (5%)	23 (96%)	1 (4%)	26	58
8	b	89/106 (84%)	88 (99%)	1 (1%)	65	80
8	c	88/106 (83%)	86 (98%)	2 (2%)	44	70
8	d	89/106 (84%)	86 (97%)	3 (3%)	32	63
8	e	88/106 (83%)	85 (97%)	3 (3%)	32	63
8	f	88/106 (83%)	88 (100%)	0	100	100
9	g	111/115 (96%)	106 (96%)	5 (4%)	24	56
9	h	111/115 (96%)	107 (96%)	4 (4%)	31	62
9	i	111/115 (96%)	103 (93%)	8 (7%)	13	40
9	j	111/115 (96%)	106 (96%)	5 (4%)	24	56
9	k	111/115 (96%)	105 (95%)	6 (5%)	20	50
9	l	111/115 (96%)	106 (96%)	5 (4%)	24	56
10	m	204/205 (100%)	199 (98%)	5 (2%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	n	204/205 (100%)	198 (97%)	6 (3%)	37	67
10	o	204/205 (100%)	198 (97%)	6 (3%)	37	67
10	p	204/205 (100%)	202 (99%)	2 (1%)	68	81
10	q	204/205 (100%)	200 (98%)	4 (2%)	48	73
11	r	63/84 (75%)	59 (94%)	4 (6%)	16	45
11	s	66/84 (79%)	64 (97%)	2 (3%)	36	66
11	t	66/84 (79%)	63 (96%)	3 (4%)	24	56
11	u	63/84 (75%)	62 (98%)	1 (2%)	55	76
11	v	63/84 (75%)	63 (100%)	0	100	100
11	w	36/84 (43%)	35 (97%)	1 (3%)	38	67
12	x	58/317 (18%)	55 (95%)	3 (5%)	21	51
All	All	13048/22951 (57%)	12603 (97%)	445 (3%)	33	63

All (445) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	40	ASP
1	D	51	LYS
1	D	62	GLN
1	D	73	ILE
1	D	113	LYS
1	D	140	TYR
1	D	334	VAL
1	D	402	MET
1	D	434	LEU
1	E	40	ASP
1	E	52	THR
1	E	73	ILE
1	E	106	ASN
1	E	113	LYS
1	E	137	VAL
1	E	140	TYR
1	E	334	VAL
1	E	351	LEU
1	E	396	GLU
1	F	40	ASP
1	F	42	TYR
1	F	43	SER

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Mol	Chain	Res	Type
1	F	45	SER
1	F	49	ASN
1	F	62	GLN
1	F	73	ILE
1	F	113	LYS
1	F	121	ASN
1	F	140	TYR
1	F	334	VAL
1	F	434	LEU
1	G	40	ASP
1	G	42	TYR
1	G	43	SER
1	G	44	ASN
1	G	73	ILE
1	G	101	ASN
1	G	113	LYS
1	G	140	TYR
1	G	334	VAL
1	G	351	LEU
1	G	352	VAL
1	G	434	LEU
1	H	42	TYR
1	H	44	ASN
1	H	53	THR
1	H	113	LYS
1	H	140	TYR
1	H	334	VAL
1	H	351	LEU
1	H	434	LEU
1	I	16	LEU
1	I	42	TYR
1	I	44	ASN
1	I	45	SER
1	I	73	ILE
1	I	113	LYS
1	I	140	TYR
1	I	334	VAL
1	I	351	LEU
1	I	396	GLU
1	I	434	LEU
1	J	16	LEU
1	J	40	ASP

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Mol	Chain	Res	Type
1	J	53	THR
1	J	54	PRO
1	J	61	SER
1	J	65	GLN
1	J	73	ILE
1	J	113	LYS
1	J	137	VAL
1	J	140	TYR
1	J	141	GLU
1	J	334	VAL
1	J	414	ARG
1	J	434	LEU
1	K	4	VAL
1	K	16	LEU
1	K	40	ASP
1	K	51	LYS
1	K	53	THR
1	K	73	ILE
1	K	113	LYS
1	K	140	TYR
1	K	141	GLU
1	K	334	VAL
1	K	351	LEU
1	K	410	ILE
1	L	16	LEU
1	L	40	ASP
1	L	51	LYS
1	L	53	THR
1	L	73	ILE
1	L	105	ARG
1	L	106	ASN
1	L	113	LYS
1	L	140	TYR
1	L	334	VAL
1	L	346	LEU
1	L	363	LYS
1	L	396	GLU
1	L	414	ARG
1	M	16	LEU
1	M	40	ASP
1	M	51	LYS
1	M	53	THR

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Mol	Chain	Res	Type
1	M	73	ILE
1	M	140	TYR
1	M	334	VAL
1	M	343	ASN
1	M	346	LEU
1	M	351	LEU
1	M	434	LEU
1	N	16	LEU
1	N	40	ASP
1	N	51	LYS
1	N	53	THR
1	N	73	ILE
1	N	106	ASN
1	N	111	LEU
1	N	113	LYS
1	N	121	ASN
1	N	140	TYR
1	N	334	VAL
1	N	351	LEU
1	N	410	ILE
1	O	16	LEU
1	O	40	ASP
1	O	45	SER
1	O	51	LYS
1	O	53	THR
1	O	73	ILE
1	O	105	ARG
1	O	106	ASN
1	O	113	LYS
1	O	140	TYR
1	O	334	VAL
1	O	363	LYS
1	O	403	THR
1	O	434	LEU
2	0	20	TYR
2	0	23	ASP
2	0	174	LYS
2	0	176	ASN
3	1	127	GLN
3	1	146	MET
3	1	166	VAL
3	1	202	GLN

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Mol	Chain	Res	Type
3	1	208	ASP
3	1	259	MET
3	2	86	THR
3	2	95	MET
3	2	149	VAL
3	2	214	LEU
3	2	220	THR
3	2	272	LEU
3	3	96	LEU
3	3	133	VAL
3	3	141	LEU
3	3	149	VAL
3	3	214	LEU
4	4	1	MET
4	4	16	MET
4	4	55	LEU
4	5	45	ASN
4	5	64	LEU
4	5	72	MET
4	5	89	TYR
4	6	1	MET
4	6	7	VAL
4	6	14	LEU
4	6	42	THR
4	6	86	GLN
4	7	88	LEU
5	8	2	GLU
5	8	47	LEU
5	8	70	ARG
5	8	102	ILE
5	8	125	LEU
5	8	192	ILE
5	8	195	LEU
5	8	207	ARG
5	8	212	LEU
5	8	214	ILE
2	9	28	PHE
6	A	45	PHE
6	A	167	ASP
6	A	192	LEU
6	A	226	ASN
7	AA	342	GLN

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Mol	Chain	Res	Type
7	AB	342	GLN
7	AD	349	ILE
7	AF	346	ASP
7	AF	351	GLN
7	AF	352	ASP
7	AF	355	GLN
7	AH	342	GLN
7	AJ	349	ILE
7	AK	330	ASN
7	AK	331	MET
7	AK	332	VAL
7	AL	339	LEU
7	AN	339	LEU
7	AN	352	ASP
7	AO	330	ASN
6	B	12	LEU
6	B	42	GLU
6	B	45	PHE
6	B	104	GLN
6	B	165	GLN
6	C	31	THR
6	C	55	GLN
6	C	60	THR
6	C	109	ASP
6	C	112	ILE
6	C	259	ASN
6	C	262	LEU
6	AP	55	GLN
6	AP	106	THR
6	AP	109	ASP
6	AP	226	ASN
6	AQ	55	GLN
6	AQ	61	GLU
6	AQ	75	VAL
6	AQ	100	ASP
6	AQ	163	ARG
6	AQ	226	ASN
6	AQ	236	GLU
6	AR	28	ASN
6	AR	38	ARG
6	AR	77	THR
6	AR	180	VAL

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Mol	Chain	Res	Type
6	AR	192	LEU
6	AR	236	GLU
6	AS	77	THR
6	AS	146	ASP
6	AS	203	GLN
6	AS	219	MET
6	AS	226	ASN
6	AS	236	GLU
6	AT	28	ASN
6	AT	37	SER
6	AT	109	ASP
6	AT	192	LEU
6	AT	226	ASN
6	AT	236	GLU
6	AT	254	MET
6	AU	37	SER
6	AU	192	LEU
6	AU	226	ASN
6	AU	236	GLU
6	AV	28	ASN
6	AV	37	SER
6	AV	49	ILE
6	AV	141	ILE
6	AV	192	LEU
6	AV	226	ASN
6	AV	236	GLU
6	AW	43	ASP
6	AW	104	GLN
6	AW	151	THR
6	AW	168	ASN
6	AW	226	ASN
6	AX	43	ASP
6	AX	55	GLN
6	AX	91	ASN
6	AX	151	THR
6	AX	168	ASN
6	AX	226	ASN
6	AY	91	ASN
6	AY	104	GLN
6	AY	148	ILE
6	AY	169	GLN
6	AY	226	ASN

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Mol	Chain	Res	Type
6	AZ	1	MET
6	AZ	91	ASN
6	AZ	148	ILE
6	AZ	228	THR
6	AZ	235	ILE
6	Aa	1	MET
6	Aa	91	ASN
6	Aa	226	ASN
6	P	1	MET
6	P	9	LYS
6	P	43	ASP
6	P	55	GLN
6	P	91	ASN
6	P	203	GLN
6	P	226	ASN
6	Q	1	MET
6	Q	91	ASN
6	Q	104	GLN
6	Q	123	ASN
6	Q	151	THR
6	Q	226	ASN
6	R	43	ASP
6	R	91	ASN
6	R	104	GLN
6	R	151	THR
6	R	226	ASN
6	S	91	ASN
6	S	151	THR
6	S	166	GLN
6	S	169	GLN
6	S	226	ASN
6	T	1	MET
6	T	91	ASN
6	T	151	THR
6	T	165	GLN
6	T	168	ASN
6	T	226	ASN
6	U	1	MET
6	U	59	ASN
6	U	89	THR
6	U	151	THR
6	U	166	GLN

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Mol	Chain	Res	Type
6	U	226	ASN
6	V	1	MET
6	V	91	ASN
6	V	146	ASP
6	V	151	THR
6	V	166	GLN
6	V	226	ASN
6	W	61	GLU
6	W	91	ASN
6	W	151	THR
6	W	203	GLN
6	W	234	MET
6	W	260	GLN
6	X	1	MET
6	X	91	ASN
6	X	226	ASN
6	Y	43	ASP
6	Y	61	GLU
6	Y	91	ASN
6	Y	151	THR
6	Y	154	THR
6	Y	168	ASN
6	Y	226	ASN
6	Z	1	MET
6	Z	43	ASP
6	Z	91	ASN
6	Z	151	THR
6	Z	168	ASN
6	Z	201	ASP
6	a	16	GLN
6	a	91	ASN
6	a	180	VAL
6	a	206	VAL
6	a	210	ASP
6	a	216	ARG
6	a	226	ASN
8	b	9	LEU
8	c	6	ASP
8	c	87	ASP
8	d	4	SER
8	d	6	ASP
8	d	7	ASN

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Mol	Chain	Res	Type
8	e	6	ASP
8	e	7	ASN
8	e	88	THR
9	g	23	THR
9	g	39	LYS
9	g	53	LEU
9	g	65	VAL
9	g	134	GLN
9	h	3	LEU
9	h	34	VAL
9	h	65	VAL
9	h	67	VAL
9	i	36	SER
9	i	39	LYS
9	i	61	ASP
9	i	62	THR
9	i	67	VAL
9	i	84	ASP
9	i	113	ARG
9	i	131	ARG
9	j	53	LEU
9	j	61	ASP
9	j	65	VAL
9	j	67	VAL
9	j	126	LYS
9	k	14	MET
9	k	40	ASP
9	k	53	LEU
9	k	65	VAL
9	k	113	ARG
9	k	134	GLN
9	l	40	ASP
9	l	43	LYS
9	l	65	VAL
9	l	126	LYS
9	l	137	GLN
10	m	7	LEU
10	m	60	GLU
10	m	72	ILE
10	m	135	LEU
10	m	218	LEU
10	n	60	GLU

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Mol	Chain	Res	Type
10	n	72	ILE
10	n	158	PHE
10	n	162	ASP
10	n	200	GLN
10	n	204	ILE
10	o	72	ILE
10	o	73	THR
10	o	101	ARG
10	o	114	THR
10	o	158	PHE
10	o	229	VAL
10	p	72	ILE
10	p	135	LEU
10	q	72	ILE
10	q	73	THR
10	q	135	LEU
10	q	204	ILE
11	r	34	ASN
11	r	37	LEU
11	r	39	LYS
11	r	67	LEU
11	s	67	LEU
11	s	98	LEU
11	t	32	ASP
11	t	35	ASP
11	t	67	LEU
11	u	67	LEU
11	w	91	LEU
12	x	48	TRP
12	x	69	ARG
12	x	86	MET
3	y	86	THR
3	y	99	LEU
3	y	113	VAL
3	y	141	LEU
3	y	254	MET
3	y	261	VAL
3	y	283	LEU
3	z	86	THR
3	z	87	LEU
3	z	113	VAL
3	z	128	THR

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Mol	Chain	Res	Type
3	z	184	LEU
3	z	192	LEU
3	z	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (620) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	21	ASN
1	D	44	ASN
1	D	62	GLN
1	D	65	GLN
1	D	99	GLN
1	D	106	ASN
1	D	343	ASN
1	D	391	ASN
1	D	428	GLN
1	D	431	GLN
1	D	432	ASN
1	D	435	GLN
1	E	49	ASN
1	E	65	GLN
1	E	106	ASN
1	E	129	GLN
1	E	372	GLN
1	E	391	ASN
1	E	428	GLN
1	E	432	ASN
1	E	435	GLN
1	F	21	ASN
1	F	27	ASN
1	F	44	ASN
1	F	59	GLN
1	F	62	GLN
1	F	106	ASN
1	F	356	ASN
1	F	415	ASN
1	F	432	ASN
1	F	435	GLN
1	G	65	GLN
1	G	100	GLN
1	G	106	ASN
1	G	372	GLN

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Mol	Chain	Res	Type
1	G	391	ASN
1	G	426	HIS
1	G	428	GLN
1	G	431	GLN
1	G	432	ASN
1	G	435	GLN
1	H	49	ASN
1	H	65	GLN
1	H	100	GLN
1	H	106	ASN
1	H	129	GLN
1	H	372	GLN
1	H	391	ASN
1	H	428	GLN
1	H	432	ASN
1	H	435	GLN
1	I	25	ASN
1	I	27	ASN
1	I	44	ASN
1	I	65	GLN
1	I	99	GLN
1	I	129	GLN
1	I	372	GLN
1	I	391	ASN
1	I	426	HIS
1	I	432	ASN
1	I	435	GLN
1	J	21	ASN
1	J	27	ASN
1	J	59	GLN
1	J	62	GLN
1	J	65	GLN
1	J	99	GLN
1	J	129	GLN
1	J	340	ASN
1	J	372	GLN
1	J	383	ASN
1	J	391	ASN
1	J	432	ASN
1	J	435	GLN
1	K	21	ASN
1	K	27	ASN

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Mol	Chain	Res	Type
1	K	106	ASN
1	K	372	GLN
1	K	383	ASN
1	K	391	ASN
1	K	404	GLN
1	K	427	ASN
1	K	428	GLN
1	K	435	GLN
1	L	21	ASN
1	L	27	ASN
1	L	44	ASN
1	L	65	GLN
1	L	106	ASN
1	L	129	GLN
1	L	383	ASN
1	L	391	ASN
1	L	428	GLN
1	L	435	GLN
1	M	21	ASN
1	M	27	ASN
1	M	62	GLN
1	M	65	GLN
1	M	99	GLN
1	M	106	ASN
1	M	129	GLN
1	M	343	ASN
1	M	372	GLN
1	M	383	ASN
1	M	391	ASN
1	M	427	ASN
1	M	428	GLN
1	M	430	GLN
1	M	435	GLN
1	N	21	ASN
1	N	65	GLN
1	N	99	GLN
1	N	106	ASN
1	N	129	GLN
1	N	340	ASN
1	N	372	GLN
1	N	391	ASN
1	N	428	GLN

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Mol	Chain	Res	Type
1	N	435	GLN
1	O	21	ASN
1	O	65	GLN
1	O	99	GLN
1	O	106	ASN
1	O	391	ASN
1	O	428	GLN
1	O	435	GLN
2	0	41	ASN
2	0	118	ASN
2	0	182	ASN
3	1	88	GLN
3	1	127	GLN
3	1	228	GLN
3	2	127	GLN
3	3	186	GLN
3	3	205	ASN
4	4	47	GLN
4	4	71	GLN
4	6	47	GLN
4	6	67	HIS
4	7	39	GLN
4	7	67	HIS
5	8	90	GLN
5	8	106	GLN
5	8	182	GLN
5	8	199	ASN
5	8	211	GLN
2	9	182	ASN
6	A	15	GLN
6	A	16	GLN
6	A	28	ASN
6	A	58	GLN
6	A	104	GLN
6	A	168	ASN
6	A	190	GLN
6	A	191	ASN
6	A	217	GLN
6	A	226	ASN
7	AH	342	GLN
7	AK	330	ASN
7	AL	341	ASN

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Mol	Chain	Res	Type
7	AL	351	GLN
7	AM	341	ASN
7	AN	342	GLN
7	AO	330	ASN
7	AO	355	GLN
6	B	24	ASN
6	B	48	ASN
6	B	55	GLN
6	B	104	GLN
6	B	181	ASN
6	B	203	GLN
6	B	217	GLN
6	B	244	ASN
6	C	28	ASN
6	C	51	GLN
6	C	104	GLN
6	C	166	GLN
6	C	169	GLN
6	C	190	GLN
6	C	217	GLN
6	C	226	ASN
6	AP	15	GLN
6	AP	24	ASN
6	AP	47	GLN
6	AP	51	GLN
6	AP	87	GLN
6	AP	119	GLN
6	AP	191	ASN
6	AP	217	GLN
6	AP	259	ASN
6	AQ	16	GLN
6	AQ	24	ASN
6	AQ	51	GLN
6	AQ	58	GLN
6	AQ	81	HIS
6	AQ	104	GLN
6	AQ	165	GLN
6	AQ	168	ASN
6	AQ	191	ASN
6	AQ	203	GLN
6	AQ	217	GLN
6	AQ	226	ASN

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Mol	Chain	Res	Type
6	AR	2	HIS
6	AR	16	GLN
6	AR	24	ASN
6	AR	87	GLN
6	AR	104	GLN
6	AR	165	GLN
6	AR	190	GLN
6	AR	191	ASN
6	AR	203	GLN
6	AR	217	GLN
6	AR	226	ASN
6	AR	260	GLN
6	AS	2	HIS
6	AS	16	GLN
6	AS	24	ASN
6	AS	25	ASN
6	AS	50	ASN
6	AS	87	GLN
6	AS	104	GLN
6	AS	165	GLN
6	AS	168	ASN
6	AS	203	GLN
6	AS	217	GLN
6	AS	260	GLN
6	AT	16	GLN
6	AT	24	ASN
6	AT	47	GLN
6	AT	51	GLN
6	AT	87	GLN
6	AT	104	GLN
6	AT	165	GLN
6	AT	191	ASN
6	AT	217	GLN
6	AT	226	ASN
6	AU	16	GLN
6	AU	24	ASN
6	AU	87	GLN
6	AU	104	GLN
6	AU	165	GLN
6	AU	190	GLN
6	AU	191	ASN
6	AU	217	GLN

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Mol	Chain	Res	Type
6	AU	226	ASN
6	AU	260	GLN
6	AV	2	HIS
6	AV	16	GLN
6	AV	24	ASN
6	AV	25	ASN
6	AV	47	GLN
6	AV	87	GLN
6	AV	104	GLN
6	AV	119	GLN
6	AV	165	GLN
6	AV	168	ASN
6	AV	217	GLN
6	AV	260	GLN
6	AW	16	GLN
6	AW	18	ASN
6	AW	24	ASN
6	AW	28	ASN
6	AW	47	GLN
6	AW	51	GLN
6	AW	87	GLN
6	AW	91	ASN
6	AW	104	GLN
6	AW	123	ASN
6	AW	165	GLN
6	AW	166	GLN
6	AW	169	GLN
6	AW	191	ASN
6	AW	217	GLN
6	AW	226	ASN
6	AW	260	GLN
6	AW	261	GLN
6	AX	2	HIS
6	AX	24	ASN
6	AX	28	ASN
6	AX	47	GLN
6	AX	51	GLN
6	AX	87	GLN
6	AX	91	ASN
6	AX	111	ASN
6	AX	166	GLN
6	AX	191	ASN

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Mol	Chain	Res	Type
6	AX	217	GLN
6	AX	260	GLN
6	AX	261	GLN
6	AY	15	GLN
6	AY	16	GLN
6	AY	18	ASN
6	AY	47	GLN
6	AY	50	ASN
6	AY	51	GLN
6	AY	58	GLN
6	AY	78	GLN
6	AY	91	ASN
6	AY	111	ASN
6	AY	123	ASN
6	AY	165	GLN
6	AY	166	GLN
6	AY	169	GLN
6	AY	190	GLN
6	AY	217	GLN
6	AY	226	ASN
6	AY	260	GLN
6	AY	261	GLN
6	AZ	15	GLN
6	AZ	16	GLN
6	AZ	18	ASN
6	AZ	24	ASN
6	AZ	47	GLN
6	AZ	51	GLN
6	AZ	58	GLN
6	AZ	91	ASN
6	AZ	104	GLN
6	AZ	111	ASN
6	AZ	119	GLN
6	AZ	123	ASN
6	AZ	169	GLN
6	AZ	190	GLN
6	AZ	203	GLN
6	AZ	217	GLN
6	AZ	226	ASN
6	AZ	260	GLN
6	AZ	261	GLN
6	Aa	15	GLN

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Mol	Chain	Res	Type
6	Aa	16	GLN
6	Aa	18	ASN
6	Aa	28	ASN
6	Aa	47	GLN
6	Aa	51	GLN
6	Aa	58	GLN
6	Aa	91	ASN
6	Aa	104	GLN
6	Aa	111	ASN
6	Aa	165	GLN
6	Aa	166	GLN
6	Aa	168	ASN
6	Aa	169	GLN
6	Aa	190	GLN
6	Aa	191	ASN
6	Aa	217	GLN
6	Aa	226	ASN
6	Aa	260	GLN
6	Aa	261	GLN
6	P	16	GLN
6	P	18	ASN
6	P	24	ASN
6	P	47	GLN
6	P	50	ASN
6	P	51	GLN
6	P	91	ASN
6	P	111	ASN
6	P	119	GLN
6	P	165	GLN
6	P	166	GLN
6	P	181	ASN
6	P	191	ASN
6	P	217	GLN
6	P	226	ASN
6	P	260	GLN
6	P	261	GLN
6	Q	16	GLN
6	Q	18	ASN
6	Q	24	ASN
6	Q	47	GLN
6	Q	51	GLN
6	Q	58	GLN

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Mol	Chain	Res	Type
6	Q	78	GLN
6	Q	83	HIS
6	Q	91	ASN
6	Q	119	GLN
6	Q	123	ASN
6	Q	165	GLN
6	Q	166	GLN
6	Q	190	GLN
6	Q	191	ASN
6	Q	217	GLN
6	Q	226	ASN
6	Q	260	GLN
6	R	18	ASN
6	R	24	ASN
6	R	28	ASN
6	R	47	GLN
6	R	51	GLN
6	R	58	GLN
6	R	87	GLN
6	R	91	ASN
6	R	119	GLN
6	R	165	GLN
6	R	166	GLN
6	R	168	ASN
6	R	169	GLN
6	R	217	GLN
6	R	260	GLN
6	R	261	GLN
6	S	24	ASN
6	S	28	ASN
6	S	47	GLN
6	S	51	GLN
6	S	58	GLN
6	S	83	HIS
6	S	87	GLN
6	S	91	ASN
6	S	165	GLN
6	S	166	GLN
6	S	168	ASN
6	S	203	GLN
6	S	217	GLN
6	S	226	ASN

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Mol	Chain	Res	Type
6	S	259	ASN
6	S	260	GLN
6	T	18	ASN
6	T	24	ASN
6	T	28	ASN
6	T	47	GLN
6	T	50	ASN
6	T	51	GLN
6	T	59	ASN
6	T	83	HIS
6	T	91	ASN
6	T	104	GLN
6	T	165	GLN
6	T	166	GLN
6	T	168	ASN
6	T	169	GLN
6	T	191	ASN
6	T	203	GLN
6	T	217	GLN
6	T	226	ASN
6	T	260	GLN
6	T	261	GLN
6	U	24	ASN
6	U	28	ASN
6	U	47	GLN
6	U	51	GLN
6	U	78	GLN
6	U	104	GLN
6	U	119	GLN
6	U	165	GLN
6	U	166	GLN
6	U	169	GLN
6	U	217	GLN
6	U	226	ASN
6	U	260	GLN
6	U	261	GLN
6	V	24	ASN
6	V	28	ASN
6	V	47	GLN
6	V	48	ASN
6	V	58	GLN
6	V	85	ASN

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Mol	Chain	Res	Type
6	V	87	GLN
6	V	91	ASN
6	V	119	GLN
6	V	165	GLN
6	V	168	ASN
6	V	169	GLN
6	V	191	ASN
6	V	203	GLN
6	V	217	GLN
6	V	226	ASN
6	V	260	GLN
6	V	261	GLN
6	W	16	GLN
6	W	24	ASN
6	W	28	ASN
6	W	47	GLN
6	W	59	ASN
6	W	91	ASN
6	W	104	GLN
6	W	119	GLN
6	W	168	ASN
6	W	169	GLN
6	W	181	ASN
6	W	191	ASN
6	W	217	GLN
6	W	260	GLN
6	W	261	GLN
6	X	18	ASN
6	X	24	ASN
6	X	28	ASN
6	X	47	GLN
6	X	50	ASN
6	X	51	GLN
6	X	55	GLN
6	X	85	ASN
6	X	91	ASN
6	X	119	GLN
6	X	165	GLN
6	X	166	GLN
6	X	169	GLN
6	X	203	GLN
6	X	217	GLN

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Mol	Chain	Res	Type
6	X	226	ASN
6	X	260	GLN
6	X	261	GLN
6	Y	24	ASN
6	Y	28	ASN
6	Y	47	GLN
6	Y	51	GLN
6	Y	58	GLN
6	Y	87	GLN
6	Y	91	ASN
6	Y	165	GLN
6	Y	168	ASN
6	Y	169	GLN
6	Y	191	ASN
6	Y	217	GLN
6	Y	226	ASN
6	Y	260	GLN
6	Z	18	ASN
6	Z	24	ASN
6	Z	28	ASN
6	Z	47	GLN
6	Z	50	ASN
6	Z	51	GLN
6	Z	58	GLN
6	Z	91	ASN
6	Z	165	GLN
6	Z	166	GLN
6	Z	168	ASN
6	Z	169	GLN
6	Z	190	GLN
6	Z	217	GLN
6	Z	226	ASN
6	Z	260	GLN
6	Z	261	GLN
6	a	16	GLN
6	a	18	ASN
6	a	24	ASN
6	a	28	ASN
6	a	47	GLN
6	a	50	ASN
6	a	51	GLN
6	a	59	ASN

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Mol	Chain	Res	Type
6	a	87	GLN
6	a	91	ASN
6	a	119	GLN
6	a	165	GLN
6	a	168	ASN
6	a	169	GLN
6	a	217	GLN
6	a	226	ASN
6	a	260	GLN
8	b	50	GLN
8	c	32	GLN
8	c	106	ASN
8	c	110	HIS
8	d	14	HIS
8	d	105	GLN
8	d	106	ASN
8	d	107	GLN
8	d	110	HIS
8	e	85	GLN
8	e	101	ASN
8	e	107	GLN
8	e	110	HIS
8	f	14	HIS
8	f	34	ASN
8	f	50	GLN
8	f	107	GLN
8	f	110	HIS
9	g	100	ASN
9	g	118	ASN
9	g	134	GLN
9	h	127	GLN
9	i	22	ASN
9	i	46	HIS
9	i	100	ASN
9	i	118	ASN
9	j	22	ASN
9	j	118	ASN
9	k	22	ASN
9	k	100	ASN
9	k	120	GLN
9	l	22	ASN
9	l	100	ASN

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Mol	Chain	Res	Type
9	l	120	GLN
10	m	24	ASN
10	m	179	ASN
10	m	200	GLN
10	m	228	GLN
10	n	15	ASN
10	n	24	ASN
10	n	102	ASN
10	n	188	ASN
10	n	200	GLN
10	o	14	GLN
10	o	40	GLN
10	o	102	ASN
10	o	200	GLN
10	o	222	GLN
10	p	17	GLN
10	p	119	HIS
10	p	200	GLN
10	p	228	GLN
10	q	15	ASN
10	q	20	GLN
10	q	40	GLN
10	q	102	ASN
10	q	200	GLN
11	r	42	ASN
11	r	86	GLN
11	s	45	ASN
11	s	86	GLN
11	s	89	ASN
11	t	45	ASN
11	t	75	ASN
11	t	86	GLN
11	u	86	GLN
11	v	55	GLN
11	v	75	ASN
3	y	186	GLN
3	z	126	GLN
3	z	127	GLN
3	z	165	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

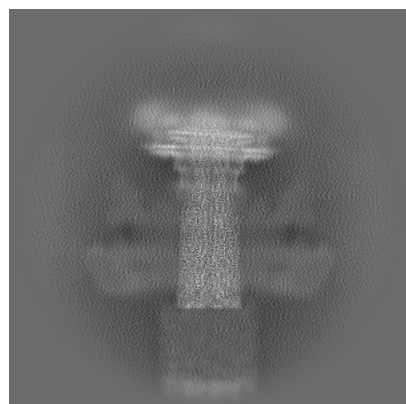
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39782. These allow visual inspection of the internal detail of the map and identification of artifacts.

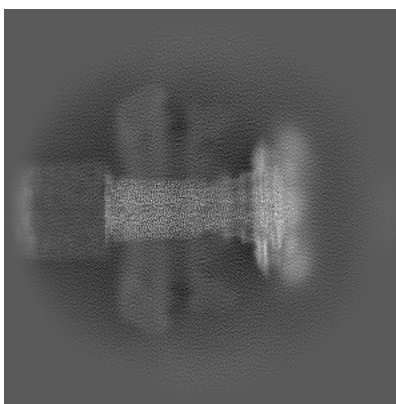
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

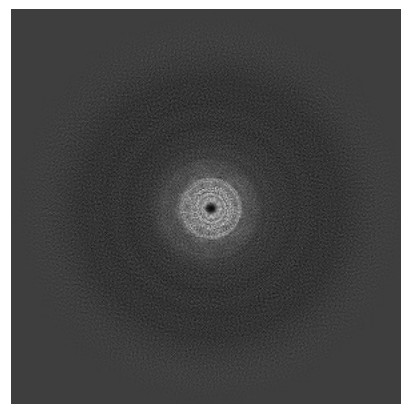
6.1.1 Primary map



X

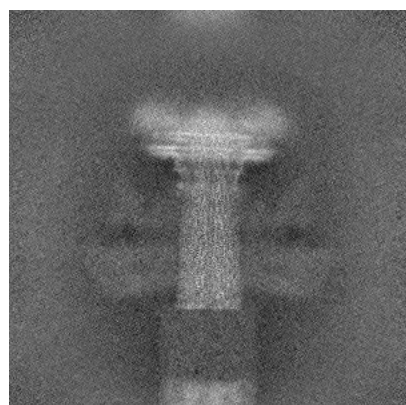


Y

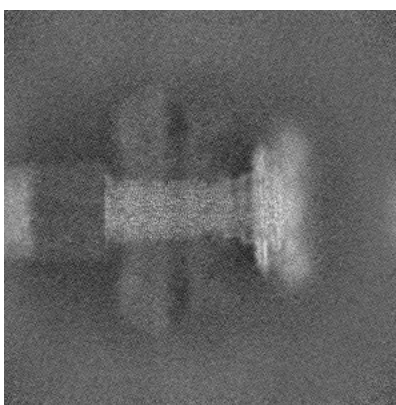


Z

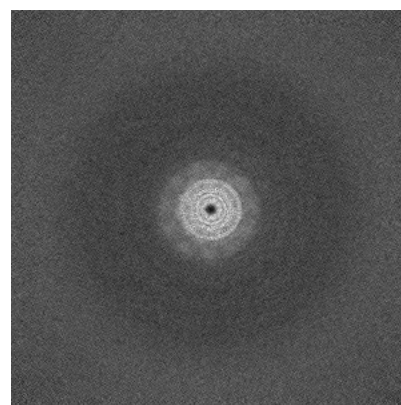
6.1.2 Raw map



X



Y

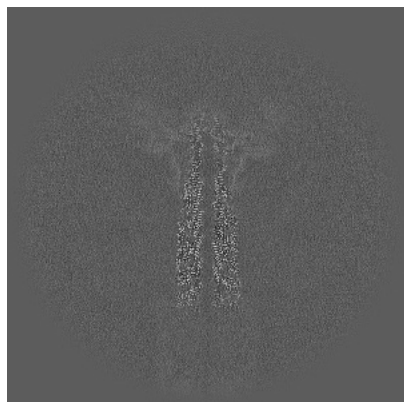


Z

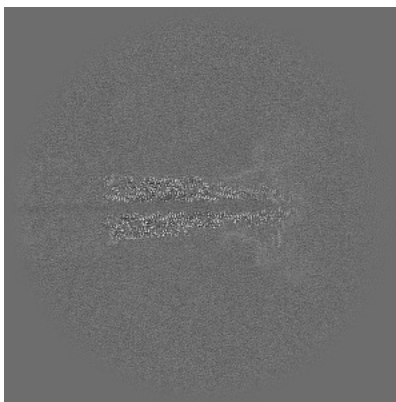
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

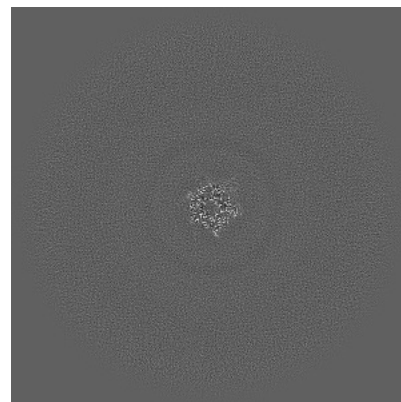
6.2.1 Primary map



X Index: 310



Y Index: 310

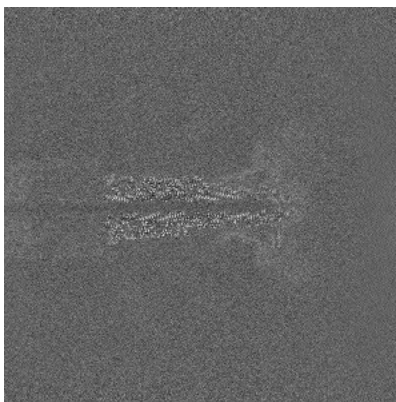


Z Index: 310

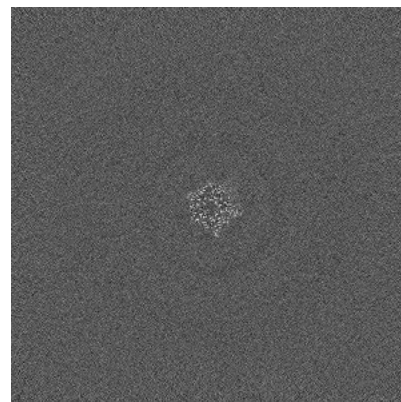
6.2.2 Raw map



X Index: 310



Y Index: 310

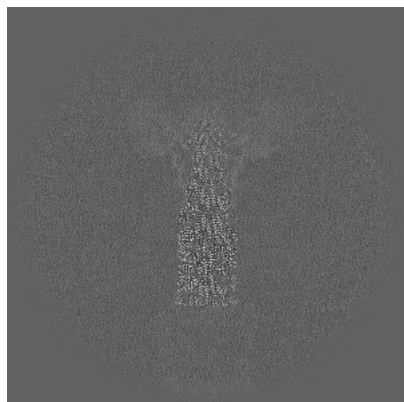


Z Index: 310

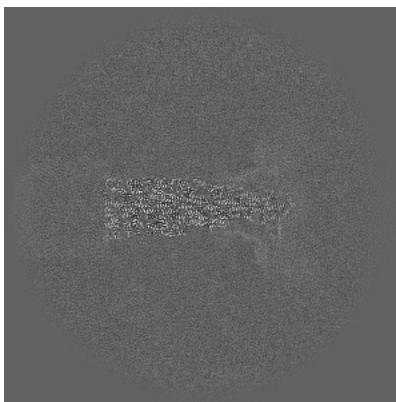
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

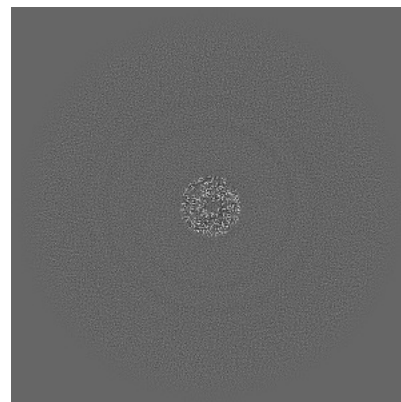
6.3.1 Primary map



X Index: 323

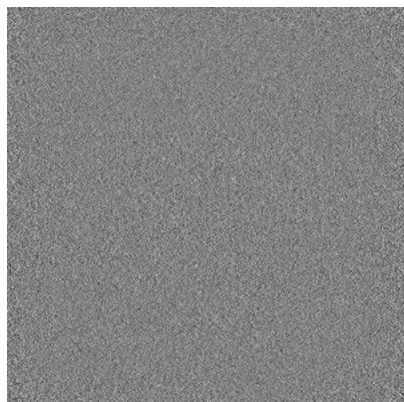


Y Index: 296

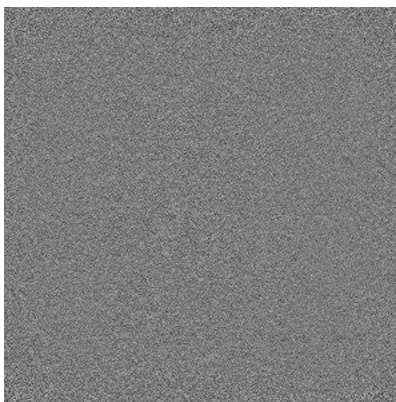


Z Index: 255

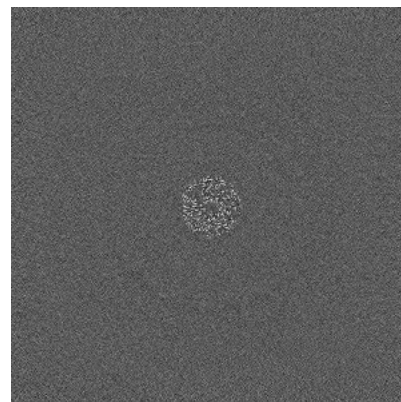
6.3.2 Raw map



X Index: 0



Y Index: 0

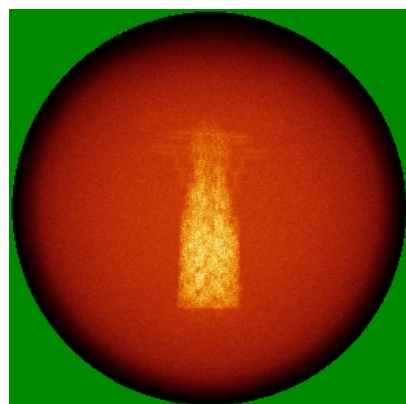


Z Index: 253

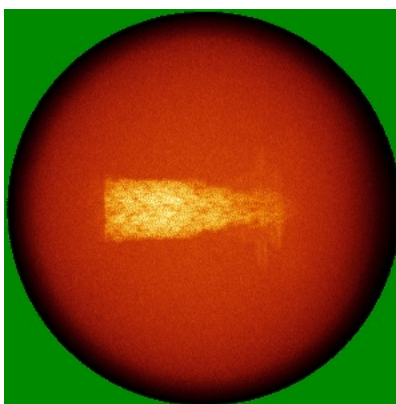
The images above show the largest variance slices of the map in three orthogonal directions.

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

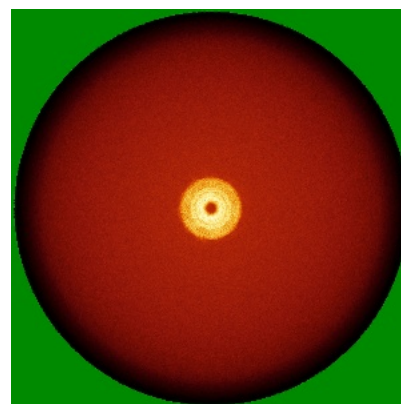
6.4.1 Primary map



X

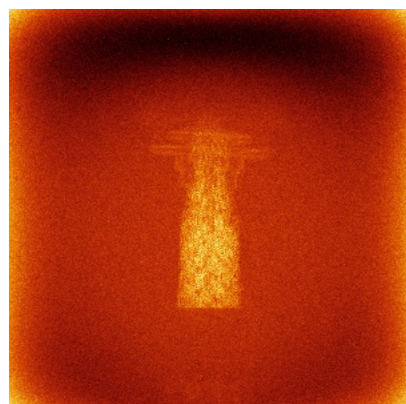


Y

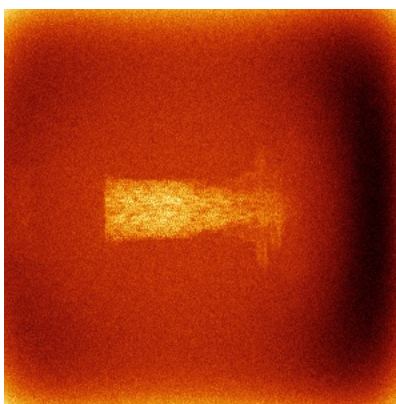


Z

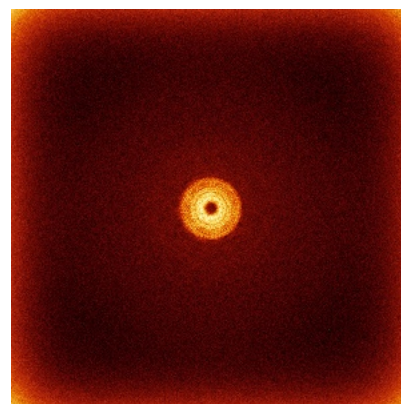
6.4.2 Raw map



X



Y

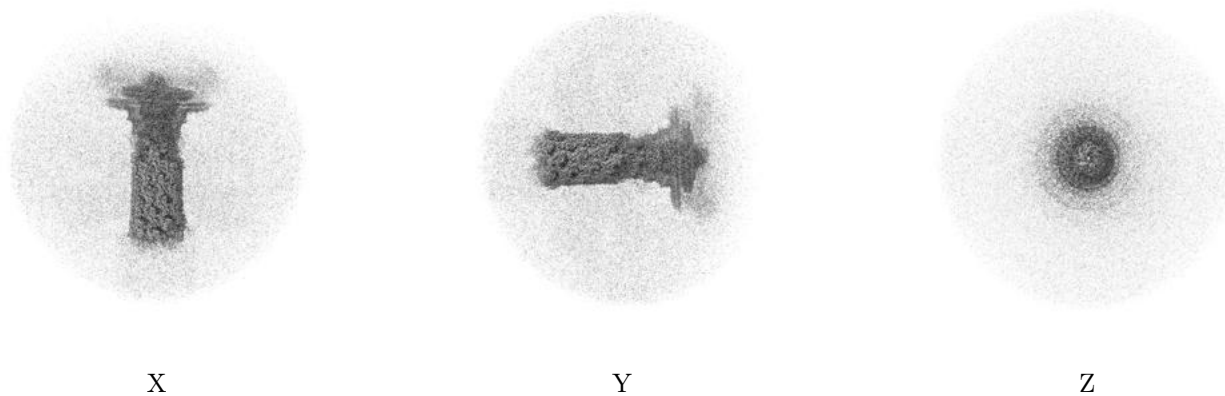


Z

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.

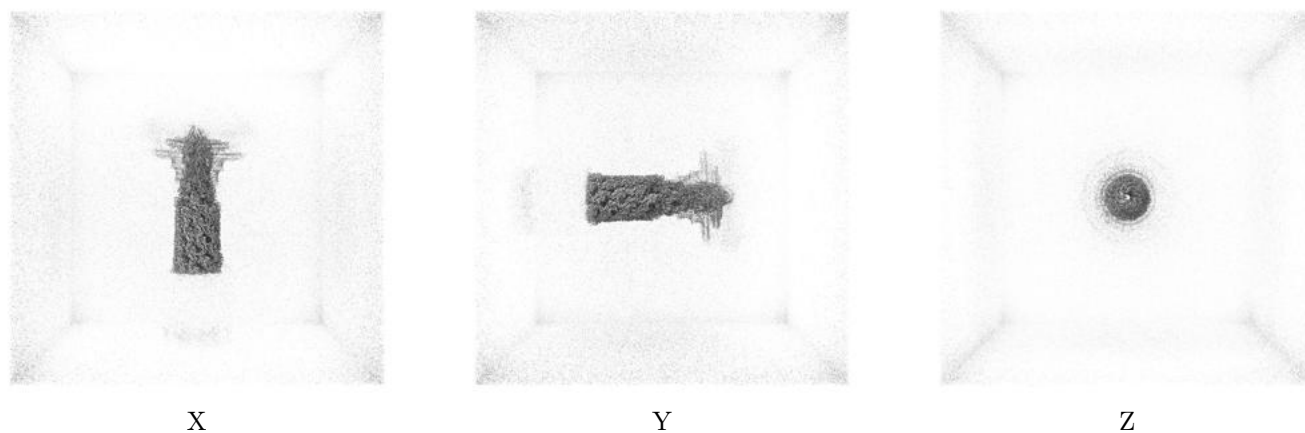
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.42. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

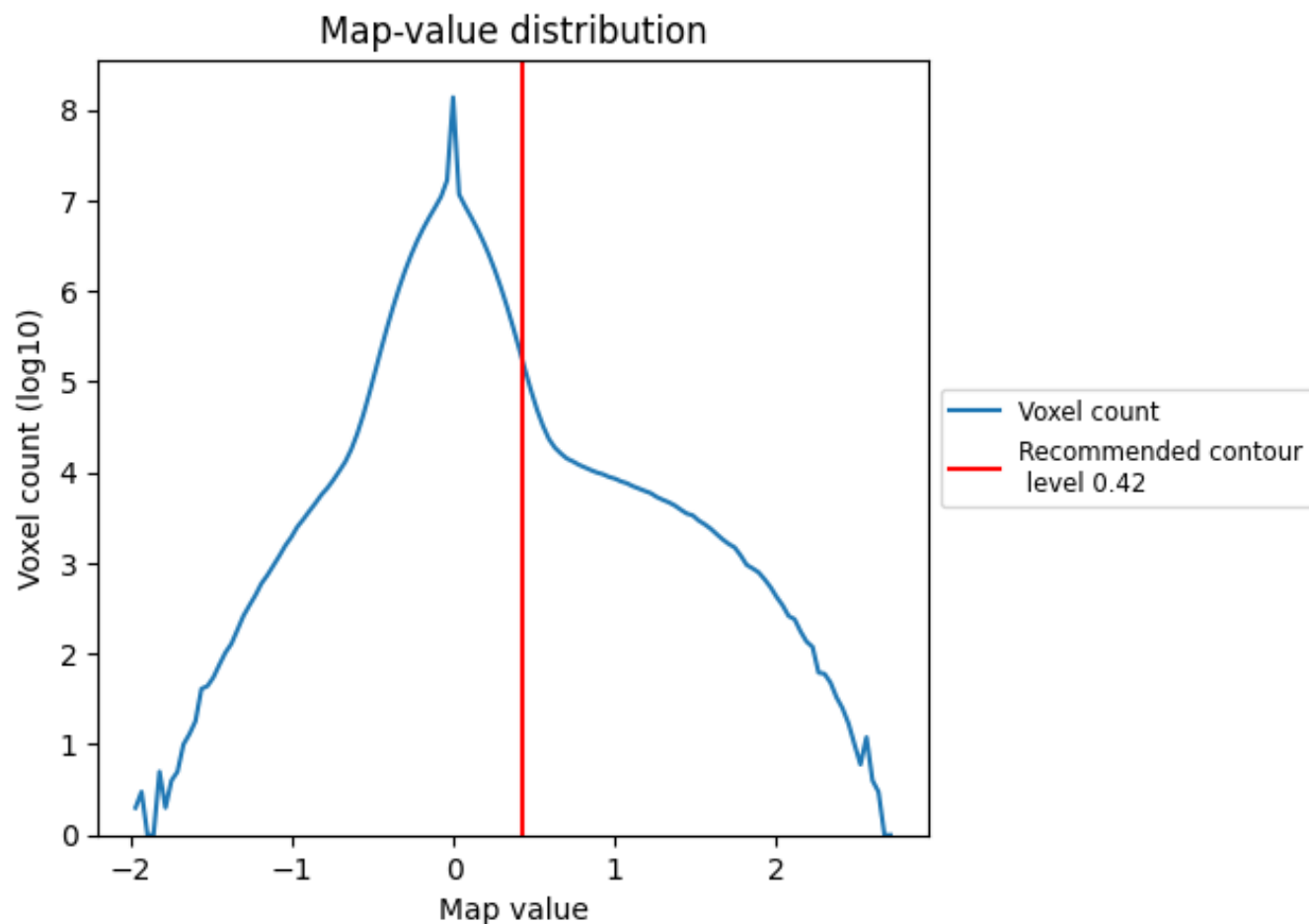
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

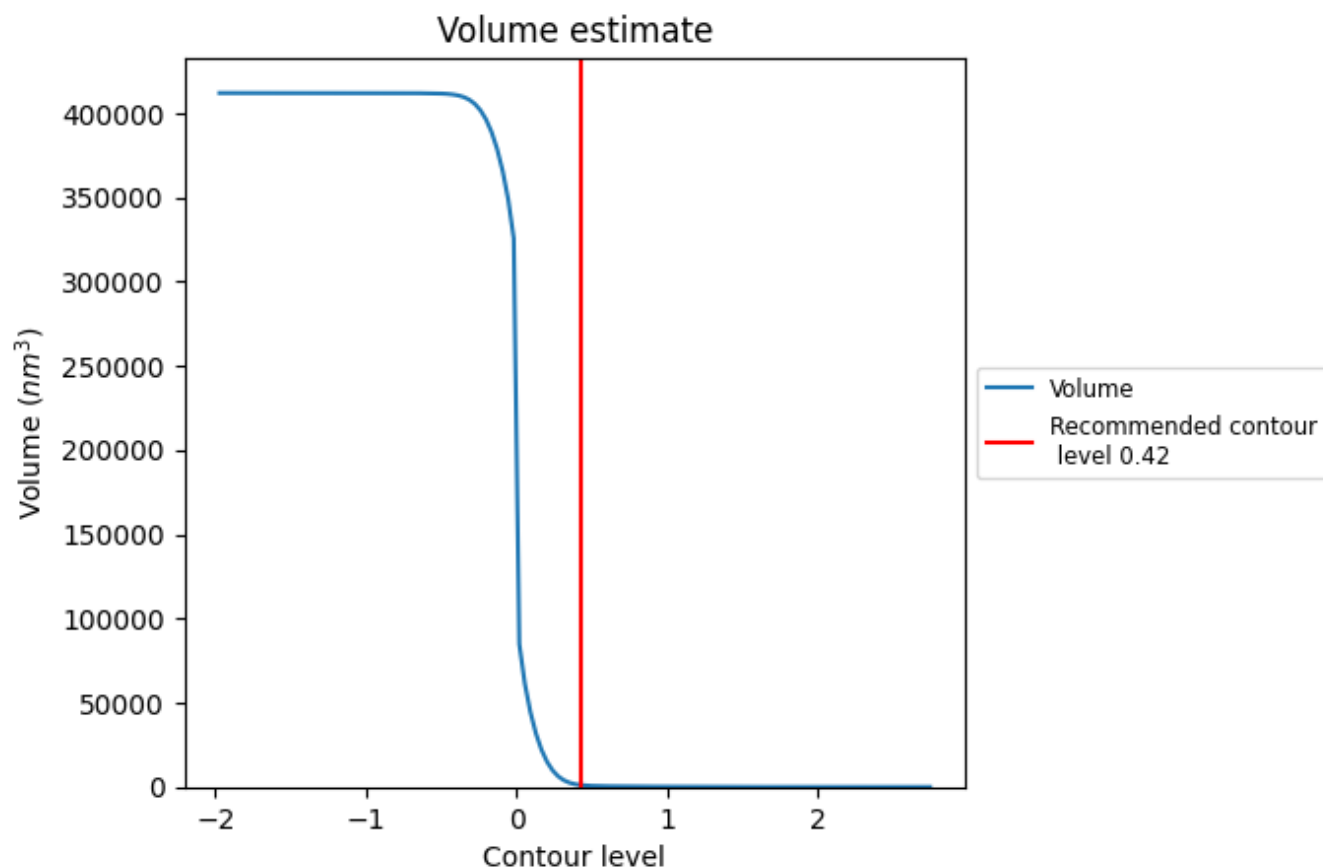
This section contains the results of statistical analysis of the map.

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.

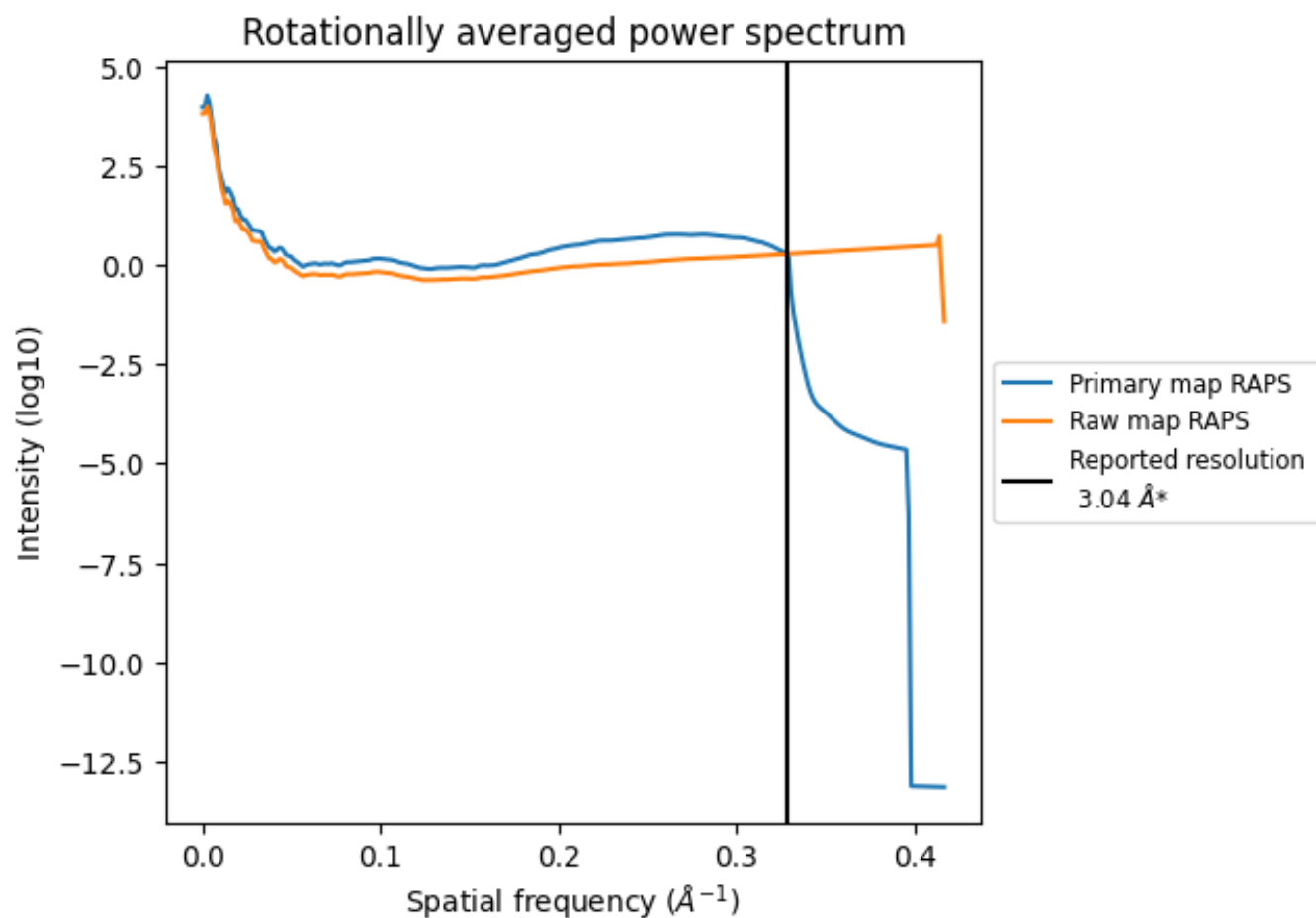
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1170 nm³; this corresponds to an approximate mass of 1057 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 ⓘ

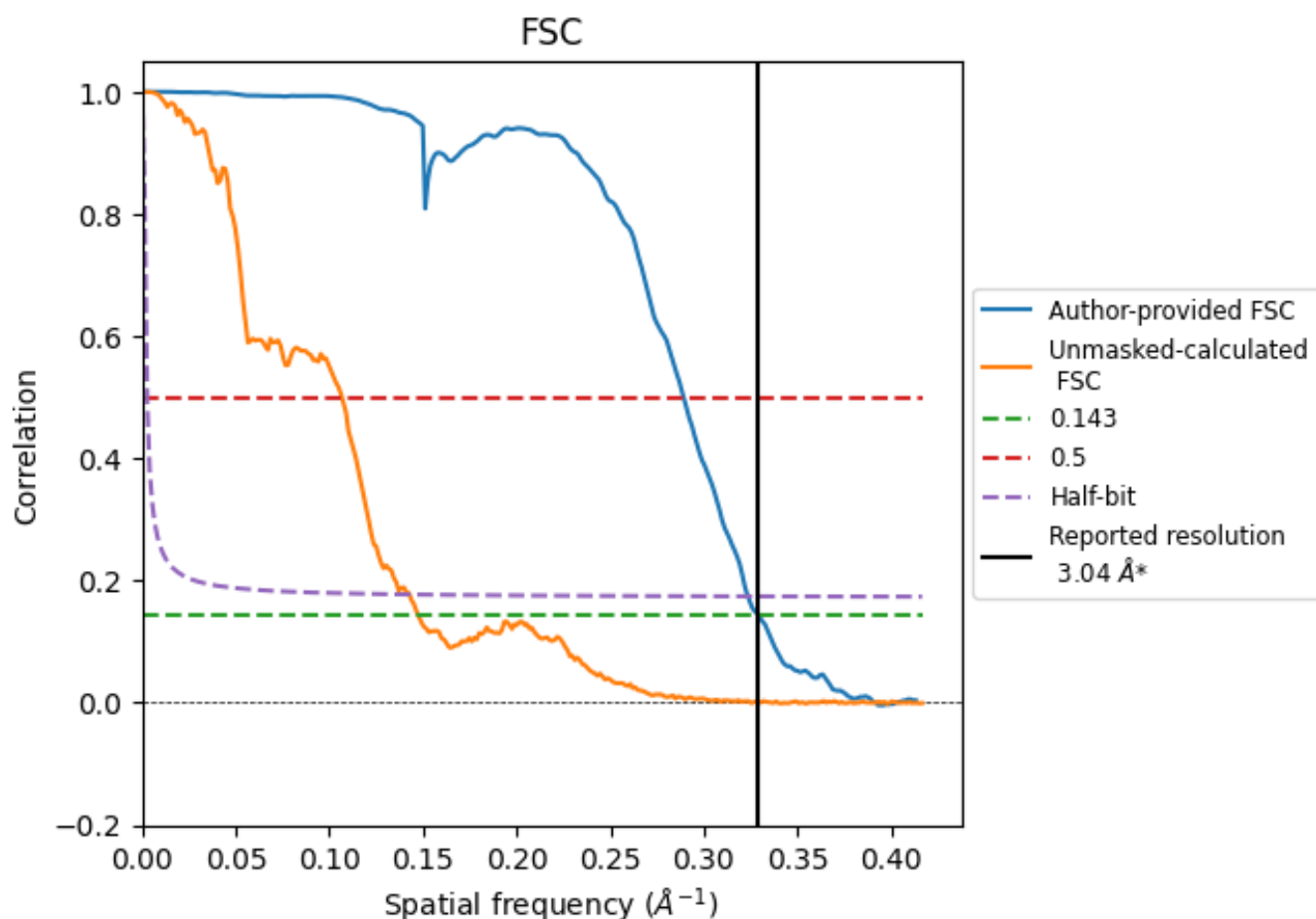


*Reported resolution corresponds to spatial frequency of 0.329 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.329 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

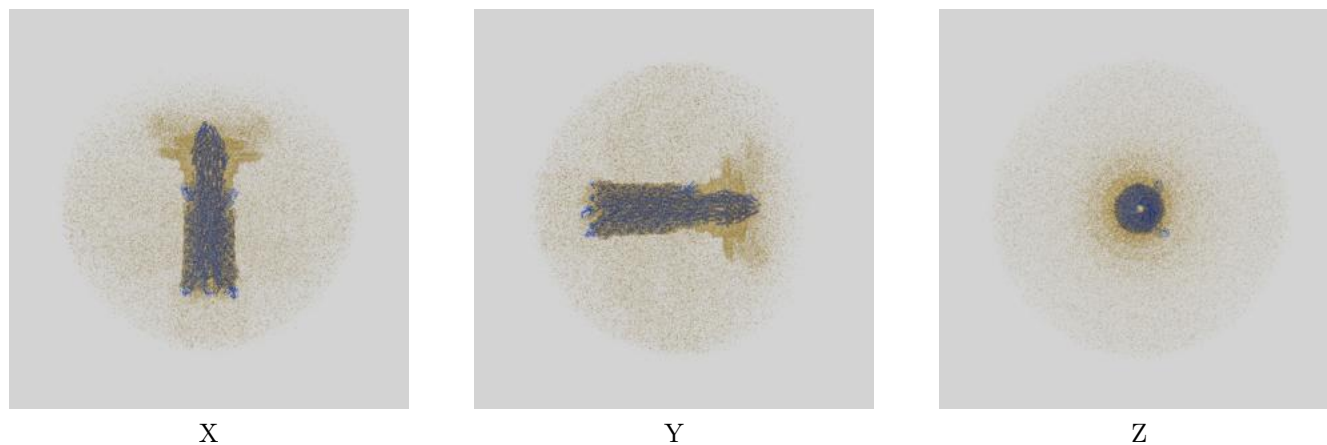
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.46	3.09
Unmasked-calculated*	6.78	9.37	7.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.78 differs from the reported value 3.04 by more than 10 %

9 Map-model fit [i](#)

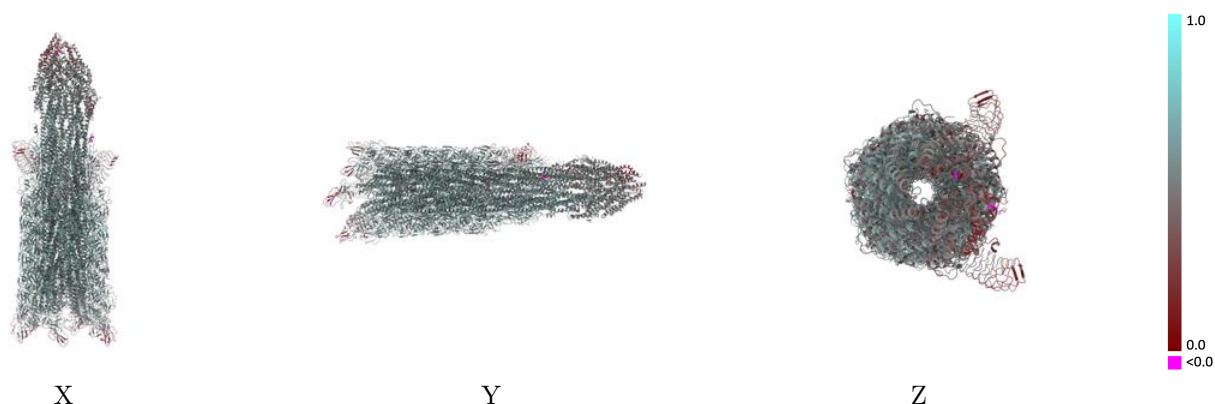
This section contains information regarding the fit between EMDB map EMD-39782 and PDB model 8Z5U. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



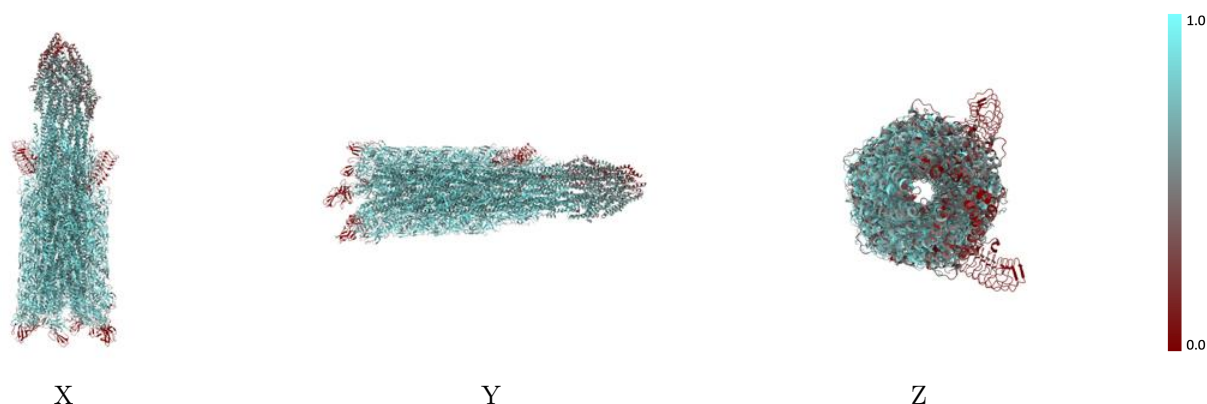
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



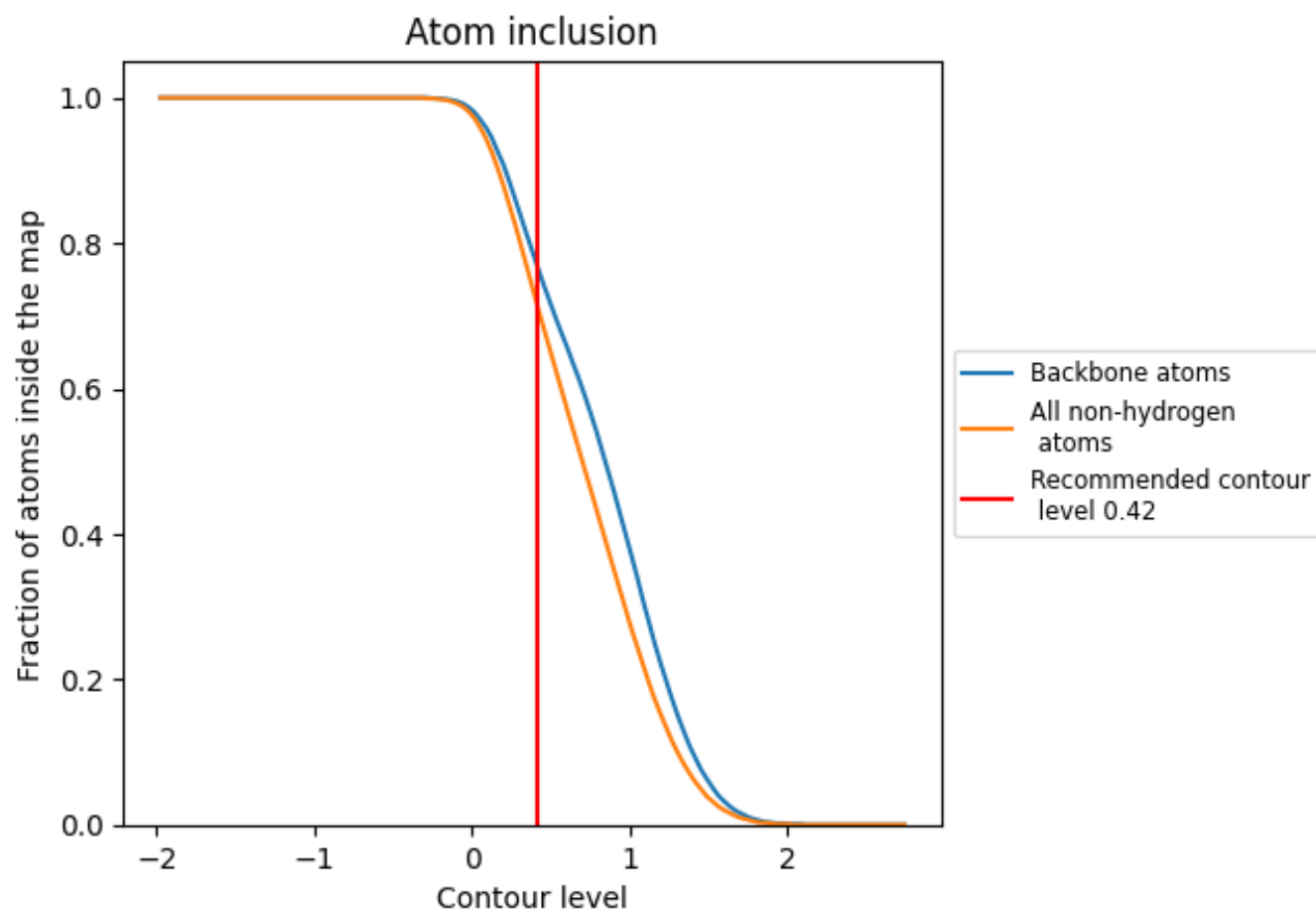
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.42).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 71% 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 (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7110	 0.5330
0	 0.0790	 0.3420
1	 0.5180	 0.4720
2	 0.6340	 0.5060
3	 0.5580	 0.4790
4	 0.4360	 0.4260
5	 0.5180	 0.4410
6	 0.4560	 0.4420
7	 0.5320	 0.4750
8	 0.4870	 0.4550
9	 0.1120	 0.3640
A	 0.7890	 0.5650
AA	 0.6890	 0.5130
AB	 0.7190	 0.5490
AC	 0.6980	 0.5370
AD	 0.7630	 0.5690
AE	 0.6000	 0.5200
AF	 0.3800	 0.4110
AG	 0.7260	 0.5260
AH	 0.7810	 0.5510
AI	 0.6300	 0.4960
AJ	 0.2940	 0.3850
AK	 0.6800	 0.5320
AL	 0.6450	 0.4940
AM	 0.7100	 0.5130
AN	 0.7190	 0.5280
AO	 0.7360	 0.5420
AP	 0.7920	 0.5630
AQ	 0.7710	 0.5530
AR	 0.8010	 0.5660
AS	 0.8160	 0.5580
AT	 0.8140	 0.5770
AU	 0.8130	 0.5760
AV	 0.8050	 0.5640
AW	 0.8070	 0.5630



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Chain	Atom inclusion	Q-score
AX	 0.8030	 0.5690
AY	 0.7490	 0.5490
AZ	 0.7880	 0.5610
Aa	 0.8040	 0.5720
B	 0.7900	 0.5720
C	 0.8060	 0.5760
D	 0.3880	 0.4380
E	 0.4520	 0.4520
F	 0.5360	 0.4880
G	 0.6060	 0.5080
H	 0.6390	 0.5000
I	 0.6600	 0.5000
J	 0.7110	 0.5230
K	 0.7270	 0.5320
L	 0.7560	 0.5430
M	 0.7650	 0.5460
N	 0.7370	 0.5190
O	 0.7520	 0.5470
P	 0.7930	 0.5560
Q	 0.7920	 0.5550
R	 0.8210	 0.5860
S	 0.7900	 0.5560
T	 0.8010	 0.5650
U	 0.8190	 0.5770
V	 0.8100	 0.5760
W	 0.7940	 0.5580
X	 0.7860	 0.5510
Y	 0.8050	 0.5630
Z	 0.8050	 0.5720
a	 0.8110	 0.5660
b	 0.7510	 0.5550
c	 0.7250	 0.5180
d	 0.7800	 0.5620
e	 0.7850	 0.5630
f	 0.7970	 0.5680
g	 0.7560	 0.5330
h	 0.7910	 0.5530
i	 0.7410	 0.5310
j	 0.8040	 0.5650
k	 0.7940	 0.5670
l	 0.7830	 0.5580
m	 0.8010	 0.5660

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Chain	Atom inclusion	Q-score
n	 0.7290	 0.5340
o	 0.7780	 0.5600
p	 0.7900	 0.5640
q	 0.7450	 0.5390
r	 0.7170	 0.5410
s	 0.6110	 0.4990
t	 0.6560	 0.5060
u	 0.7150	 0.5370
v	 0.6860	 0.5340
w	 0.6830	 0.5240
x	 0.1910	 0.2950
y	 0.6510	 0.5070
z	 0.6720	 0.5190