



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 09:05 PM UTC

PDB ID : 7E82 / pdb_00007e82
EMDB ID : EMD-31008
Title : Cryo-EM structure of the flagellar rod with partial hook from Salmonella
Authors : Tan, J.X.; Chang, S.H.; Wang, X.F.; Xu, C.H.; Zhou, Y.; Zhang, X.; Zhu, Y.Q.
Deposited on : 2021-02-28
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

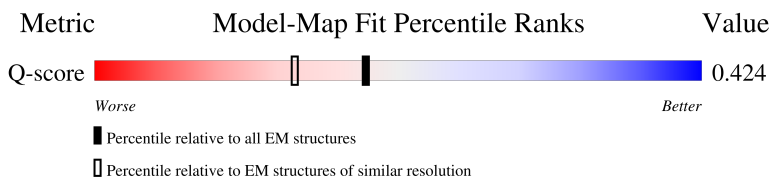
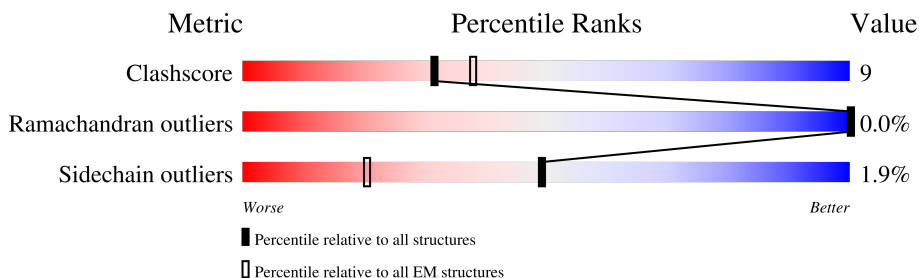
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	260	13% 77% 23%
1	B	260	24% 74% 25%
1	C	260	14% 77% 22%
1	D	260	12% 75% 25%

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Mol	Chain	Length	Quality of chain
1	E	260	12% 74% 25% .
1	F	260	11% 75% 24% .
1	G	260	11% 74% 25% .
1	H	260	10% 77% 23% .
1	I	260	8% 79% 20% .
1	J	260	9% 79% 19% .
1	K	260	8% 81% 18% .
1	L	260	8% 78% 21% .
1	M	260	10% 83% 17% .
1	N	260	7% 76% 20% .
1	O	260	11% 76% 20% ..
1	P	260	8% 76% 20% 5%
1	Q	260	8% 77% 17% 5%
1	R	260	9% 76% 19% ..
1	S	260	9% 75% 19% 5%
1	T	260	8% 78% 19% .
1	U	260	8% 78% 21% .
1	V	260	8% 75% 24% .
1	W	260	11% 78% 20% .
1	X	260	18% 82% 18% .
2	a	251	10% 77% 22% .
2	b	251	25% 74% 24% ..
2	c	251	11% 75% 24% .
2	d	251	13% 79% 19% ..
2	e	251	27% 80% 19% .

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Mol	Chain	Length	Quality of chain
3	0	15	40% 100%
3	1	15	67% 87% 13%
3	2	15	33% 87% 13%
3	3	15	40% 93% 7%
3	4	15	60% 80% 20%
4	5	21	14% 90% 10%
4	6	21	86% 95% 5%
4	7	21	14% 81% 19%
4	8	21	38% 90% 10%
4	9	21	86% 86% 14%
5	f	134	13% 67% 28% .
5	g	134	30% 66% 28% ..
5	h	134	7% 65% 29% ..
5	i	134	11% 76% 20% .
5	j	134	13% 75% 19% 5%
5	p	134	31% 72% 24% .
6	k	138	14% 62% 17% 22%
6	l	138	22% 61% 15% 23%
6	m	138	16% 54% 22% 23%
6	n	138	20% 57% 20% 22%
6	o	138	40% 62% 17% 21%
7	q	104	30% 60% 9% 32%
7	r	104	37% 56% 12% 33%
7	s	104	28% 63% 6% 31%
7	t	104	25% 62% 8% 31%

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Mol	Chain	Length	Quality of chain
7	u	104	
7	v	104	
8	DA	403	
8	DB	403	
8	DC	403	
8	DD	403	
8	DE	403	
8	DF	403	
8	DG	403	
8	DH	403	
8	DI	403	
8	DJ	403	
8	DK	403	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 101606 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 basal-body rod protein FlgG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	B	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	C	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	D	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	E	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	F	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	G	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	H	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	I	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	J	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	K	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	L	259	Total 1941	C 1197	N 340	O 399	S 5	0	0
1	M	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	N	251	Total 1887	C 1167	N 330	O 384	S 6	0	0
1	O	252	Total 1894	C 1172	N 331	O 385	S 6	0	0
1	P	248	Total 1862	C 1151	N 327	O 379	S 5	0	0
1	Q	247	Total 1858	C 1149	N 326	O 378	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	250	Total	C	N	O	S	0	0
			1875	1159	329	382	5		
1	S	247	Total	C	N	O	S	0	0
			1858	1149	326	378	5		
1	T	253	Total	C	N	O	S	0	0
			1902	1176	333	388	5		
1	U	259	Total	C	N	O	S	0	0
			1941	1197	340	399	5		
1	V	259	Total	C	N	O	S	0	0
			1941	1197	340	399	5		
1	W	259	Total	C	N	O	S	0	0
			1941	1197	340	399	5		
1	X	259	Total	C	N	O	S	0	0
			1941	1197	340	399	5		

- Molecule 2 is a protein called Flagellar basal-body rod protein FlgF.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
2	b	248	Total	C	N	O	S	0	0
			1804	1106	324	367	7		
2	c	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
2	d	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
2	e	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		

- Molecule 3 is a protein called Flagellar MS ring L2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	0	15	Total	C	N	O	0	0
			75	45	15	15		
3	1	15	Total	C	N	O	0	0
			75	45	15	15		
3	2	15	Total	C	N	O	0	0
			75	45	15	15		
3	3	15	Total	C	N	O	0	0
			75	45	15	15		
3	4	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 4 is a protein called Flagellar MS ring L1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	5	21	Total	C	N	O	0	0
			140	88	24	28		
4	6	21	Total	C	N	O	0	0
			140	88	24	28		
4	7	21	Total	C	N	O	0	0
			140	88	24	28		
4	9	21	Total	C	N	O	0	0
			140	88	24	28		
4	8	21	Total	C	N	O	0	0
			140	88	24	28		

- Molecule 5 is a protein called Flagellar basal-body rod protein FlgC.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	128	Total	C	N	O	S	0	0
			936	585	160	186	5		
5	g	130	Total	C	N	O	S	0	0
			949	592	163	189	5		
5	h	128	Total	C	N	O	S	0	0
			935	584	160	186	5		
5	j	127	Total	C	N	O	S	0	0
			931	582	159	185	5		
5	p	129	Total	C	N	O	S	0	0
			940	587	161	187	5		
5	i	129	Total	C	N	O	S	0	0
			944	589	162	188	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	l	106	Total	C	N	O	S	0	0
			833	515	150	163	5		
6	m	106	Total	C	N	O	S	0	0
			833	515	150	163	5		
6	o	109	Total	C	N	O	S	0	0
			856	529	156	166	5		
6	k	108	Total	C	N	O	S	0	0
			852	527	155	165	5		
6	n	107	Total	C	N	O	S	0	0
			844	521	154	164	5		

- Molecule 7 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	71	Total	C	N	O	S	0	0
			536	330	98	102	6		
7	r	70	Total	C	N	O	S	0	0
			526	323	97	100	6		
7	s	72	Total	C	N	O	S	0	0
			543	335	99	103	6		
7	t	72	Total	C	N	O	S	0	0
			543	335	99	103	6		
7	u	72	Total	C	N	O	S	0	0
			543	335	99	103	6		
7	v	38	Total	C	N	O	S	0	0
			289	178	50	55	6		

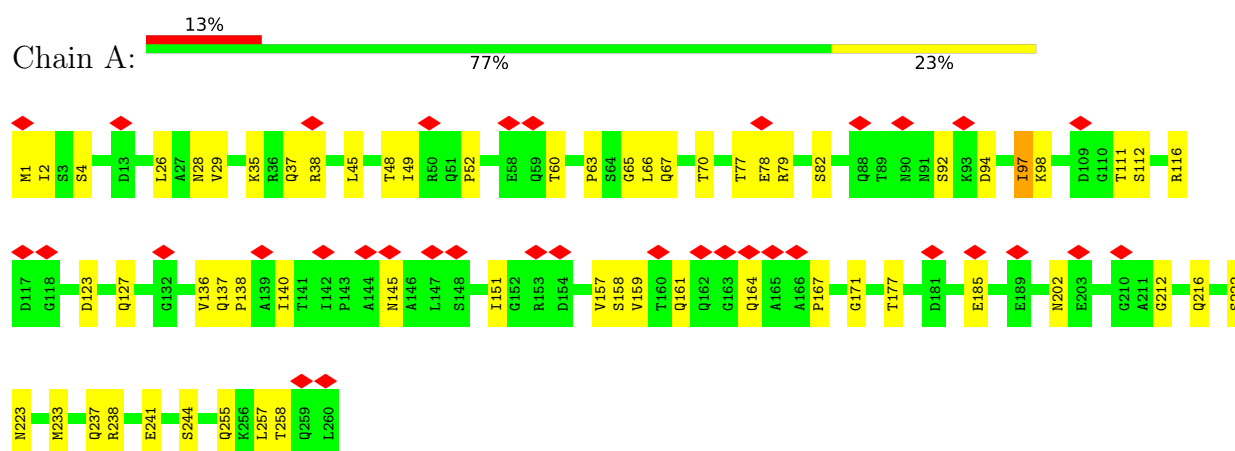
- Molecule 8 is a protein called Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	DA	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DB	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DC	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DD	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DE	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DF	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DG	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DH	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DI	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DJ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DK	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		

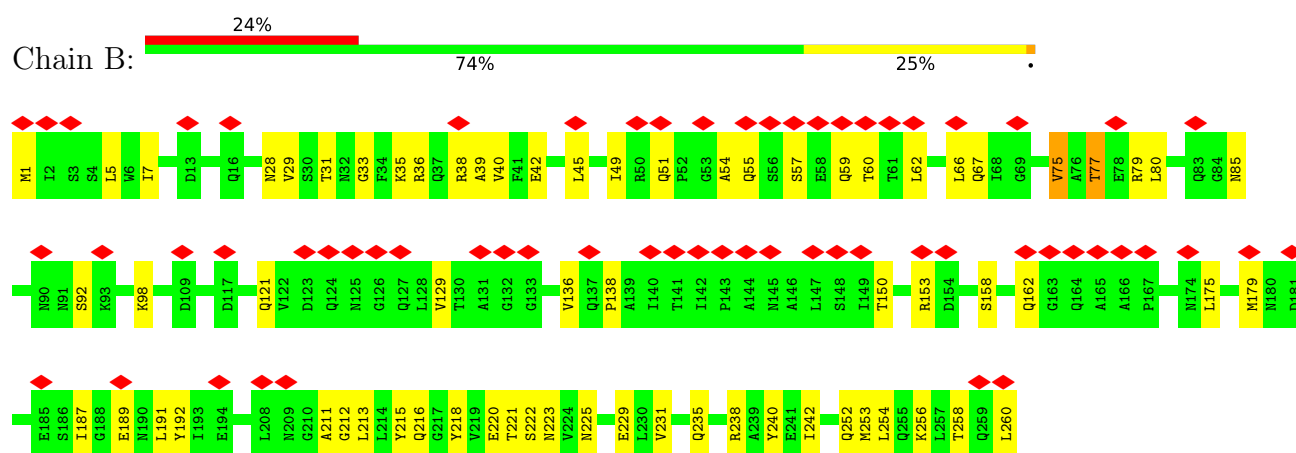
3 Residue-property plots

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

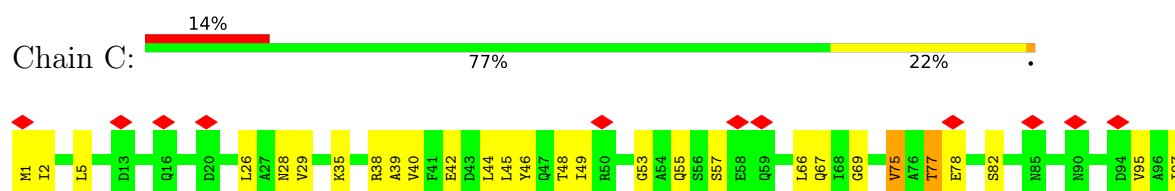
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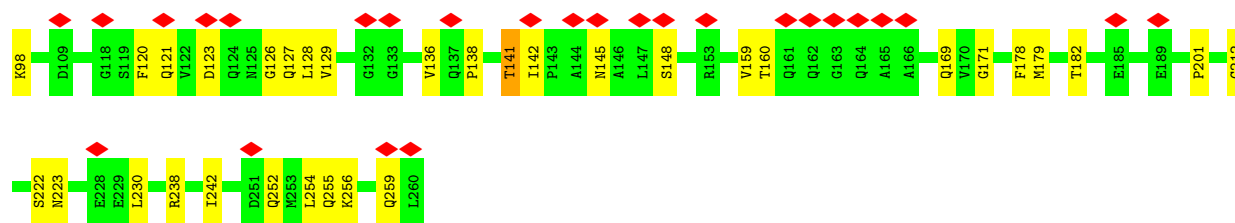


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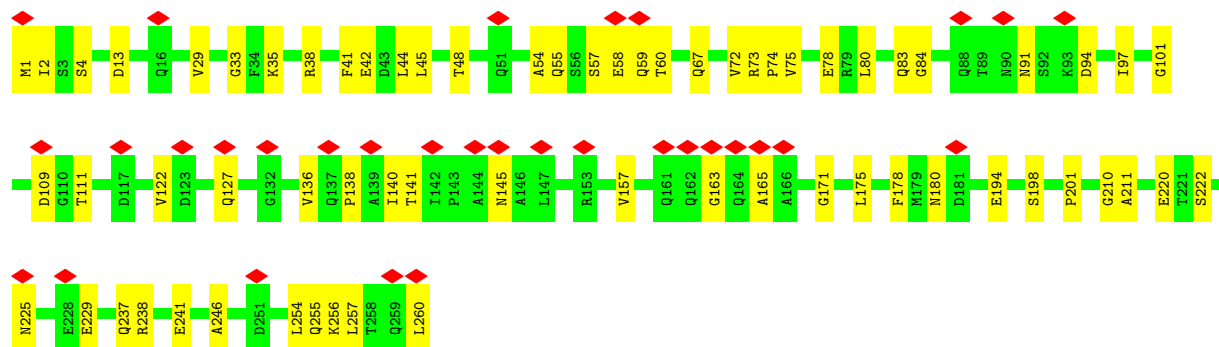
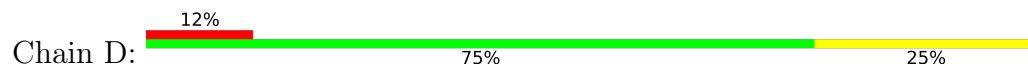


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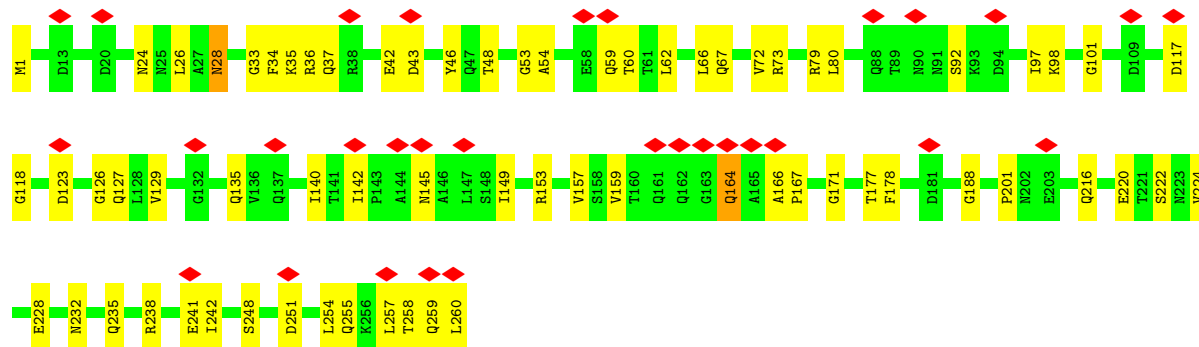
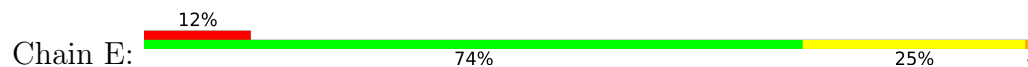




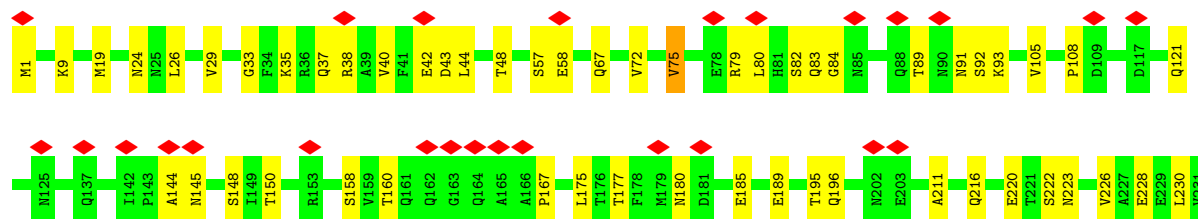
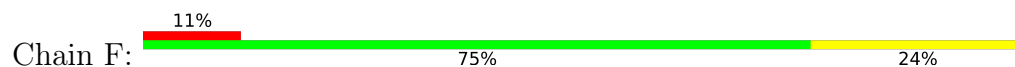
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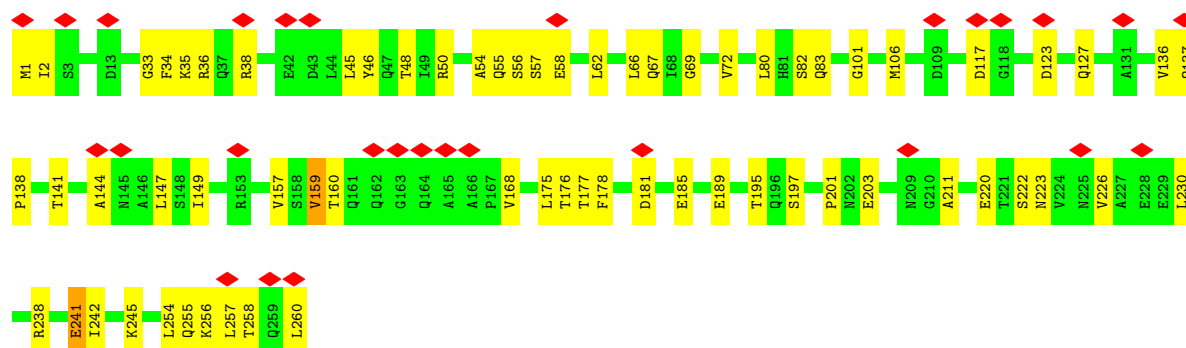
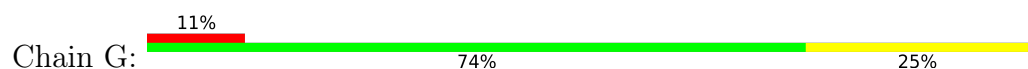


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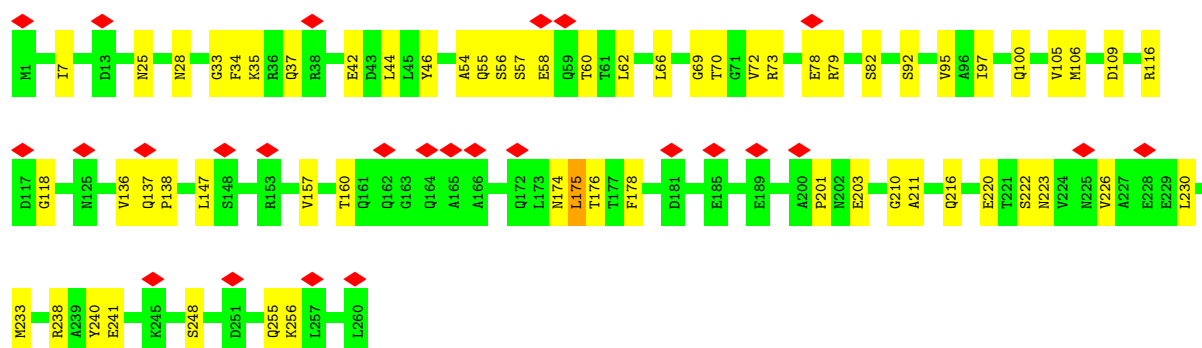
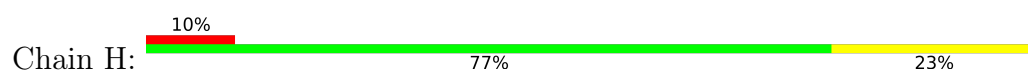




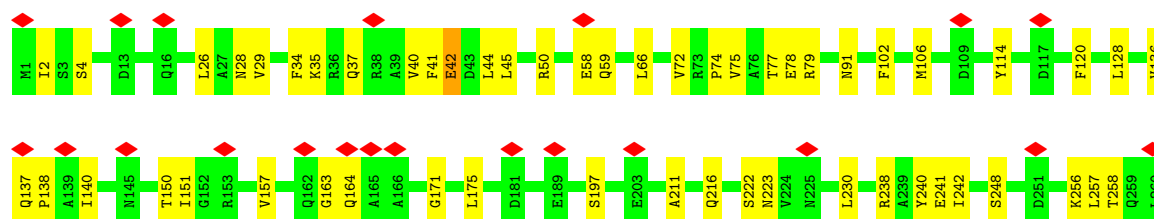
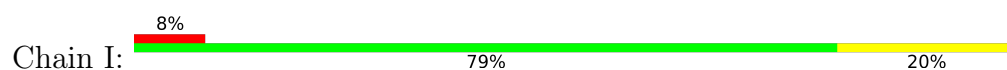
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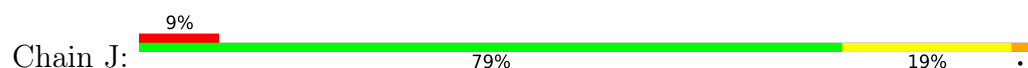
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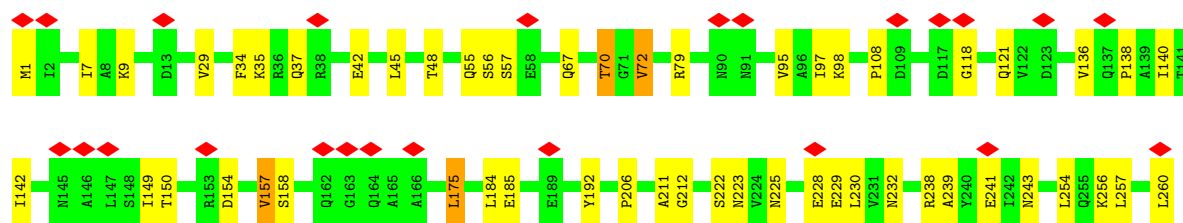


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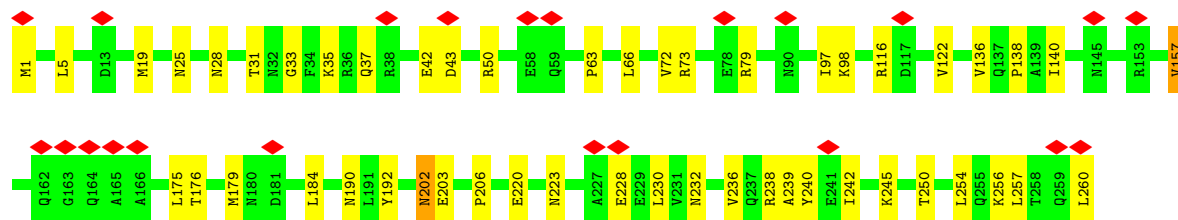
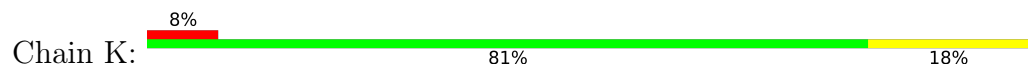


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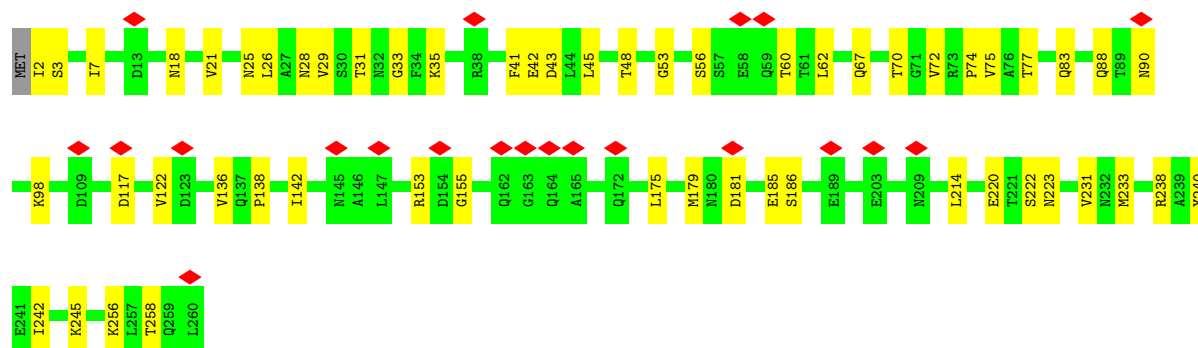
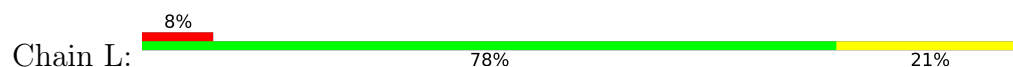




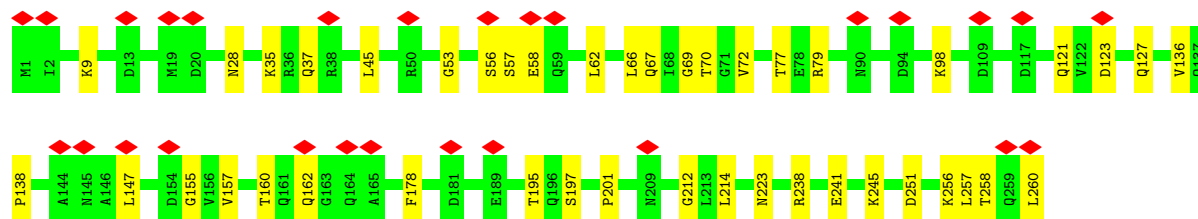
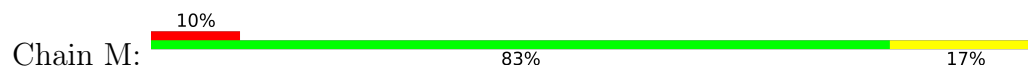
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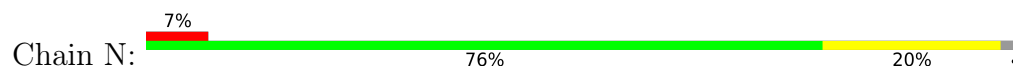
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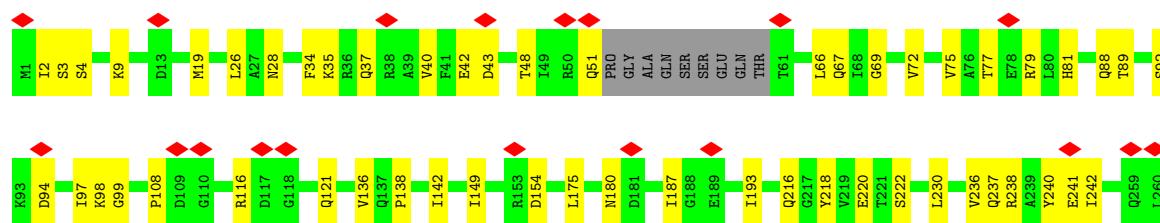


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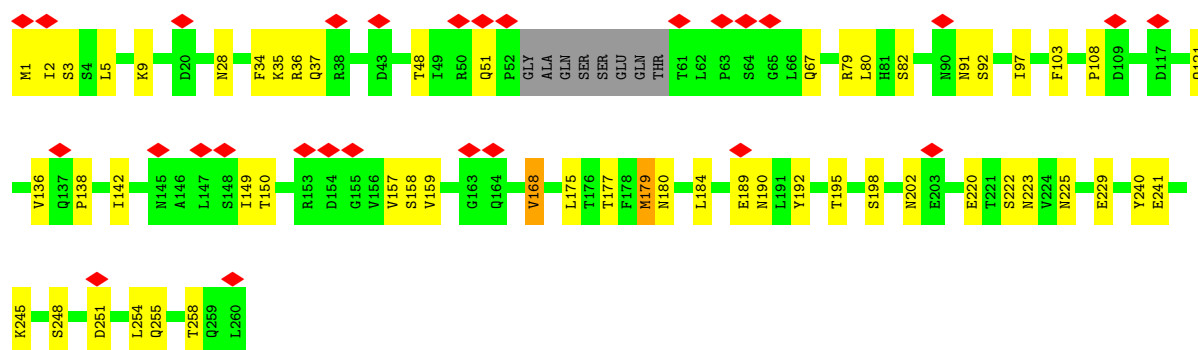
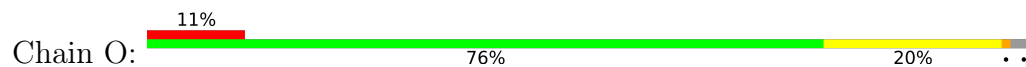


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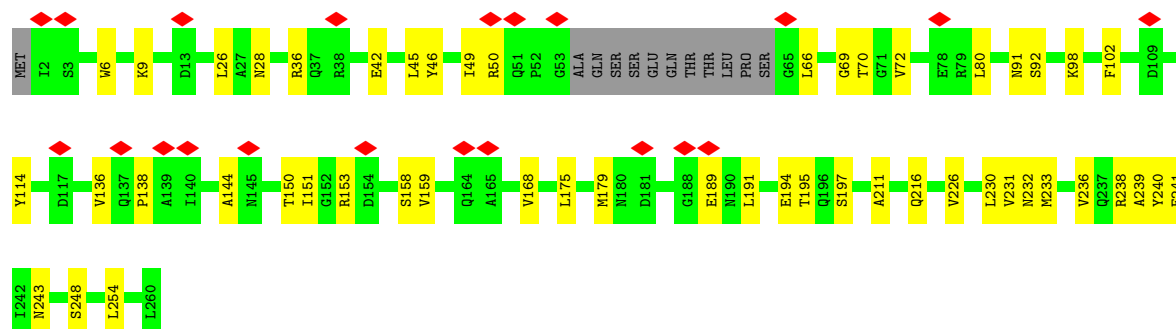
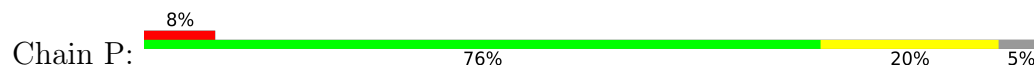




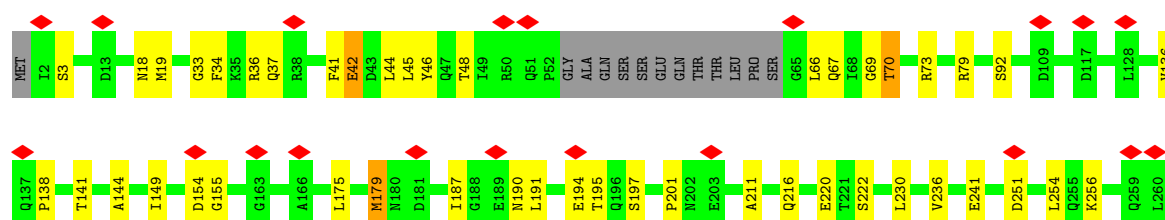
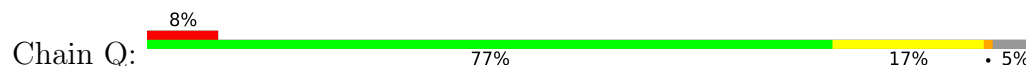
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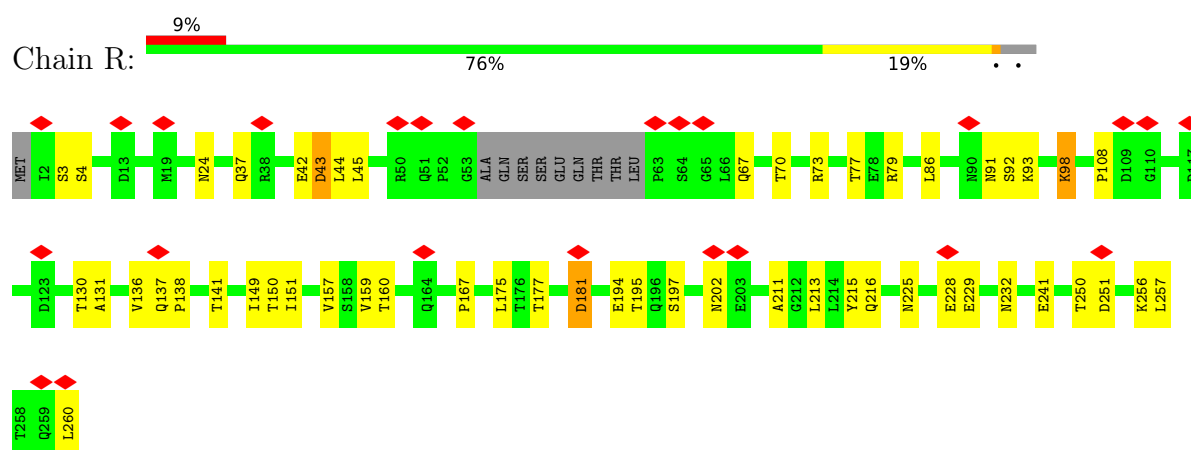
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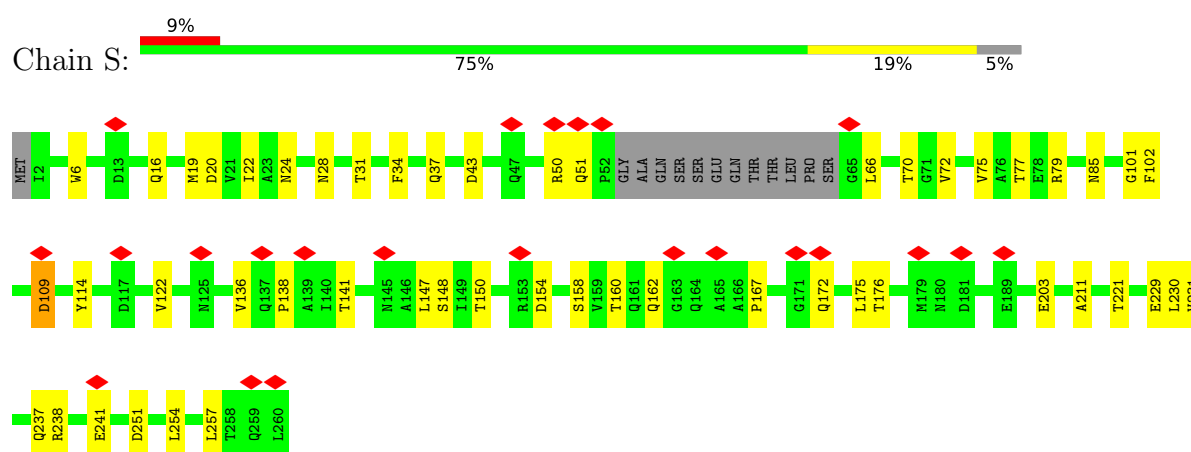
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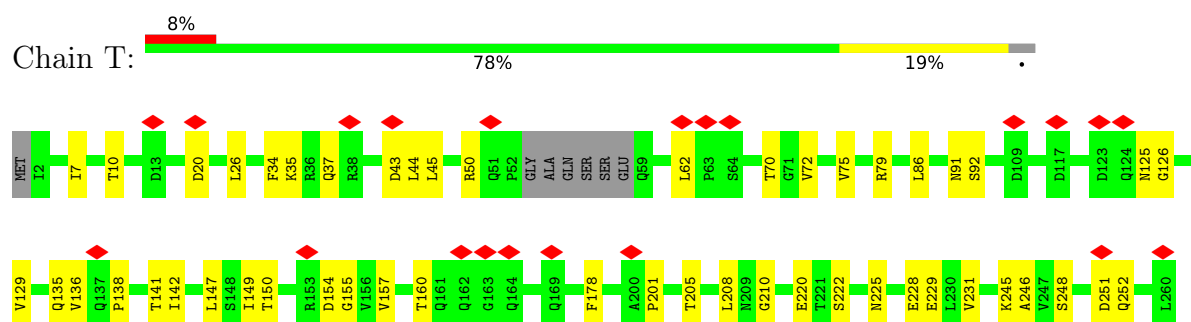
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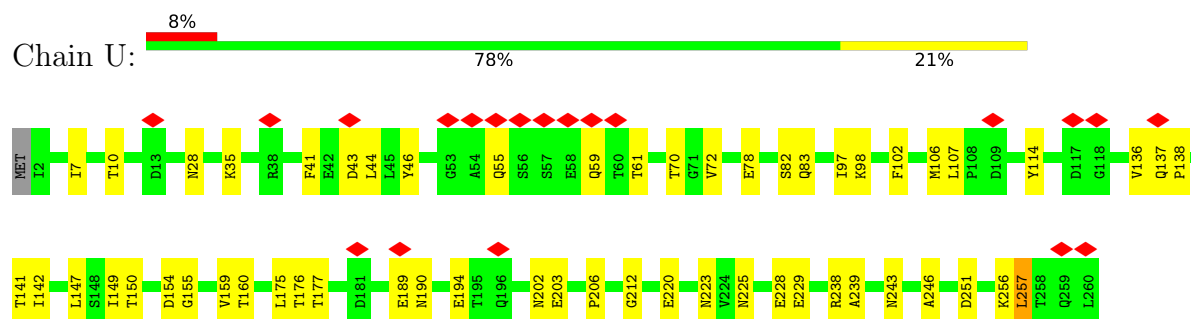
• Molecule 1: Flagellar basal-body rod protein FlgG



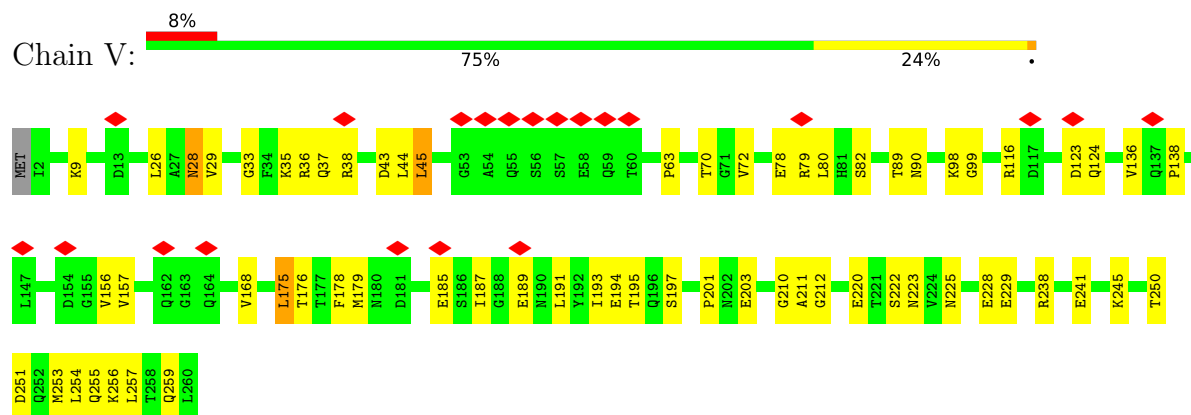
• Molecule 1: Flagellar basal-body rod protein FlgG



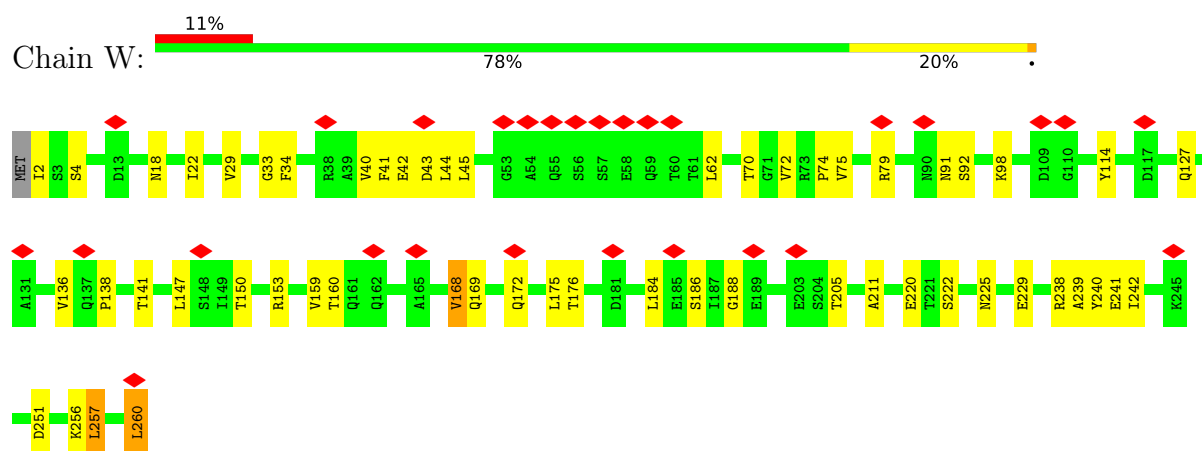
• Molecule 1: Flagellar basal-body rod protein FlgG



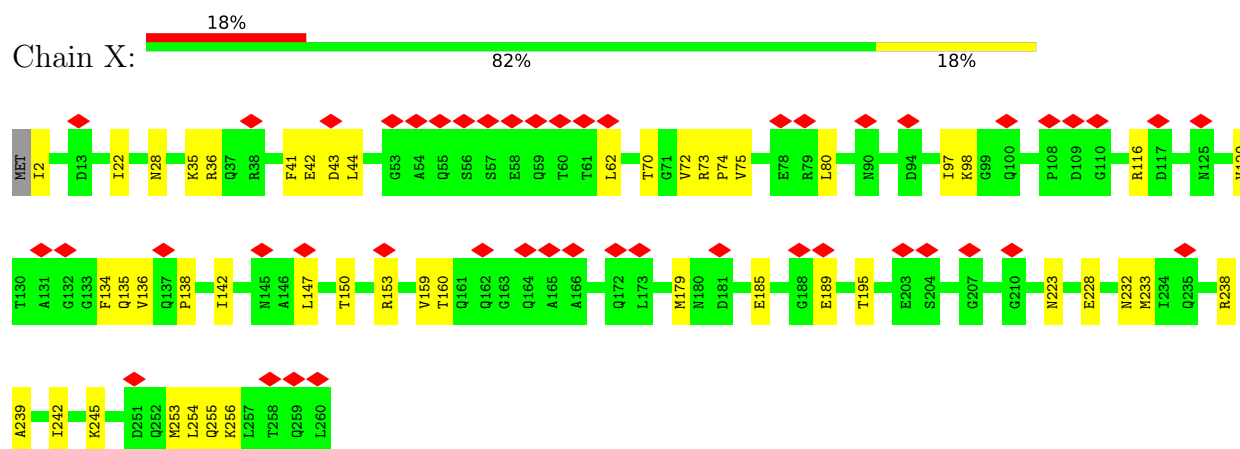
- Molecule 1: Flagellar basal-body rod protein FlgG



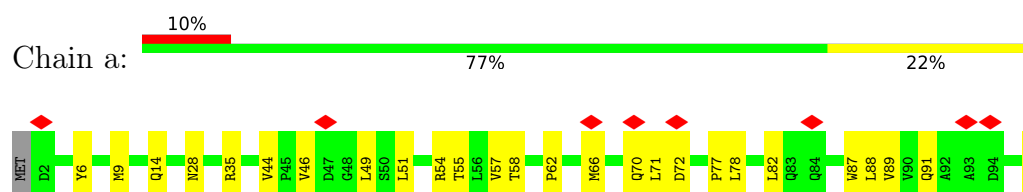
- Molecule 1: Flagellar basal-body rod protein FlgG

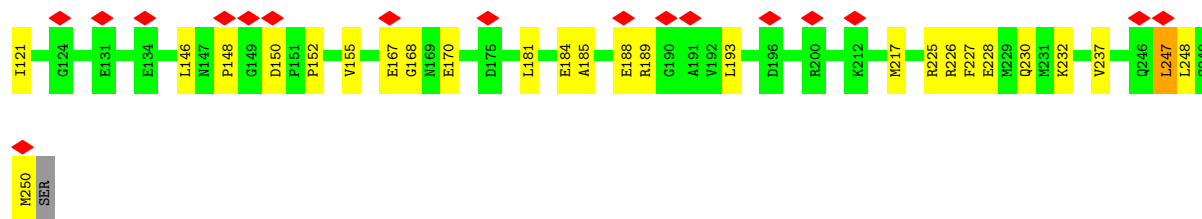


- Molecule 1: Flagellar basal-body rod protein FlgG

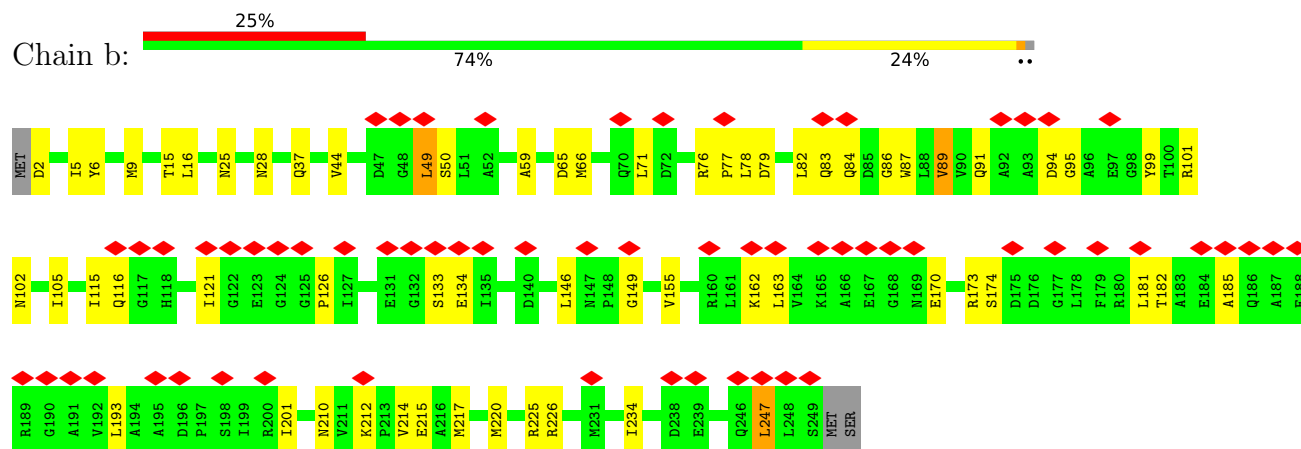


- Molecule 2: Flagellar basal-body rod protein FlgF

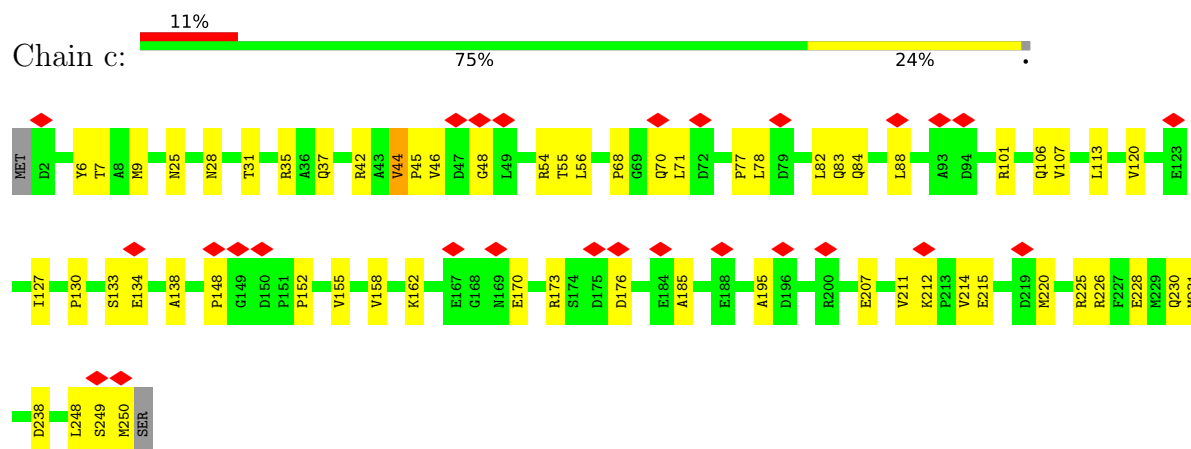




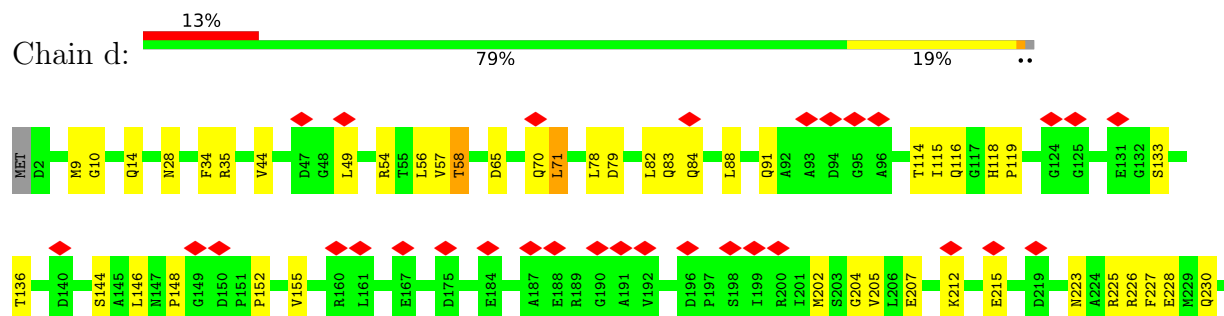
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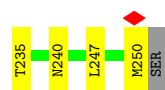


• Molecule 2: Flagellar basal-body rod protein FlgF

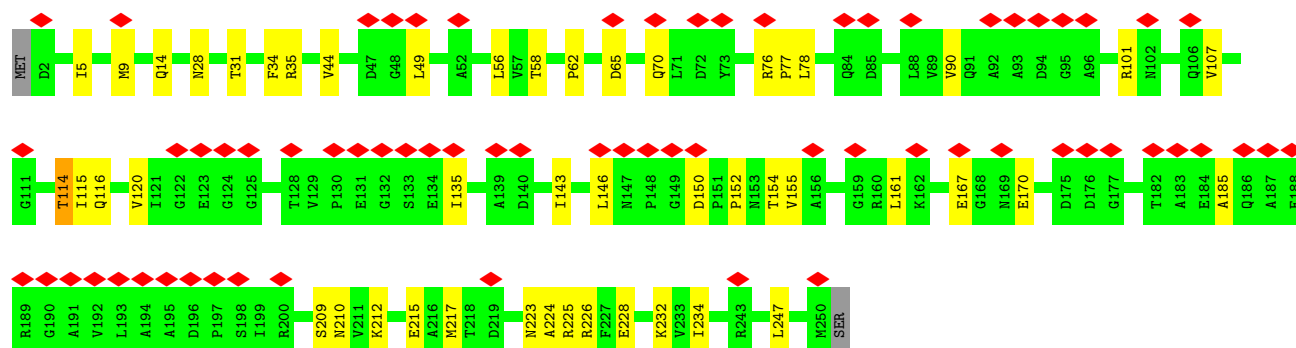
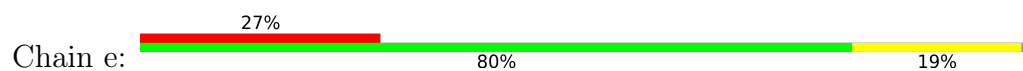


• Molecule 2: Flagellar basal-body rod protein FlgF

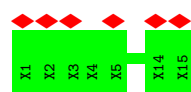
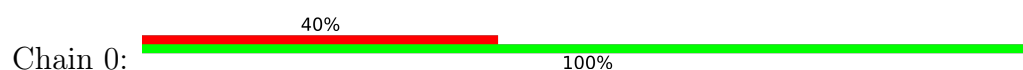




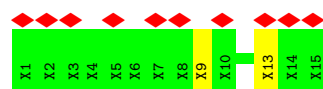
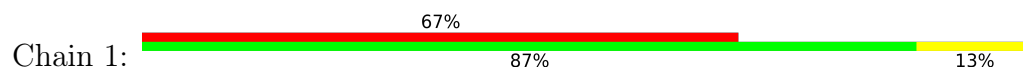
- Molecule 2: Flagellar basal-body rod protein FlgF



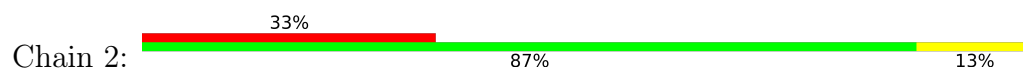
- Molecule 3: Flagellar MS ring L2



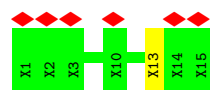
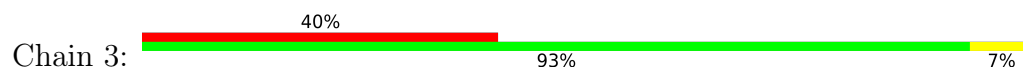
- Molecule 3: Flagellar MS ring L2



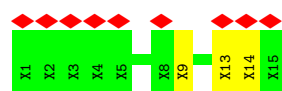
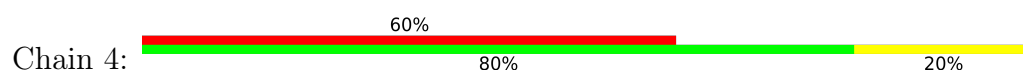
- Molecule 3: Flagellar MS ring L2



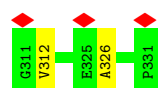
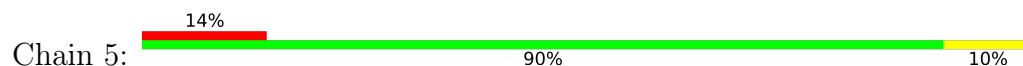
- Molecule 3: Flagellar MS ring L2



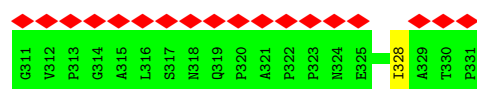
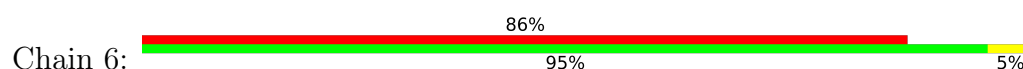
- Molecule 3: Flagellar MS ring L2



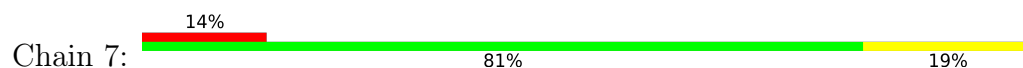
- Molecule 4: Flagellar MS ring L1



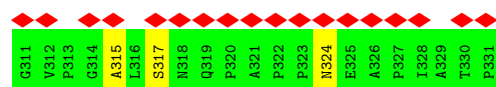
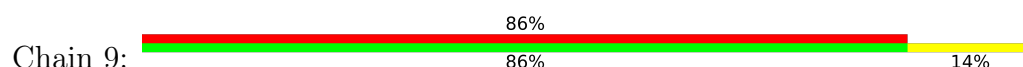
- Molecule 4: Flagellar MS ring L1



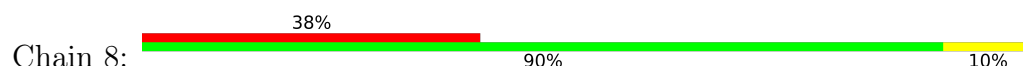
- Molecule 4: Flagellar MS ring L1



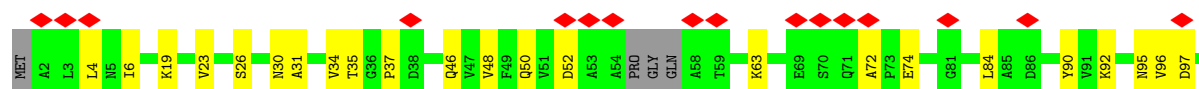
- Molecule 4: Flagellar MS ring L1



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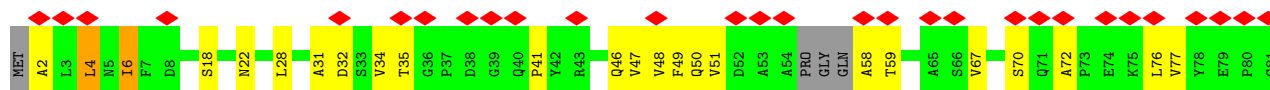


- Molecule 5: Flagellar basal-body rod protein FlgC





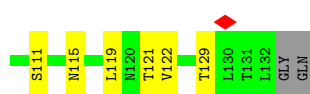
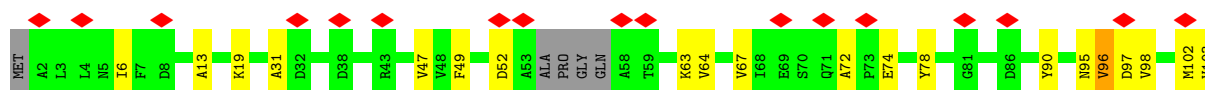
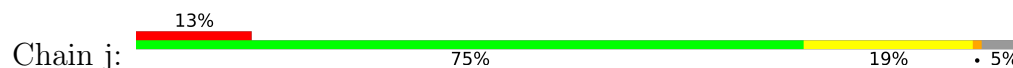
• Molecule 5: Flagellar basal-body rod protein FlgC



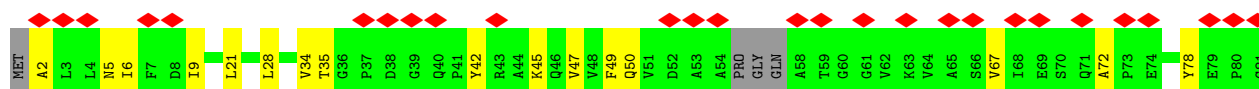
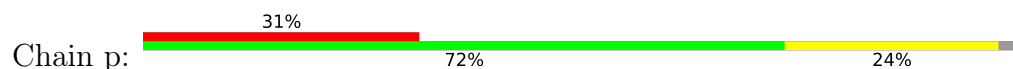
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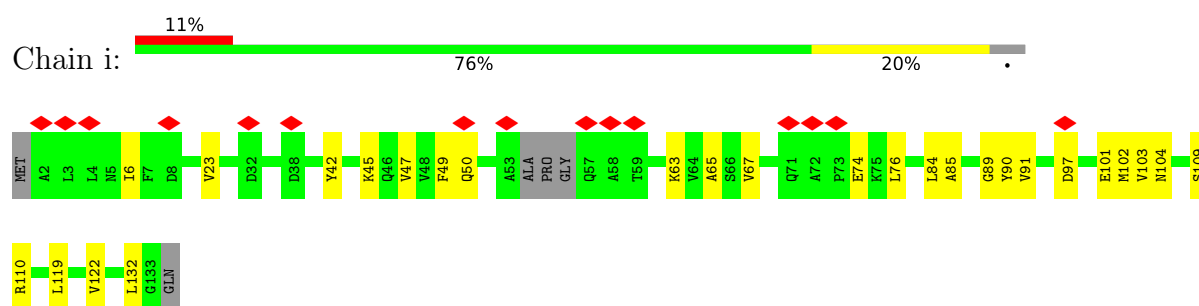
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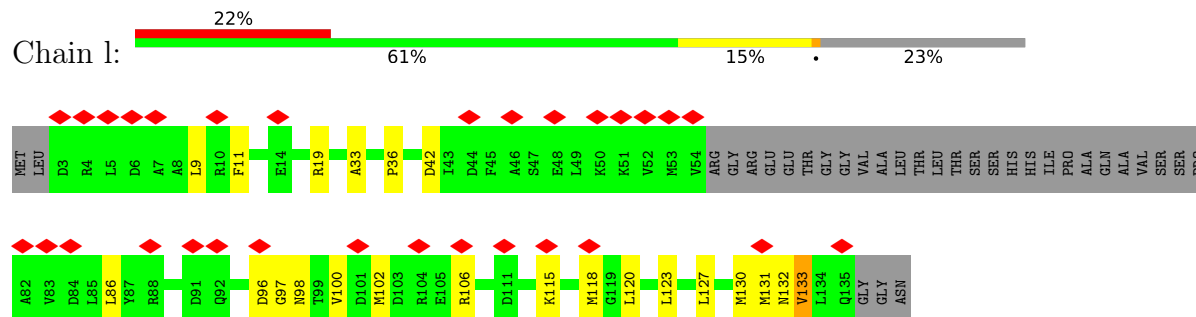
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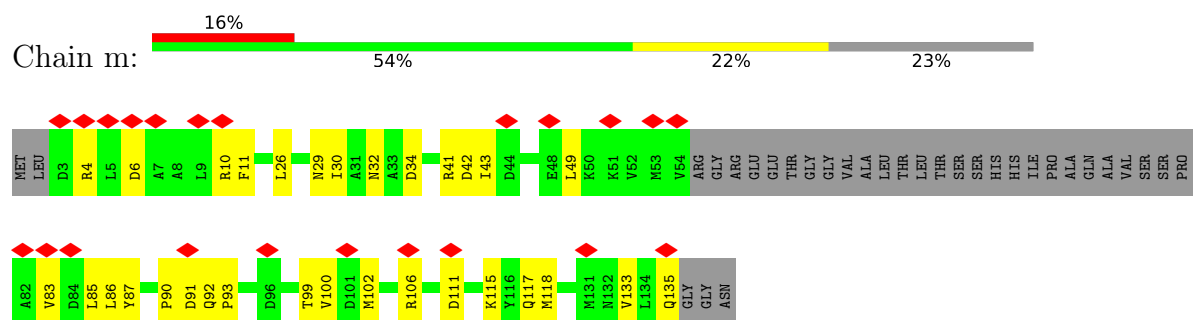
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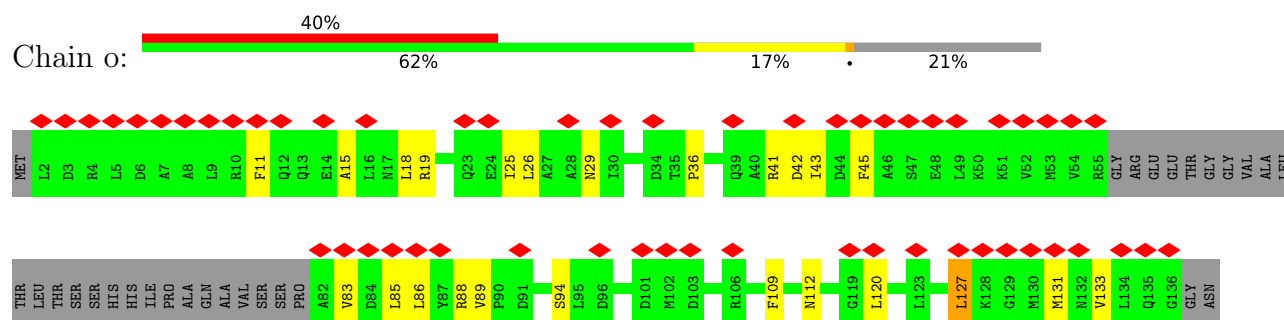
- Molecule 6: Flagellar basal body rod protein FlgB



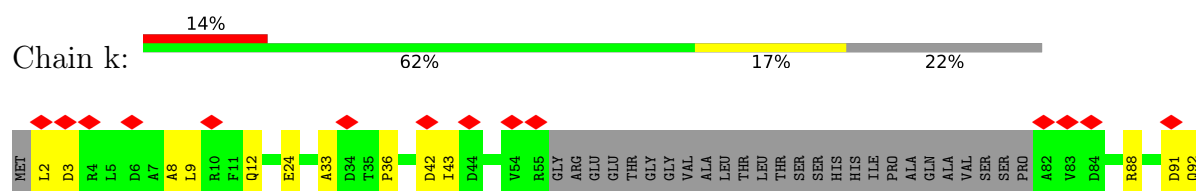
- Molecule 6: Flagellar basal body rod protein FlgB



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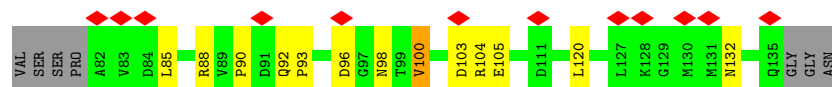
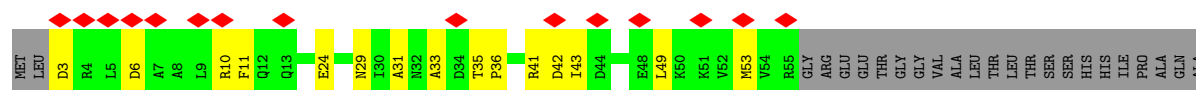


- Molecule 6: Flagellar basal body rod protein FlgB

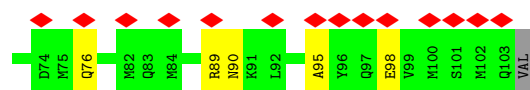
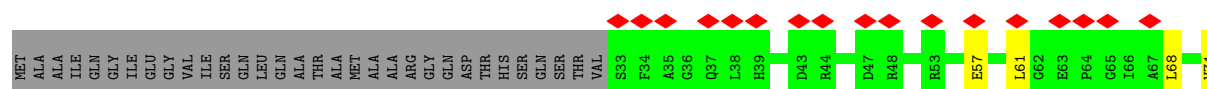




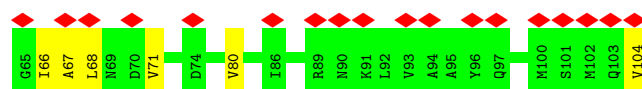
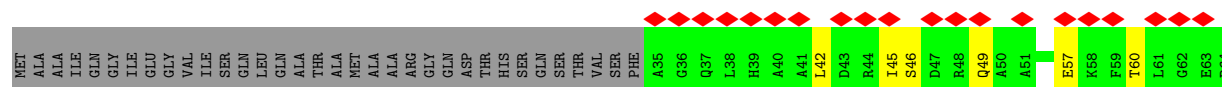
- Molecule 6: Flagellar basal body rod protein FlgB



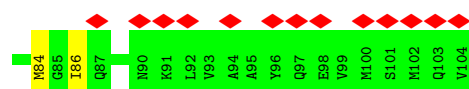
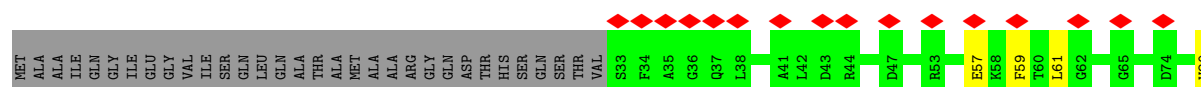
- Molecule 7: Flagellar hook-basal body complex protein FliE



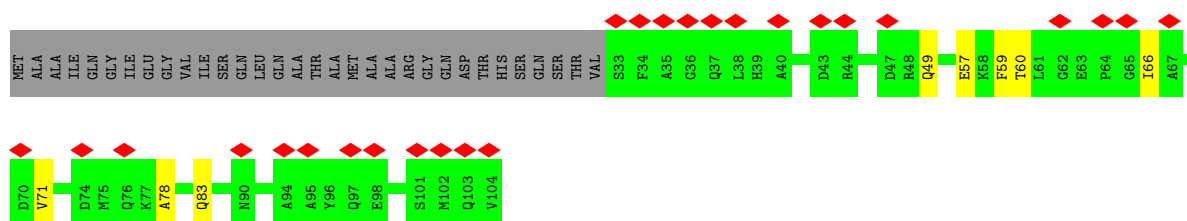
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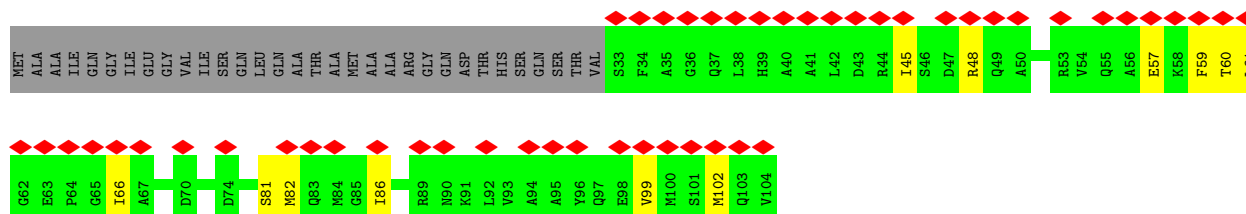
- Molecule 7: Flagellar hook-basal body complex protein FliE



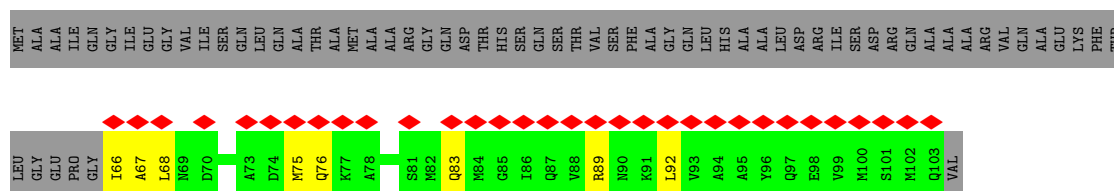
- Molecule 7: Flagellar hook-basal body complex protein FliE



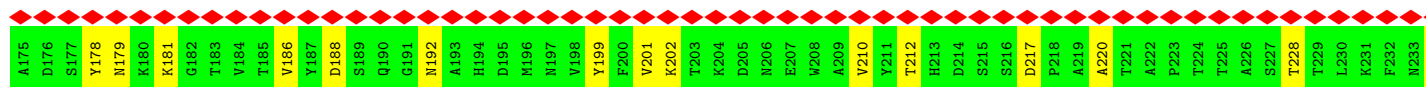
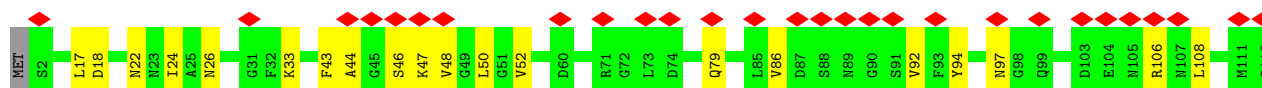
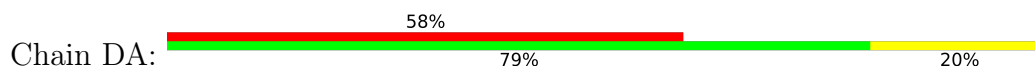
• Molecule 7: Flagellar hook-basal body complex protein FliE

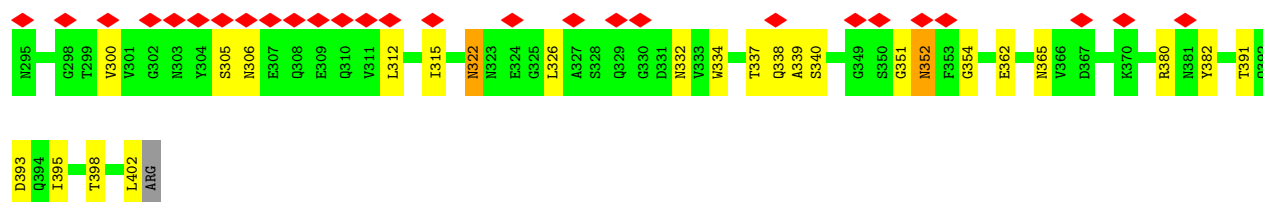


• Molecule 7: Flagellar hook-basal body complex protein FliE

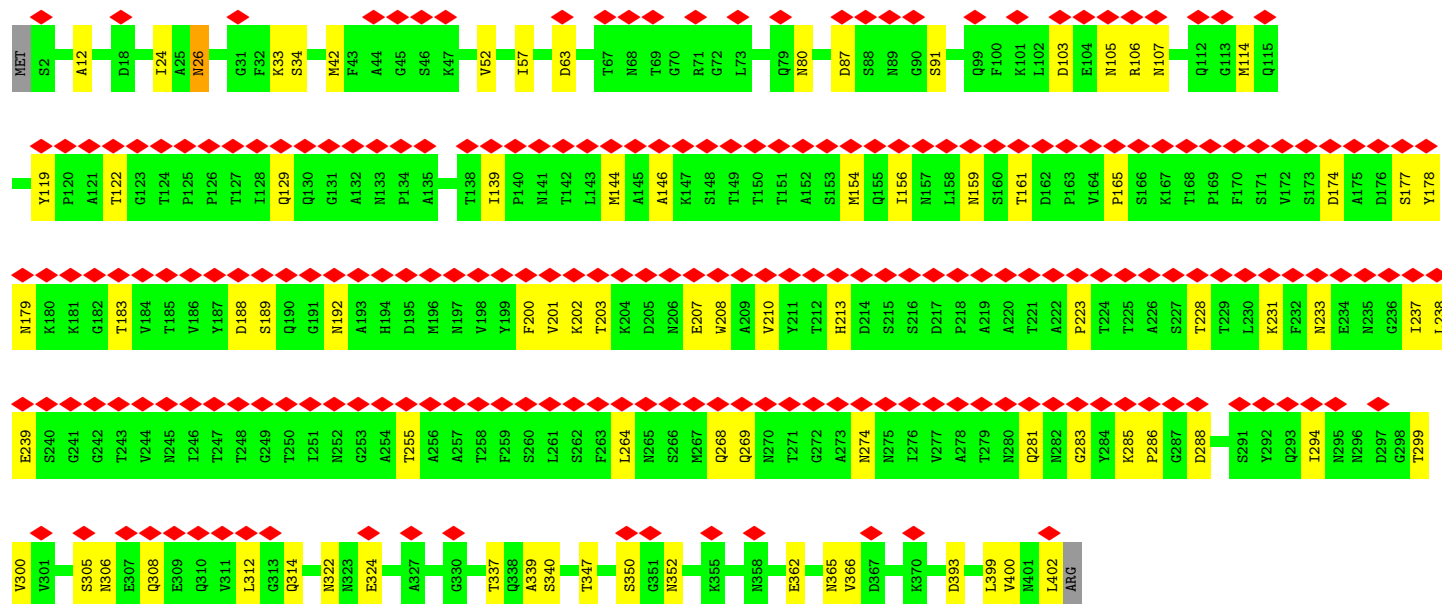
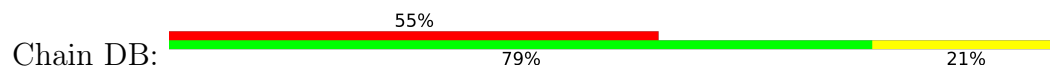


• Molecule 8: Flagellar hook protein FlgE

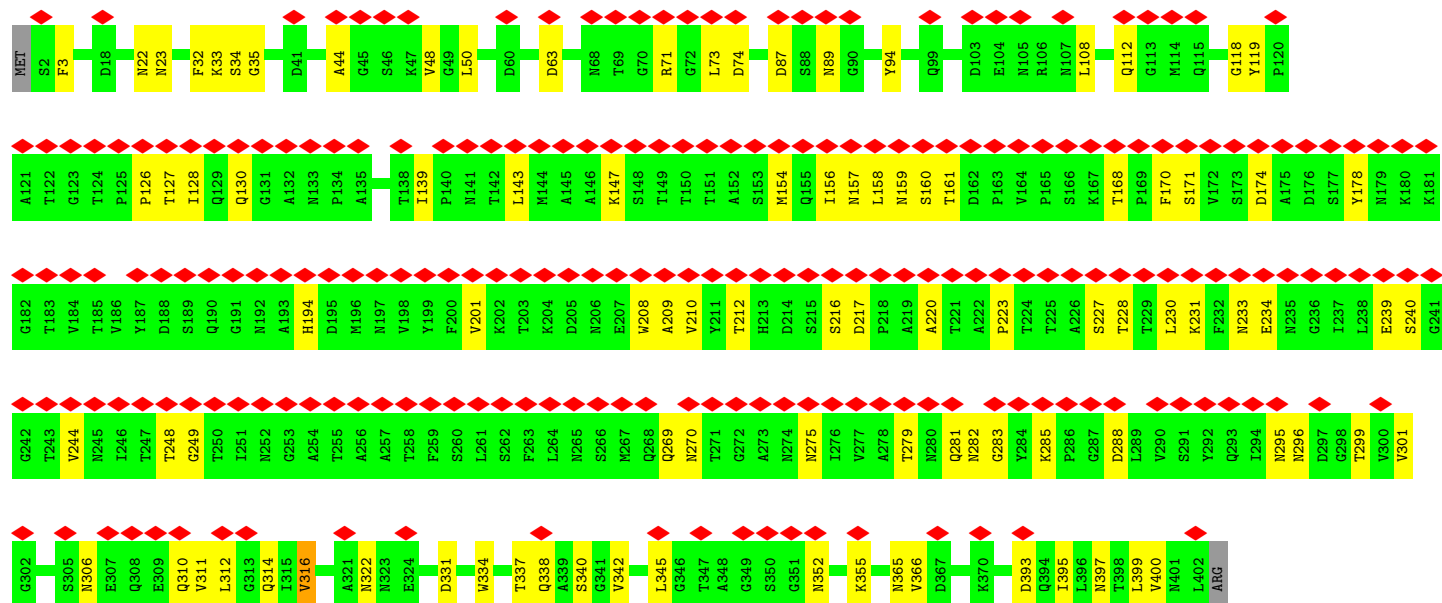
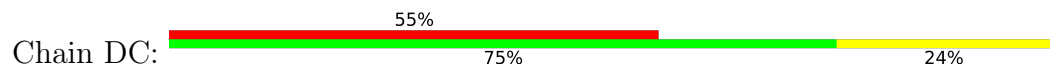




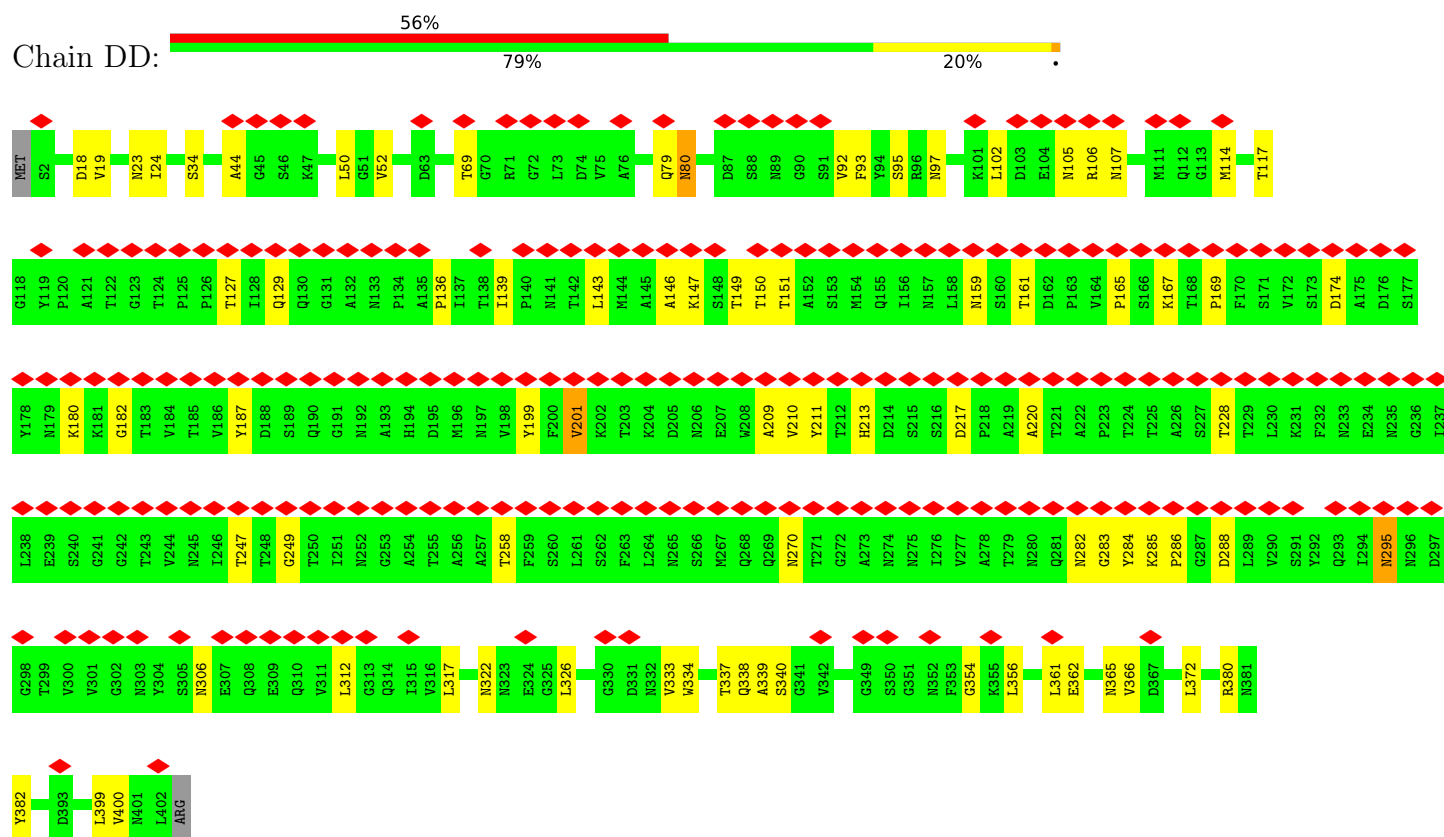
• Molecule 8: Flagellar hook protein FlgE



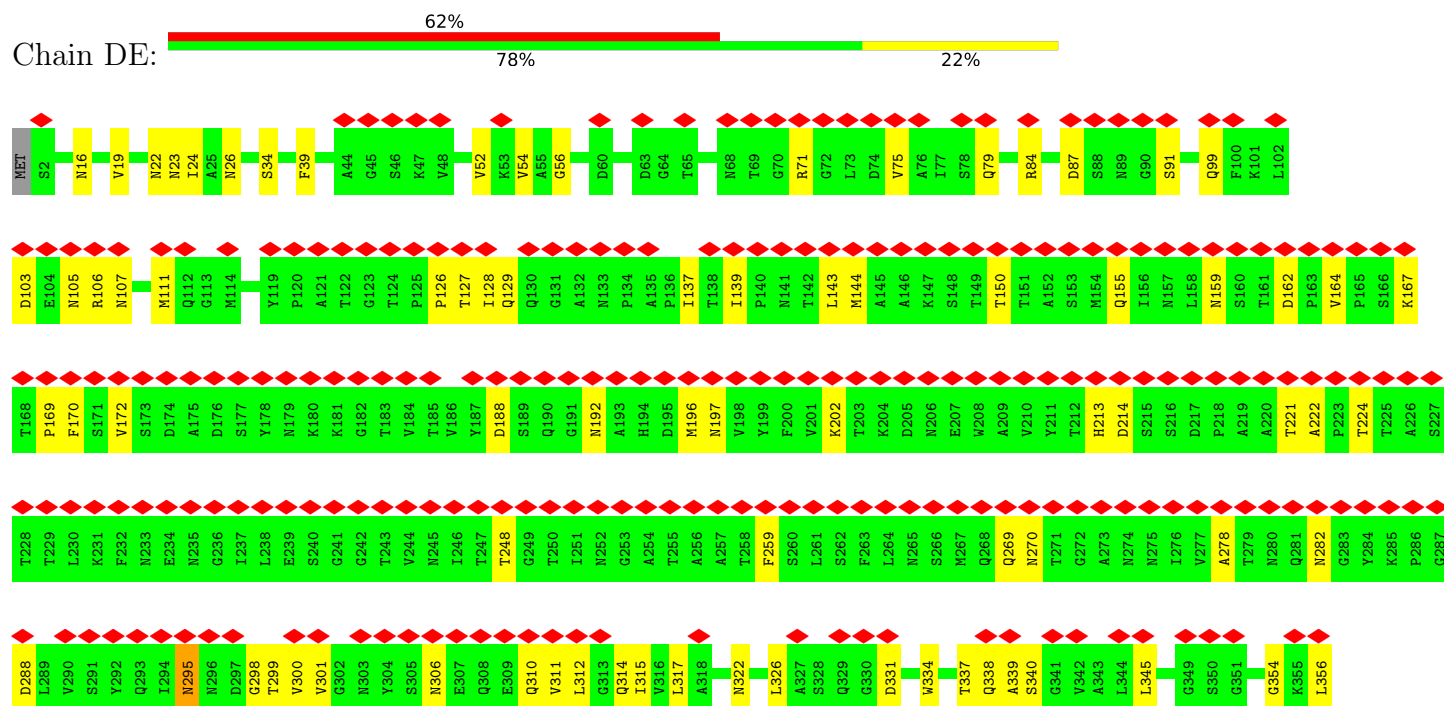
• Molecule 8: Flagellar hook protein FlgE

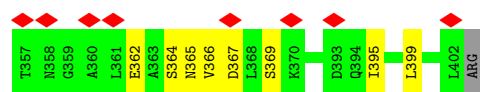


● Molecule 8: Flagellar hook protein FlgE

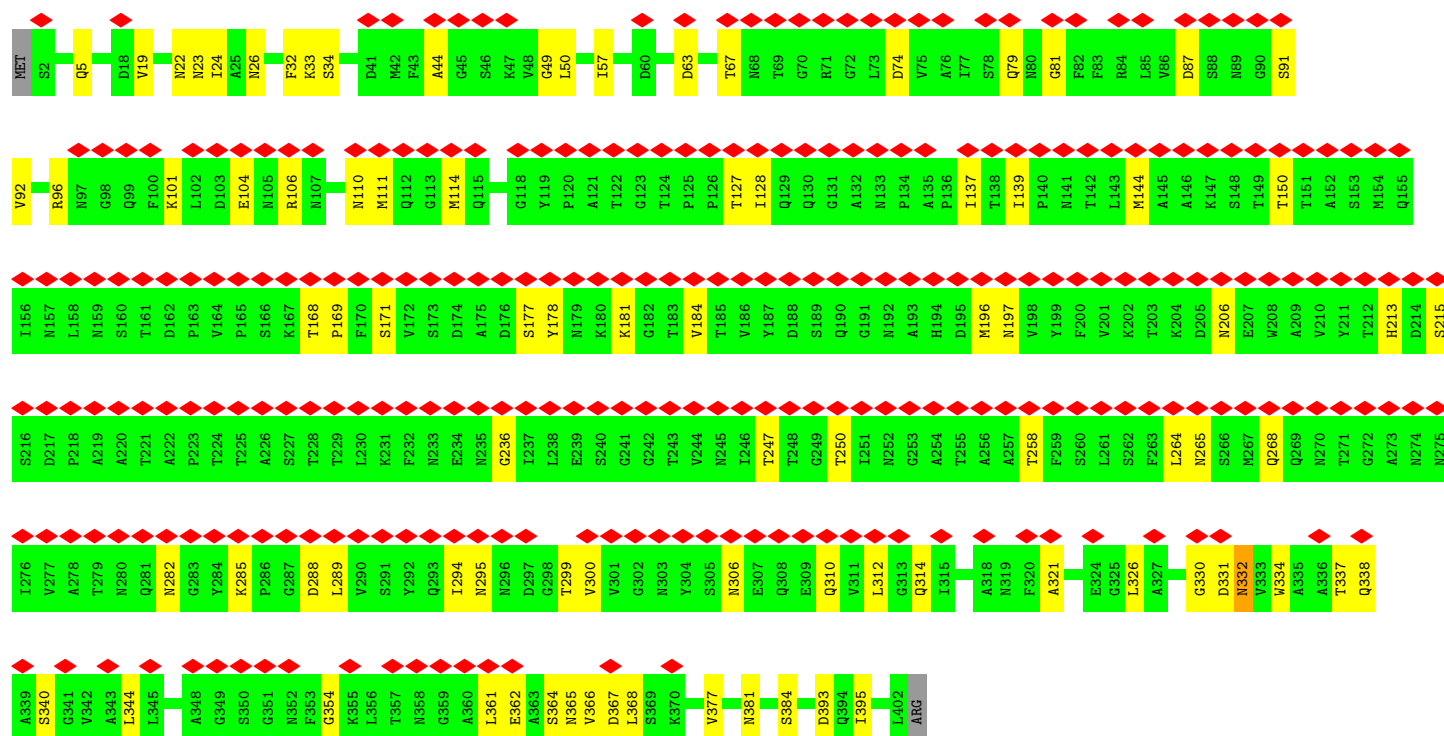
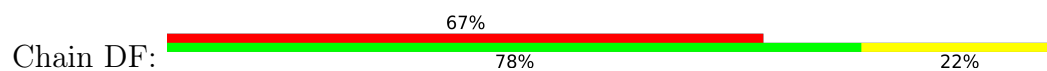


● Molecule 8: Flagellar hook protein FlgE

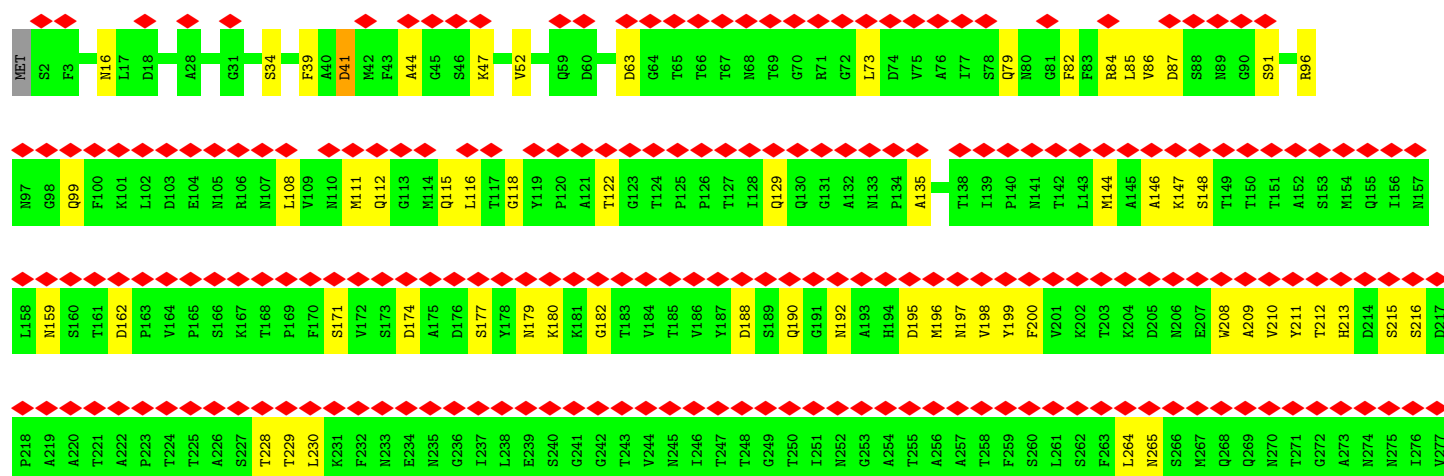
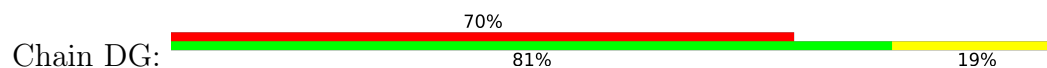


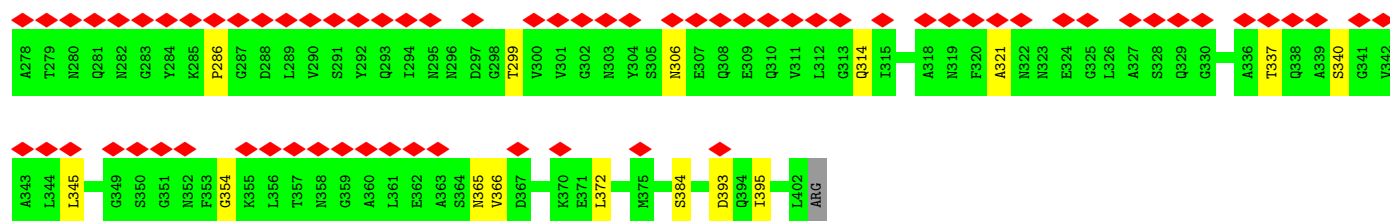


• Molecule 8: Flagellar hook protein FlgE

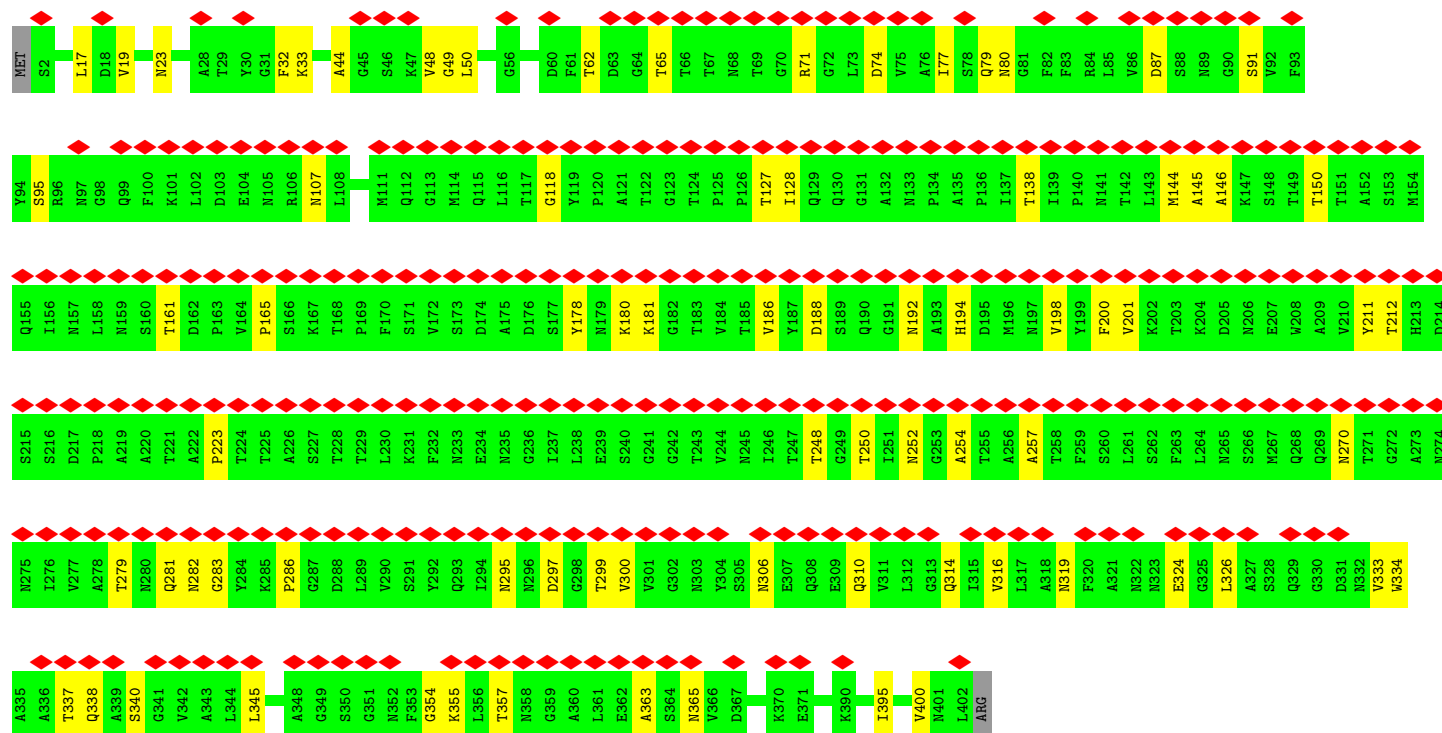
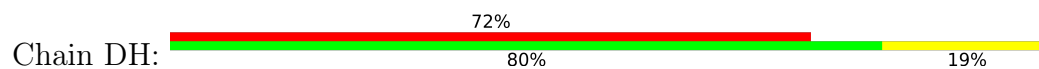


• Molecule 8: Flagellar hook protein FlgE

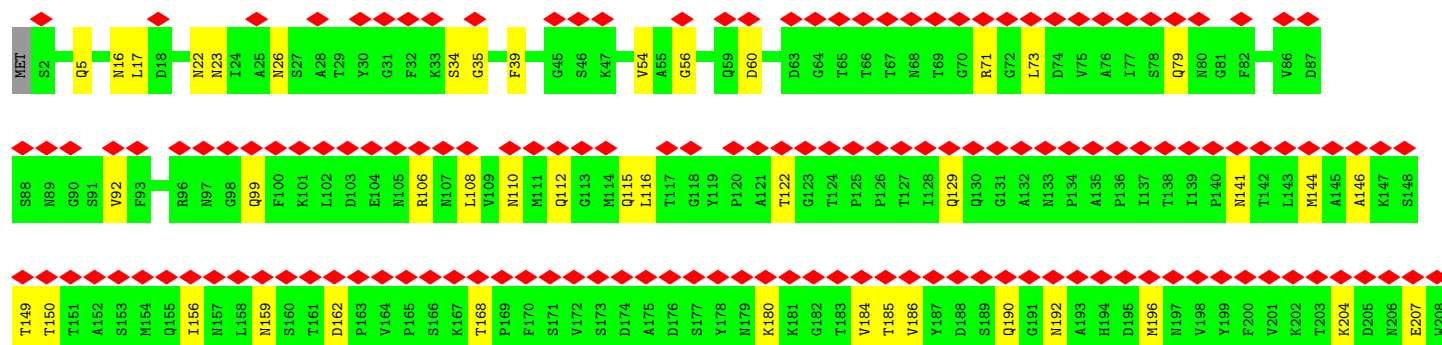
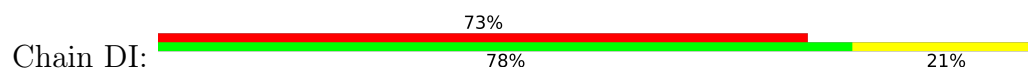


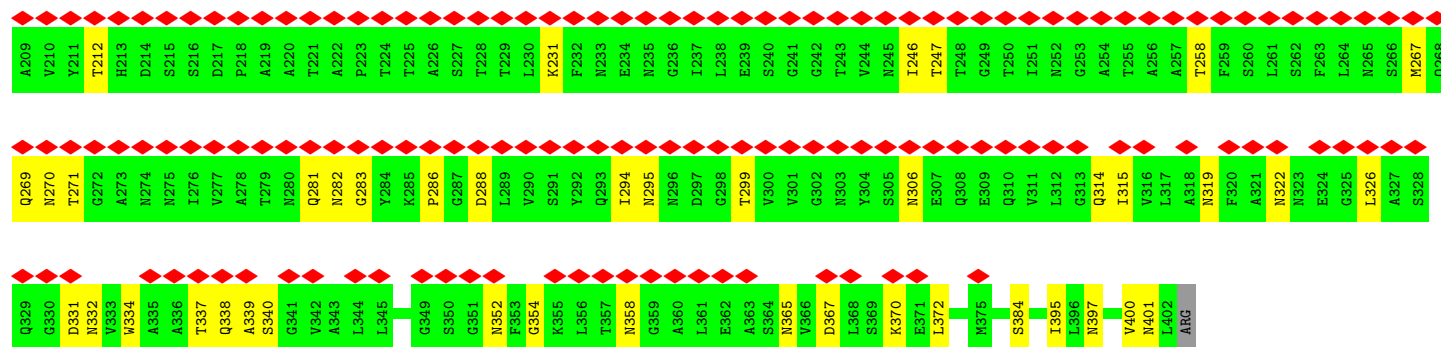


• Molecule 8: Flagellar hook protein FlgE

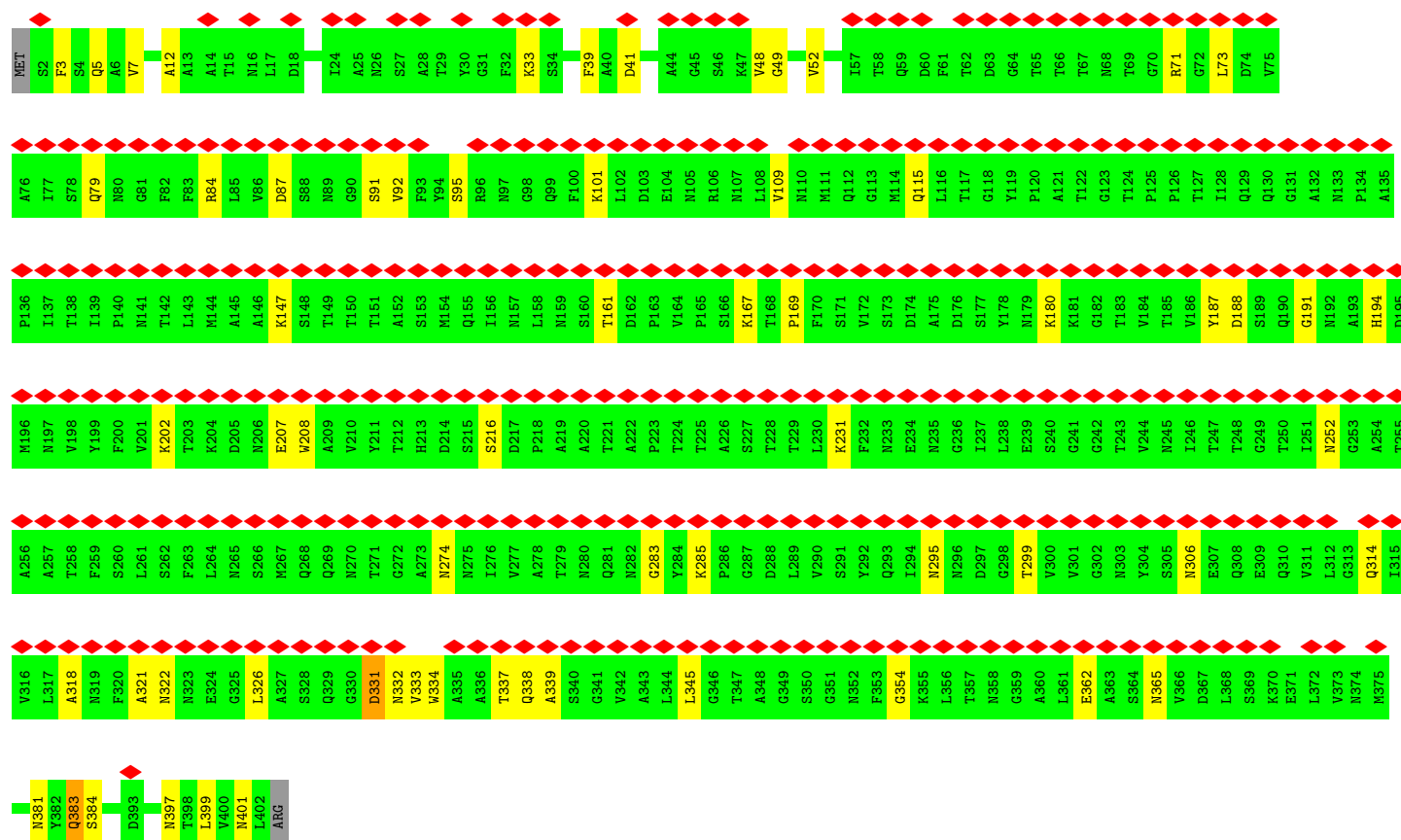
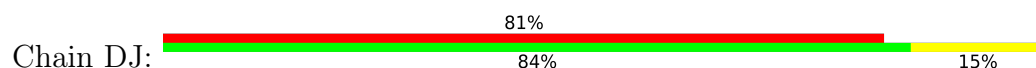


• Molecule 8: Flagellar hook protein FlgE

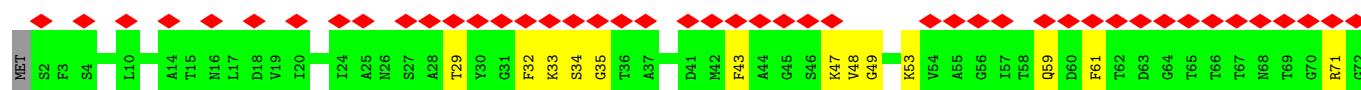
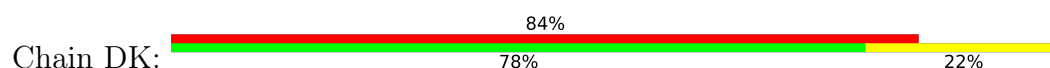




• Molecule 8: Flagellar hook protein FlgE



• Molecule 8: Flagellar hook protein FlgE





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102044	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 ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.722	Depositor
Minimum map value	-1.395	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.65	Depositor
Map size (Å)	669.184, 669.184, 669.184	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/1973	0.28	0/2682
1	B	0.14	0/1973	0.27	0/2682
1	C	0.15	0/1973	0.26	0/2682
1	D	0.16	0/1973	0.28	0/2682
1	E	0.15	0/1973	0.30	0/2682
1	F	0.16	0/1973	0.28	0/2682
1	G	0.16	0/1973	0.27	0/2682
1	H	0.16	0/1973	0.28	0/2682
1	I	0.16	0/1973	0.29	0/2682
1	J	0.16	0/1973	0.28	0/2682
1	K	0.16	0/1973	0.27	0/2682
1	L	0.15	0/1965	0.25	0/2672
1	M	0.16	0/1973	0.27	0/2682
1	N	0.16	0/1909	0.26	0/2593
1	O	0.16	0/1917	0.26	0/2605
1	P	0.16	0/1884	0.29	0/2559
1	Q	0.17	0/1880	0.28	0/2554
1	R	0.16	0/1898	0.29	0/2578
1	S	0.15	0/1880	0.27	0/2554
1	T	0.15	0/1925	0.25	0/2617
1	U	0.16	0/1965	0.27	0/2672
1	V	0.16	0/1965	0.29	0/2672
1	W	0.22	0/1965	0.35	0/2672
1	X	0.16	0/1965	0.31	0/2672
2	a	0.15	0/1836	0.29	0/2502
2	b	0.15	0/1828	0.28	0/2492
2	c	0.15	0/1836	0.25	0/2502
2	d	0.15	0/1836	0.29	0/2502
2	e	0.14	0/1836	0.33	0/2502
4	5	0.14	0/145	0.23	0/203
4	6	0.10	0/145	0.24	0/203
4	7	0.52	0/145	0.85	0/203
4	8	0.13	0/145	0.23	0/203
4	9	0.13	0/145	0.28	0/203

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	f	0.15	0/946	0.24	0/1285
5	g	0.15	0/959	0.29	0/1302
5	h	0.16	0/945	0.26	0/1283
5	i	0.16	0/954	0.28	0/1295
5	j	0.16	0/941	0.27	0/1278
5	p	0.13	0/950	0.25	0/1290
6	k	0.15	0/859	0.28	0/1156
6	l	0.14	0/840	0.25	0/1131
6	m	0.16	0/840	0.26	0/1131
6	n	0.15	0/851	0.25	0/1145
6	o	0.13	0/863	0.28	0/1161
7	q	0.12	0/540	0.25	0/723
7	r	0.16	0/529	0.31	0/709
7	s	0.12	0/547	0.23	0/733
7	t	0.11	0/547	0.28	0/733
7	u	0.12	0/547	0.29	0/733
7	v	0.11	0/289	0.22	0/385
8	DA	0.15	0/2991	0.27	0/4076
8	DB	0.12	0/2991	0.25	0/4076
8	DC	0.12	0/2991	0.25	0/4076
8	DD	0.12	0/2991	0.25	0/4076
8	DE	0.11	0/2991	0.23	0/4076
8	DF	0.11	0/2991	0.23	0/4076
8	DG	0.12	0/2991	0.25	0/4076
8	DH	0.14	0/2991	0.27	0/4076
8	DI	0.15	0/2991	0.32	2/4076 (0.0%)
8	DJ	0.20	0/2991	0.37	2/4076 (0.0%)
8	DK	0.16	0/2991	0.28	1/4076 (0.0%)
All	All	0.15	0/102539	0.28	5/139428 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DJ	383	GLN	CB-CA-C	-7.47	99.15	110.88
8	DI	270	ASN	CA-C-N	-6.39	110.45	122.27
8	DI	270	ASN	C-N-CA	-6.39	110.45	122.27
8	DJ	381	ASN	N-CA-C	-5.82	104.94	111.28
8	DK	104	GLU	CB-CA-C	5.46	121.16	110.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1949	0	1926	44	0
1	B	1949	0	1926	57	0
1	C	1949	0	1926	41	0
1	D	1949	0	1926	44	0
1	E	1949	0	1926	53	0
1	F	1949	0	1926	53	0
1	G	1949	0	1926	54	0
1	H	1949	0	1926	45	0
1	I	1949	0	1926	42	0
1	J	1949	0	1926	49	0
1	K	1949	0	1926	40	0
1	L	1941	0	1914	43	0
1	M	1949	0	1926	33	0
1	N	1887	0	1871	42	0
1	O	1894	0	1878	43	0
1	P	1862	0	1839	40	0
1	Q	1858	0	1836	31	0
1	R	1875	0	1852	39	0
1	S	1858	0	1836	41	0
1	T	1902	0	1881	33	0
1	U	1941	0	1914	43	0
1	V	1941	0	1914	47	0
1	W	1941	0	1914	46	0
1	X	1941	0	1914	35	0
2	a	1812	0	1800	46	0
2	b	1804	0	1791	45	0
2	c	1812	0	1800	46	0
2	d	1812	0	1800	47	0
2	e	1812	0	1800	38	0
3	0	75	0	18	0	0
3	1	75	0	17	2	0
3	2	75	0	17	4	0
3	3	75	0	18	4	0
3	4	75	0	19	4	0
4	5	140	0	136	1	0
4	6	140	0	136	1	0
4	7	140	0	136	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	8	140	0	136	4	0
4	9	140	0	136	3	0
5	f	936	0	951	26	0
5	g	949	0	962	36	0
5	h	935	0	949	31	0
5	i	944	0	957	19	0
5	j	931	0	946	20	0
5	p	940	0	954	31	0
6	k	852	0	855	21	0
6	l	833	0	831	16	0
6	m	833	0	831	23	0
6	n	844	0	844	22	0
6	o	856	0	858	24	0
7	q	536	0	541	5	0
7	r	526	0	536	10	0
7	s	543	0	550	7	0
7	t	543	0	550	4	0
7	u	543	0	550	10	0
7	v	289	0	299	8	0
8	DA	2947	0	2839	52	0
8	DB	2947	0	2839	54	0
8	DC	2947	0	2839	65	0
8	DD	2947	0	2839	55	0
8	DE	2947	0	2839	65	0
8	DF	2947	0	2839	60	0
8	DG	2947	0	2839	49	0
8	DH	2947	0	2839	45	0
8	DI	2947	0	2839	52	0
8	DJ	2947	0	2839	44	0
8	DK	2947	0	2839	58	0
All	All	101606	0	99628	1753	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 9.

All (1753) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:44:VAL:HG11	4:8:328:ILE:HD13	1.50	0.90
2:b:226:ARG:NH1	5:g:32:ASP:OD2	2.06	0.88
3:3:13:UNK:CB	6:n:35:THR:HG23	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DG:199:TYR:HB2	8:DG:211:TYR:HB2	1.61	0.82
1:D:122:VAL:O	8:DC:322:ASN:ND2	2.12	0.82
1:B:98:LYS:O	1:B:212:GLY:HA3	1.80	0.81
1:V:136:VAL:HG12	1:V:138:PRO:HD2	1.62	0.81
1:K:136:VAL:HG12	1:K:138:PRO:HD2	1.63	0.81
1:P:136:VAL:HG12	1:P:138:PRO:HD2	1.63	0.81
1:S:136:VAL:HG12	1:S:138:PRO:HD2	1.63	0.81
1:A:98:LYS:O	1:A:212:GLY:HA3	1.80	0.81
1:G:260:LEU:O	1:M:245:LYS:NZ	2.14	0.80
8:DF:33:LYS:HA	8:DF:365:ASN:HD21	1.48	0.79
1:V:185:GLU:HG3	1:V:193:ILE:HG13	1.66	0.79
4:9:324:ASN:ND2	6:o:94:SER:O	2.17	0.77
8:DF:57:ILE:HG12	8:DK:47:LYS:HB3	1.64	0.77
1:M:136:VAL:HG12	1:M:138:PRO:HD2	1.67	0.77
1:N:136:VAL:HG12	1:N:138:PRO:HD2	1.66	0.76
1:T:136:VAL:HG12	1:T:138:PRO:HD2	1.67	0.76
8:DB:269:GLN:HE22	8:DH:145:ALA:HB1	1.51	0.76
1:H:78:GLU:OE1	1:M:121:GLN:NE2	2.20	0.75
1:J:136:VAL:HG12	1:J:138:PRO:HD2	1.69	0.75
8:DJ:95:SER:HB3	8:DJ:333:VAL:HG23	1.69	0.75
8:DA:106:ARG:HD3	8:DF:321:ALA:HB1	1.66	0.75
1:C:256:LYS:HD3	1:G:241:GLU:HG2	1.69	0.74
1:M:98:LYS:O	1:M:212:GLY:HA3	1.87	0.74
5:g:34:VAL:HG13	5:g:35:THR:HG22	1.69	0.74
1:H:136:VAL:HG12	1:H:138:PRO:HD2	1.70	0.74
1:R:136:VAL:HG12	1:R:138:PRO:HD2	1.69	0.74
1:C:136:VAL:HG12	1:C:138:PRO:HD2	1.68	0.74
1:A:136:VAL:HG12	1:A:138:PRO:HD2	1.68	0.74
5:h:6:ILE:HG21	5:h:122:VAL:HG21	1.69	0.74
5:p:6:ILE:HG21	5:p:122:VAL:HG21	1.70	0.74
1:V:98:LYS:O	1:V:212:GLY:HA3	1.88	0.73
1:U:98:LYS:O	1:U:212:GLY:HA3	1.88	0.73
8:DE:106:ARG:NH1	8:DJ:321:ALA:HB1	2.03	0.73
8:DA:146:ALA:HB2	8:DA:286:PRO:HD3	1.70	0.73
8:DH:146:ALA:HB2	8:DH:286:PRO:HD3	1.71	0.73
1:A:258:THR:O	1:K:245:LYS:NZ	2.21	0.73
1:W:136:VAL:HG12	1:W:138:PRO:HD2	1.70	0.73
1:G:258:THR:O	1:M:245:LYS:NZ	2.21	0.72
8:DF:144:MET:SD	8:DF:310:GLN:NE2	2.62	0.72
1:A:78:GLU:OE1	1:J:121:GLN:NE2	2.22	0.72
1:B:67:GLN:HE22	1:F:185:GLU:HG3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ILE:HD12	1:F:230:LEU:HD21	1.71	0.72
1:G:55:GLN:HG2	1:W:169:GLN:HE22	1.53	0.72
1:H:37:GLN:HG2	1:H:79:ARG:HG2	1.70	0.72
6:l:36:PRO:HB3	6:l:96:ASP:HB2	1.71	0.72
1:B:45:LEU:HB3	1:L:98:LYS:HD2	1.72	0.72
1:I:37:GLN:HG2	1:I:79:ARG:HG2	1.72	0.72
8:DD:147:LYS:HB3	8:DD:283:GLY:HA2	1.70	0.71
1:O:136:VAL:HG12	1:O:138:PRO:HD2	1.72	0.71
1:Q:37:GLN:HG2	1:Q:79:ARG:HG2	1.72	0.71
2:a:232:LYS:HG2	5:h:102:MET:HE1	1.70	0.71
5:h:44:ALA:HB2	5:h:96:VAL:HG22	1.72	0.71
1:H:97:ILE:HD11	1:H:116:ARG:HG3	1.73	0.71
5:p:34:VAL:HG23	5:p:35:THR:HG22	1.71	0.71
1:I:42:GLU:HG2	1:I:75:VAL:HB	1.71	0.71
1:Q:136:VAL:HG12	1:Q:138:PRO:HD2	1.72	0.71
6:o:11:PHE:CZ	7:u:57:GLU:HG3	2.24	0.71
1:L:136:VAL:HG12	1:L:138:PRO:HD2	1.73	0.71
6:n:36:PRO:HB3	6:n:96:ASP:HB2	1.72	0.71
2:a:248:LEU:HD22	6:k:106:ARG:HG2	1.71	0.71
8:DI:184:VAL:HB	8:DI:196:MET:HB3	1.71	0.70
8:DD:217:ASP:HB2	8:DD:220:ALA:HB2	1.73	0.70
1:T:37:GLN:HG2	1:T:79:ARG:HG2	1.73	0.70
1:N:72:VAL:HB	1:S:28:ASN:HB3	1.74	0.70
1:O:3:SER:HA	2:c:70:GLN:HE21	1.57	0.70
1:Q:73:ARG:HD3	2:d:202:MET:HE2	1.74	0.70
2:d:49:LEU:HD22	4:8:322:PRO:HD2	1.72	0.70
5:j:6:ILE:HG21	5:j:122:VAL:HG21	1.73	0.70
7:r:104:VAL:HG23	7:v:89:ARG:HH22	1.57	0.70
1:J:257:LEU:HB2	1:O:240:TYR:HE1	1.58	0.69
2:a:146:LEU:HB2	2:a:155:VAL:HG12	1.74	0.69
2:a:188:GLU:HG3	2:a:189:ARG:HG3	1.72	0.69
1:G:176:THR:HB	1:G:203:GLU:HG3	1.72	0.69
1:J:98:LYS:O	1:J:212:GLY:HA3	1.92	0.69
1:O:1:MET:SD	2:c:70:GLN:NE2	2.64	0.69
2:a:170:GLU:HB2	2:a:185:ALA:HB2	1.74	0.69
1:A:1:MET:HE1	1:K:239:ALA:N	2.07	0.69
8:DI:319:ASN:ND2	8:DI:352:ASN:O	2.26	0.69
2:d:228:GLU:HG2	1:W:256:LYS:HZ3	1.56	0.69
8:DA:351:GLY:O	8:DA:352:ASN:ND2	2.24	0.69
1:U:136:VAL:HG12	1:U:138:PRO:HD2	1.74	0.69
8:DE:106:ARG:CZ	8:DJ:321:ALA:HB1	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:m:135:GLN:OE1	7:t:83:GLN:NE2	2.26	0.69
1:X:136:VAL:HG12	1:X:138:PRO:HD2	1.74	0.69
8:DA:24:ILE:HD11	8:DF:384:SER:HB3	1.75	0.68
1:E:164:GLN:NE2	1:E:166:ALA:O	2.27	0.68
8:DC:217:ASP:HB2	8:DC:220:ALA:HB2	1.74	0.68
1:B:252:GLN:OE1	1:F:237:GLN:NE2	2.21	0.68
1:J:260:LEU:HD22	1:O:248:SER:HB3	1.75	0.68
1:S:251:ASP:OD1	2:b:225:ARG:NH1	2.25	0.68
1:U:256:LYS:HG2	2:c:228:GLU:HG2	1.74	0.68
1:E:260:LEU:HD22	1:I:248:SER:HB2	1.76	0.68
1:K:242:ILE:HD13	1:P:226:VAL:HG11	1.76	0.68
1:G:67:GLN:NE2	1:L:185:GLU:OE1	2.23	0.67
1:B:253:MET:HE1	1:F:19:MET:HG2	1.77	0.67
1:N:19:MET:HB2	1:N:236:VAL:HG11	1.77	0.67
5:i:6:ILE:HD11	6:k:24:GLU:HA	1.76	0.67
8:DH:107:ASN:HB3	8:DH:138:THR:HG22	1.74	0.67
1:I:136:VAL:HG12	1:I:138:PRO:HD2	1.76	0.67
1:Q:3:SER:HA	2:d:70:GLN:HG3	1.75	0.67
1:U:176:THR:HG22	1:U:203:GLU:HG3	1.76	0.67
8:DI:322:ASN:ND2	8:DI:339:ALA:O	2.27	0.67
1:U:251:ASP:OD1	2:a:225:ARG:NH1	2.28	0.67
1:R:160:THR:HG22	1:R:167:PRO:HB3	1.78	0.66
8:DF:295:ASN:ND2	8:DF:299:THR:OG1	2.29	0.66
8:DH:295:ASN:ND2	8:DH:297:ASP:OD1	2.28	0.66
8:DE:137:ILE:HD11	8:DE:300:VAL:HG11	1.78	0.66
2:c:55:THR:OG1	5:f:26:SER:OG	2.13	0.66
3:2:9:UNK:O	5:i:104:ASN:ND2	2.26	0.66
8:DC:143:LEU:HD22	8:DC:288:ASP:HA	1.77	0.66
1:V:176:THR:HG22	1:V:203:GLU:HG2	1.78	0.66
8:DH:144:MET:SD	8:DH:310:GLN:NE2	2.68	0.66
5:j:47:VAL:HG12	5:j:67:VAL:HG22	1.78	0.66
5:j:129:THR:HA	6:n:120:LEU:HD11	1.77	0.66
8:DF:294:ILE:HG12	8:DF:300:VAL:HG12	1.77	0.66
1:R:37:GLN:HG2	1:R:79:ARG:HG2	1.76	0.65
8:DD:322:ASN:ND2	8:DD:339:ALA:O	2.30	0.65
1:U:239:ALA:O	1:U:243:ASN:ND2	2.30	0.65
5:h:20:ARG:NH1	6:m:34:ASP:OD2	2.30	0.65
8:DK:153:SER:HB3	8:DK:280:ASN:HB2	1.78	0.65
5:i:47:VAL:HG12	5:i:67:VAL:HG22	1.78	0.65
1:A:241:GLU:HG2	8:DA:398:THR:HG21	1.78	0.65
3:3:13:UNK:CB	6:n:36:PRO:HD2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:37:GLN:HG2	1:J:79:ARG:HG2	1.80	0.64
5:p:85:ALA:HB1	5:p:89:GLY:HA2	1.78	0.64
8:DA:322:ASN:ND2	8:DA:339:ALA:O	2.30	0.64
8:DB:281:GLN:OE1	8:DB:283:GLY:N	2.28	0.64
6:k:42:ASP:OD2	6:k:88:ARG:NH2	2.30	0.64
8:DE:170:PHE:HB3	8:DE:224:THR:HG23	1.79	0.64
1:A:98:LYS:O	1:A:212:GLY:CA	2.45	0.64
8:DE:79:GLN:HB2	8:DE:354:GLY:HA3	1.78	0.64
5:i:6:ILE:HG21	5:i:122:VAL:HG21	1.78	0.64
1:K:116:ARG:NH1	1:K:220:GLU:OE1	2.31	0.64
8:DB:322:ASN:ND2	8:DB:339:ALA:O	2.29	0.64
8:DB:146:ALA:HB2	8:DB:286:PRO:HD3	1.80	0.64
1:U:98:LYS:O	1:U:212:GLY:CA	2.45	0.64
8:DA:285:LYS:O	8:DA:306:ASN:ND2	2.31	0.64
8:DJ:207:GLU:OE2	8:DJ:231:LYS:NZ	2.30	0.64
8:DF:22:ASN:OD1	8:DF:26:ASN:ND2	2.31	0.64
8:DK:326:LEU:HB3	8:DK:334:TRP:HB3	1.78	0.64
1:D:136:VAL:HG12	1:D:138:PRO:HD2	1.80	0.64
8:DA:210:VAL:HB	8:DA:228:THR:HB	1.78	0.64
1:D:57:SER:HB3	1:D:60:THR:HG22	1.79	0.63
1:E:1:MET:HE1	1:J:239:ALA:N	2.13	0.63
1:N:66:LEU:HA	1:S:77:THR:HG22	1.79	0.63
1:O:195:THR:HG22	2:c:152:PRO:HB2	1.80	0.63
8:DD:285:LYS:O	8:DD:306:ASN:ND2	2.32	0.63
2:a:226:ARG:NH2	5:h:32:ASP:OD2	2.29	0.63
2:d:227:PHE:HE2	1:W:257:LEU:HB2	1.63	0.63
8:DK:294:ILE:HG12	8:DK:300:VAL:HG12	1.81	0.63
8:DH:150:THR:OG1	8:DH:282:ASN:ND2	2.31	0.63
2:e:31:THR:HG22	1:X:41:PHE:HB2	1.81	0.63
8:DE:150:THR:OG1	8:DE:282:ASN:ND2	2.28	0.63
8:DH:65:THR:H	8:DH:363:ALA:H	1.45	0.63
6:l:118:MET:HE1	7:r:60:THR:HG22	1.80	0.63
8:DK:35:GLY:HA2	8:DK:59:GLN:HA	1.80	0.63
1:E:66:LEU:HA	1:I:77:THR:HG22	1.80	0.63
1:P:9:LYS:NZ	2:a:72:ASP:OD1	2.22	0.63
1:R:42:GLU:OE2	1:R:73:ARG:NH1	2.32	0.63
6:m:102:MET:HB3	6:m:106:ARG:HH21	1.64	0.63
8:DB:156:ILE:HG21	8:DB:200:PHE:HE2	1.64	0.63
8:DH:165:PRO:HG2	8:DH:201:VAL:HG23	1.81	0.63
8:DI:22:ASN:OD1	8:DI:26:ASN:ND2	2.32	0.63
1:D:48:THR:HG22	1:D:67:GLN:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:180:ASN:HB3	1:O:198:SER:HA	1.80	0.63
7:q:89:ARG:NH2	7:q:90:ASN:OD1	2.30	0.63
1:C:169:GLN:NE2	1:C:171:GLY:O	2.32	0.62
5:g:31:ALA:HA	5:g:96:VAL:HG21	1.79	0.62
1:A:38:ARG:NH1	1:A:78:GLU:OE2	2.32	0.62
1:M:45:LEU:HB3	1:X:98:LYS:HE3	1.81	0.62
8:DB:122:THR:OG1	8:DB:129:GLN:NE2	2.32	0.62
8:DB:174:ASP:HB3	8:DB:177:SER:HB2	1.81	0.62
1:N:99:GLY:O	1:N:116:ARG:NH2	2.32	0.62
1:T:251:ASP:OD1	2:c:225:ARG:NH1	2.32	0.62
8:DD:161:THR:HG22	8:DJ:252:ASN:ND2	2.14	0.62
1:D:127:GLN:HA	1:D:141:THR:HA	1.80	0.62
1:G:55:GLN:HG2	1:W:169:GLN:NE2	2.14	0.62
8:DE:34:SER:HB3	8:DE:366:VAL:HG22	1.79	0.62
8:DE:159:ASN:ND2	8:DE:270:ASN:OD1	2.32	0.62
8:DF:285:LYS:O	8:DF:306:ASN:ND2	2.32	0.62
8:DK:33:LYS:HG2	8:DK:59:GLN:HB3	1.80	0.62
1:D:180:ASN:HB3	1:D:198:SER:HA	1.81	0.62
1:K:256:LYS:HG2	1:P:241:GLU:HG3	1.80	0.62
2:b:146:LEU:HB2	2:b:155:VAL:HG12	1.80	0.62
4:7:316:LEU:HD23	6:m:86:LEU:HD12	1.81	0.62
1:Q:19:MET:HB2	1:Q:236:VAL:HG11	1.81	0.62
2:c:25:ASN:HD21	2:c:37:GLN:H	1.45	0.62
5:g:85:ALA:HB1	5:g:89:GLY:HA2	1.82	0.62
1:D:42:GLU:OE2	1:D:73:ARG:NH2	2.32	0.62
1:E:28:ASN:HB3	8:DB:52:VAL:HG12	1.80	0.62
1:U:78:GLU:OE1	2:c:106:GLN:NE2	2.31	0.62
8:DE:19:VAL:O	8:DE:23:ASN:ND2	2.33	0.62
8:DF:22:ASN:CG	8:DK:49:GLY:HA3	2.25	0.62
8:DK:101:LYS:NZ	8:DK:110:ASN:O	2.33	0.62
1:U:142:ILE:HD13	1:U:149:ILE:HG12	1.82	0.62
8:DB:165:PRO:HG2	8:DB:201:VAL:HG23	1.82	0.62
8:DD:95:SER:HB2	8:DD:333:VAL:HG12	1.81	0.62
1:R:98:LYS:HD3	1:R:215:TYR:HE2	1.64	0.61
2:a:28:ASN:HD22	1:V:43:ASP:HB3	1.64	0.61
1:V:36:ARG:NH2	1:V:228:GLU:OE2	2.33	0.61
2:b:82:LEU:HD11	2:b:163:LEU:HD22	1.82	0.61
7:u:48:ARG:NH2	7:u:81:SER:OG	2.32	0.61
8:DI:295:ASN:ND2	8:DI:299:THR:OG1	2.34	0.61
1:A:177:THR:OG1	1:A:202:ASN:OD1	2.17	0.61
8:DD:18:ASP:OD1	8:DI:5:GLN:NE2	2.23	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:167:GLU:N	2:a:170:GLU:OE2	2.33	0.61
1:B:238:ARG:NE	8:DF:393:ASP:OD1	2.33	0.61
2:d:28:ASN:HB3	1:W:72:VAL:HB	1.82	0.61
5:j:6:ILE:HD11	6:n:24:GLU:HA	1.81	0.61
2:b:76:ARG:NH1	2:b:79:ASP:OD1	2.32	0.61
2:e:28:ASN:HB3	1:X:72:VAL:HB	1.82	0.61
8:DA:337:THR:O	8:DA:340:SER:OG	2.17	0.61
8:DG:196:MET:SD	8:DG:212:THR:OG1	2.58	0.61
8:DI:337:THR:O	8:DI:340:SER:OG	2.17	0.61
1:B:136:VAL:HG12	1:B:138:PRO:HD2	1.81	0.61
1:H:100:GLN:NE2	1:H:210:GLY:O	2.34	0.61
1:L:256:LYS:HG2	1:Q:241:GLU:HG2	1.83	0.61
1:M:98:LYS:O	1:M:212:GLY:CA	2.49	0.61
5:h:12:SER:OG	5:h:62:VAL:O	2.17	0.61
8:DB:203:THR:OG1	8:DB:207:GLU:OE2	2.18	0.61
1:O:36:ARG:HD3	1:O:80:LEU:HD12	1.82	0.61
1:Q:48:THR:HG22	1:Q:67:GLN:HG2	1.83	0.61
5:i:84:LEU:HD11	1:W:62:LEU:HD22	1.82	0.61
8:DF:206:ASN:ND2	8:DF:268:GLN:OE1	2.30	0.61
1:A:60:THR:HG21	1:O:108:PRO:HG3	1.83	0.60
1:I:78:GLU:OE1	1:N:121:GLN:NE2	2.33	0.60
1:E:188:GLY:HA2	8:DB:42:MET:HA	1.83	0.60
1:U:44:LEU:HB2	1:U:70:THR:HB	1.82	0.60
8:DD:146:ALA:HB2	8:DD:286:PRO:HD3	1.83	0.60
8:DK:102:LEU:HD23	8:DK:106:ARG:HE	1.66	0.60
1:B:92:SER:O	1:B:216:GLN:NE2	2.33	0.60
2:e:225:ARG:NH1	1:W:251:ASP:OD1	2.34	0.60
1:A:1:MET:HG3	1:A:2:ILE:HG12	1.83	0.60
1:E:241:GLU:HG2	8:DC:400:VAL:HG11	1.82	0.60
8:DB:105:ASN:OD1	8:DB:107:ASN:ND2	2.35	0.60
1:G:54:ALA:HB1	1:W:150:THR:HG21	1.81	0.60
1:H:174:ASN:ND2	1:H:203:GLU:OE2	2.34	0.60
2:b:170:GLU:HB2	2:b:185:ALA:HB2	1.83	0.60
5:g:72:ALA:HB3	5:g:95:ASN:HD22	1.67	0.60
5:p:72:ALA:O	5:p:95:ASN:ND2	2.35	0.60
1:V:98:LYS:O	1:V:212:GLY:CA	2.48	0.60
8:DJ:33:LYS:NZ	8:DJ:362:GLU:OE2	2.34	0.60
1:G:38:ARG:HH12	1:G:80:LEU:HD21	1.66	0.60
2:c:248:LEU:HD13	6:m:106:ARG:HG2	1.82	0.60
8:DE:16:ASN:HB2	8:DE:39:PHE:HZ	1.66	0.60
8:DF:184:VAL:HB	8:DF:196:MET:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DI:79:GLN:HB2	8:DI:354:GLY:HA3	1.83	0.60
8:DI:326:LEU:HB3	8:DI:334:TRP:HB3	1.83	0.60
1:A:123:ASP:OD1	1:A:127:GLN:N	2.35	0.60
7:r:46:SER:O	7:r:49:GLN:NE2	2.33	0.60
1:B:153:ARG:HD2	1:B:213:LEU:HD13	1.84	0.60
1:K:35:LYS:NZ	1:K:220:GLU:OE2	2.34	0.60
1:E:228:GLU:OE1	1:E:232:ASN:ND2	2.35	0.60
1:L:21:VAL:O	1:L:25:ASN:ND2	2.35	0.60
8:DD:317:LEU:HD11	8:DD:356:LEU:HD21	1.83	0.60
8:DF:19:VAL:O	8:DF:23:ASN:ND2	2.33	0.60
1:C:1:MET:N	1:C:1:MET:SD	2.75	0.59
1:F:1:MET:SD	1:F:1:MET:N	2.74	0.59
1:H:147:LEU:HB2	1:H:160:THR:HG23	1.84	0.59
1:S:6:TRP:CZ3	5:g:77:VAL:HG11	2.36	0.59
1:S:50:ARG:HE	1:S:51:GLN:H	1.50	0.59
8:DK:143:LEU:HD12	8:DK:286:PRO:HB2	1.83	0.59
1:F:48:THR:HG22	1:F:67:GLN:HG2	1.84	0.59
1:U:35:LYS:NZ	1:U:220:GLU:OE2	2.36	0.59
1:A:67:GLN:HE22	1:J:185:GLU:HG3	1.66	0.59
1:I:72:VAL:HB	1:N:28:ASN:HB3	1.83	0.59
1:U:106:MET:SD	1:U:137:GLN:NE2	2.76	0.59
8:DC:285:LYS:O	8:DC:306:ASN:ND2	2.34	0.59
8:DE:143:LEU:HD22	8:DE:288:ASP:HA	1.83	0.59
8:DE:150:THR:HG1	8:DE:282:ASN:HD21	1.47	0.59
8:DE:367:ASP:OD2	8:DE:369:SER:OG	2.17	0.59
1:A:238:ARG:NH1	8:DB:393:ASP:OD1	2.35	0.59
1:B:175:LEU:HD11	1:B:211:ALA:HB1	1.84	0.59
1:D:54:ALA:HB1	1:S:150:THR:HG21	1.84	0.59
2:a:148:PRO:HB2	1:V:210:GLY:HA3	1.83	0.59
6:o:41:ARG:HB3	6:o:85:LEU:HD12	1.83	0.59
1:R:3:SER:O	2:e:70:GLN:NE2	2.36	0.59
8:DA:149:THR:HB	8:DA:186:VAL:HG13	1.83	0.59
8:DI:184:VAL:N	8:DI:196:MET:O	2.35	0.59
1:U:41:PHE:HB2	2:c:31:THR:HG22	1.85	0.59
8:DG:199:TYR:HE2	8:DG:213:HIS:HB3	1.68	0.59
8:DD:105:ASN:OD1	8:DD:107:ASN:ND2	2.36	0.59
1:M:66:LEU:HA	1:R:77:THR:HG22	1.85	0.58
2:a:55:THR:OG1	5:h:30:ASN:ND2	2.36	0.58
8:DF:326:LEU:HB3	8:DF:334:TRP:HB3	1.84	0.58
1:D:38:ARG:NH2	1:D:78:GLU:OE2	2.32	0.58
1:K:25:ASN:HD21	1:K:37:GLN:H	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:82:SER:OG	1:O:223:ASN:ND2	2.37	0.58
3:1:9:UNK:O	5:f:104:ASN:ND2	2.33	0.58
8:DI:269:GLN:O	8:DI:271:THR:N	2.36	0.58
1:B:35:LYS:NZ	1:B:220:GLU:OE2	2.36	0.58
1:T:43:ASP:OD1	2:b:28:ASN:ND2	2.34	0.58
8:DD:19:VAL:O	8:DD:23:ASN:ND2	2.36	0.58
8:DG:73:LEU:HD11	8:DG:108:LEU:HD11	1.84	0.58
8:DI:23:ASN:ND2	8:DI:35:GLY:O	2.34	0.58
1:S:237:GLN:O	1:S:241:GLU:HG2	2.04	0.58
8:DA:288:ASP:OD1	8:DA:305:SER:OG	2.21	0.58
8:DB:337:THR:O	8:DB:340:SER:OG	2.20	0.58
8:DE:362:GLU:N	8:DE:362:GLU:OE1	2.35	0.58
1:C:98:LYS:O	1:C:212:GLY:HA3	2.04	0.58
1:C:148:SER:OG	1:C:160:THR:OG1	2.20	0.58
1:Q:92:SER:O	1:Q:216:GLN:NE2	2.36	0.58
1:R:256:LYS:HG2	1:W:241:GLU:HG2	1.84	0.58
8:DC:159:ASN:ND2	8:DC:270:ASN:OD1	2.36	0.58
1:D:83:GLN:NE2	1:D:84:GLY:O	2.36	0.58
2:a:91:GLN:HB3	2:a:119:PRO:HG2	1.85	0.58
1:V:38:ARG:NH2	1:V:78:GLU:OE2	2.37	0.58
1:F:144:ALA:O	1:F:145:ASN:ND2	2.36	0.58
2:c:54:ARG:NH2	6:m:92:GLN:OE1	2.37	0.58
1:X:44:LEU:HB2	1:X:70:THR:HB	1.84	0.58
8:DF:79:GLN:HB2	8:DF:354:GLY:HA3	1.85	0.58
8:DF:81:GLY:O	8:DF:96:ARG:NH1	2.37	0.58
1:H:82:SER:OG	1:H:223:ASN:ND2	2.32	0.58
1:Q:42:GLU:HG3	1:V:189:GLU:HA	1.85	0.58
2:b:44:VAL:HG11	4:6:328:ILE:HD13	1.86	0.58
2:d:240:ASN:HD21	5:i:109:SER:HA	1.67	0.58
8:DF:101:LYS:NZ	8:DF:110:ASN:O	2.37	0.58
1:B:260:LEU:HD22	1:F:248:SER:HB3	1.86	0.58
1:G:36:ARG:HD2	1:G:80:LEU:HD12	1.85	0.58
1:G:72:VAL:HB	1:L:28:ASN:HB3	1.86	0.58
1:L:88:GLN:NE2	1:L:90:ASN:OD1	2.34	0.58
2:b:9:MET:HB3	5:f:103:VAL:HG11	1.86	0.58
2:e:115:ILE:HG22	2:e:116:GLN:HG3	1.86	0.58
6:n:88:ARG:NH1	6:n:105:GLU:OE2	2.37	0.58
1:E:242:ILE:HD12	1:I:230:LEU:HD21	1.86	0.57
1:V:175:LEU:HD11	1:V:211:ALA:HB1	1.86	0.57
8:DD:149:THR:HA	8:DD:283:GLY:HA3	1.85	0.57
1:A:140:ILE:HD12	1:A:171:GLY:HA3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:19:MET:HB2	1:K:236:VAL:HG11	1.86	0.57
5:g:51:VAL:HG11	5:p:42:TYR:CD1	2.39	0.57
1:K:73:ARG:NH2	1:P:189:GLU:OE1	2.37	0.57
1:Q:44:LEU:HD11	2:d:205:VAL:HG11	1.86	0.57
2:d:83:GLN:HG3	2:d:84:GLN:H	1.69	0.57
1:C:242:ILE:HD12	1:G:230:LEU:HD21	1.86	0.57
1:F:228:GLU:OE1	1:F:232:ASN:ND2	2.37	0.57
1:S:37:GLN:HG2	1:S:79:ARG:HG2	1.85	0.57
2:a:106:GLN:NE2	1:V:78:GLU:OE1	2.35	0.57
2:d:136:THR:OG1	2:d:144:SER:OG	2.21	0.57
7:r:104:VAL:HA	7:v:89:ARG:HH12	1.70	0.57
8:DG:99:GLN:HG3	8:DG:111:MET:HE3	1.85	0.57
8:DI:144:MET:SD	8:DI:306:ASN:ND2	2.65	0.57
1:S:43:ASP:N	1:S:43:ASP:OD1	2.36	0.57
2:d:114:THR:OG1	2:d:115:ILE:O	2.19	0.57
6:m:42:ASP:OD1	6:m:43:ILE:N	2.37	0.57
8:DE:87:ASP:OD1	8:DE:91:SER:N	2.37	0.57
8:DG:299:THR:HG22	8:DG:314:GLN:HB3	1.85	0.57
1:A:151:ILE:HG12	1:A:157:VAL:HG12	1.86	0.57
1:B:54:ALA:HB3	1:B:62:LEU:HD12	1.87	0.57
1:K:176:THR:HG22	1:K:203:GLU:HG2	1.85	0.57
1:N:116:ARG:NH1	1:N:220:GLU:OE1	2.37	0.57
1:N:237:GLN:O	1:N:241:GLU:HG2	2.05	0.57
2:e:90:VAL:HG12	2:e:120:VAL:HA	1.87	0.57
5:h:85:ALA:HB1	5:h:89:GLY:HA2	1.85	0.57
5:j:52:ASP:HB3	5:j:63:LYS:HD3	1.87	0.57
6:o:127:LEU:HD11	7:v:76:GLN:HB3	1.86	0.57
1:B:231:VAL:O	1:B:235:GLN:HG2	2.05	0.57
1:E:54:ALA:HB3	1:E:62:LEU:HD13	1.87	0.57
1:G:1:MET:N	1:G:1:MET:SD	2.78	0.57
8:DC:23:ASN:ND2	8:DC:35:GLY:O	2.36	0.57
8:DI:207:GLU:HG3	8:DI:231:LYS:HG2	1.87	0.57
2:a:247:LEU:HB2	5:h:116:ILE:HG23	1.87	0.57
8:DD:210:VAL:HB	8:DD:228:THR:HB	1.87	0.57
1:G:82:SER:HB3	1:G:223:ASN:HD22	1.70	0.56
1:K:228:GLU:OE1	1:K:232:ASN:ND2	2.38	0.56
1:S:257:LEU:CD1	5:g:99:VAL:HG12	2.35	0.56
2:a:237:VAL:HG22	5:h:21:LEU:HD21	1.87	0.56
2:c:130:PRO:HD3	2:c:158:VAL:HG21	1.87	0.56
6:k:42:ASP:OD1	6:k:43:ILE:N	2.35	0.56
8:DA:18:ASP:OD1	8:DF:5:GLN:NE2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:THR:HG22	1:C:67:GLN:HG2	1.86	0.56
2:d:82:LEU:HD21	2:d:88:LEU:HG	1.87	0.56
8:DJ:331:ASP:O	8:DJ:333:VAL:N	2.39	0.56
1:C:230:LEU:HD12	8:DJ:399:LEU:HG	1.87	0.56
1:E:153:ARG:NH2	8:DC:112:GLN:O	2.39	0.56
1:J:108:PRO:HG2	1:P:153:ARG:HH21	1.70	0.56
1:R:251:ASP:OD1	1:X:238:ARG:NH2	2.39	0.56
2:d:223:ASN:OD1	2:d:226:ARG:NH2	2.38	0.56
1:V:28:ASN:O	1:V:28:ASN:ND2	2.34	0.56
1:V:123:ASP:OD1	1:V:124:GLN:N	2.35	0.56
8:DC:160:SER:HB2	8:DI:192:ASN:HD21	1.70	0.56
8:DG:146:ALA:HB2	8:DG:286:PRO:HD3	1.86	0.56
8:DI:299:THR:HG22	8:DI:314:GLN:HB3	1.87	0.56
1:J:48:THR:HG22	1:J:67:GLN:HG2	1.88	0.56
8:DA:178:TYR:HA	8:DA:201:VAL:HG22	1.87	0.56
8:DD:102:LEU:HD23	8:DD:106:ARG:HD2	1.87	0.56
8:DK:317:LEU:HD12	8:DK:353:PHE:HB3	1.86	0.56
1:B:55:GLN:NE2	1:B:57:SER:O	2.38	0.56
1:G:230:LEU:HD12	8:DE:399:LEU:HG	1.88	0.56
8:DH:33:LYS:HA	8:DH:365:ASN:HD21	1.70	0.56
1:O:35:LYS:NZ	1:O:220:GLU:OE2	2.39	0.56
6:o:45:PHE:HE2	7:u:61:LEU:HA	1.70	0.56
8:DC:87:ASP:OD2	8:DC:89:ASN:ND2	2.35	0.56
8:DH:188:ASP:OD1	8:DH:192:ASN:N	2.37	0.56
1:D:29:VAL:O	1:D:222:SER:OG	2.20	0.56
1:P:6:TRP:CE3	2:a:70:GLN:HG2	2.40	0.56
1:R:92:SER:O	1:R:216:GLN:NE2	2.39	0.56
8:DB:285:LYS:O	8:DB:306:ASN:ND2	2.39	0.56
1:F:180:ASN:ND2	1:K:122:VAL:O	2.39	0.56
1:J:238:ARG:NH1	1:J:241:GLU:OE1	2.35	0.56
1:O:37:GLN:HG2	1:O:79:ARG:HG2	1.88	0.56
8:DJ:397:ASN:OD1	8:DJ:401:ASN:ND2	2.39	0.56
1:B:162:GLN:OE1	8:DK:89:ASN:ND2	2.39	0.56
1:B:218:TYR:OH	8:DK:53:LYS:NZ	2.33	0.56
1:D:175:LEU:HD11	1:D:211:ALA:HB1	1.86	0.56
2:d:146:LEU:HB2	2:d:155:VAL:HG12	1.86	0.56
5:i:132:LEU:HD21	6:k:123:LEU:HD22	1.87	0.56
8:DJ:326:LEU:HB3	8:DJ:334:TRP:HB3	1.87	0.56
1:E:60:THR:HG21	1:N:108:PRO:HG3	1.87	0.56
1:Q:254:LEU:HD23	1:W:238:ARG:HG3	1.88	0.56
5:j:19:LYS:HD2	5:j:64:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DD:80:ASN:OD1	8:DD:80:ASN:N	2.34	0.56
8:DI:149:THR:HG21	8:DI:186:VAL:HG12	1.87	0.56
1:N:34:PHE:HB3	1:N:222:SER:HB3	1.87	0.55
1:W:79:ARG:NH2	1:W:184:LEU:O	2.39	0.55
1:H:256:LYS:HG2	1:M:241:GLU:HG2	1.88	0.55
5:i:76:LEU:HD12	5:i:90:TYR:HB3	1.87	0.55
1:B:49:ILE:HB	1:B:66:LEU:HD23	1.88	0.55
1:I:140:ILE:HD12	1:I:171:GLY:HA3	1.89	0.55
1:R:194:GLU:OE1	1:R:194:GLU:N	2.39	0.55
5:f:6:ILE:HG21	5:f:122:VAL:HG21	1.86	0.55
5:h:19:LYS:NZ	6:k:91:ASP:OD1	2.39	0.55
1:E:42:GLU:OE2	1:E:73:ARG:NE	2.39	0.55
1:G:56:SER:O	1:W:153:ARG:N	2.39	0.55
8:DA:150:THR:OG1	8:DA:282:ASN:ND2	2.30	0.55
8:DE:172:VAL:HG11	8:DE:222:ALA:HB1	1.87	0.55
1:N:37:GLN:HB3	1:N:79:ARG:HG2	1.89	0.55
8:DF:22:ASN:ND2	8:DK:49:GLY:HA3	2.22	0.55
1:H:54:ALA:HB1	1:X:150:THR:HG21	1.89	0.55
2:b:25:ASN:ND2	2:b:37:GLN:O	2.37	0.55
2:c:162:LYS:HG3	2:c:195:ALA:HB2	1.88	0.55
8:DC:157:ASN:HB2	8:DC:275:ASN:HB3	1.87	0.55
1:A:35:LYS:O	1:A:79:ARG:NH1	2.40	0.55
1:A:185:GLU:OE1	8:DA:46:SER:HB2	2.06	0.55
1:U:154:ASP:OD1	1:U:155:GLY:N	2.34	0.55
2:b:86:GLY:O	2:b:101:ARG:NH1	2.40	0.55
8:DB:188:ASP:OD1	8:DB:192:ASN:N	2.40	0.55
8:DC:73:LEU:HD11	8:DC:108:LEU:HD11	1.88	0.55
1:A:98:LYS:HE3	8:DG:44:ALA:HA	1.88	0.55
1:I:175:LEU:HD11	1:I:211:ALA:HB1	1.89	0.55
1:R:44:LEU:HB2	1:R:70:THR:HG23	1.89	0.55
1:B:57:SER:HA	1:Q:154:ASP:CG	2.31	0.55
1:D:59:GLN:N	1:D:59:GLN:OE1	2.40	0.55
1:H:210:GLY:N	1:M:162:GLN:OE1	2.34	0.55
2:d:58:THR:HG21	4:8:328:ILE:HD12	1.89	0.55
8:DD:127:THR:O	8:DD:129:GLN:NE2	2.40	0.55
8:DD:150:THR:HG22	8:DD:151:THR:HG23	1.89	0.55
8:DH:33:LYS:NZ	8:DH:62:THR:O	2.36	0.55
8:DI:71:ARG:NH1	8:DI:99:GLN:OE1	2.40	0.55
1:E:54:ALA:HB1	1:T:150:THR:HG21	1.88	0.54
1:S:175:LEU:HD11	1:S:211:ALA:HB1	1.87	0.54
2:c:77:PRO:HG2	2:c:78:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:114:THR:OG1	2:e:115:ILE:O	2.24	0.54
1:E:59:GLN:OE1	1:E:59:GLN:N	2.41	0.54
5:f:35:THR:HB	5:f:84:LEU:HD21	1.90	0.54
8:DC:299:THR:HG22	8:DC:314:GLN:HB3	1.90	0.54
5:g:58:ALA:O	5:p:45:LYS:HE3	2.06	0.54
8:DA:156:ILE:O	8:DA:266:SER:OG	2.15	0.54
1:K:72:VAL:HB	1:P:28:ASN:HB3	1.89	0.54
1:U:203:GLU:OE1	1:U:203:GLU:N	2.40	0.54
2:c:82:LEU:HD21	2:c:88:LEU:HG	1.88	0.54
2:c:133:SER:HA	2:c:148:PRO:HD3	1.90	0.54
1:V:82:SER:OG	1:V:223:ASN:ND2	2.40	0.54
8:DD:167:LYS:HG3	8:DD:169:PRO:HD2	1.89	0.54
8:DE:22:ASN:OD1	8:DE:26:ASN:ND2	2.41	0.54
8:DK:97:ASN:OD1	8:DK:332:ASN:ND2	2.40	0.54
1:D:194:GLU:OE1	1:D:194:GLU:N	2.31	0.54
1:F:1:MET:HE1	1:L:238:ARG:HB2	1.88	0.54
1:F:82:SER:OG	1:F:223:ASN:ND2	2.39	0.54
1:H:72:VAL:HB	1:M:28:ASN:HB3	1.88	0.54
1:S:147:LEU:HB2	1:S:160:THR:HG23	1.89	0.54
5:g:6:ILE:HG12	5:g:122:VAL:HG21	1.88	0.54
5:j:97:ASP:OD1	5:j:98:VAL:N	2.40	0.54
8:DC:154:MET:HE1	8:DC:156:ILE:HB	1.90	0.54
8:DG:337:THR:O	8:DG:340:SER:OG	2.22	0.54
8:DK:159:ASN:ND2	8:DK:270:ASN:OD1	2.40	0.54
1:E:145:ASN:HA	8:DB:352:ASN:HD22	1.71	0.54
5:j:111:SER:O	5:j:115:ASN:ND2	2.40	0.54
1:X:43:ASP:N	1:X:43:ASP:OD1	2.41	0.54
8:DC:126:PRO:HG2	8:DC:310:GLN:HE22	1.73	0.54
8:DD:34:SER:HB3	8:DD:366:VAL:HG22	1.90	0.54
8:DD:117:THR:HA	8:DD:136:PRO:HA	1.89	0.54
8:DF:171:SER:N	8:DF:177:SER:OG	2.39	0.54
5:j:78:TYR:HB2	5:j:90:TYR:HE1	1.73	0.54
8:DB:238:LEU:HD23	8:DB:264:LEU:HA	1.90	0.54
8:DE:301:VAL:HG22	8:DE:311:VAL:HG22	1.89	0.54
8:DH:19:VAL:O	8:DH:23:ASN:ND2	2.29	0.54
1:B:240:TYR:CG	8:DE:395:ILE:HD11	2.43	0.54
1:T:142:ILE:HD13	1:T:149:ILE:HD13	1.90	0.54
5:f:111:SER:O	5:f:115:ASN:ND2	2.41	0.54
2:d:225:ARG:HG3	1:V:254:LEU:HD23	1.89	0.54
8:DK:337:THR:O	8:DK:340:SER:OG	2.23	0.54
1:M:53:GLY:HA2	1:R:197:SER:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:13:UNK:H	6:o:36:PRO:HG2	1.73	0.54
4:9:315:ALA:O	6:o:88:ARG:HG3	2.08	0.54
5:g:41:PRO:HG2	5:g:92:LYS:HD3	1.89	0.54
1:V:37:GLN:OE1	1:V:79:ARG:NH2	2.39	0.54
8:DD:362:GLU:OE1	8:DD:362:GLU:N	2.40	0.54
8:DF:150:THR:OG1	8:DF:282:ASN:ND2	2.36	0.54
1:E:257:LEU:HB2	1:I:240:TYR:HE1	1.72	0.53
1:P:175:LEU:HD11	1:P:211:ALA:HB1	1.90	0.53
8:DB:189:SER:HG	8:DB:255:THR:HG1	1.56	0.53
8:DF:5:GLN:NE2	8:DF:49:GLY:O	2.41	0.53
1:E:35:LYS:NZ	1:E:220:GLU:OE2	2.41	0.53
1:J:1:MET:N	1:J:1:MET:SD	2.81	0.53
1:K:140:ILE:HD13	1:K:157:VAL:HG11	1.89	0.53
2:a:228:GLU:HG2	1:V:256:LYS:HG2	1.89	0.53
8:DK:74:ASP:N	8:DK:74:ASP:OD1	2.41	0.53
1:K:175:LEU:HD13	1:K:206:PRO:HG3	1.89	0.53
1:M:147:LEU:HB2	1:M:160:THR:HG23	1.90	0.53
1:B:28:ASN:HB3	8:DE:52:VAL:HB	1.91	0.53
2:d:207:GLU:OE1	2:d:207:GLU:N	2.34	0.53
8:DB:178:TYR:HA	8:DB:201:VAL:HB	1.89	0.53
1:A:94:ASP:N	1:A:94:ASP:OD1	2.40	0.53
1:E:48:THR:HG22	1:E:67:GLN:HG2	1.89	0.53
1:F:92:SER:HA	1:F:216:GLN:HE21	1.72	0.53
1:I:238:ARG:NH1	1:I:241:GLU:OE1	2.41	0.53
8:DI:247:THR:HG22	8:DI:258:THR:HA	1.89	0.53
8:DJ:101:LYS:N	8:DJ:109:VAL:O	2.41	0.53
6:l:42:ASP:OD1	6:l:42:ASP:N	2.41	0.53
6:o:120:LEU:HD11	5:p:129:THR:HA	1.90	0.53
8:DG:122:THR:OG1	8:DG:129:GLN:NE2	2.42	0.53
1:F:43:ASP:HA	1:F:72:VAL:HA	1.90	0.53
1:J:42:GLU:HB3	1:O:189:GLU:HA	1.91	0.53
1:K:1:MET:N	1:K:1:MET:SD	2.81	0.53
2:a:227:PHE:HE1	1:V:257:LEU:HB2	1.73	0.53
2:e:224:ALA:HA	1:X:253:MET:SD	2.49	0.53
8:DD:295:ASN:OD1	8:DD:295:ASN:N	2.41	0.53
1:E:98:LYS:HE3	8:DH:44:ALA:HA	1.91	0.53
2:c:55:THR:O	5:f:30:ASN:ND2	2.40	0.53
1:V:195:THR:HG23	1:V:197:SER:H	1.73	0.53
1:B:29:VAL:O	1:B:222:SER:OG	2.21	0.53
1:I:2:ILE:HG22	1:I:4:SER:H	1.74	0.53
1:I:257:LEU:HB2	1:N:240:TYR:HE1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:45:LEU:O	1:Q:70:THR:OG1	2.25	0.53
2:d:228:GLU:HG2	1:W:256:LYS:NZ	2.24	0.53
1:X:228:GLU:O	1:X:232:ASN:ND2	2.31	0.53
8:DE:331:ASP:OD1	8:DE:331:ASP:N	2.40	0.53
8:DH:355:LYS:NZ	8:DH:357:THR:OG1	2.34	0.53
8:DK:143:LEU:HD23	8:DK:143:LEU:H	1.74	0.53
1:T:154:ASP:OD1	1:T:155:GLY:N	2.34	0.53
8:DD:159:ASN:ND2	8:DD:270:ASN:OD1	2.42	0.53
8:DG:171:SER:N	8:DG:177:SER:OG	2.40	0.53
1:B:85:ASN:OD1	1:B:221:THR:OG1	2.27	0.52
1:E:53:GLY:HA2	1:I:197:SER:HB3	1.90	0.52
1:G:36:ARG:HH11	1:G:80:LEU:HD12	1.74	0.52
1:S:154:ASP:O	1:S:172:GLN:NE2	2.41	0.52
2:a:247:LEU:HD11	5:h:119:LEU:HD13	1.90	0.52
1:H:57:SER:OG	1:H:60:THR:OG1	2.25	0.52
1:I:50:ARG:HH12	1:N:75:VAL:HG23	1.74	0.52
1:I:151:ILE:HG12	1:I:157:VAL:HG22	1.91	0.52
1:J:239:ALA:O	1:J:243:ASN:ND2	2.40	0.52
2:a:35:ARG:HH11	2:a:101:ARG:HD3	1.73	0.52
2:e:247:LEU:HD11	5:j:119:LEU:HD13	1.92	0.52
5:g:110:ARG:CZ	1:X:255:GLN:HB2	2.39	0.52
8:DI:73:LEU:HD11	8:DI:108:LEU:HD11	1.90	0.52
1:O:91:ASN:OD1	1:O:92:SER:N	2.39	0.52
1:U:102:PHE:HB3	1:U:114:TYR:HB3	1.91	0.52
5:f:109:SER:O	5:f:113:GLN:HG2	2.09	0.52
6:k:127:LEU:HD13	7:q:76:GLN:HB3	1.91	0.52
8:DC:159:ASN:HA	8:DC:270:ASN:HA	1.91	0.52
8:DG:162:ASP:OD2	8:DG:179:ASN:ND2	2.41	0.52
1:E:238:ARG:NE	8:DC:393:ASP:OD1	2.40	0.52
5:g:59:THR:HG22	5:p:45:LYS:HD2	1.91	0.52
8:DC:212:THR:HG22	8:DC:227:SER:HB3	1.91	0.52
8:DG:16:ASN:HB2	8:DG:39:PHE:HZ	1.75	0.52
1:J:29:VAL:O	1:J:222:SER:OG	2.27	0.52
1:N:9:LYS:NZ	1:T:228:GLU:OE2	2.42	0.52
6:k:98:ASN:OD1	6:k:100:VAL:HG12	2.10	0.52
1:F:33:GLY:N	1:F:220:GLU:O	2.43	0.52
1:F:93:LYS:HD3	1:F:121:GLN:HA	1.92	0.52
1:K:257:LEU:HD22	1:P:240:TYR:OH	2.09	0.52
5:p:111:SER:O	5:p:115:ASN:ND2	2.42	0.52
1:V:29:VAL:O	1:V:222:SER:OG	2.21	0.52
8:DA:94:TYR:O	8:DA:334:TRP:N	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DC:139:ILE:HA	8:DC:312:LEU:HD22	1.90	0.52
8:DD:199:TYR:HB2	8:DD:211:TYR:HB2	1.91	0.52
8:DH:95:SER:HB2	8:DH:333:VAL:HG12	1.92	0.52
1:H:56:SER:O	1:X:153:ARG:N	2.41	0.52
1:P:233:MET:HA	1:P:236:VAL:HG22	1.91	0.52
6:n:85:LEU:HD23	6:n:85:LEU:H	1.74	0.52
1:E:117:ASP:OD1	1:E:118:GLY:N	2.43	0.52
1:K:79:ARG:HH22	1:K:184:LEU:HB2	1.74	0.52
6:n:42:ASP:OD1	6:n:43:ILE:N	2.43	0.52
8:DC:301:VAL:HG22	8:DC:311:VAL:HG12	1.92	0.52
8:DI:159:ASN:HB3	8:DI:162:ASP:HB2	1.92	0.52
1:B:256:LYS:HG2	1:F:241:GLU:HG2	1.92	0.52
5:p:126:MET:HG3	7:v:68:LEU:CD2	2.39	0.52
6:n:33:ALA:HA	6:n:100:VAL:HG11	1.91	0.52
1:V:33:GLY:N	1:V:220:GLU:O	2.42	0.52
1:V:44:LEU:HB2	1:V:70:THR:HB	1.91	0.52
1:W:91:ASN:OD1	1:W:92:SER:N	2.43	0.52
8:DH:299:THR:HG22	8:DH:314:GLN:HB3	1.90	0.52
8:DI:397:ASN:OD1	8:DI:401:ASN:ND2	2.43	0.52
1:B:98:LYS:O	1:B:212:GLY:CA	2.55	0.52
1:B:242:ILE:HG13	1:F:226:VAL:HG11	1.91	0.52
1:I:66:LEU:HD12	1:N:77:THR:HG23	1.92	0.52
1:J:56:SER:C	2:c:138:ALA:HB1	2.34	0.52
8:DB:33:LYS:NZ	8:DB:362:GLU:OE2	2.43	0.52
8:DD:151:THR:OG1	8:DD:282:ASN:ND2	2.38	0.52
8:DE:326:LEU:HB3	8:DE:334:TRP:HB3	1.92	0.52
1:T:72:VAL:HB	2:b:28:ASN:HB3	1.92	0.51
2:e:223:ASN:OD1	2:e:226:ARG:NH2	2.43	0.51
5:g:125:MET:HE2	5:p:109:SER:HA	1.91	0.51
1:X:253:MET:HE2	1:X:253:MET:HA	1.91	0.51
8:DF:377:VAL:O	8:DF:381:ASN:ND2	2.41	0.51
8:DI:116:LEU:HD21	8:DI:315:ILE:HG12	1.91	0.51
2:a:9:MET:HB3	5:i:103:VAL:HG21	1.92	0.51
5:p:2:ALA:HB2	7:v:66:ILE:O	2.10	0.51
8:DF:337:THR:O	8:DF:340:SER:OG	2.24	0.51
8:DJ:322:ASN:ND2	8:DJ:339:ALA:O	2.44	0.51
1:C:28:ASN:HB3	8:DD:52:VAL:HB	1.91	0.51
1:E:255:GLN:HB2	1:J:238:ARG:NH2	2.26	0.51
1:F:83:GLN:NE2	1:F:84:GLY:O	2.38	0.51
1:H:62:LEU:O	1:M:197:SER:OG	2.27	0.51
1:N:187:ILE:HD13	1:N:193:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:72:VAL:HB	1:U:28:ASN:HB3	1.93	0.51
2:d:215:GLU:OE1	1:V:9:LYS:NZ	2.41	0.51
8:DE:317:LEU:HD11	8:DE:356:LEU:HD21	1.92	0.51
1:J:175:LEU:HD11	1:J:211:ALA:HB1	1.92	0.51
1:N:51:GLN:NE2	1:S:75:VAL:O	2.33	0.51
5:f:34:VAL:HG13	5:f:35:THR:HG22	1.93	0.51
8:DF:367:ASP:OD1	8:DF:367:ASP:N	2.40	0.51
1:R:43:ASP:OD1	1:R:43:ASP:N	2.24	0.51
2:a:66:MET:HG3	2:a:168:GLY:HA3	1.90	0.51
5:g:111:SER:O	5:g:115:ASN:ND2	2.38	0.51
6:l:33:ALA:O	6:l:98:ASN:ND2	2.44	0.51
6:m:118:MET:HE2	7:s:59:PHE:HE2	1.75	0.51
6:k:33:ALA:O	6:k:98:ASN:ND2	2.44	0.51
8:DE:197:ASN:HB2	8:DE:213:HIS:HB3	1.92	0.51
8:DE:337:THR:O	8:DE:340:SER:OG	2.26	0.51
8:DF:299:THR:HA	8:DF:314:GLN:HA	1.92	0.51
8:DI:269:GLN:OE1	8:DI:269:GLN:N	2.43	0.51
1:K:33:GLY:N	1:K:220:GLU:O	2.40	0.51
1:T:245:LYS:HG2	2:b:217:MET:HE1	1.93	0.51
6:m:11:PHE:CZ	7:s:57:GLU:HG3	2.45	0.51
1:C:49:ILE:HB	1:C:66:LEU:HD22	1.93	0.51
1:F:38:ARG:HD3	1:F:80:LEU:HD11	1.92	0.51
1:K:260:LEU:HD12	1:P:248:SER:HB2	1.91	0.51
2:b:121:ILE:HA	2:b:126:PRO:HA	1.91	0.51
1:J:9:LYS:HG2	1:P:231:VAL:HG21	1.93	0.51
1:L:48:THR:HG22	1:L:67:GLN:HG2	1.92	0.51
2:e:14:GLN:HG3	2:e:58:THR:HA	1.92	0.51
8:DA:33:LYS:NZ	8:DA:362:GLU:OE2	2.44	0.51
8:DD:210:VAL:N	8:DD:228:THR:O	2.37	0.51
1:F:37:GLN:HG2	1:F:79:ARG:HG2	1.92	0.51
1:H:35:LYS:NZ	1:H:220:GLU:OE2	2.43	0.51
5:f:102:MET:O	5:f:106:MET:HG2	2.11	0.51
5:h:34:VAL:HG12	5:h:93:MET:HE1	1.92	0.51
6:m:6:ASP:O	6:m:10:ARG:HB2	2.11	0.51
8:DE:26:ASN:OD1	8:DJ:41:ASP:HB3	2.10	0.51
8:DI:212:THR:HG21	8:DI:246:ILE:HG13	1.92	0.51
8:DJ:383:GLN:OE1	8:DJ:383:GLN:HA	2.10	0.51
8:DK:365:ASN:O	8:DK:365:ASN:ND2	2.43	0.51
1:G:149:ILE:HG22	1:G:159:VAL:HB	1.92	0.50
2:b:247:LEU:HD13	5:g:119:LEU:HD13	1.92	0.50
8:DE:295:ASN:OD1	8:DE:295:ASN:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DK:79:GLN:HG2	8:DK:354:GLY:HA3	1.93	0.50
1:G:66:LEU:HA	1:L:77:THR:HG22	1.94	0.50
1:J:98:LYS:O	1:J:212:GLY:CA	2.59	0.50
1:S:6:TRP:CE3	5:g:77:VAL:HG11	2.46	0.50
1:U:141:THR:HG23	1:U:141:THR:O	2.11	0.50
1:W:147:LEU:HB2	1:W:160:THR:HG23	1.93	0.50
8:DA:365:ASN:ND2	8:DA:365:ASN:O	2.43	0.50
8:DD:143:LEU:HD22	8:DD:288:ASP:HA	1.93	0.50
8:DH:337:THR:OG1	8:DH:338:GLN:N	2.43	0.50
8:DI:106:ARG:HH12	8:DI:141:ASN:HB2	1.75	0.50
1:G:255:GLN:HE22	1:G:256:LYS:HE3	1.75	0.50
1:H:60:THR:HG21	1:R:108:PRO:HB3	1.93	0.50
2:c:45:PRO:HB3	2:c:55:THR:HG22	1.93	0.50
2:e:9:MET:HB3	5:p:103:VAL:HG21	1.93	0.50
3:4:14:UNK:O	5:p:50:GLN:NE2	2.43	0.50
1:V:35:LYS:NZ	1:V:220:GLU:OE2	2.35	0.50
1:X:189:GLU:OE1	1:X:189:GLU:N	2.42	0.50
8:DB:34:SER:HB3	8:DB:366:VAL:HG22	1.93	0.50
8:DB:179:ASN:OD1	8:DB:202:LYS:N	2.44	0.50
8:DC:331:ASP:OD1	8:DC:331:ASP:N	2.44	0.50
8:DE:337:THR:OG1	8:DE:338:GLN:N	2.45	0.50
1:P:151:ILE:N	1:P:216:GLN:OE1	2.39	0.50
8:DH:337:THR:O	8:DH:340:SER:OG	2.24	0.50
1:A:37:GLN:HG2	1:A:79:ARG:HD3	1.94	0.50
1:K:184:LEU:HB3	1:K:192:TYR:HB3	1.94	0.50
5:g:2:ALA:HA	7:r:67:ALA:HA	1.92	0.50
8:DI:150:THR:N	8:DI:282:ASN:OD1	2.30	0.50
1:B:1:MET:HB2	1:B:5:LEU:HD23	1.94	0.50
1:E:33:GLY:N	1:E:220:GLU:O	2.45	0.50
1:H:46:TYR:CD1	1:H:69:GLY:HA2	2.47	0.50
2:a:62:PRO:HA	1:V:63:PRO:HG2	1.94	0.50
2:e:143:ILE:HD11	2:e:161:LEU:HG	1.92	0.50
8:DC:32:PHE:O	8:DC:365:ASN:ND2	2.43	0.50
8:DD:151:THR:HG1	8:DD:282:ASN:HD21	1.55	0.50
8:DF:44:ALA:H	8:DF:50:LEU:HD13	1.76	0.50
8:DK:188:ASP:OD1	8:DK:192:ASN:N	2.39	0.50
1:B:187:ILE:HG13	1:B:191:LEU:HB2	1.94	0.50
1:F:9:LYS:HG2	1:L:231:VAL:HG21	1.94	0.50
1:J:230:LEU:HD12	8:DB:399:LEU:HG	1.93	0.50
1:O:254:LEU:HD23	1:U:238:ARG:HG3	1.93	0.50
3:4:13:UNK:CB	5:p:49:PHE:H	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:62:LEU:HD23	1:X:62:LEU:H	1.75	0.50
8:DA:86:VAL:HG12	8:DA:92:VAL:HG22	1.94	0.50
8:DE:103:ASP:OD1	8:DE:107:ASN:N	2.39	0.50
8:DJ:299:THR:HG22	8:DJ:314:GLN:HB3	1.93	0.50
1:E:34:PHE:HB3	1:E:222:SER:HB3	1.94	0.50
1:K:5:LEU:HG	1:K:250:THR:HG21	1.94	0.50
1:P:194:GLU:OE1	1:P:194:GLU:N	2.32	0.50
2:d:228:GLU:HA	1:W:256:LYS:HD2	1.93	0.50
5:h:128:LYS:HZ3	6:m:117:GLN:CD	2.14	0.50
6:n:42:ASP:OD2	6:n:88:ARG:NH2	2.45	0.50
8:DD:93:PHE:HD2	8:DD:114:MET:HE1	1.76	0.50
1:I:29:VAL:O	1:I:222:SER:OG	2.29	0.50
1:K:179:MET:HE1	1:P:144:ALA:HA	1.93	0.50
2:a:82:LEU:HD21	2:a:88:LEU:HG	1.94	0.50
8:DA:139:ILE:HA	8:DA:312:LEU:HD13	1.93	0.50
8:DB:294:ILE:HG12	8:DB:300:VAL:HG12	1.94	0.50
8:DF:362:GLU:OE1	8:DF:362:GLU:N	2.43	0.50
8:DG:159:ASN:HB3	8:DG:162:ASP:HB2	1.94	0.50
8:DK:188:ASP:HA	8:DK:257:ALA:HB2	1.93	0.50
1:A:2:ILE:HG22	1:A:4:SER:H	1.77	0.49
1:A:28:ASN:HB3	8:DA:52:VAL:HB	1.94	0.49
1:A:237:GLN:HG3	8:DA:395:ILE:HG22	1.94	0.49
1:R:225:ASN:O	1:R:229:GLU:HG2	2.12	0.49
2:a:181:LEU:HD11	2:a:193:LEU:HG	1.94	0.49
5:g:18:SER:O	5:g:22:ASN:ND2	2.31	0.49
6:o:15:ALA:O	6:o:19:ARG:HG2	2.12	0.49
1:W:43:ASP:OD1	1:W:43:ASP:N	2.44	0.49
1:X:2:ILE:HG13	1:X:254:LEU:HD21	1.94	0.49
8:DC:208:TRP:HB2	8:DC:230:LEU:HB2	1.94	0.49
8:DG:79:GLN:HB2	8:DG:354:GLY:HA3	1.94	0.49
8:DH:180:LYS:HB3	8:DH:200:PHE:HB2	1.93	0.49
8:DI:16:ASN:HB2	8:DI:39:PHE:HZ	1.77	0.49
8:DJ:318:ALA:HB2	8:DJ:345:LEU:HD13	1.93	0.49
1:H:92:SER:O	1:H:216:GLN:NE2	2.41	0.49
1:H:176:THR:HG22	1:H:203:GLU:HB2	1.94	0.49
1:O:150:THR:OG1	1:O:158:SER:OG	2.30	0.49
5:f:23:VAL:HG11	5:f:46:GLN:HA	1.92	0.49
5:g:113:GLN:O	5:g:116:ILE:HG22	2.13	0.49
8:DD:165:PRO:HG2	8:DD:201:VAL:HG23	1.94	0.49
1:A:63:PRO:HB2	1:O:121:GLN:OE1	2.12	0.49
1:E:251:ASP:OD1	1:J:238:ARG:NE	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:256:LYS:HE3	1:O:241:GLU:OE2	2.13	0.49
1:L:33:GLY:N	1:L:220:GLU:O	2.44	0.49
2:d:225:ARG:NH1	1:V:251:ASP:OD1	2.45	0.49
8:DD:139:ILE:HA	8:DD:312:LEU:HD22	1.94	0.49
8:DE:322:ASN:ND2	8:DE:339:ALA:O	2.40	0.49
1:C:127:GLN:HA	1:C:141:THR:HA	1.95	0.49
1:C:179:MET:HE1	1:G:144:ALA:HA	1.93	0.49
1:I:230:LEU:HD12	8:DC:399:LEU:HG	1.94	0.49
1:J:257:LEU:HD22	1:O:240:TYR:OH	2.11	0.49
2:b:181:LEU:HD21	2:b:193:LEU:HD11	1.92	0.49
8:DI:331:ASP:OD1	8:DI:332:ASN:N	2.38	0.49
1:D:101:GLY:HA3	1:D:175:LEU:HD13	1.93	0.49
1:E:140:ILE:HD12	1:E:171:GLY:HA3	1.95	0.49
1:F:254:LEU:HD23	1:L:238:ARG:HG3	1.94	0.49
1:G:147:LEU:HB2	1:G:160:THR:HG23	1.93	0.49
1:M:35:LYS:HA	1:M:223:ASN:OD1	2.12	0.49
2:a:184:GLU:OE1	2:a:184:GLU:N	2.44	0.49
2:b:77:PRO:HG2	2:b:78:LEU:HD23	1.94	0.49
2:d:9:MET:HB2	5:j:103:VAL:HG11	1.94	0.49
1:P:6:TRP:HE3	2:a:70:GLN:HG2	1.76	0.49
6:o:85:LEU:HD23	6:o:85:LEU:H	1.77	0.49
8:DD:151:THR:HG1	8:DD:282:ASN:ND2	2.11	0.49
1:A:145:ASN:OD1	1:A:161:GLN:NE2	2.45	0.49
1:E:24:ASN:ND2	1:E:37:GLN:OE1	2.43	0.49
1:M:251:ASP:OD1	1:S:238:ARG:NH2	2.38	0.49
5:g:49:PHE:O	5:p:34:VAL:O	2.29	0.49
1:W:225:ASN:O	1:W:229:GLU:HG2	2.13	0.49
1:E:72:VAL:HB	1:I:28:ASN:HB3	1.94	0.49
1:J:72:VAL:HG22	1:O:28:ASN:HB3	1.95	0.49
1:N:92:SER:O	1:N:216:GLN:NE2	2.46	0.49
8:DA:235:ASN:O	8:DA:269:GLN:NE2	2.45	0.49
8:DI:54:VAL:HG12	8:DI:56:GLY:H	1.78	0.49
1:C:123:ASP:OD1	1:C:127:GLN:N	2.35	0.49
1:G:33:GLY:N	1:G:220:GLU:O	2.42	0.49
1:R:181:ASP:OD1	1:R:181:ASP:N	2.37	0.49
1:S:257:LEU:HD13	5:g:99:VAL:HG12	1.94	0.49
5:f:19:LYS:NZ	6:m:91:ASP:HB2	2.28	0.49
8:DG:365:ASN:O	8:DG:365:ASN:ND2	2.45	0.49
1:E:254:LEU:HD23	1:J:238:ARG:HG3	1.95	0.49
1:S:109:ASP:OD1	1:S:109:ASP:N	2.46	0.49
8:DC:44:ALA:HB2	8:DC:50:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLN:HB2	1:K:238:ARG:CZ	2.43	0.48
1:D:33:GLY:N	1:D:220:GLU:O	2.45	0.48
1:E:123:ASP:OD1	1:E:127:GLN:N	2.34	0.48
1:F:83:GLN:HG2	8:DF:44:ALA:HB1	1.94	0.48
1:G:181:ASP:OD1	1:G:181:ASP:N	2.44	0.48
1:I:58:GLU:HG2	1:I:59:GLN:HG2	1.95	0.48
1:I:258:THR:O	1:O:245:LYS:NZ	2.45	0.48
1:P:102:PHE:HB3	1:P:114:TYR:HB3	1.94	0.48
1:W:33:GLY:N	1:W:220:GLU:O	2.43	0.48
8:DJ:84:ARG:HD2	8:DJ:345:LEU:HD11	1.94	0.48
1:N:3:SER:HB2	1:S:20:ASP:OD1	2.13	0.48
1:T:35:LYS:NZ	1:T:220:GLU:OE2	2.37	0.48
2:d:91:GLN:HB3	2:d:119:PRO:HG2	1.94	0.48
2:d:247:LEU:HD11	5:i:119:LEU:HD13	1.95	0.48
6:l:131:MET:HE2	7:s:80:VAL:HG22	1.94	0.48
8:DA:382:TYR:CD2	8:DF:395:ILE:HD11	2.47	0.48
8:DD:174:ASP:N	8:DD:174:ASP:OD1	2.45	0.48
1:C:29:VAL:O	1:C:222:SER:OG	2.29	0.48
1:G:48:THR:HG22	1:G:67:GLN:HG2	1.95	0.48
1:K:98:LYS:HZ1	8:DA:43:PHE:C	2.21	0.48
2:a:55:THR:HG1	5:h:26:SER:HG	1.61	0.48
3:3:13:UNK:N	6:n:36:PRO:CG	2.77	0.48
5:j:78:TYR:HB2	5:j:90:TYR:CE1	2.49	0.48
8:DA:79:GLN:HB2	8:DA:354:GLY:HA2	1.95	0.48
8:DF:295:ASN:ND2	8:DF:299:THR:HG1	2.10	0.48
8:DG:209:ALA:HA	8:DG:229:THR:HA	1.96	0.48
8:DH:107:ASN:HA	8:DH:138:THR:HA	1.94	0.48
1:C:126:GLY:O	1:C:142:ILE:N	2.43	0.48
1:D:238:ARG:NH1	1:D:241:GLU:OE1	2.46	0.48
2:a:181:LEU:HD21	2:a:193:LEU:HD11	1.95	0.48
2:e:150:ASP:OD1	2:e:154:THR:OG1	2.28	0.48
8:DC:118:GLY:HA2	8:DC:316:VAL:HG12	1.95	0.48
8:DG:299:THR:HA	8:DG:314:GLN:HA	1.95	0.48
1:J:45:LEU:HD13	1:U:98:LYS:HG2	1.95	0.48
1:J:228:GLU:HG2	1:J:232:ASN:ND2	2.29	0.48
5:f:31:ALA:HA	5:f:96:VAL:HG21	1.95	0.48
6:m:26:LEU:HA	6:m:29:ASN:HD21	1.78	0.48
6:o:42:ASP:OD2	6:o:88:ARG:NH2	2.46	0.48
1:X:97:ILE:HG23	1:X:116:ARG:HE	1.79	0.48
8:DE:269:GLN:OE1	8:DK:145:ALA:HA	2.13	0.48
8:DI:295:ASN:OD1	8:DI:299:THR:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:SER:OG	1:D:58:GLU:N	2.47	0.48
1:J:79:ARG:NH2	1:J:184:LEU:O	2.47	0.48
1:O:251:ASP:OD1	1:U:238:ARG:NH2	2.46	0.48
2:c:35:ARG:HH12	2:c:68:PRO:HA	1.79	0.48
5:g:125:MET:HE1	5:p:21:LEU:HD22	1.96	0.48
1:W:127:GLN:HG2	1:W:141:THR:HG22	1.96	0.48
8:DE:19:VAL:HG12	8:DE:23:ASN:HD21	1.79	0.48
8:DK:301:VAL:HG22	8:DK:311:VAL:HG12	1.95	0.48
1:F:40:VAL:HG23	1:F:75:VAL:HG13	1.95	0.48
1:J:254:LEU:HD23	1:P:238:ARG:HG3	1.96	0.48
1:L:155:GLY:HA2	1:L:214:LEU:HD12	1.96	0.48
2:e:9:MET:CB	5:p:103:VAL:HG21	2.44	0.48
8:DD:24:ILE:HD11	8:DI:384:SER:HB2	1.94	0.48
1:H:34:PHE:HB3	1:H:222:SER:HB3	1.96	0.48
1:N:154:ASP:OD1	1:N:154:ASP:N	2.45	0.48
1:O:2:ILE:HG23	1:O:5:LEU:HB2	1.96	0.48
1:V:179:MET:N	1:V:179:MET:SD	2.87	0.48
8:DB:12:ALA:HB2	8:DB:52:VAL:HG21	1.95	0.48
8:DC:231:LYS:HB3	8:DC:240:SER:HB3	1.96	0.48
8:DC:296:ASN:HB3	8:DC:355:LYS:HE3	1.94	0.48
8:DI:146:ALA:HB2	8:DI:286:PRO:HD3	1.96	0.48
1:O:177:THR:OG1	1:O:202:ASN:OD1	2.27	0.48
1:P:36:ARG:HH21	1:P:80:LEU:HD22	1.78	0.48
2:a:77:PRO:HG2	2:a:78:LEU:HD23	1.95	0.48
5:f:52:ASP:HB2	5:f:63:LYS:HB2	1.95	0.48
1:V:38:ARG:HH12	1:V:80:LEU:HD11	1.79	0.48
8:DB:119:TYR:HD2	8:DB:314:GLN:HE21	1.62	0.48
8:DG:188:ASP:OD1	8:DG:192:ASN:N	2.46	0.48
8:DH:178:TYR:CE1	8:DH:181:LYS:HB2	2.49	0.48
8:DI:367:ASP:HB3	8:DI:370:LYS:HB2	1.95	0.48
1:D:2:ILE:HG22	1:D:4:SER:H	1.79	0.48
1:K:35:LYS:HA	1:K:223:ASN:OD1	2.14	0.48
1:K:50:ARG:HB2	1:K:66:LEU:H	1.79	0.48
1:Q:18:ASN:HB2	1:Q:41:PHE:HZ	1.79	0.48
1:R:45:LEU:HD23	1:W:188:GLY:HA3	1.96	0.48
5:j:72:ALA:O	5:j:95:ASN:ND2	2.46	0.48
6:n:11:PHE:HB2	6:n:53:MET:HE1	1.96	0.48
8:DF:247:THR:HG22	8:DF:258:THR:HG22	1.96	0.48
8:DG:41:ASP:OD1	8:DG:41:ASP:N	2.33	0.48
8:DG:174:ASP:HB3	8:DG:177:SER:HB2	1.96	0.48
8:DI:110:ASN:ND2	8:DI:112:GLN:OE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:TYR:CD1	1:C:69:GLY:HA2	2.49	0.47
1:D:145:ASN:HA	8:DC:352:ASN:ND2	2.29	0.47
1:E:37:GLN:HB3	1:E:79:ARG:HD3	1.96	0.47
1:P:50:ARG:HH22	5:h:81:GLY:HA2	1.79	0.47
1:R:44:LEU:HD21	1:R:73:ARG:HB3	1.94	0.47
4:7:330:THR:HG23	5:f:37:PRO:HB2	1.96	0.47
5:g:46:GLN:HE22	5:g:70:SER:HB2	1.79	0.47
5:g:47:VAL:HG12	5:g:67:VAL:HG12	1.95	0.47
1:X:129:VAL:HG12	1:X:135:GLN:HB3	1.96	0.47
8:DF:331:ASP:OD1	8:DF:331:ASP:N	2.46	0.47
1:F:175:LEU:HD11	1:F:211:ALA:HB1	1.95	0.47
1:G:82:SER:OG	1:G:83:GLN:N	2.47	0.47
1:H:66:LEU:HD12	1:M:77:THR:HG22	1.94	0.47
1:H:175:LEU:HD11	1:H:211:ALA:HB1	1.96	0.47
1:I:137:GLN:HB3	1:I:138:PRO:HD3	1.96	0.47
1:L:41:PHE:HA	1:L:74:PRO:HA	1.96	0.47
1:N:242:ILE:HD12	1:S:230:LEU:HD21	1.95	0.47
1:Q:36:ARG:NH2	1:V:89:THR:O	2.47	0.47
2:d:14:GLN:HG3	2:d:58:THR:HA	1.96	0.47
5:h:111:SER:O	5:h:115:ASN:ND2	2.45	0.47
8:DH:74:ASP:N	8:DH:74:ASP:OD1	2.46	0.47
1:A:49:ILE:HB	1:A:66:LEU:HD23	1.97	0.47
1:D:225:ASN:O	1:D:229:GLU:HG2	2.15	0.47
1:J:150:THR:OG1	1:J:158:SER:OG	2.32	0.47
1:M:37:GLN:HB3	1:M:79:ARG:HG2	1.96	0.47
2:b:89:VAL:HG11	2:b:162:LYS:HD3	1.96	0.47
2:e:217:MET:HE1	1:X:245:LYS:HD3	1.96	0.47
6:o:133:VAL:HA	7:u:86:ILE:HD12	1.94	0.47
6:k:33:ALA:HB1	6:k:102:MET:HE1	1.95	0.47
1:W:29:VAL:O	1:W:222:SER:OG	2.29	0.47
8:DE:106:ARG:NH1	8:DJ:321:ALA:CB	2.76	0.47
8:DF:139:ILE:HD13	8:DF:312:LEU:HD22	1.96	0.47
8:DG:208:TRP:HB3	8:DG:230:LEU:HB2	1.96	0.47
1:F:238:ARG:NE	8:DA:393:ASP:OD1	2.42	0.47
1:T:147:LEU:HB2	1:T:160:THR:HG23	1.96	0.47
1:U:43:ASP:OD1	1:U:43:ASP:N	2.47	0.47
1:U:82:SER:HB3	1:U:223:ASN:HD22	1.79	0.47
6:o:25:ILE:O	6:o:29:ASN:ND2	2.47	0.47
5:p:130:LEU:HD22	7:v:68:LEU:HD21	1.97	0.47
5:i:85:ALA:HB1	5:i:89:GLY:HA2	1.97	0.47
8:DG:144:MET:SD	8:DG:306:ASN:ND2	2.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLY:N	1:B:220:GLU:O	2.47	0.47
1:B:40:VAL:HG23	1:B:75:VAL:HG13	1.97	0.47
1:G:2:ILE:HD11	1:G:254:LEU:HD13	1.96	0.47
1:P:239:ALA:O	1:P:243:ASN:ND2	2.38	0.47
2:c:113:LEU:HD12	2:c:127:ILE:HG13	1.96	0.47
5:f:74:GLU:OE2	5:f:92:LYS:NZ	2.40	0.47
1:X:42:GLU:HG3	1:X:75:VAL:HG11	1.95	0.47
8:DA:129:GLN:HG3	8:DA:131:GLY:H	1.79	0.47
8:DD:326:LEU:HB3	8:DD:334:TRP:HB3	1.97	0.47
8:DI:365:ASN:ND2	8:DI:365:ASN:O	2.47	0.47
1:C:178:PHE:CE1	1:C:201:PRO:HB3	2.49	0.47
1:P:50:ARG:H	1:P:50:ARG:HD3	1.79	0.47
1:R:67:GLN:NE2	1:W:186:SER:O	2.47	0.47
1:T:210:GLY:HA2	2:b:149:GLY:HA3	1.96	0.47
2:b:83:GLN:HG2	2:b:84:GLN:H	1.80	0.47
2:e:170:GLU:OE1	2:e:170:GLU:N	2.47	0.47
1:V:99:GLY:O	1:V:116:ARG:NH2	2.34	0.47
8:DC:156:ILE:HD11	8:DC:158:LEU:HD21	1.97	0.47
1:C:42:GLU:HB2	1:G:189:GLU:HA	1.96	0.47
1:D:72:VAL:HB	1:H:28:ASN:HB3	1.97	0.47
1:D:257:LEU:HB2	1:H:240:TYR:HE2	1.80	0.47
1:I:102:PHE:HB3	1:I:114:TYR:HB3	1.96	0.47
1:M:69:GLY:HA3	1:R:24:ASN:ND2	2.30	0.47
1:R:151:ILE:HG12	1:R:157:VAL:HG22	1.97	0.47
2:e:212:LYS:HB2	2:e:215:GLU:HB3	1.95	0.47
5:h:86:ASP:OD1	5:h:90:TYR:N	2.47	0.47
5:j:74:GLU:HA	5:j:95:ASN:HB3	1.97	0.47
6:l:96:ASP:OD1	6:l:97:GLY:N	2.47	0.47
8:DB:365:ASN:O	8:DB:365:ASN:ND2	2.48	0.47
8:DC:239:GLU:OE1	8:DC:239:GLU:N	2.47	0.47
8:DC:337:THR:O	8:DC:340:SER:OG	2.28	0.47
8:DJ:71:ARG:HH11	8:DJ:73:LEU:HB3	1.79	0.47
1:B:238:ARG:HA	1:B:238:ARG:HD3	1.67	0.47
1:C:45:LEU:HB2	1:M:98:LYS:NZ	2.29	0.47
1:U:257:LEU:HA	2:c:231:MET:HE3	1.96	0.47
8:DE:22:ASN:CG	8:DJ:49:GLY:HA3	2.40	0.47
8:DG:112:GLN:OE1	8:DG:112:GLN:N	2.47	0.47
8:DI:156:ILE:HD11	8:DI:180:LYS:HG2	1.97	0.47
8:DJ:188:ASP:OD1	8:DJ:191:GLY:N	2.48	0.47
1:C:55:GLN:NE2	1:C:57:SER:O	2.47	0.47
1:C:82:SER:HB3	1:C:223:ASN:HD22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:4:SER:HB3	1:S:19:MET:HG3	1.97	0.47
2:a:227:PHE:CE1	1:V:257:LEU:HB2	2.50	0.47
8:DB:213:HIS:HB2	8:DB:223:PRO:HG3	1.97	0.47
8:DF:63:ASP:N	8:DF:63:ASP:OD1	2.44	0.47
8:DF:332:ASN:N	8:DF:332:ASN:OD1	2.47	0.47
8:DG:208:TRP:N	8:DG:230:LEU:O	2.42	0.47
1:B:225:ASN:O	1:B:229:GLU:HG2	2.16	0.47
1:G:54:ALA:HB3	1:G:62:LEU:HD12	1.96	0.47
1:G:175:LEU:HD11	1:G:211:ALA:HB1	1.97	0.47
1:J:140:ILE:HD13	1:J:157:VAL:HG11	1.96	0.47
1:L:35:LYS:NZ	1:L:220:GLU:OE2	2.45	0.47
1:N:69:GLY:HA3	1:S:24:ASN:ND2	2.30	0.47
1:P:42:GLU:OE2	1:U:190:ASN:N	2.48	0.47
2:a:6:TYR:HA	2:a:9:MET:HG3	1.96	0.47
2:a:14:GLN:HG3	2:a:58:THR:HA	1.96	0.47
1:W:175:LEU:HD11	1:W:211:ALA:HB1	1.96	0.47
8:DC:157:ASN:O	8:DC:275:ASN:N	2.44	0.47
8:DE:84:ARG:HD2	8:DE:345:LEU:HD11	1.97	0.47
8:DG:210:VAL:N	8:DG:228:THR:O	2.41	0.47
1:J:228:GLU:HG2	1:J:232:ASN:HD21	1.80	0.46
1:K:63:PRO:O	1:P:197:SER:OG	2.27	0.46
1:O:79:ARG:NH2	1:O:184:LEU:O	2.48	0.46
1:P:45:LEU:O	1:P:70:THR:OG1	2.24	0.46
2:a:44:VAL:HG12	4:5:326:ALA:HB1	1.97	0.46
6:l:102:MET:HE2	6:l:102:MET:HA	1.97	0.46
6:o:43:ILE:HG22	6:o:85:LEU:HA	1.96	0.46
8:DB:57:ILE:HB	8:DG:47:LYS:HB3	1.96	0.46
8:DH:79:GLN:HG3	8:DH:80:ASN:H	1.80	0.46
1:F:42:GLU:OE1	1:K:190:ASN:ND2	2.48	0.46
6:l:19:ARG:NH1	6:l:115:LYS:HB3	2.29	0.46
8:DB:63:ASP:N	8:DB:63:ASP:OD1	2.48	0.46
8:DH:250:THR:OG1	8:DH:254:ALA:O	2.29	0.46
8:DK:112:GLN:N	8:DK:112:GLN:OE1	2.48	0.46
1:B:42:GLU:CG	1:F:189:GLU:HA	2.45	0.46
1:B:150:THR:OG1	1:B:158:SER:OG	2.18	0.46
1:F:242:ILE:HD12	1:K:230:LEU:HD11	1.95	0.46
1:H:33:GLY:N	1:H:220:GLU:O	2.43	0.46
1:J:56:SER:O	2:c:138:ALA:HB1	2.15	0.46
1:J:154:ASP:HA	1:J:206:PRO:HB2	1.96	0.46
1:P:46:TYR:CD1	1:P:69:GLY:HA2	2.49	0.46
1:P:91:ASN:OD1	1:P:92:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:7:ILE:O	1:T:10:THR:OG1	2.31	0.46
6:o:26:LEU:HA	6:o:29:ASN:HD21	1.80	0.46
5:i:23:VAL:HG21	5:i:47:VAL:HG13	1.96	0.46
6:k:2:LEU:HB3	6:k:3:ASP:H	1.59	0.46
8:DI:269:GLN:N	8:DI:269:GLN:CD	2.74	0.46
8:DK:155:GLN:HB3	8:DK:278:ALA:HB3	1.96	0.46
8:DK:156:ILE:HD11	8:DK:180:LYS:HG2	1.97	0.46
8:DK:299:THR:HA	8:DK:314:GLN:HA	1.97	0.46
1:G:50:ARG:NH1	1:L:75:VAL:O	2.48	0.46
1:H:66:LEU:HA	1:M:77:THR:HG22	1.97	0.46
1:Q:46:TYR:CD1	1:Q:69:GLY:HA2	2.50	0.46
1:R:260:LEU:O	1:X:245:LYS:HE3	2.16	0.46
1:T:91:ASN:OD1	1:T:92:SER:N	2.45	0.46
8:DC:119:TYR:HD2	8:DC:314:GLN:HE21	1.63	0.46
8:DE:164:VAL:HG12	8:DE:202:LYS:HD3	1.97	0.46
8:DF:67:THR:N	8:DF:361:LEU:O	2.44	0.46
1:A:82:SER:HB2	1:A:223:ASN:HD22	1.81	0.46
1:L:45:LEU:HB2	1:W:98:LYS:HE2	1.97	0.46
2:e:115:ILE:HG22	2:e:116:GLN:H	1.81	0.46
5:h:75:LYS:HE2	5:h:95:ASN:HA	1.97	0.46
1:V:35:LYS:HA	1:V:223:ASN:OD1	2.16	0.46
8:DH:281:GLN:HG2	8:DH:283:GLY:H	1.80	0.46
1:A:92:SER:HA	1:A:216:GLN:HE21	1.80	0.46
1:B:42:GLU:HG2	1:F:189:GLU:OE1	2.16	0.46
1:K:202:ASN:OD1	1:K:202:ASN:N	2.49	0.46
1:L:29:VAL:O	1:L:222:SER:OG	2.33	0.46
1:P:232:ASN:O	1:P:236:VAL:HG13	2.16	0.46
1:R:175:LEU:HD11	1:R:211:ALA:HB1	1.97	0.46
1:T:44:LEU:HB2	1:T:70:THR:HB	1.97	0.46
1:T:50:ARG:NH2	2:b:59:ALA:O	2.49	0.46
6:n:33:ALA:O	6:n:98:ASN:ND2	2.48	0.46
8:DA:382:TYR:CG	8:DF:395:ILE:HD11	2.51	0.46
8:DE:159:ASN:OD1	8:DE:162:ASP:N	2.49	0.46
8:DH:127:THR:OG1	8:DH:128:ILE:N	2.47	0.46
1:E:126:GLY:O	1:E:142:ILE:N	2.37	0.46
1:E:129:VAL:HG12	1:E:135:GLN:HB3	1.96	0.46
1:G:123:ASP:OD1	1:G:127:GLN:N	2.49	0.46
1:L:18:ASN:HB2	1:L:41:PHE:HZ	1.81	0.46
1:U:225:ASN:O	1:U:229:GLU:HG2	2.16	0.46
2:b:173:ARG:HG2	2:b:174:SER:H	1.81	0.46
2:d:250:MET:HE3	5:j:121:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DB:299:THR:HG22	8:DB:314:GLN:HB3	1.98	0.46
8:DC:22:ASN:ND2	8:DH:49:GLY:HA3	2.31	0.46
8:DJ:285:LYS:O	8:DJ:306:ASN:ND2	2.33	0.46
1:C:38:ARG:NH1	1:C:78:GLU:OE2	2.49	0.46
1:E:167:PRO:HG3	8:DH:338:GLN:HB2	1.98	0.46
1:Q:34:PHE:HB3	1:Q:222:SER:HB3	1.98	0.46
1:R:195:THR:HG22	2:e:152:PRO:HB2	1.98	0.46
1:U:177:THR:OG1	1:U:202:ASN:OD1	2.29	0.46
2:b:181:LEU:HD11	2:b:193:LEU:HG	1.98	0.46
8:DE:99:GLN:HG3	8:DE:111:MET:HE3	1.98	0.46
8:DK:33:LYS:HD3	8:DK:61:PHE:HA	1.98	0.46
8:DK:392:GLN:HA	8:DK:395:ILE:HG22	1.98	0.46
1:D:13:ASP:OD2	1:N:88:GLN:NE2	2.49	0.46
1:G:57:SER:OG	1:G:58:GLU:N	2.48	0.46
1:M:67:GLN:H	1:R:77:THR:HG21	1.81	0.46
1:S:22:ILE:HG23	1:S:229:GLU:HG3	1.98	0.46
1:S:101:GLY:HA3	1:S:175:LEU:HD13	1.98	0.46
2:b:15:THR:OG1	2:b:226:ARG:NE	2.38	0.46
2:c:25:ASN:HD21	2:c:37:GLN:N	2.13	0.46
2:d:115:ILE:HG22	2:d:116:GLN:H	1.81	0.46
6:o:131:MET:HE2	7:v:83:GLN:HE22	1.80	0.46
8:DC:33:LYS:HA	8:DC:365:ASN:HD21	1.81	0.46
8:DD:69:THR:HG21	8:DD:361:LEU:HD12	1.96	0.46
8:DE:71:ARG:NH1	8:DE:99:GLN:OE1	2.48	0.46
8:DF:106:ARG:HE	8:DK:321:ALA:HB1	1.81	0.46
1:B:45:LEU:HD11	1:L:83:GLN:HG2	1.98	0.46
1:D:55:GLN:NE2	1:D:57:SER:O	2.47	0.46
1:D:210:GLY:HA2	1:H:147:LEU:HD21	1.98	0.46
1:F:57:SER:OG	1:F:58:GLU:N	2.48	0.46
2:e:228:GLU:HG3	1:X:253:MET:HE1	1.96	0.46
6:m:41:ARG:HB3	6:m:85:LEU:HD12	1.97	0.46
6:m:133:VAL:HA	7:s:86:ILE:HD12	1.97	0.46
1:A:233:MET:HG2	8:DA:391:THR:HG21	1.97	0.45
1:E:238:ARG:NH2	8:DC:397:ASN:HB2	2.31	0.45
1:Q:33:GLY:N	1:Q:220:GLU:O	2.42	0.45
2:b:9:MET:HG2	5:f:103:VAL:HG21	1.96	0.45
6:k:12:GLN:HB3	6:k:123:LEU:HD12	1.98	0.45
8:DD:161:THR:HG22	8:DJ:252:ASN:CG	2.41	0.45
8:DF:87:ASP:HB2	8:DF:114:MET:HE1	1.99	0.45
8:DG:195:ASP:HB2	8:DG:216:SER:H	1.80	0.45
1:B:67:GLN:NE2	1:F:185:GLU:HG3	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:PHE:HA	1:D:75:VAL:H	1.80	0.45
1:F:72:VAL:HB	1:K:28:ASN:HB3	1.98	0.45
1:G:35:LYS:HA	1:G:223:ASN:OD1	2.16	0.45
1:L:35:LYS:HA	1:L:223:ASN:OD1	2.17	0.45
1:L:56:SER:HB2	1:L:62:LEU:HD12	1.97	0.45
1:N:42:GLU:HG2	1:N:75:VAL:HB	1.98	0.45
1:N:88:GLN:HB3	1:N:218:TYR:CE2	2.51	0.45
1:Q:194:GLU:HG3	1:Q:201:PRO:HD3	1.97	0.45
1:R:228:GLU:O	1:R:232:ASN:ND2	2.31	0.45
1:S:257:LEU:HD11	5:g:99:VAL:HG12	1.99	0.45
1:T:45:LEU:HD23	5:f:90:TYR:CE2	2.51	0.45
2:b:210:ASN:OD1	2:b:210:ASN:N	2.50	0.45
2:c:170:GLU:OE1	2:c:170:GLU:N	2.49	0.45
2:e:146:LEU:HB2	2:e:155:VAL:HG12	1.98	0.45
6:n:41:ARG:HB3	6:n:85:LEU:HD12	1.97	0.45
8:DA:108:LEU:HB2	8:DA:137:ILE:HG23	1.98	0.45
8:DB:26:ASN:HA	8:DG:52:VAL:HG11	1.98	0.45
8:DE:196:MET:HG3	8:DE:259:PHE:HZ	1.81	0.45
8:DF:236:GLY:HA2	8:DF:268:GLN:HE21	1.81	0.45
1:Q:195:THR:HG22	2:d:152:PRO:HB2	1.98	0.45
1:Q:251:ASP:OD1	1:W:238:ARG:NH2	2.34	0.45
2:c:25:ASN:ND2	2:c:37:GLN:H	2.10	0.45
8:DC:171:SER:HB3	8:DC:174:ASP:HB3	1.98	0.45
1:W:44:LEU:HB2	1:W:70:THR:HB	1.98	0.45
1:W:238:ARG:HA	1:W:238:ARG:HD3	1.77	0.45
1:J:35:LYS:HA	1:J:223:ASN:OD1	2.16	0.45
2:b:134:GLU:OE1	2:b:134:GLU:N	2.49	0.45
2:d:34:PHE:O	2:d:35:ARG:NE	2.48	0.45
5:f:72:ALA:O	5:f:95:ASN:ND2	2.49	0.45
1:W:114:TYR:HE1	1:W:176:THR:HG21	1.82	0.45
7:u:59:PHE:HB2	7:u:66:ILE:HG21	1.98	0.45
8:DC:178:TYR:HA	8:DC:201:VAL:HG12	1.99	0.45
1:B:79:ARG:NH2	1:B:192:TYR:OH	2.49	0.45
1:F:195:THR:OG1	1:F:196:GLN:N	2.48	0.45
1:G:136:VAL:HG12	1:G:138:PRO:HD2	1.98	0.45
1:J:55:GLN:HG3	1:J:57:SER:O	2.16	0.45
1:O:142:ILE:HD13	1:O:149:ILE:HG12	1.98	0.45
2:d:54:ARG:NH1	6:n:93:PRO:O	2.43	0.45
2:d:133:SER:HA	2:d:148:PRO:HD3	1.99	0.45
2:e:135:ILE:HG23	2:e:143:ILE:HG23	1.99	0.45
8:DA:188:ASP:OD1	8:DA:192:ASN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DB:207:GLU:HB3	8:DB:231:LYS:HG2	1.98	0.45
8:DB:288:ASP:N	8:DB:288:ASP:OD1	2.49	0.45
8:DG:87:ASP:OD1	8:DG:91:SER:N	2.49	0.45
1:A:29:VAL:O	1:A:222:SER:OG	2.31	0.45
1:D:45:LEU:HD22	1:N:98:LYS:HG3	1.99	0.45
1:D:246:ALA:HA	1:H:233:MET:HE3	1.99	0.45
1:J:225:ASN:O	1:J:229:GLU:HG2	2.17	0.45
1:N:2:ILE:HD12	1:S:16:GLN:HE22	1.81	0.45
1:O:51:GLN:NE2	1:T:75:VAL:O	2.46	0.45
2:b:66:MET:HE2	2:b:87:TRP:HZ2	1.80	0.45
2:c:249:SER:O	5:f:123:LYS:NZ	2.47	0.45
2:d:44:VAL:HG23	2:d:56:LEU:HB2	1.99	0.45
2:d:79:ASP:O	2:d:204:GLY:N	2.36	0.45
2:e:35:ARG:HH11	2:e:101:ARG:HD3	1.82	0.45
2:e:228:GLU:HG2	1:X:256:LYS:HG2	1.99	0.45
5:j:74:GLU:OE1	5:j:74:GLU:N	2.50	0.45
6:m:49:LEU:HD22	7:s:61:LEU:HD21	1.99	0.45
1:V:250:THR:HA	1:V:253:MET:HG2	1.99	0.45
8:DC:288:ASP:OD1	8:DC:288:ASP:N	2.49	0.45
8:DC:345:LEU:H	8:DC:345:LEU:HD12	1.81	0.45
8:DF:34:SER:HB2	8:DF:366:VAL:HG22	1.98	0.45
8:DJ:187:TYR:HB3	8:DJ:191:GLY:HA2	1.99	0.45
1:M:67:GLN:H	1:R:77:THR:CG2	2.29	0.45
1:U:35:LYS:HA	1:U:223:ASN:OD1	2.17	0.45
2:b:102:ASN:ND2	2:b:116:GLN:OE1	2.44	0.45
5:h:50:GLN:OE1	5:h:63:LYS:NZ	2.50	0.45
8:DC:170:PHE:CE2	8:DC:223:PRO:HG2	2.52	0.45
1:D:1:MET:N	1:D:1:MET:SD	2.90	0.45
1:S:66:LEU:HD11	1:X:74:PRO:HB2	1.99	0.45
2:c:35:ARG:O	2:c:173:ARG:NH2	2.43	0.45
8:DH:87:ASP:OD1	8:DH:91:SER:N	2.50	0.45
8:DJ:180:LYS:HD3	8:DJ:274:ASN:HB3	1.99	0.45
1:F:167:PRO:HD2	8:DF:338:GLN:HE21	1.81	0.45
1:L:238:ARG:HD3	1:L:238:ARG:HA	1.75	0.45
1:T:178:PHE:CE2	1:T:201:PRO:HB3	2.51	0.45
2:c:42:ARG:NH1	4:7:328:ILE:O	2.40	0.45
2:c:48:GLY:HA3	6:m:93:PRO:HB3	1.97	0.45
5:g:50:GLN:HG2	5:p:35:THR:O	2.17	0.45
8:DB:208:TRP:HE1	8:DB:268:GLN:HG3	1.82	0.45
8:DC:154:MET:HB3	8:DC:279:THR:HG23	1.97	0.45
8:DC:159:ASN:HD21	8:DC:161:THR:HG22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:179:MET:HE2	1:Q:179:MET:HB3	1.83	0.44
4:9:317:SER:O	6:o:86:LEU:HB3	2.17	0.44
6:o:11:PHE:CE2	7:u:57:GLU:HG3	2.51	0.44
6:o:19:ARG:HH21	6:o:112:ASN:HA	1.82	0.44
1:V:43:ASP:N	1:V:43:ASP:OD1	2.41	0.44
7:u:57:GLU:O	7:u:60:THR:HG22	2.16	0.44
1:B:45:LEU:HD13	1:L:98:LYS:HG3	1.99	0.44
1:E:164:GLN:HE21	1:E:164:GLN:HB3	1.61	0.44
1:O:9:LYS:HD3	1:U:228:GLU:OE1	2.17	0.44
2:b:212:LYS:HB2	2:b:215:GLU:HB2	2.00	0.44
2:c:83:GLN:HG2	2:c:84:GLN:H	1.82	0.44
5:p:78:TYR:CZ	1:X:73:ARG:HD3	2.52	0.44
8:DC:127:THR:OG1	8:DC:128:ILE:N	2.51	0.44
8:DC:201:VAL:HG22	8:DC:209:ALA:HB3	1.98	0.44
8:DC:295:ASN:ND2	8:DC:299:THR:OG1	2.40	0.44
8:DI:34:SER:H	8:DI:365:ASN:HD21	1.65	0.44
8:DK:322:ASN:ND2	8:DK:339:ALA:O	2.49	0.44
8:DK:337:THR:OG1	8:DK:338:GLN:N	2.49	0.44
1:M:9:LYS:HD3	1:S:231:VAL:HG11	1.98	0.44
1:M:245:LYS:HE3	1:M:245:LYS:HB2	1.84	0.44
1:P:189:GLU:O	1:P:191:LEU:HG	2.17	0.44
2:b:87:TRP:HB3	2:b:99:TYR:HB3	1.99	0.44
2:c:212:LYS:HB2	2:c:215:GLU:HB2	1.99	0.44
2:d:235:THR:HG23	1:W:260:LEU:HD12	1.99	0.44
8:DD:247:THR:HG22	8:DD:258:THR:HB	1.98	0.44
8:DF:178:TYR:CE1	8:DF:181:LYS:HB2	2.52	0.44
8:DH:144:MET:HE3	8:DH:306:ASN:HD21	1.82	0.44
1:D:255:GLN:HB2	1:I:238:ARG:NH2	2.32	0.44
1:D:260:LEU:HD22	1:H:248:SER:HB3	1.99	0.44
1:L:56:SER:HB3	1:L:60:THR:HG23	1.99	0.44
2:d:28:ASN:HD22	1:W:43:ASP:HB3	1.82	0.44
6:n:103:ASP:OD1	6:n:104:ARG:N	2.49	0.44
8:DB:87:ASP:OD1	8:DB:91:SER:N	2.50	0.44
8:DG:180:LYS:HB3	8:DG:200:PHE:HB2	1.99	0.44
8:DH:295:ASN:OD1	8:DH:299:THR:OG1	2.31	0.44
8:DK:71:ARG:HH21	8:DK:73:LEU:HB2	1.82	0.44
1:F:238:ARG:HD3	1:F:238:ARG:HA	1.67	0.44
1:H:95:VAL:O	1:H:118:GLY:HA3	2.17	0.44
1:O:1:MET:HE3	2:c:211:VAL:O	2.17	0.44
1:O:34:PHE:HB3	1:O:222:SER:HB3	1.99	0.44
1:P:150:THR:HG23	1:P:158:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:13:UNK:CB	6:k:36:PRO:HD2	2.47	0.44
3:2:13:UNK:O	6:k:36:PRO:HG2	2.18	0.44
6:k:33:ALA:HA	6:k:100:VAL:HG11	1.99	0.44
8:DA:44:ALA:HB2	8:DA:50:LEU:HD11	2.00	0.44
8:DC:130:GLN:OE1	8:DC:130:GLN:N	2.50	0.44
8:DC:210:VAL:O	8:DC:227:SER:OG	2.32	0.44
8:DE:127:THR:OG1	8:DE:128:ILE:N	2.48	0.44
8:DG:63:ASP:OD1	8:DG:63:ASP:N	2.48	0.44
8:DK:29:THR:HB	8:DK:32:PHE:HB2	1.99	0.44
1:A:257:LEU:HG	1:P:230:LEU:HD12	1.99	0.44
5:h:27:ASN:OD1	5:h:42:TYR:OH	2.29	0.44
6:n:49:LEU:HD23	7:q:61:LEU:HD23	2.00	0.44
8:DD:180:LYS:HZ3	8:DD:182:GLY:HA3	1.81	0.44
8:DE:144:MET:SD	8:DE:306:ASN:ND2	2.70	0.44
8:DE:365:ASN:O	8:DE:365:ASN:ND2	2.50	0.44
8:DF:197:ASN:HB2	8:DF:213:HIS:HB3	2.00	0.44
8:DG:197:ASN:N	8:DG:213:HIS:O	2.42	0.44
8:DH:186:VAL:HG13	8:DH:194:HIS:HB2	1.98	0.44
8:DK:194:HIS:HB3	8:DK:196:MET:HE3	1.99	0.44
1:B:121:GLN:N	1:B:129:VAL:O	2.45	0.44
1:I:45:LEU:HD23	1:I:45:LEU:H	1.83	0.44
5:f:97:ASP:O	5:f:101:GLU:HG2	2.17	0.44
5:f:129:THR:HA	6:l:120:LEU:HD11	1.99	0.44
5:j:13:ALA:HB2	6:n:31:ALA:HB1	1.98	0.44
5:j:31:ALA:HA	5:j:96:VAL:HG11	1.99	0.44
6:n:6:ASP:O	6:n:10:ARG:HB2	2.17	0.44
1:V:225:ASN:O	1:V:229:GLU:HG2	2.17	0.44
8:DI:267:MET:HB3	8:DI:269:GLN:OE1	2.18	0.44
8:DJ:337:THR:OG1	8:DJ:338:GLN:N	2.50	0.44
1:D:35:LYS:HB3	1:D:80:LEU:O	2.17	0.44
1:I:106:MET:HE2	1:I:137:GLN:HA	2.00	0.44
1:N:9:LYS:HD3	1:T:231:VAL:HG11	2.00	0.44
1:O:184:LEU:HB3	1:O:192:TYR:HB3	2.00	0.44
1:R:108:PRO:HG2	1:X:153:ARG:NH2	2.33	0.44
2:c:226:ARG:O	2:c:230:GLN:HG2	2.18	0.44
3:3:13:UNK:CB	5:j:49:PHE:HB2	2.48	0.44
6:l:33:ALA:HA	6:l:100:VAL:HG11	1.99	0.44
8:DA:217:ASP:HB2	8:DA:220:ALA:HB2	1.98	0.44
8:DD:187:TYR:CD2	8:DD:285:LYS:HB3	2.52	0.44
8:DK:237:ILE:HD13	8:DK:267:MET:HE1	1.99	0.44
1:B:36:ARG:NH1	1:B:223:ASN:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:ARG:HD3	1:D:238:ARG:HA	1.68	0.44
1:I:35:LYS:HA	1:I:223:ASN:OD1	2.18	0.44
1:O:3:SER:OG	1:T:20:ASP:OD2	2.36	0.44
1:Q:154:ASP:OD1	1:Q:155:GLY:N	2.51	0.44
2:a:55:THR:OG1	5:h:26:SER:OG	2.30	0.44
2:e:65:ASP:O	2:e:210:ASN:ND2	2.51	0.44
8:DA:179:ASN:OD1	8:DA:202:LYS:N	2.43	0.44
8:DA:326:LEU:HB3	8:DA:334:TRP:HB3	2.00	0.44
8:DE:105:ASN:OD1	8:DE:107:ASN:ND2	2.51	0.44
8:DH:44:ALA:H	8:DH:50:LEU:HD23	1.83	0.44
8:DJ:147:LYS:HB2	8:DJ:283:GLY:HA2	2.00	0.44
8:DJ:365:ASN:O	8:DJ:365:ASN:ND2	2.50	0.44
1:C:40:VAL:HG23	1:C:75:VAL:HG13	1.99	0.43
1:E:92:SER:O	1:E:216:GLN:NE2	2.44	0.43
1:G:34:PHE:HB3	1:G:222:SER:HB3	2.00	0.43
1:G:178:PHE:CE2	1:G:201:PRO:HB3	2.53	0.43
1:I:151:ILE:N	1:I:216:GLN:OE1	2.42	0.43
1:U:147:LEU:HB2	1:U:160:THR:HG23	2.00	0.43
2:b:16:LEU:HD23	2:b:16:LEU:HA	1.88	0.43
2:e:76:ARG:HG3	2:e:77:PRO:HD2	1.99	0.43
6:o:42:ASP:OD1	6:o:43:ILE:N	2.48	0.43
1:W:239:ALA:O	1:W:242:ILE:HG22	2.17	0.43
8:DD:306:ASN:OD1	8:DD:306:ASN:N	2.51	0.43
8:DF:330:GLY:HA2	8:DK:43:PHE:H	1.82	0.43
8:DJ:194:HIS:ND1	8:DJ:216:SER:OG	2.44	0.43
1:D:256:LYS:HB3	1:H:241:GLU:OE1	2.18	0.43
1:U:43:ASP:HB3	2:c:28:ASN:HD22	1.82	0.43
6:m:111:ASP:OD1	6:m:115:LYS:NZ	2.51	0.43
5:i:74:GLU:H	5:i:74:GLU:CD	2.25	0.43
8:DC:63:ASP:N	8:DC:63:ASP:OD1	2.48	0.43
8:DC:310:GLN:NE2	8:DC:311:VAL:O	2.51	0.43
8:DE:22:ASN:ND2	8:DJ:49:GLY:HA3	2.33	0.43
8:DK:295:ASN:ND2	8:DK:299:THR:OG1	2.39	0.43
1:D:140:ILE:HD12	1:D:171:GLY:HA3	2.00	0.43
1:D:237:GLN:HA	8:DC:395:ILE:HD11	1.99	0.43
1:G:176:THR:HA	1:G:203:GLU:HA	2.00	0.43
1:I:45:LEU:HD21	1:T:86:LEU:HD13	1.99	0.43
1:T:225:ASN:O	1:T:229:GLU:HG2	2.17	0.43
1:V:194:GLU:H	1:V:194:GLU:CD	2.27	0.43
1:V:255:GLN:O	1:V:259:GLN:HG2	2.18	0.43
8:DA:234:GLU:O	8:DG:190:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DC:281:GLN:HG2	8:DC:283:GLY:H	1.82	0.43
8:DD:382:TYR:CD2	8:DI:395:ILE:HD11	2.53	0.43
8:DE:167:LYS:HE2	8:DE:169:PRO:HG2	1.99	0.43
8:DF:264:LEU:HD23	8:DF:265:ASN:HB2	2.00	0.43
8:DH:345:LEU:H	8:DH:345:LEU:HD12	1.84	0.43
1:E:101:GLY:HA2	1:E:177:THR:HG22	2.00	0.43
1:F:238:ARG:O	1:F:242:ILE:HG12	2.18	0.43
1:I:34:PHE:HB3	1:I:222:SER:HB3	1.99	0.43
1:J:142:ILE:HD13	1:J:149:ILE:HD13	1.99	0.43
1:M:57:SER:OG	1:M:58:GLU:N	2.52	0.43
1:M:238:ARG:HA	1:M:238:ARG:HD3	1.79	0.43
1:N:142:ILE:HD13	1:N:149:ILE:HG12	2.00	0.43
1:R:91:ASN:OD1	1:R:93:LYS:N	2.44	0.43
1:S:31:THR:HG23	1:S:34:PHE:HB2	2.00	0.43
2:a:28:ASN:HB3	1:V:72:VAL:HB	1.99	0.43
2:e:34:PHE:HB3	2:e:209:SER:HB2	2.00	0.43
3:4:9:UNK:HA	5:p:104:ASN:HD21	1.84	0.43
5:f:50:GLN:N	5:f:63:LYS:O	2.52	0.43
6:o:109:PHE:HE1	5:p:121:THR:HG21	1.84	0.43
5:i:42:TYR:OH	5:i:45:LYS:NZ	2.51	0.43
8:DA:181:LYS:HG3	8:DA:199:TYR:HE1	1.83	0.43
8:DB:26:ASN:OD1	8:DG:41:ASP:HB3	2.18	0.43
8:DE:214:ASP:OD2	8:DE:248:THR:OG1	2.36	0.43
8:DF:24:ILE:HG13	8:DF:368:LEU:HD22	2.01	0.43
8:DH:192:ASN:OD1	8:DH:252:ASN:ND2	2.42	0.43
8:DK:34:SER:HB3	8:DK:366:VAL:HG12	2.00	0.43
1:J:42:GLU:OE1	1:O:190:ASN:ND2	2.52	0.43
1:Q:66:LEU:HD23	1:Q:66:LEU:H	1.82	0.43
1:S:102:PHE:HB3	1:S:114:TYR:HB3	2.00	0.43
1:S:176:THR:HG22	1:S:203:GLU:HG2	2.01	0.43
1:U:7:ILE:O	1:U:10:THR:OG1	2.33	0.43
2:a:89:VAL:HG12	2:a:121:ILE:HD11	2.00	0.43
2:d:212:LYS:HB2	2:d:215:GLU:HB3	2.00	0.43
5:g:82:ASN:ND2	5:g:84:LEU:HB2	2.34	0.43
8:DC:337:THR:OG1	8:DC:338:GLN:N	2.50	0.43
1:C:121:GLN:N	1:C:129:VAL:O	2.50	0.43
1:K:256:LYS:HA	1:K:256:LYS:HD2	1.77	0.43
1:P:42:GLU:CG	1:U:189:GLU:HA	2.48	0.43
1:P:49:ILE:HB	1:P:66:LEU:HD22	1.99	0.43
1:U:59:GLN:HB3	1:U:61:THR:HG23	2.00	0.43
2:a:250:MET:HA	5:h:123:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:250:MET:HE3	2:c:250:MET:HB3	1.96	0.43
3:1:13:UNK:HA	5:f:48:VAL:HG13	2.00	0.43
1:X:35:LYS:HA	1:X:223:ASN:OD1	2.19	0.43
1:X:36:ARG:HE	1:X:80:LEU:HD12	1.84	0.43
8:DA:97:ASN:HD21	8:DA:332:ASN:HD21	1.66	0.43
8:DB:103:ASP:OD1	8:DB:107:ASN:N	2.48	0.43
8:DB:288:ASP:OD1	8:DB:305:SER:OG	2.34	0.43
8:DC:71:ARG:NH2	8:DH:324:GLU:OE1	2.51	0.43
8:DD:211:TYR:HB3	8:DD:213:HIS:HE1	1.84	0.43
8:DJ:202:LYS:HB2	8:DJ:208:TRP:CZ3	2.53	0.43
8:DK:87:ASP:OD1	8:DK:91:SER:N	2.52	0.43
8:DK:101:LYS:HB3	8:DK:111:MET:HE1	2.00	0.43
1:A:158:SER:OG	1:A:167:PRO:HB2	2.19	0.43
1:B:240:TYR:CD2	8:DE:395:ILE:HD11	2.54	0.43
1:C:35:LYS:HA	1:C:223:ASN:OD1	2.19	0.43
1:F:150:THR:OG1	1:F:158:SER:OG	2.36	0.43
1:H:238:ARG:HD3	1:H:238:ARG:HA	1.89	0.43
1:K:25:ASN:ND2	1:K:37:GLN:H	2.17	0.43
1:R:4:SER:OG	1:R:250:THR:OG1	2.19	0.43
8:DB:106:ARG:HD3	8:DG:321:ALA:HB1	2.00	0.43
8:DD:365:ASN:O	8:DD:365:ASN:ND2	2.52	0.43
8:DE:129:GLN:OE1	8:DE:129:GLN:N	2.52	0.43
8:DJ:79:GLN:HB3	8:DJ:354:GLY:HA3	2.01	0.43
1:A:45:LEU:HG	1:A:70:THR:HG21	2.00	0.43
1:I:242:ILE:HD12	1:N:230:LEU:HD11	2.00	0.43
1:K:43:ASP:HA	1:K:72:VAL:HA	2.01	0.43
1:T:125:ASN:OD1	1:T:126:GLY:N	2.51	0.43
2:b:49:LEU:HD23	2:b:50:SER:N	2.34	0.43
6:o:120:LEU:HG	5:p:132:LEU:HD12	1.99	0.43
8:DA:140:PRO:HD2	8:DA:312:LEU:HD13	2.01	0.43
8:DB:24:ILE:HD11	8:DG:384:SER:HB2	2.01	0.43
8:DC:94:TYR:O	8:DC:334:TRP:N	2.45	0.43
8:DG:86:VAL:HG23	8:DG:115:GLN:HB2	2.01	0.43
8:DJ:5:GLN:NE2	8:DJ:49:GLY:O	2.42	0.43
1:B:39:ALA:HA	1:B:77:THR:HA	2.01	0.43
1:C:78:GLU:HB2	1:C:182:THR:HG23	2.01	0.43
1:C:145:ASN:O	1:C:145:ASN:ND2	2.52	0.43
1:E:80:LEU:HD22	1:I:91:ASN:ND2	2.34	0.43
1:F:89:THR:OG1	1:F:91:ASN:OD1	2.26	0.43
1:H:58:GLU:OE1	1:H:58:GLU:N	2.45	0.43
1:L:2:ILE:HD12	1:L:2:ILE:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:35:LYS:HG3	1:N:81:HIS:CE1	2.54	0.43
1:O:5:LEU:HD23	1:O:5:LEU:HA	1.81	0.43
1:O:48:THR:HG22	1:O:67:GLN:HG2	2.00	0.43
1:U:82:SER:OG	1:U:83:GLN:N	2.52	0.43
1:U:107:LEU:HD23	1:U:107:LEU:HA	1.86	0.43
2:c:6:TYR:O	2:c:9:MET:HG3	2.18	0.43
2:e:167:GLU:H	2:e:167:GLU:CD	2.27	0.43
5:g:2:ALA:C	7:r:67:ALA:HA	2.43	0.43
1:V:225:ASN:O	1:V:228:GLU:HG3	2.19	0.43
1:W:159:VAL:HG12	1:W:168:VAL:HG22	2.00	0.43
8:DB:159:ASN:N	8:DB:274:ASN:OD1	2.52	0.43
8:DG:34:SER:HB3	8:DG:366:VAL:HG12	2.01	0.43
8:DH:77:ILE:HG22	8:DH:79:GLN:H	1.84	0.43
8:DH:248:THR:OG1	8:DH:257:ALA:N	2.52	0.43
8:DK:298:GLY:O	8:DK:315:ILE:HG12	2.18	0.43
1:B:7:ILE:HG21	1:F:24:ASN:HA	2.01	0.43
1:C:53:GLY:HA2	1:G:197:SER:HB3	2.00	0.43
1:C:77:THR:O	1:C:77:THR:OG1	2.37	0.43
1:C:252:GLN:O	1:C:256:LYS:HG2	2.19	0.43
1:E:257:LEU:HD22	1:I:240:TYR:OH	2.19	0.43
1:H:7:ILE:HG12	1:H:70:THR:O	2.19	0.43
1:L:26:LEU:HD12	1:L:233:MET:HE3	2.01	0.43
1:L:181:ASP:OD1	1:L:181:ASP:N	2.49	0.43
1:Q:256:LYS:HE2	1:V:241:GLU:HG3	2.00	0.43
2:e:5:ILE:HG13	2:e:234:ILE:HD13	2.00	0.43
5:g:82:ASN:HD21	5:g:84:LEU:HD13	1.84	0.43
6:k:8:ALA:HB3	6:k:9:LEU:HD12	2.00	0.43
8:DD:201:VAL:HG13	8:DD:209:ALA:HB3	2.00	0.43
8:DH:80:ASN:ND2	8:DH:319:ASN:OD1	2.52	0.43
1:A:45:LEU:HD22	1:P:98:LYS:HG3	2.01	0.42
1:E:26:LEU:HD23	1:E:26:LEU:HA	1.86	0.42
1:H:35:LYS:HA	1:H:223:ASN:OD1	2.18	0.42
2:a:170:GLU:OE1	2:a:170:GLU:N	2.52	0.42
2:b:2:ASP:O	2:b:5:ILE:HG22	2.19	0.42
2:d:54:ARG:NH2	6:n:92:GLN:OE1	2.51	0.42
8:DA:300:VAL:HG23	8:DA:312:LEU:HB2	2.01	0.42
8:DD:284:TYR:HB2	8:DD:306:ASN:HD22	1.83	0.42
8:DK:197:ASN:HB2	8:DK:213:HIS:HB3	2.01	0.42
1:B:38:ARG:HD3	1:B:80:LEU:HD21	2.00	0.42
1:E:43:ASP:OD2	1:E:46:TYR:OH	2.31	0.42
1:F:35:LYS:HA	1:F:223:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:GLN:NE2	1:H:57:SER:O	2.52	0.42
1:J:238:ARG:HD3	1:J:238:ARG:HA	1.73	0.42
1:N:43:ASP:N	1:N:43:ASP:OD1	2.49	0.42
1:T:34:PHE:HB3	1:T:222:SER:HB3	2.00	0.42
2:e:116:GLN:HG3	2:e:116:GLN:H	1.71	0.42
7:t:49:GLN:HG2	7:t:78:ALA:HB1	2.02	0.42
8:DG:84:ARG:HD2	8:DG:345:LEU:HD11	2.00	0.42
8:DK:94:TYR:O	8:DK:334:TRP:N	2.38	0.42
8:DK:158:LEU:HD13	8:DK:208:TRP:CD2	2.54	0.42
1:C:255:GLN:O	1:C:259:GLN:HG2	2.20	0.42
1:D:41:PHE:HA	1:D:74:PRO:HA	2.00	0.42
1:E:260:LEU:CD2	1:I:248:SER:HB2	2.49	0.42
1:F:108:PRO:HG2	1:L:153:ARG:NH1	2.34	0.42
1:G:46:TYR:CD1	1:G:69:GLY:HA2	2.53	0.42
1:L:7:ILE:HG12	1:L:70:THR:O	2.18	0.42
1:N:40:VAL:HG23	1:N:75:VAL:HG13	2.00	0.42
1:O:175:LEU:HD23	1:O:175:LEU:H	1.84	0.42
1:O:225:ASN:O	1:O:229:GLU:HG2	2.19	0.42
1:U:175:LEU:HD22	1:U:206:PRO:HG3	2.00	0.42
2:b:6:TYR:HA	2:b:9:MET:HG3	2.01	0.42
2:e:115:ILE:HG13	2:e:120:VAL:HG22	2.01	0.42
5:h:118:VAL:HG21	6:m:30:ILE:HG21	2.00	0.42
6:m:90:PRO:HB3	6:m:99:THR:OG1	2.19	0.42
6:k:102:MET:HG3	6:k:106:ARG:CZ	2.48	0.42
7:u:99:VAL:HA	7:u:102:MET:HE3	2.02	0.42
8:DC:34:SER:HB3	8:DC:366:VAL:HG22	2.00	0.42
8:DE:75:VAL:HG21	8:DE:356:LEU:HD13	2.01	0.42
8:DF:32:PHE:O	8:DF:365:ASN:ND2	2.53	0.42
1:C:238:ARG:O	1:C:242:ILE:HG12	2.19	0.42
1:D:254:LEU:HD23	1:D:254:LEU:HA	1.94	0.42
1:E:36:ARG:HB3	1:E:224:VAL:HG22	2.02	0.42
1:H:230:LEU:HD12	8:DD:399:LEU:HG	2.00	0.42
1:L:258:THR:OG1	1:R:241:GLU:HG2	2.19	0.42
1:R:257:LEU:HB2	1:W:240:TYR:HE1	1.84	0.42
2:d:10:GLY:O	2:d:14:GLN:HG2	2.19	0.42
2:e:170:GLU:HB2	2:e:185:ALA:HB2	2.00	0.42
5:g:119:LEU:HD23	5:g:119:LEU:HA	1.91	0.42
5:h:101:GLU:OE1	5:h:101:GLU:N	2.52	0.42
6:o:11:PHE:HZ	7:u:57:GLU:HG3	1.81	0.42
8:DA:155:GLN:OE1	8:DA:265:ASN:ND2	2.52	0.42
8:DC:248:THR:OG1	8:DC:249:GLY:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DF:104:GLU:HB3	8:DK:339:ALA:HA	2.01	0.42
8:DK:213:HIS:CE1	8:DK:215:SER:HB3	2.55	0.42
1:A:77:THR:HB	8:DA:47:LYS:HG2	2.02	0.42
1:J:230:LEU:HD13	8:DB:400:VAL:HA	2.02	0.42
1:M:257:LEU:O	1:M:260:LEU:HB3	2.19	0.42
1:T:248:SER:O	1:T:252:GLN:HG2	2.19	0.42
2:c:170:GLU:HB2	2:c:185:ALA:HB2	2.01	0.42
6:l:130:MET:O	6:l:133:VAL:HG12	2.20	0.42
5:p:97:ASP:OD1	5:p:97:ASP:N	2.46	0.42
6:n:3:ASP:N	6:n:6:ASP:HB3	2.35	0.42
8:DD:337:THR:OG1	8:DD:338:GLN:N	2.53	0.42
8:DD:380:ARG:NH2	8:DJ:397:ASN:HB2	2.35	0.42
1:B:260:LEU:HD21	1:F:244:SER:HB2	2.02	0.42
1:F:44:LEU:HD23	1:F:44:LEU:HA	1.92	0.42
1:L:122:VAL:HG11	1:L:142:ILE:HD12	2.02	0.42
1:O:9:LYS:HD3	1:U:228:GLU:CD	2.44	0.42
2:d:227:PHE:CE2	1:W:257:LEU:HB2	2.49	0.42
5:i:90:TYR:CE2	1:V:45:LEU:HD22	2.55	0.42
8:DD:44:ALA:HB2	8:DD:50:LEU:HD11	2.02	0.42
8:DE:26:ASN:CG	8:DJ:52:VAL:HG12	2.45	0.42
8:DE:54:VAL:HG12	8:DE:56:GLY:H	1.84	0.42
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.86	0.42
1:I:120:PHE:HB3	1:I:128:LEU:HD11	2.02	0.42
1:L:28:ASN:HB2	1:L:31:THR:OG1	2.20	0.42
1:P:179:MET:HE3	1:P:179:MET:HB3	1.82	0.42
5:h:51:VAL:HG12	6:m:32:ASN:ND2	2.34	0.42
5:p:5:ASN:O	5:p:9:ILE:HG12	2.20	0.42
7:q:95:ALA:O	7:q:98:GLU:HG3	2.20	0.42
8:DA:158:LEU:HB2	8:DA:268:GLN:HA	2.01	0.42
8:DH:198:VAL:HA	8:DH:211:TYR:O	2.20	0.42
8:DI:115:GLN:CD	8:DI:115:GLN:H	2.27	0.42
8:DK:180:LYS:HD3	8:DK:274:ASN:HB3	2.01	0.42
1:B:42:GLU:HG2	1:F:189:GLU:HA	2.02	0.42
1:D:178:PHE:CZ	1:D:201:PRO:HB3	2.55	0.42
1:E:67:GLN:H	1:I:77:THR:HG21	1.84	0.42
1:G:45:LEU:HD21	1:R:86:LEU:HD13	2.01	0.42
1:R:213:LEU:HD13	1:R:213:LEU:HA	1.89	0.42
2:a:54:ARG:HH21	6:k:92:GLN:HG3	1.85	0.42
2:a:87:TRP:HB3	2:a:99:TYR:HB3	2.01	0.42
2:a:226:ARG:O	2:a:230:GLN:HG2	2.20	0.42
2:d:114:THR:OG1	2:d:118:HIS:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l:118:MET:HE3	6:l:118:MET:HB3	1.97	0.42
1:W:45:LEU:O	1:W:70:THR:OG1	2.31	0.42
8:DA:22:ASN:OD1	8:DA:26:ASN:ND2	2.53	0.42
8:DE:139:ILE:HD13	8:DE:312:LEU:HD22	2.01	0.42
8:DE:298:GLY:O	8:DE:315:ILE:HG22	2.20	0.42
8:DF:337:THR:OG1	8:DF:338:GLN:N	2.52	0.42
8:DH:212:THR:O	8:DH:223:PRO:HG2	2.19	0.42
8:DI:267:MET:HB3	8:DI:269:GLN:HE22	1.83	0.42
1:C:238:ARG:HA	1:C:238:ARG:HD3	1.75	0.42
1:F:29:VAL:O	1:F:222:SER:OG	2.34	0.42
1:F:257:LEU:HB2	1:K:240:TYR:HE1	1.85	0.42
1:H:178:PHE:CE1	1:H:201:PRO:HB3	2.54	0.42
1:H:255:GLN:HB2	1:N:238:ARG:CZ	2.50	0.42
1:H:255:GLN:HB2	1:N:238:ARG:NH2	2.34	0.42
1:N:89:THR:OG1	1:N:94:ASP:OD2	2.32	0.42
1:N:97:ILE:HD12	1:N:175:LEU:HD22	2.02	0.42
1:S:85:ASN:O	1:S:221:THR:HG22	2.20	0.42
2:e:62:PRO:HG3	1:X:62:LEU:HD12	2.02	0.42
1:V:178:PHE:CE1	1:V:201:PRO:HB3	2.55	0.42
1:X:22:ILE:HG21	1:X:233:MET:HG3	2.02	0.42
8:DD:95:SER:OG	8:DD:97:ASN:OD1	2.32	0.42
8:DG:197:ASN:OD1	8:DG:215:SER:HB2	2.20	0.42
8:DG:208:TRP:O	8:DG:230:LEU:N	2.31	0.42
8:DG:264:LEU:HD23	8:DG:265:ASN:HB2	2.02	0.42
8:DK:295:ASN:HD21	8:DK:299:THR:HG1	1.62	0.42
1:B:31:THR:HG22	8:DE:39:PHE:HB2	2.02	0.42
1:G:255:GLN:NE2	1:G:256:LYS:HE3	2.35	0.42
1:K:254:LEU:HA	1:K:254:LEU:HD23	1.84	0.42
1:L:185:GLU:OE1	1:L:186:SER:N	2.52	0.42
1:S:158:SER:OG	1:S:167:PRO:HB2	2.20	0.42
5:g:28:LEU:HD23	5:g:28:LEU:HA	1.89	0.42
6:l:11:PHE:CZ	7:r:57:GLU:HG2	2.55	0.42
1:V:187:ILE:HG13	1:V:191:LEU:HB2	2.01	0.42
7:r:42:LEU:HA	7:r:45:ILE:HG12	2.01	0.42
8:DC:228:THR:HG21	8:DC:244:VAL:HG21	2.01	0.42
8:DD:79:GLN:HB2	8:DD:354:GLY:HA3	2.02	0.42
8:DD:217:ASP:CG	8:DD:249:GLY:HA3	2.45	0.42
8:DE:155:GLN:HB3	8:DE:278:ALA:HB3	2.01	0.42
8:DK:105:ASN:ND2	8:DK:107:ASN:HD21	2.18	0.42
1:I:163:GLY:O	1:I:164:GLN:HG2	2.20	0.41
1:L:53:GLY:HA2	1:Q:197:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:155:GLY:HA2	1:M:214:LEU:HD12	2.02	0.41
1:M:178:PHE:CZ	1:M:201:PRO:HB3	2.55	0.41
1:N:48:THR:HG22	1:N:67:GLN:HG2	2.01	0.41
1:R:177:THR:OG1	1:R:202:ASN:OD1	2.25	0.41
2:b:5:ILE:HG13	2:b:234:ILE:HD13	2.02	0.41
2:b:82:LEU:HD13	2:b:201:ILE:HG22	2.02	0.41
2:c:44:VAL:HG23	2:c:56:LEU:HB2	2.02	0.41
2:c:134:GLU:OE1	2:c:134:GLU:N	2.48	0.41
2:e:232:LYS:HD3	5:j:102:MET:HE1	2.01	0.41
8:DB:139:ILE:HA	8:DB:312:LEU:HD13	2.02	0.41
8:DJ:87:ASP:OD1	8:DJ:91:SER:N	2.53	0.41
1:B:98:LYS:NZ	1:B:215:TYR:OH	2.31	0.41
1:G:177:THR:OG1	1:G:178:PHE:N	2.53	0.41
1:G:238:ARG:HA	1:G:238:ARG:HD3	1.77	0.41
1:K:242:ILE:HD13	1:P:226:VAL:CG1	2.48	0.41
2:a:57:VAL:HG22	5:h:30:ASN:OD1	2.20	0.41
1:W:34:PHE:HB3	1:W:222:SER:HB3	2.01	0.41
1:W:41:PHE:HD1	1:W:74:PRO:HA	1.85	0.41
7:r:66:ILE:HG22	7:r:68:LEU:H	1.86	0.41
7:t:59:PHE:HB2	7:t:66:ILE:HG21	2.02	0.41
8:DA:380:ARG:HD3	8:DA:380:ARG:HA	1.88	0.41
8:DB:233:ASN:N	8:DB:237:ILE:O	2.27	0.41
8:DE:26:ASN:OD1	8:DJ:52:VAL:HG12	2.21	0.41
8:DE:126:PRO:HG2	8:DE:310:GLN:NE2	2.35	0.41
8:DF:144:MET:HE3	8:DF:306:ASN:HD21	1.84	0.41
8:DI:281:GLN:HG2	8:DI:283:GLY:H	1.85	0.41
2:b:133:SER:OG	2:b:146:LEU:N	2.53	0.41
1:W:42:GLU:HG2	1:W:75:VAL:HG11	2.02	0.41
8:DF:197:ASN:OD1	8:DF:215:SER:HB2	2.21	0.41
8:DI:122:THR:OG1	8:DI:129:GLN:NE2	2.53	0.41
1:A:111:THR:OG1	1:A:112:SER:N	2.54	0.41
1:A:244:SER:O	8:DA:402:LEU:HD11	2.20	0.41
1:J:184:LEU:HB3	1:J:192:TYR:HB3	2.00	0.41
1:L:2:ILE:HG13	1:L:3:SER:H	1.85	0.41
1:O:255:GLN:HA	1:O:258:THR:HG22	2.00	0.41
1:T:246:ALA:HB2	2:b:220:MET:HE1	2.03	0.41
2:a:217:MET:HE1	1:V:245:LYS:HE2	2.02	0.41
2:c:176:ASP:OD1	2:c:176:ASP:N	2.53	0.41
2:e:65:ASP:OD1	2:e:65:ASP:N	2.45	0.41
5:h:47:VAL:HG12	5:h:67:VAL:HG22	2.03	0.41
1:V:26:LEU:HD23	1:V:26:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:239:ALA:O	1:X:242:ILE:HG22	2.21	0.41
8:DB:200:PHE:HE1	8:DB:210:VAL:HG13	1.85	0.41
8:DE:197:ASN:O	8:DE:213:HIS:N	2.54	0.41
8:DE:299:THR:HG22	8:DE:314:GLN:HB3	2.03	0.41
8:DH:118:GLY:HA2	8:DH:316:VAL:HG13	2.02	0.41
8:DH:326:LEU:HB3	8:DH:334:TRP:HB3	2.02	0.41
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.93	0.41
1:E:235:GLN:NE2	8:DC:3:PHE:HB3	2.35	0.41
1:G:45:LEU:HD13	1:R:98:LYS:HD2	2.02	0.41
1:G:106:MET:HE1	1:G:137:GLN:HA	2.03	0.41
1:L:43:ASP:HA	1:L:72:VAL:HA	2.03	0.41
1:Q:175:LEU:HD11	1:Q:211:ALA:HB1	2.02	0.41
1:S:148:SER:H	1:S:160:THR:HG22	1.84	0.41
1:U:194:GLU:H	1:U:194:GLU:CD	2.29	0.41
2:d:228:GLU:HG2	1:W:256:LYS:HD3	2.02	0.41
5:p:2:ALA:HA	7:v:67:ALA:HA	2.02	0.41
8:DG:372:LEU:HD23	8:DG:372:LEU:HA	1.94	0.41
8:DJ:167:LYS:HE3	8:DJ:169:PRO:HG2	2.02	0.41
1:B:51:GLN:NE2	1:F:185:GLU:OE1	2.53	0.41
1:B:189:GLU:HG2	1:B:191:LEU:HG	2.02	0.41
1:G:101:GLY:HA3	1:G:175:LEU:HD13	2.03	0.41
1:H:25:ASN:HD21	1:H:37:GLN:H	1.68	0.41
1:H:44:LEU:HD21	1:H:73:ARG:HD3	2.02	0.41
1:I:44:LEU:HD23	1:I:44:LEU:HA	1.85	0.41
1:M:123:ASP:OD1	1:M:127:GLN:N	2.53	0.41
1:R:137:GLN:HB3	1:R:138:PRO:HD3	2.02	0.41
1:S:72:VAL:CG1	1:X:28:ASN:HB3	2.51	0.41
1:S:72:VAL:HG11	1:X:28:ASN:HB3	2.03	0.41
8:DF:127:THR:OG1	8:DF:128:ILE:N	2.54	0.41
8:DI:288:ASP:OD1	8:DI:288:ASP:N	2.51	0.41
8:DJ:41:ASP:OD1	8:DJ:41:ASP:N	2.53	0.41
1:E:255:GLN:HB2	1:J:238:ARG:CZ	2.50	0.41
1:E:258:THR:HG21	1:J:241:GLU:CD	2.45	0.41
1:F:148:SER:OG	1:F:160:THR:OG1	2.32	0.41
1:G:242:ILE:HG21	1:L:26:LEU:HD22	2.03	0.41
1:J:34:PHE:HB3	1:J:222:SER:HB3	2.02	0.41
1:J:260:LEU:CD2	1:O:248:SER:HB3	2.48	0.41
1:K:28:ASN:HB2	1:K:31:THR:OG1	2.20	0.41
2:b:94:ASP:OD1	2:b:95:GLY:N	2.53	0.41
4:7:320:PRO:HD3	6:m:87:TYR:CE2	2.56	0.41
6:l:102:MET:O	6:l:106:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:257:LEU:O	1:W:260:LEU:HB3	2.21	0.41
8:DE:221:THR:OG1	8:DE:222:ALA:N	2.54	0.41
8:DG:85:LEU:HD13	8:DG:116:LEU:HA	2.01	0.41
8:DH:79:GLN:HB3	8:DH:354:GLY:HA3	2.02	0.41
1:A:137:GLN:HB3	1:A:138:PRO:HD3	2.02	0.41
1:B:1:MET:HE3	1:G:238:ARG:CB	2.50	0.41
1:C:254:LEU:HD12	1:C:254:LEU:HA	1.90	0.41
1:E:149:ILE:HG13	1:E:159:VAL:HG23	2.03	0.41
1:F:93:LYS:HE2	1:F:93:LYS:HB3	1.90	0.41
1:R:130:THR:OG1	1:R:131:ALA:N	2.54	0.41
2:d:44:VAL:HG11	4:8:328:ILE:CD1	2.36	0.41
6:o:26:LEU:HA	6:o:29:ASN:ND2	2.36	0.41
1:W:172:GLN:HE21	1:W:205:THR:HG23	1.85	0.41
8:DB:87:ASP:HB3	8:DB:114:MET:HE3	2.01	0.41
8:DB:144:MET:HE1	8:DB:308:GLN:HB2	2.01	0.41
8:DE:24:ILE:HD11	8:DJ:384:SER:HB3	2.02	0.41
8:DE:188:ASP:OD2	8:DE:192:ASN:HB2	2.21	0.41
8:DF:364:SER:O	8:DF:365:ASN:ND2	2.54	0.41
8:DI:294:ILE:HG23	8:DI:358:ASN:HD22	1.86	0.41
8:DK:186:VAL:HG21	8:DK:259:PHE:CZ	2.56	0.41
1:A:48:THR:HG22	1:A:67:GLN:HG2	2.03	0.41
1:A:97:ILE:HG23	1:A:116:ARG:HE	1.85	0.41
1:B:258:THR:O	1:G:245:LYS:NZ	2.54	0.41
1:C:2:ILE:HG23	1:C:5:LEU:H	1.85	0.41
1:C:39:ALA:HA	1:C:77:THR:HA	2.03	0.41
1:D:91:ASN:HB2	1:D:94:ASP:OD1	2.21	0.41
1:G:255:GLN:HA	1:G:258:THR:HG22	2.03	0.41
1:G:257:LEU:HB2	1:L:240:TYR:HE1	1.86	0.41
1:P:26:LEU:HD23	1:P:26:LEU:HA	1.87	0.41
1:Q:187:ILE:HG13	1:Q:191:LEU:HB2	2.03	0.41
2:b:65:ASP:OD1	2:b:65:ASP:N	2.52	0.41
2:b:91:GLN:HB2	2:b:121:ILE:HG13	2.02	0.41
2:c:101:ARG:NH2	2:c:207:GLU:OE1	2.45	0.41
2:d:49:LEU:HD23	6:n:90:PRO:HD2	2.03	0.41
3:2:13:UNK:CB	5:i:49:PHE:HB2	2.51	0.41
5:h:23:VAL:HG13	5:h:45:LYS:HG3	2.03	0.41
6:l:127:LEU:HD23	6:l:127:LEU:HA	1.93	0.41
5:i:50:GLN:N	5:i:63:LYS:O	2.54	0.41
8:DA:264:LEU:HD23	8:DA:265:ASN:HB2	2.03	0.41
8:DA:337:THR:OG1	8:DA:338:GLN:N	2.54	0.41
8:DB:154:MET:HE1	8:DB:156:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DB:239:GLU:OE1	8:DB:239:GLU:N	2.54	0.41
8:DB:347:THR:HG23	8:DB:350:SER:H	1.86	0.41
8:DC:147:LYS:NZ	8:DC:282:ASN:O	2.33	0.41
8:DC:269:GLN:HG2	8:DI:190:GLN:HA	2.01	0.41
8:DE:364:SER:O	8:DE:366:VAL:HG23	2.21	0.41
8:DG:82:PHE:HE1	8:DG:96:ARG:HD2	1.86	0.41
8:DI:204:LYS:HE3	8:DI:204:LYS:HB2	1.94	0.41
8:DJ:5:GLN:OE1	8:DJ:5:GLN:N	2.51	0.41
8:DJ:12:ALA:HB1	8:DJ:39:PHE:CE1	2.56	0.41
8:DJ:109:VAL:HG22	8:DJ:115:GLN:HA	2.03	0.41
8:DK:108:LEU:HD13	8:DK:108:LEU:HA	1.94	0.41
8:DK:248:THR:OG1	8:DK:249:GLY:N	2.54	0.41
1:L:242:ILE:HD12	1:Q:230:LEU:HD21	2.03	0.41
1:T:26:LEU:HD23	1:T:26:LEU:HA	1.93	0.41
1:U:72:VAL:HB	2:c:28:ASN:HB3	2.03	0.41
1:U:246:ALA:HA	2:c:220:MET:HE3	2.02	0.41
2:c:107:VAL:HG22	2:c:113:LEU:HD23	2.02	0.41
5:f:4:LEU:HD13	5:f:4:LEU:HA	1.89	0.41
5:g:110:ARG:HA	5:g:110:ARG:HD3	1.76	0.41
5:h:28:LEU:HD23	5:h:28:LEU:HA	1.80	0.41
5:p:28:LEU:HD23	5:p:28:LEU:HA	1.94	0.41
7:s:84:MET:HE3	7:s:84:MET:HB3	1.93	0.41
8:DG:118:GLY:N	8:DG:135:ALA:O	2.53	0.41
8:DG:182:GLY:N	8:DG:198:VAL:O	2.44	0.41
1:B:35:LYS:HB3	1:B:80:LEU:O	2.21	0.40
1:C:120:PHE:HB3	1:C:128:LEU:HD11	2.02	0.40
1:D:109:ASP:OD1	1:D:111:THR:HG22	2.21	0.40
1:E:178:PHE:CE2	1:E:201:PRO:HB3	2.57	0.40
1:E:248:SER:HB2	8:DB:402:LEU:HG	2.03	0.40
1:H:106:MET:HB2	1:H:137:GLN:OE1	2.21	0.40
1:L:179:MET:HE1	1:Q:144:ALA:HB2	2.03	0.40
1:P:195:THR:HG22	2:a:152:PRO:HB2	2.03	0.40
1:S:70:THR:HG21	5:g:76:LEU:O	2.21	0.40
1:T:129:VAL:HG12	1:T:135:GLN:HA	2.03	0.40
6:m:118:MET:HE2	7:s:59:PHE:CE2	2.55	0.40
1:W:40:VAL:O	1:W:75:VAL:HG12	2.21	0.40
8:DA:116:LEU:HD21	8:DA:315:ILE:HD12	2.03	0.40
8:DC:233:ASN:OD1	8:DC:234:GLU:N	2.50	0.40
8:DJ:3:PHE:O	8:DJ:7:VAL:HG12	2.21	0.40
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.88	0.40
1:B:59:GLN:HG2	1:B:60:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:HD23	1:C:26:LEU:HA	1.82	0.40
1:I:26:LEU:HD23	1:I:26:LEU:HA	1.88	0.40
1:J:7:ILE:HG12	1:J:70:THR:O	2.22	0.40
1:N:180:ASN:ND2	1:S:122:VAL:O	2.53	0.40
1:O:97:ILE:HD11	1:O:103:PHE:CE2	2.57	0.40
1:U:46:TYR:OH	2:c:173:ARG:NH1	2.55	0.40
2:b:99:TYR:HE2	2:b:181:LEU:HG	1.87	0.40
2:d:71:LEU:HA	2:d:207:GLU:HA	2.02	0.40
2:e:44:VAL:HG23	2:e:56:LEU:HB2	2.04	0.40
5:g:2:ALA:C	5:g:4:LEU:H	2.29	0.40
6:l:9:LEU:HD23	6:l:123:LEU:HD11	2.03	0.40
1:X:147:LEU:HB2	1:X:160:THR:HG23	2.02	0.40
7:t:57:GLU:HA	7:t:60:THR:HG22	2.04	0.40
7:u:45:ILE:HD11	7:u:82:MET:HA	2.04	0.40
8:DA:143:LEU:HD22	8:DA:288:ASP:HA	2.04	0.40
8:DD:337:THR:O	8:DD:340:SER:OG	2.32	0.40
8:DF:288:ASP:OD1	8:DF:289:LEU:N	2.54	0.40
8:DI:246:ILE:HD13	8:DI:246:ILE:HA	1.93	0.40
8:DI:337:THR:OG1	8:DI:338:GLN:N	2.53	0.40
8:DK:318:ALA:HB2	8:DK:345:LEU:HD13	2.04	0.40
1:F:19:MET:HB2	1:F:236:VAL:HG11	2.04	0.40
1:G:256:LYS:HA	1:G:256:LYS:HD3	1.84	0.40
1:J:95:VAL:O	1:J:118:GLY:HA3	2.21	0.40
1:L:42:GLU:CD	1:Q:190:ASN:HB2	2.46	0.40
1:S:254:LEU:HD23	2:b:225:ARG:HG3	2.02	0.40
1:T:205:THR:HG23	1:T:208:LEU:HD13	2.03	0.40
1:U:55:GLN:N	1:U:55:GLN:OE1	2.55	0.40
2:d:65:ASP:OD1	2:d:65:ASP:N	2.54	0.40
2:e:9:MET:HE3	5:p:100:GLY:HA2	2.02	0.40
5:i:50:GLN:HG3	5:i:65:ALA:HB2	2.03	0.40
5:i:110:ARG:HA	5:i:110:ARG:HD3	1.83	0.40
6:k:102:MET:O	6:k:105:GLU:HG3	2.22	0.40
1:W:2:ILE:HG22	1:W:4:SER:H	1.87	0.40
1:W:18:ASN:O	1:W:22:ILE:HG12	2.21	0.40
1:X:134:PHE:CE2	1:X:189:GLU:HG3	2.56	0.40
7:q:68:LEU:HA	7:q:71:VAL:HG12	2.03	0.40
8:DB:80:ASN:OD1	8:DB:80:ASN:N	2.54	0.40
8:DF:74:ASP:OD1	8:DF:74:ASP:N	2.52	0.40
8:DF:87:ASP:N	8:DF:91:SER:O	2.47	0.40
8:DI:372:LEU:HD23	8:DI:372:LEU:HA	1.96	0.40
1:D:163:GLY:C	1:D:165:ALA:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:41:PHE:HA	1:I:74:PRO:HA	2.04	0.40
1:M:178:PHE:CE2	1:M:201:PRO:HB3	2.57	0.40
1:O:159:VAL:HG13	1:O:168:VAL:HG13	2.03	0.40
1:O:179:MET:HE1	1:T:126:GLY:HA2	2.03	0.40
5:f:6:ILE:H	5:f:6:ILE:HG12	1.72	0.40
6:k:101:ASP:OD1	6:k:102:MET:N	2.50	0.40
8:DC:194:HIS:HA	8:DC:216:SER:OG	2.21	0.40
8:DG:147:LYS:HD2	8:DG:148:SER:O	2.21	0.40
8:DK:71:ARG:NH2	8:DK:73:LEU:HB2	2.37	0.40
8:DK:382:TYR:O	8:DK:382:TYR:CG	2.73	0.40
1:A:52:PRO:HB3	1:A:65:GLY:H	1.87	0.40
1:C:67:GLN:HE22	1:G:185:GLU:HG3	1.86	0.40
1:D:44:LEU:HD23	1:D:44:LEU:HA	1.85	0.40
1:F:26:LEU:HA	1:F:26:LEU:HD23	1.83	0.40
1:H:109:ASP:OD2	1:S:162:GLN:NE2	2.54	0.40
1:M:56:SER:HB2	1:M:62:LEU:HG	2.04	0.40
1:N:26:LEU:HD23	1:N:26:LEU:HA	1.89	0.40
1:T:62:LEU:HD21	5:g:83:PRO:HD2	2.03	0.40
2:b:105:ILE:HG12	2:b:115:ILE:HD11	2.03	0.40
2:d:226:ARG:O	2:d:230:GLN:HG2	2.21	0.40
5:h:85:ALA:HA	5:h:91:VAL:HG12	2.04	0.40
5:p:47:VAL:HG12	5:p:67:VAL:HG12	2.04	0.40
5:p:126:MET:HE3	7:r:80:VAL:HG21	2.03	0.40
6:k:36:PRO:HB3	6:k:96:ASP:HB2	2.04	0.40
1:V:238:ARG:HD3	1:V:238:ARG:HA	1.81	0.40
8:DC:74:ASP:OD1	8:DC:74:ASP:N	2.54	0.40
8:DF:168:THR:N	8:DF:169:PRO:HD2	2.37	0.40
8:DH:32:PHE:O	8:DH:365:ASN:ND2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/260 (99%)	249 (96%)	9 (4%)	0	100	100
1	B	258/260 (99%)	247 (96%)	11 (4%)	0	100	100
1	C	258/260 (99%)	247 (96%)	11 (4%)	0	100	100
1	D	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	E	258/260 (99%)	246 (95%)	12 (5%)	0	100	100
1	F	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	G	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	H	258/260 (99%)	245 (95%)	13 (5%)	0	100	100
1	I	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	J	258/260 (99%)	252 (98%)	6 (2%)	0	100	100
1	K	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	L	257/260 (99%)	250 (97%)	7 (3%)	0	100	100
1	M	258/260 (99%)	247 (96%)	11 (4%)	0	100	100
1	N	247/260 (95%)	240 (97%)	7 (3%)	0	100	100
1	O	248/260 (95%)	240 (97%)	8 (3%)	0	100	100
1	P	244/260 (94%)	236 (97%)	8 (3%)	0	100	100
1	Q	243/260 (94%)	237 (98%)	6 (2%)	0	100	100
1	R	246/260 (95%)	238 (97%)	8 (3%)	0	100	100
1	S	243/260 (94%)	235 (97%)	8 (3%)	0	100	100
1	T	249/260 (96%)	241 (97%)	8 (3%)	0	100	100
1	U	257/260 (99%)	243 (95%)	14 (5%)	0	100	100
1	V	257/260 (99%)	249 (97%)	8 (3%)	0	100	100
1	W	257/260 (99%)	242 (94%)	15 (6%)	0	100	100
1	X	257/260 (99%)	244 (95%)	13 (5%)	0	100	100
2	a	247/251 (98%)	236 (96%)	11 (4%)	0	100	100
2	b	246/251 (98%)	236 (96%)	10 (4%)	0	100	100
2	c	247/251 (98%)	237 (96%)	10 (4%)	0	100	100
2	d	247/251 (98%)	232 (94%)	15 (6%)	0	100	100
2	e	247/251 (98%)	231 (94%)	16 (6%)	0	100	100
4	5	19/21 (90%)	19 (100%)	0	0	100	100
4	6	19/21 (90%)	19 (100%)	0	0	100	100
4	7	19/21 (90%)	19 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	8	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
4	9	19/21 (90%)	19 (100%)	0	0	100	100
5	f	124/134 (92%)	120 (97%)	4 (3%)	0	100	100
5	g	126/134 (94%)	121 (96%)	5 (4%)	0	100	100
5	h	124/134 (92%)	120 (97%)	4 (3%)	0	100	100
5	i	125/134 (93%)	121 (97%)	4 (3%)	0	100	100
5	j	123/134 (92%)	119 (97%)	4 (3%)	0	100	100
5	p	125/134 (93%)	120 (96%)	5 (4%)	0	100	100
6	k	104/138 (75%)	99 (95%)	5 (5%)	0	100	100
6	l	102/138 (74%)	101 (99%)	1 (1%)	0	100	100
6	m	102/138 (74%)	99 (97%)	3 (3%)	0	100	100
6	n	103/138 (75%)	99 (96%)	4 (4%)	0	100	100
6	o	105/138 (76%)	103 (98%)	2 (2%)	0	100	100
7	q	69/104 (66%)	68 (99%)	1 (1%)	0	100	100
7	r	68/104 (65%)	64 (94%)	4 (6%)	0	100	100
7	s	70/104 (67%)	70 (100%)	0	0	100	100
7	t	70/104 (67%)	69 (99%)	1 (1%)	0	100	100
7	u	70/104 (67%)	70 (100%)	0	0	100	100
7	v	36/104 (35%)	36 (100%)	0	0	100	100
8	DA	399/403 (99%)	377 (94%)	22 (6%)	0	100	100
8	DB	399/403 (99%)	377 (94%)	22 (6%)	0	100	100
8	DC	399/403 (99%)	375 (94%)	24 (6%)	0	100	100
8	DD	399/403 (99%)	378 (95%)	21 (5%)	0	100	100
8	DE	399/403 (99%)	380 (95%)	19 (5%)	0	100	100
8	DF	399/403 (99%)	376 (94%)	23 (6%)	0	100	100
8	DG	399/403 (99%)	382 (96%)	17 (4%)	0	100	100
8	DH	399/403 (99%)	379 (95%)	18 (4%)	2 (0%)	24	55
8	DI	399/403 (99%)	381 (96%)	18 (4%)	0	100	100
8	DJ	399/403 (99%)	375 (94%)	23 (6%)	1 (0%)	36	65
8	DK	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
All	All	13465/14151 (95%)	12899 (96%)	563 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	DJ	332	ASN
8	DH	270	ASN
8	DH	71	ARG

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	A	215/215 (100%)	212 (99%)	3 (1%)	59	73
1	B	215/215 (100%)	212 (99%)	3 (1%)	59	73
1	C	215/215 (100%)	209 (97%)	6 (3%)	38	62
1	D	215/215 (100%)	213 (99%)	2 (1%)	70	78
1	E	215/215 (100%)	210 (98%)	5 (2%)	44	66
1	F	215/215 (100%)	212 (99%)	3 (1%)	59	73
1	G	215/215 (100%)	207 (96%)	8 (4%)	30	58
1	H	215/215 (100%)	210 (98%)	5 (2%)	44	66
1	I	215/215 (100%)	211 (98%)	4 (2%)	50	68
1	J	215/215 (100%)	210 (98%)	5 (2%)	44	66
1	K	215/215 (100%)	211 (98%)	4 (2%)	50	68
1	L	214/215 (100%)	211 (99%)	3 (1%)	59	73
1	M	215/215 (100%)	209 (97%)	6 (3%)	38	62
1	N	208/215 (97%)	208 (100%)	0	100	100
1	O	209/215 (97%)	206 (99%)	3 (1%)	59	73
1	P	204/215 (95%)	201 (98%)	3 (2%)	57	72
1	Q	204/215 (95%)	199 (98%)	5 (2%)	42	64
1	R	206/215 (96%)	199 (97%)	7 (3%)	32	59
1	S	204/215 (95%)	202 (99%)	2 (1%)	68	76
1	T	210/215 (98%)	208 (99%)	2 (1%)	68	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	214/215 (100%)	210 (98%)	4 (2%)	50	68
1	V	214/215 (100%)	207 (97%)	7 (3%)	33	59
1	W	214/215 (100%)	211 (99%)	3 (1%)	59	73
1	X	214/215 (100%)	209 (98%)	5 (2%)	44	66
2	a	191/193 (99%)	185 (97%)	6 (3%)	35	60
2	b	190/193 (98%)	184 (97%)	6 (3%)	34	60
2	c	191/193 (99%)	183 (96%)	8 (4%)	26	55
2	d	191/193 (99%)	187 (98%)	4 (2%)	47	67
2	e	191/193 (99%)	187 (98%)	4 (2%)	47	67
4	5	15/15 (100%)	14 (93%)	1 (7%)	15	42
4	6	15/15 (100%)	15 (100%)	0	100	100
4	7	15/15 (100%)	15 (100%)	0	100	100
4	8	15/15 (100%)	15 (100%)	0	100	100
4	9	15/15 (100%)	15 (100%)	0	100	100
5	f	101/105 (96%)	98 (97%)	3 (3%)	36	61
5	g	102/105 (97%)	98 (96%)	4 (4%)	28	56
5	h	101/105 (96%)	99 (98%)	2 (2%)	48	68
5	i	102/105 (97%)	98 (96%)	4 (4%)	28	56
5	j	101/105 (96%)	100 (99%)	1 (1%)	68	76
5	p	101/105 (96%)	101 (100%)	0	100	100
6	k	91/113 (80%)	90 (99%)	1 (1%)	65	76
6	l	89/113 (79%)	86 (97%)	3 (3%)	32	59
6	m	89/113 (79%)	86 (97%)	3 (3%)	32	59
6	n	90/113 (80%)	87 (97%)	3 (3%)	33	59
6	o	91/113 (80%)	87 (96%)	4 (4%)	25	54
7	q	55/79 (70%)	54 (98%)	1 (2%)	51	70
7	r	54/79 (68%)	53 (98%)	1 (2%)	50	68
7	s	56/79 (71%)	56 (100%)	0	100	100
7	t	56/79 (71%)	55 (98%)	1 (2%)	51	70
7	u	56/79 (71%)	56 (100%)	0	100	100
7	v	32/79 (40%)	30 (94%)	2 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	DA	321/323 (99%)	315 (98%)	6 (2%)	50	68
8	DB	321/323 (99%)	316 (98%)	5 (2%)	55	72
8	DC	321/323 (99%)	317 (99%)	4 (1%)	63	75
8	DD	321/323 (99%)	315 (98%)	6 (2%)	50	68
8	DE	321/323 (99%)	320 (100%)	1 (0%)	86	86
8	DF	321/323 (99%)	315 (98%)	6 (2%)	50	68
8	DG	321/323 (99%)	318 (99%)	3 (1%)	70	78
8	DH	321/323 (99%)	314 (98%)	7 (2%)	45	66
8	DI	321/323 (99%)	315 (98%)	6 (2%)	50	68
8	DJ	321/323 (99%)	316 (98%)	5 (2%)	55	72
8	DK	321/323 (99%)	318 (99%)	3 (1%)	70	78
All	All	11022/11422 (96%)	10810 (98%)	212 (2%)	49	68

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ILE
1	A	159	VAL
1	A	164	GLN
1	B	75	VAL
1	B	77	THR
1	B	179	MET
1	C	75	VAL
1	C	77	THR
1	C	95	VAL
1	C	97	ILE
1	C	141	THR
1	C	159	VAL
1	D	97	ILE
1	D	157	VAL
1	E	28	ASN
1	E	97	ILE
1	E	157	VAL
1	E	164	GLN
1	E	259	GLN
1	F	75	VAL
1	F	105	VAL
1	F	177	THR

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Mol	Chain	Res	Type
1	G	117	ASP
1	G	141	THR
1	G	157	VAL
1	G	159	VAL
1	G	168	VAL
1	G	195	THR
1	G	226	VAL
1	G	241	GLU
1	H	42	GLU
1	H	105	VAL
1	H	157	VAL
1	H	175	LEU
1	H	226	VAL
1	I	40	VAL
1	I	42	GLU
1	I	150	THR
1	I	256	LYS
1	J	70	THR
1	J	72	VAL
1	J	97	ILE
1	J	157	VAL
1	J	175	LEU
1	K	42	GLU
1	K	97	ILE
1	K	157	VAL
1	K	202	ASN
1	L	117	ASP
1	L	175	LEU
1	L	245	LYS
1	M	70	THR
1	M	72	VAL
1	M	157	VAL
1	M	195	THR
1	M	256	LYS
1	M	258	THR
1	O	157	VAL
1	O	168	VAL
1	O	179	MET
1	P	159	VAL
1	P	168	VAL
1	P	254	LEU
1	Q	42	GLU

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Mol	Chain	Res	Type
1	Q	70	THR
1	Q	141	THR
1	Q	149	ILE
1	Q	179	MET
1	R	43	ASP
1	R	98	LYS
1	R	141	THR
1	R	149	ILE
1	R	150	THR
1	R	159	VAL
1	R	181	ASP
1	S	109	ASP
1	S	141	THR
1	T	141	THR
1	T	157	VAL
1	U	97	ILE
1	U	150	THR
1	U	159	VAL
1	U	257	LEU
2	a	46	VAL
2	a	49	LEU
2	a	51	LEU
2	a	71	LEU
2	a	150	ASP
2	a	247	LEU
2	b	49	LEU
2	b	71	LEU
2	b	89	VAL
2	b	182	THR
2	b	214	VAL
2	b	247	LEU
2	c	7	THR
2	c	44	VAL
2	c	46	VAL
2	c	71	LEU
2	c	120	VAL
2	c	155	VAL
2	c	214	VAL
2	c	238	ASP
2	d	57	VAL
2	d	58	THR
2	d	71	LEU

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Mol	Chain	Res	Type
2	d	78	LEU
2	e	49	LEU
2	e	78	LEU
2	e	107	VAL
2	e	114	THR
4	5	312	VAL
5	f	119	LEU
5	f	125	MET
5	f	132	LEU
5	g	4	LEU
5	g	6	ILE
5	g	48	VAL
5	g	116	ILE
5	h	91	VAL
5	h	119	LEU
5	j	96	VAL
6	l	86	LEU
6	l	132	ASN
6	l	133	VAL
6	m	4	ARG
6	m	83	VAL
6	m	100	VAL
6	o	18	LEU
6	o	83	VAL
6	o	89	VAL
6	o	127	LEU
5	i	91	VAL
5	i	97	ASP
5	i	101	GLU
5	i	102	MET
6	k	111	ASP
6	n	29	ASN
6	n	100	VAL
6	n	132	ASN
1	V	28	ASN
1	V	45	LEU
1	V	90	ASN
1	V	156	VAL
1	V	157	VAL
1	V	168	VAL
1	V	175	LEU
1	W	168	VAL

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Mol	Chain	Res	Type
1	W	257	LEU
1	W	260	LEU
1	X	142	ILE
1	X	159	VAL
1	X	179	MET
1	X	185	GLU
1	X	195	THR
7	q	57	GLU
7	r	71	VAL
7	t	71	VAL
7	v	75	MET
7	v	92	LEU
8	DA	17	LEU
8	DA	48	VAL
8	DA	157	ASN
8	DA	212	THR
8	DA	322	ASN
8	DA	352	ASN
8	DB	26	ASN
8	DB	161	THR
8	DB	183	THR
8	DB	228	THR
8	DB	324	GLU
8	DC	48	VAL
8	DC	168	THR
8	DC	316	VAL
8	DC	342	VAL
8	DD	80	ASN
8	DD	92	VAL
8	DD	201	VAL
8	DD	295	ASN
8	DD	372	LEU
8	DD	400	VAL
8	DE	295	ASN
8	DF	92	VAL
8	DF	111	MET
8	DF	137	ILE
8	DF	250	THR
8	DF	332	ASN
8	DF	344	LEU
8	DG	41	ASP
8	DG	393	ASP

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Mol	Chain	Res	Type
8	DG	395	ILE
8	DH	17	LEU
8	DH	48	VAL
8	DH	161	THR
8	DH	279	THR
8	DH	300	VAL
8	DH	395	ILE
8	DH	400	VAL
8	DI	17	LEU
8	DI	60	ASP
8	DI	92	VAL
8	DI	168	THR
8	DI	185	THR
8	DI	400	VAL
8	DJ	48	VAL
8	DJ	92	VAL
8	DJ	161	THR
8	DJ	295	ASN
8	DJ	331	ASP
8	DK	48	VAL
8	DK	104	GLU
8	DK	168	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	209	ASN
1	B	37	GLN
1	B	174	ASN
1	B	235	GLN
1	C	37	GLN
1	C	172	GLN
1	C	174	ASN
1	D	90	ASN
1	D	180	ASN
1	D	209	ASN
1	E	209	ASN
1	F	16	GLN
1	F	85	ASN
1	F	145	ASN
1	F	161	GLN

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Mol	Chain	Res	Type
1	F	255	GLN
1	G	190	ASN
1	G	209	ASN
1	G	255	GLN
1	G	259	GLN
1	H	25	ASN
1	H	88	GLN
1	H	190	ASN
1	I	24	ASN
1	I	174	ASN
1	I	237	GLN
1	K	25	ASN
1	K	145	ASN
1	K	161	GLN
1	L	28	ASN
1	L	47	GLN
1	L	67	GLN
1	L	202	ASN
1	M	32	ASN
1	M	37	GLN
1	M	47	GLN
1	M	209	ASN
1	M	235	GLN
1	N	16	GLN
1	N	37	GLN
1	O	15	GLN
1	P	209	ASN
1	Q	174	ASN
1	Q	232	ASN
1	R	24	ASN
1	R	32	ASN
1	S	15	GLN
1	S	24	ASN
1	S	32	ASN
1	S	81	HIS
1	S	127	GLN
1	S	190	ASN
1	T	24	ASN
1	T	135	GLN
1	T	172	GLN
1	T	180	ASN
1	T	235	GLN

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Mol	Chain	Res	Type
1	U	15	GLN
1	U	47	GLN
1	U	237	GLN
2	a	3	HIS
2	a	14	GLN
2	a	28	ASN
2	a	102	ASN
2	a	116	GLN
2	b	19	GLN
2	c	14	GLN
2	c	19	GLN
2	c	28	ASN
2	c	70	GLN
2	d	70	GLN
2	d	83	GLN
2	d	106	GLN
2	d	147	ASN
2	d	230	GLN
2	e	169	ASN
2	e	230	GLN
5	g	46	GLN
5	g	82	ASN
5	h	22	ASN
5	j	30	ASN
6	m	29	ASN
6	m	32	ASN
6	m	135	GLN
6	o	29	ASN
5	i	5	ASN
6	k	132	ASN
1	V	81	HIS
1	V	190	ASN
1	W	15	GLN
1	W	169	GLN
1	W	209	ASN
1	W	255	GLN
1	X	67	GLN
1	X	127	GLN
1	X	255	GLN
1	X	259	GLN
7	t	83	GLN
7	u	83	GLN

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Mol	Chain	Res	Type
8	DA	97	ASN
8	DA	197	ASN
8	DA	265	ASN
8	DA	275	ASN
8	DB	22	ASN
8	DB	89	ASN
8	DB	107	ASN
8	DB	115	GLN
8	DB	129	GLN
8	DB	352	ASN
8	DB	385	ASN
8	DC	107	ASN
8	DC	213	HIS
8	DC	296	ASN
8	DC	310	GLN
8	DC	314	GLN
8	DC	365	ASN
8	DD	59	GLN
8	DD	107	ASN
8	DD	192	ASN
8	DD	358	ASN
8	DE	23	ASN
8	DE	107	ASN
8	DE	192	ASN
8	DE	245	ASN
8	DE	268	GLN
8	DF	22	ASN
8	DF	26	ASN
8	DF	107	ASN
8	DF	179	ASN
8	DF	213	HIS
8	DF	322	ASN
8	DF	338	GLN
8	DF	358	ASN
8	DF	365	ASN
8	DF	392	GLN
8	DG	129	GLN
8	DG	133	ASN
8	DH	133	ASN
8	DH	179	ASN
8	DH	197	ASN
8	DH	245	ASN

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Mol	Chain	Res	Type
8	DH	293	GLN
8	DH	310	GLN
8	DH	365	ASN
8	DH	381	ASN
8	DI	129	GLN
8	DI	133	ASN
8	DI	179	ASN
8	DI	245	ASN
8	DI	280	ASN
8	DI	323	ASN
8	DI	358	ASN
8	DI	401	ASN
8	DJ	79	GLN
8	DJ	133	ASN
8	DJ	179	ASN
8	DJ	252	ASN
8	DJ	268	GLN
8	DJ	303	ASN
8	DJ	323	ASN
8	DJ	352	ASN
8	DJ	392	GLN
8	DK	97	ASN
8	DK	107	ASN
8	DK	133	ASN
8	DK	303	ASN
8	DK	332	ASN
8	DK	383	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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.

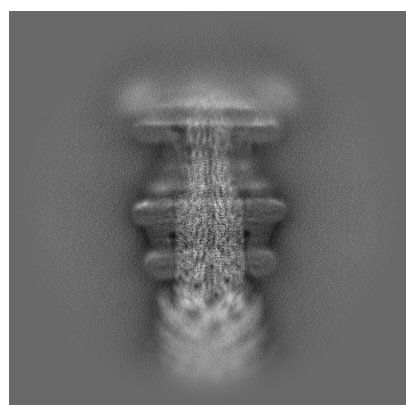
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31008. These allow visual inspection of the internal detail of the map and identification of artifacts.

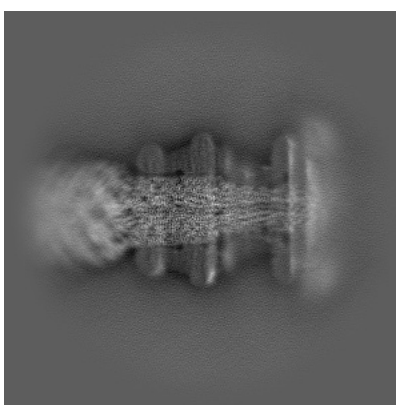
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

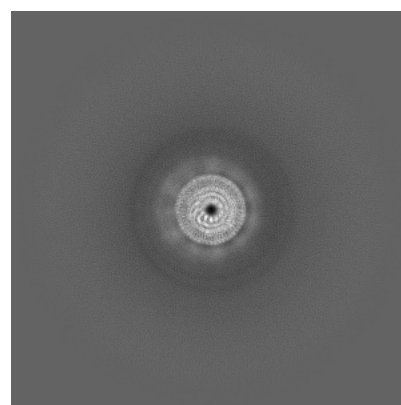
6.1.1 Primary map



X



Y

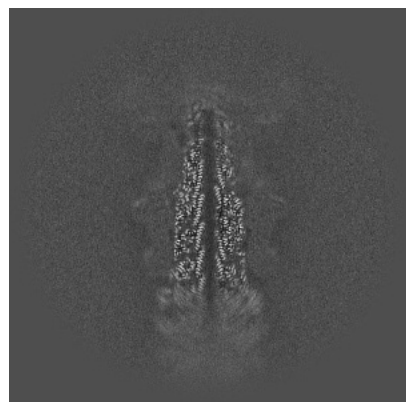


Z

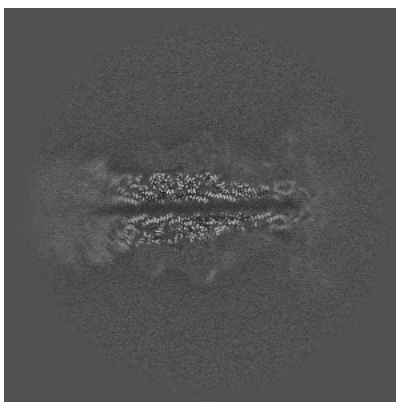
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

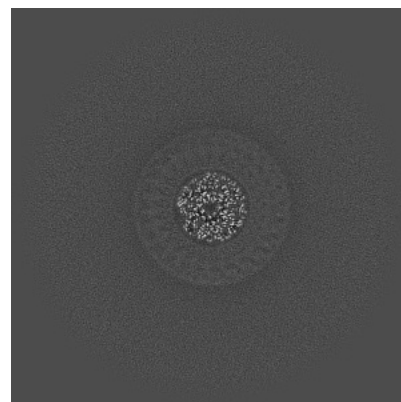
6.2.1 Primary map



X Index: 256



Y Index: 256

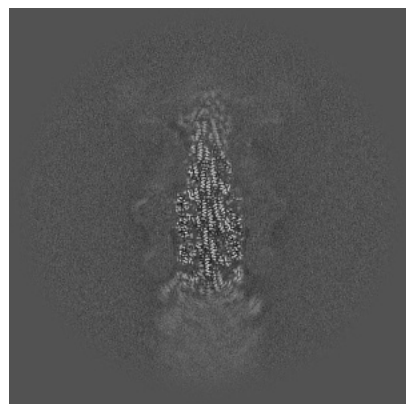


Z Index: 256

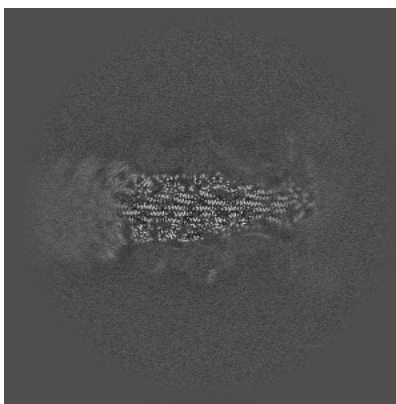
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

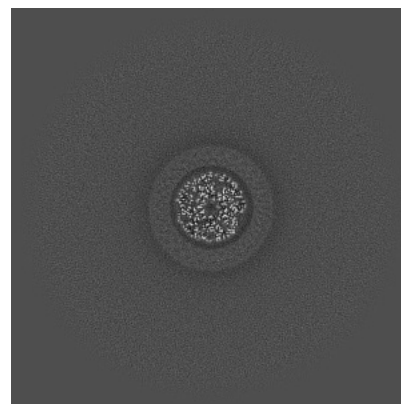
6.3.1 Primary map



X Index: 269



Y Index: 243

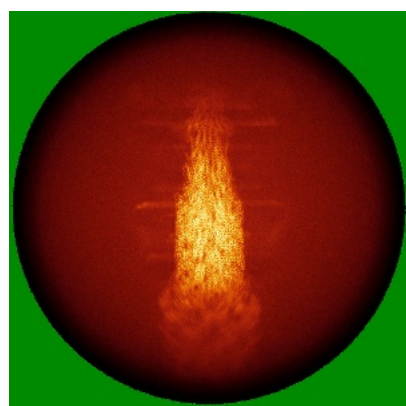


Z Index: 224

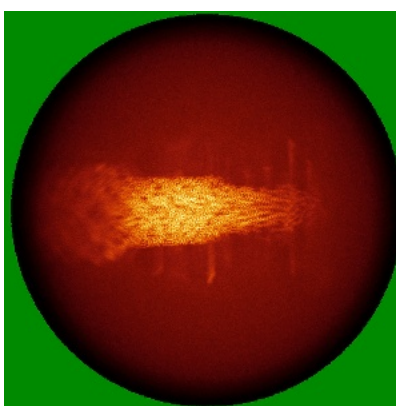
The images above show the largest variance slices of the map in three orthogonal directions.

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

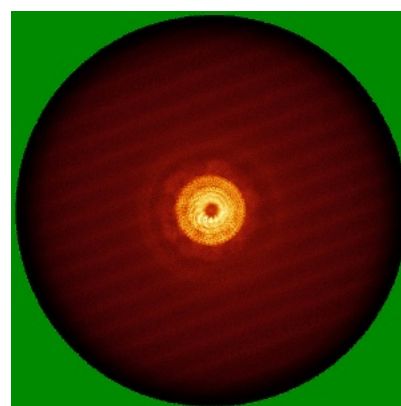
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

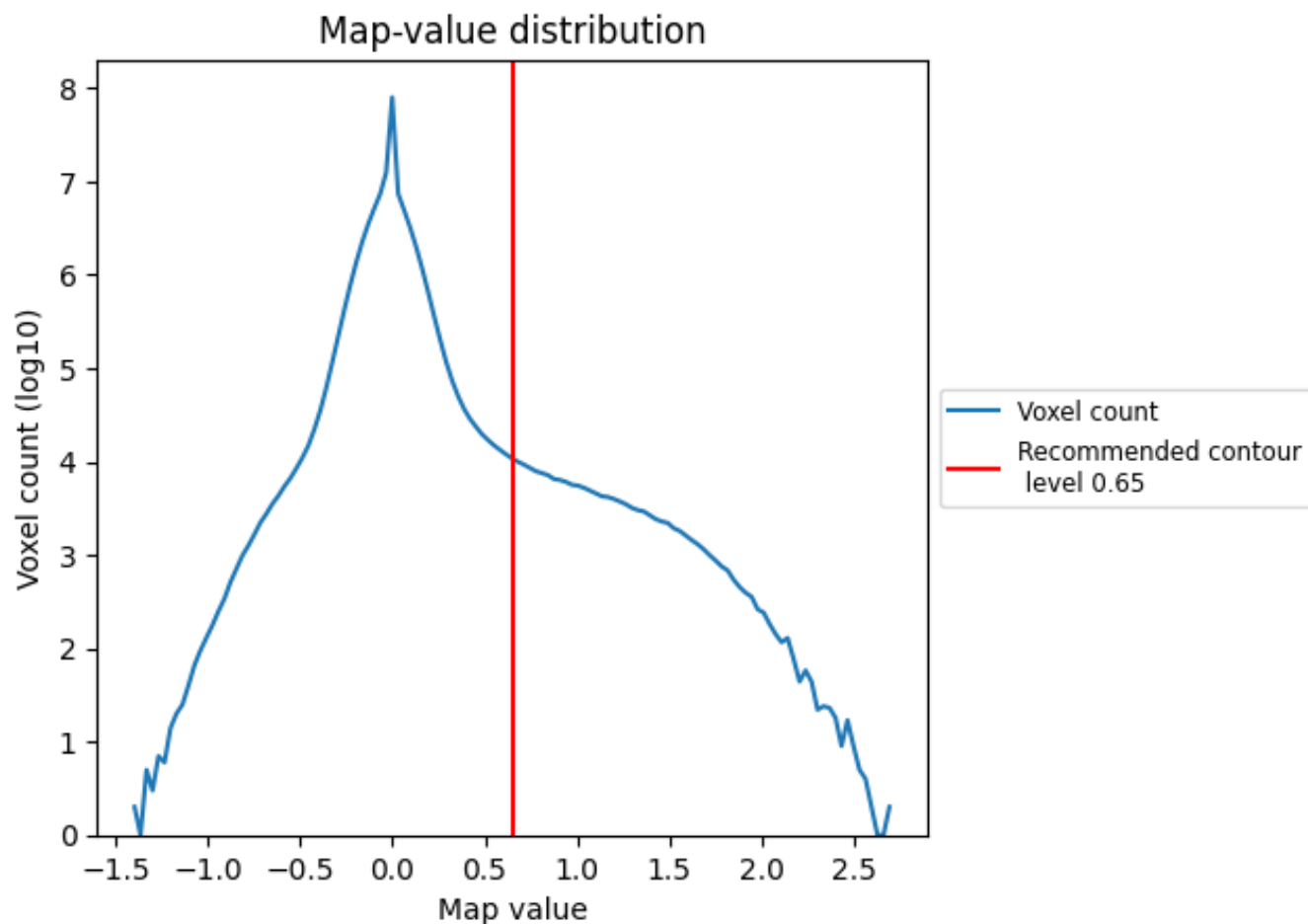
6.6 Mask visualisation

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

7 Map analysis [i](#)

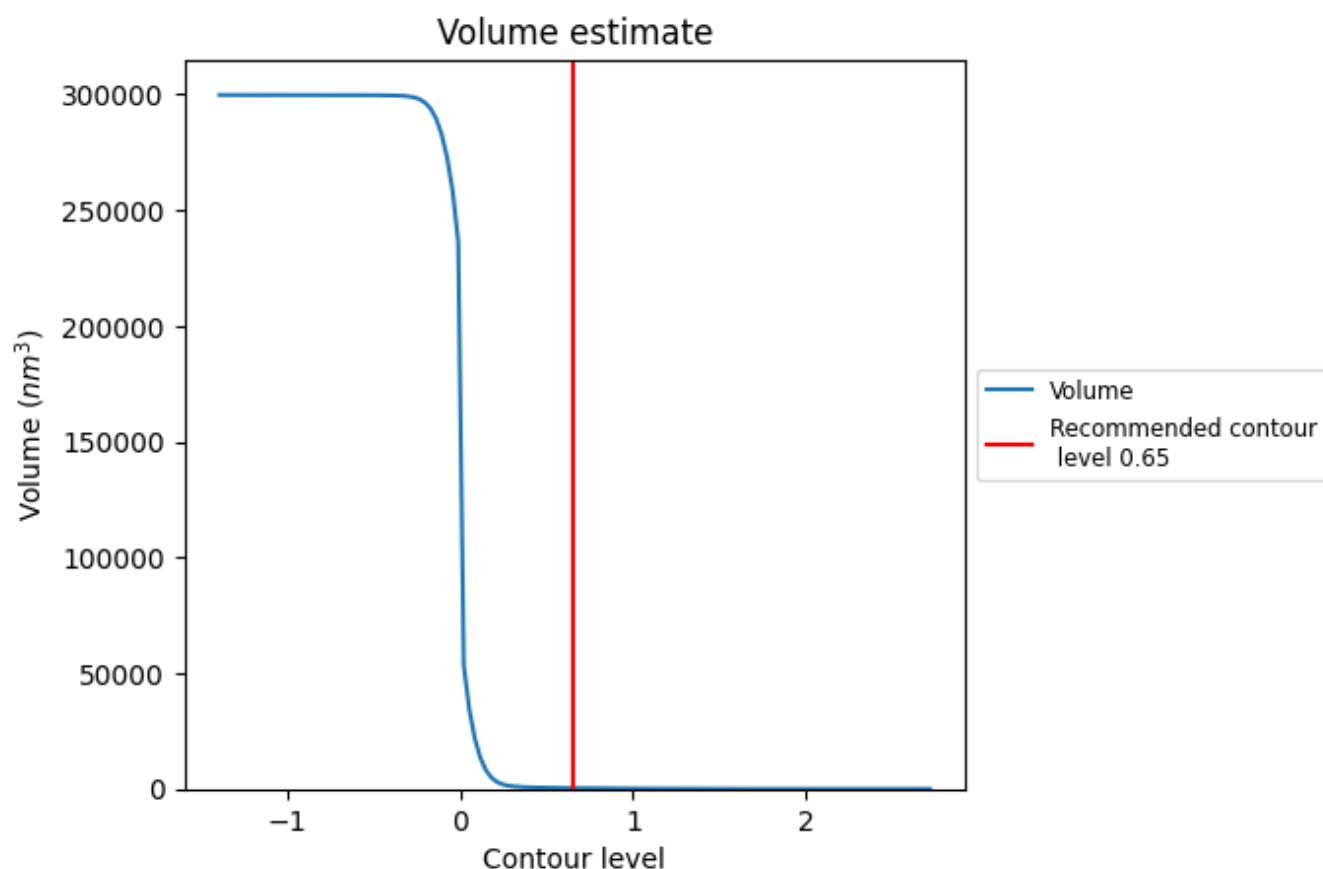
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

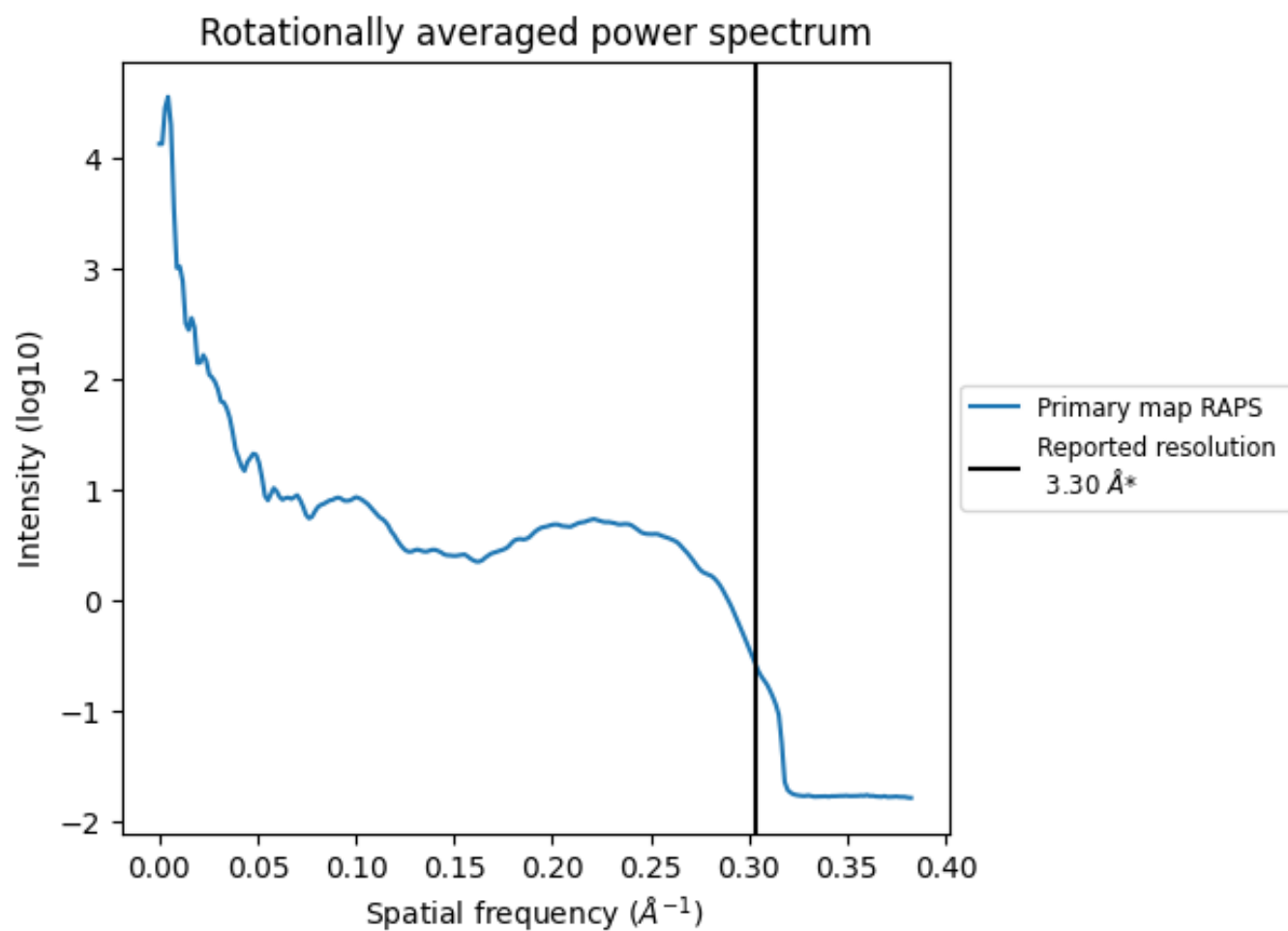
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm³; this corresponds to an approximate mass of 321 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 0.303 Å⁻¹

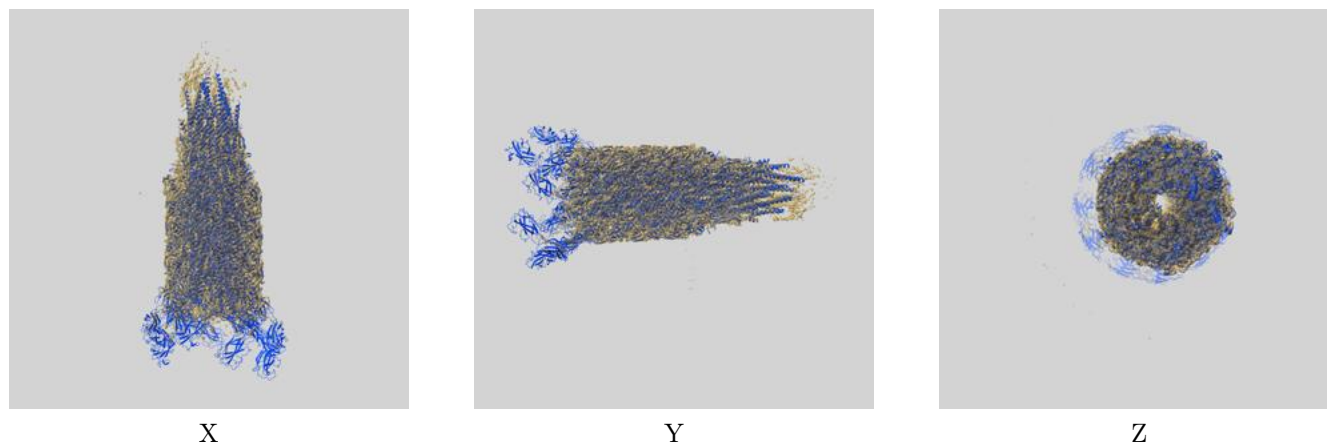
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

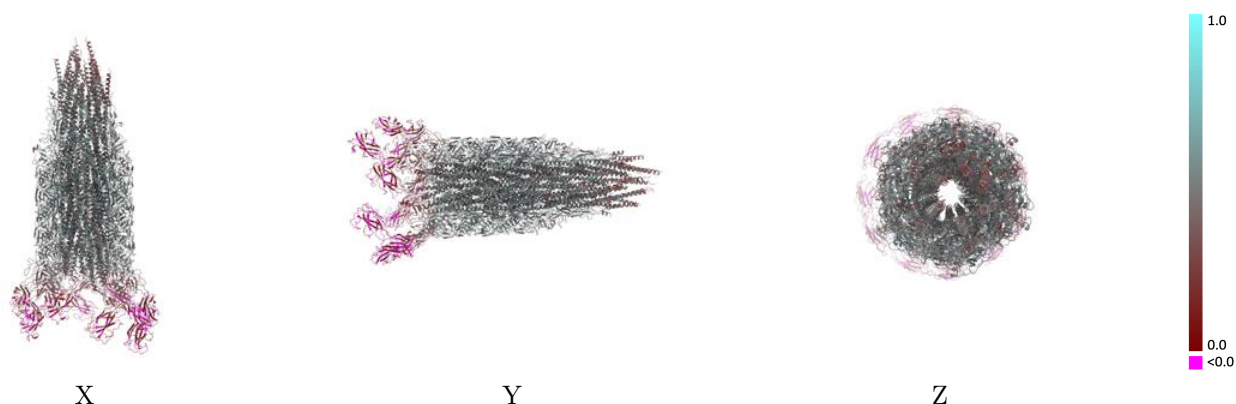
This section contains information regarding the fit between EMDB map EMD-31008 and PDB model 7E82. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



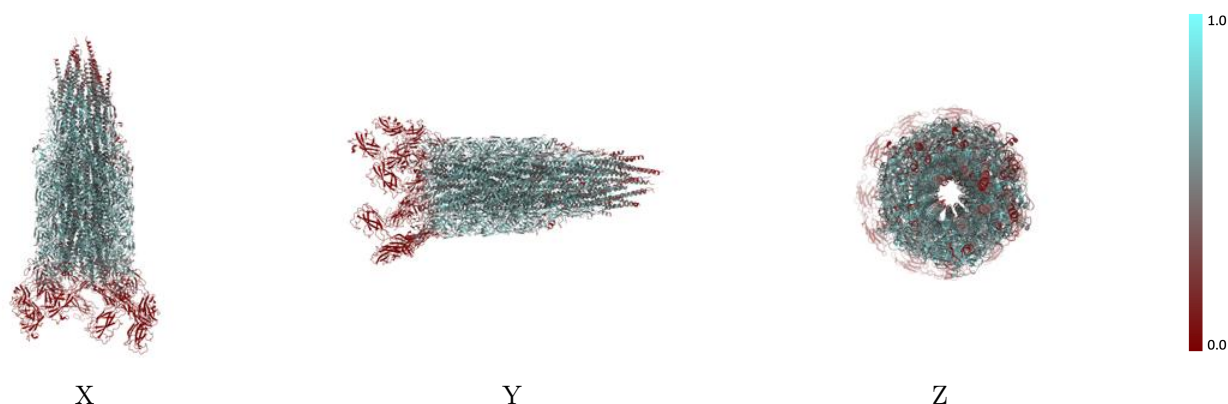
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



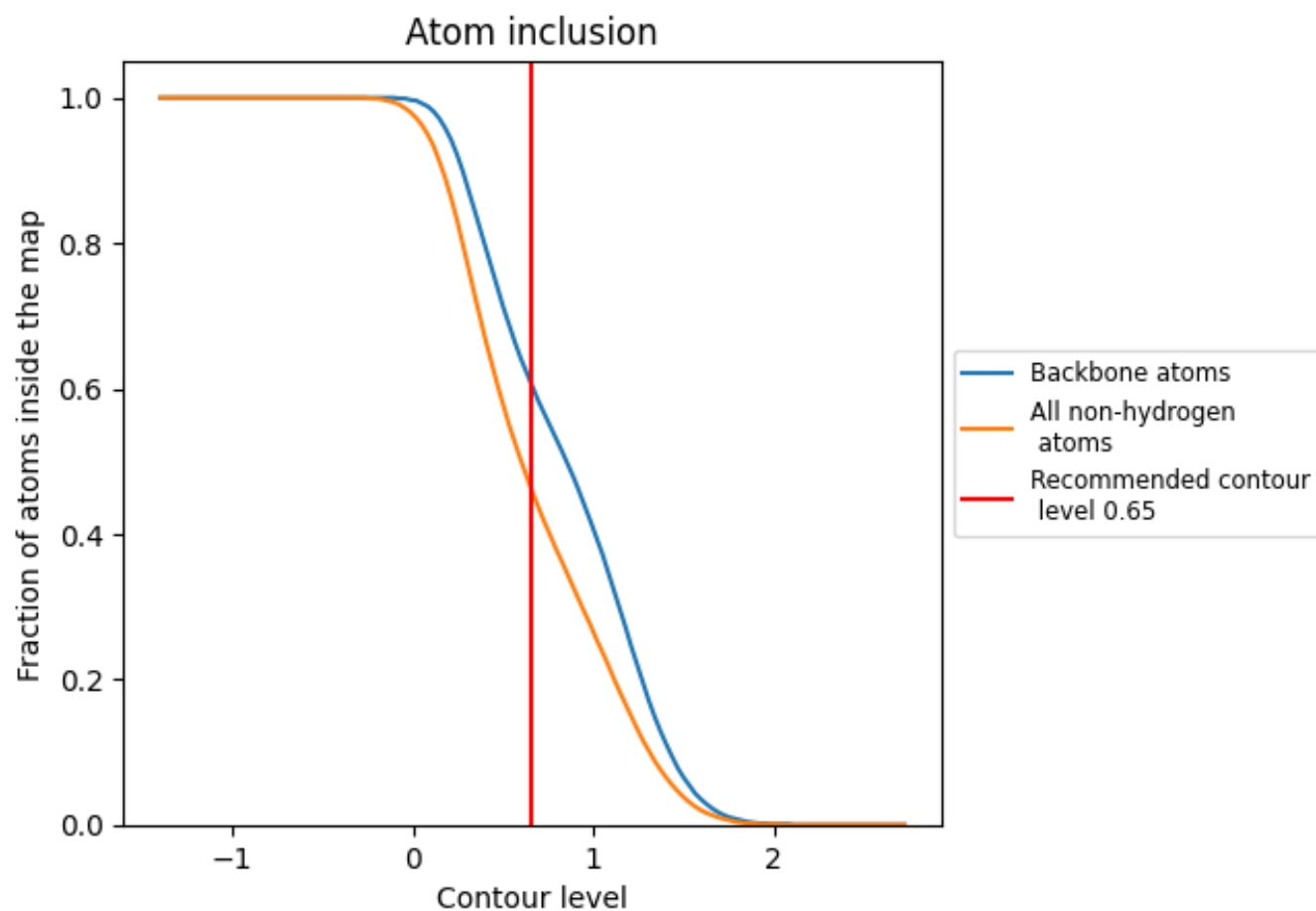
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.65).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 47% 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 (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4660	 0.4240
0	 0.5470	 0.4520
1	 0.3730	 0.4130
2	 0.5600	 0.5110
3	 0.5470	 0.4350
4	 0.4130	 0.4530
5	 0.5640	 0.5040
6	 0.1930	 0.4650
7	 0.5140	 0.4840
8	 0.4000	 0.4600
9	 0.1140	 0.4370
A	 0.5780	 0.4880
B	 0.5120	 0.4690
C	 0.5710	 0.4810
D	 0.5850	 0.4880
DA	 0.2960	 0.3420
DB	 0.3240	 0.3580
DC	 0.3340	 0.3520
DD	 0.3090	 0.3200
DE	 0.2830	 0.3180
DF	 0.2560	 0.3140
DG	 0.2330	 0.3020
DH	 0.2150	 0.2900
DI	 0.1960	 0.2680
DJ	 0.1460	 0.1970
DK	 0.1250	 0.2390
E	 0.5850	 0.4860
F	 0.5960	 0.4880
G	 0.6060	 0.4920
H	 0.5980	 0.4970
I	 0.5920	 0.4980
J	 0.6000	 0.5010
K	 0.6100	 0.5000
L	 0.6070	 0.5020
M	 0.5970	 0.5010



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Chain	Atom inclusion	Q-score
N	 0.6160	 0.5060
O	 0.5850	 0.4900
P	 0.5970	 0.4940
Q	 0.6080	 0.4980
R	 0.6010	 0.4990
S	 0.5880	 0.4940
T	 0.5900	 0.4980
U	 0.5990	 0.4970
V	 0.6050	 0.4960
W	 0.5890	 0.5000
X	 0.5400	 0.4830
a	 0.6240	 0.4960
b	 0.5320	 0.4680
c	 0.6150	 0.5000
d	 0.6040	 0.4940
e	 0.5080	 0.4750
f	 0.5820	 0.4740
g	 0.4950	 0.4310
h	 0.6160	 0.4860
i	 0.6040	 0.4810
j	 0.5930	 0.4790
k	 0.5850	 0.4640
l	 0.4850	 0.4440
m	 0.5630	 0.4550
n	 0.5380	 0.4540
o	 0.4180	 0.4250
p	 0.4840	 0.4490
q	 0.4020	 0.4150
r	 0.3830	 0.3380
s	 0.4180	 0.4050
t	 0.4420	 0.4180
u	 0.3200	 0.3950
v	 0.2240	 0.3270