



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 06:18 AM UTC

PDB ID : 7CBM / pdb_00007cbm
EMDB ID : EMD-30336
Title : Cryo-EM structure of the flagellar distal 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 : 2020-06-12
Resolution : 3.20 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:

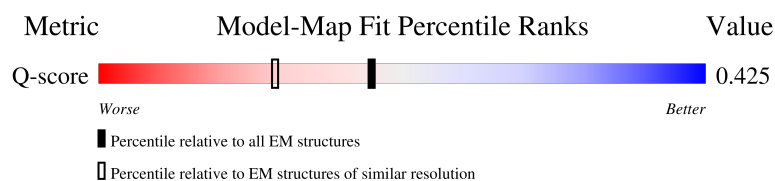
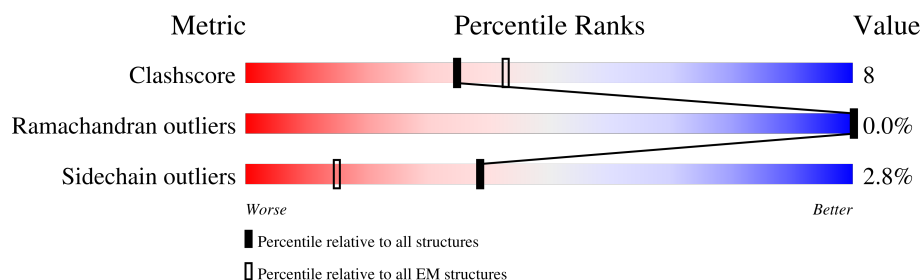
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.20 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	15020 (2.70 - 3.70)

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	7% 80% 20%
1	B	260	15% 76% 22% .
1	C	260	10% 77% 23%
1	D	260	9% 77% 23%

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Mol	Chain	Length	Quality of chain	
1	E	260	8% 79%	20% .
1	F	260	7% 78%	22%
1	G	260	6% 78%	22% .
1	H	260	7% 78%	22%
1	I	260	7% 79%	21%
1	J	260	8% 81%	17% .
1	K	260	. 81%	19%
1	L	260	5% 86%	12% .
1	M	260	6% 84%	15% .
1	N	260	7% 78%	17% . .
1	O	260	7% 81%	16% .
1	P	260	6% 79%	16% 5%
1	Q	260	7% 77%	17% . 5%
1	R	260	5% 77%	18% . .
1	S	260	6% 76%	18% 5%
1	T	260	5% 80%	17% . .
1	U	260	10% 79%	20%
1	V	260	10% 78%	21%
1	W	260	12% 82%	17% .
1	X	260	18% 79%	20%
2	a	251	17% 82%	18% .
2	b	251	23% 75%	24% .
2	c	251	16% 73%	27% .
2	d	251	20% 81%	17% . .
2	e	251	38% 80%	18% . .

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Mol	Chain	Length	Quality of chain
3	DA	403	52% 79% 20%
3	DB	403	51% 78% 20%
3	DC	403	53% 76% 23%
3	DD	403	54% 76% 21%
3	DE	403	59% 78% 21%
3	DF	403	67% 74% 25%
3	DG	403	72% 82% 17%
3	DH	403	76% 77% 22%
3	DI	403	80% 79% 20%
3	DJ	403	82% 82% 17%
3	DK	403	88% 79% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 87698 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 hook protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	DA	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
3	DB	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
3	DC	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
3	DD	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
3	DE	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		

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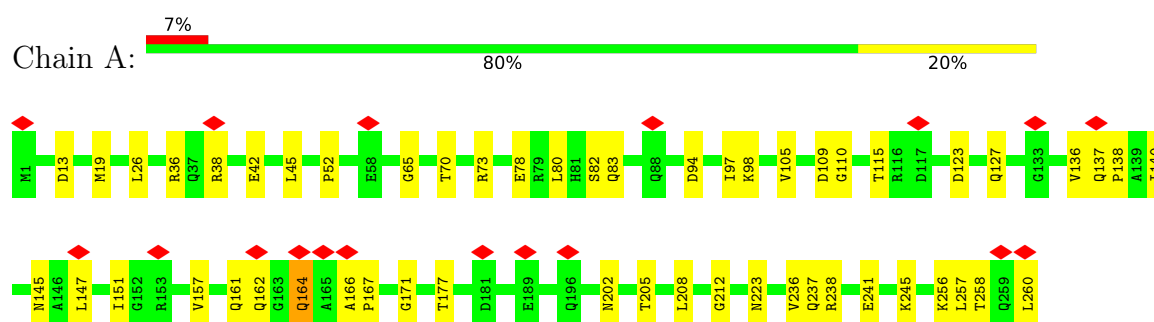
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Mol	Chain	Residues	Atoms					AltConf	Trace
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3	DG	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
3	DH	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
3	DI	401	Total 2947	C 1814	N 507	O 618	S 8	0	0
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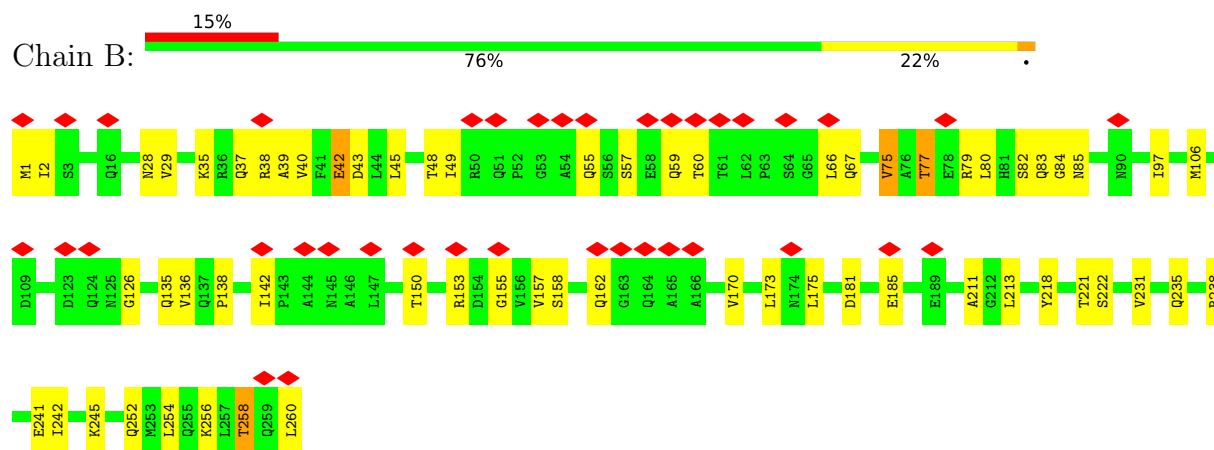
3 Residue-property plots

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

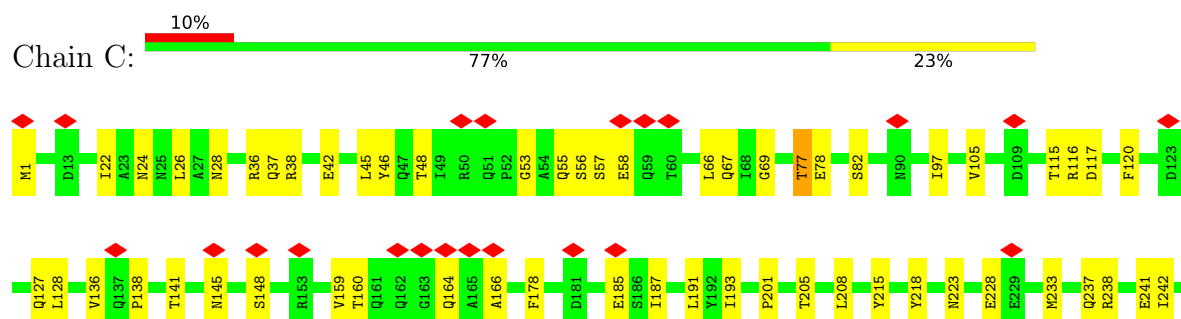
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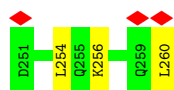


- Molecule 1: Flagellar basal-body rod protein FlgG

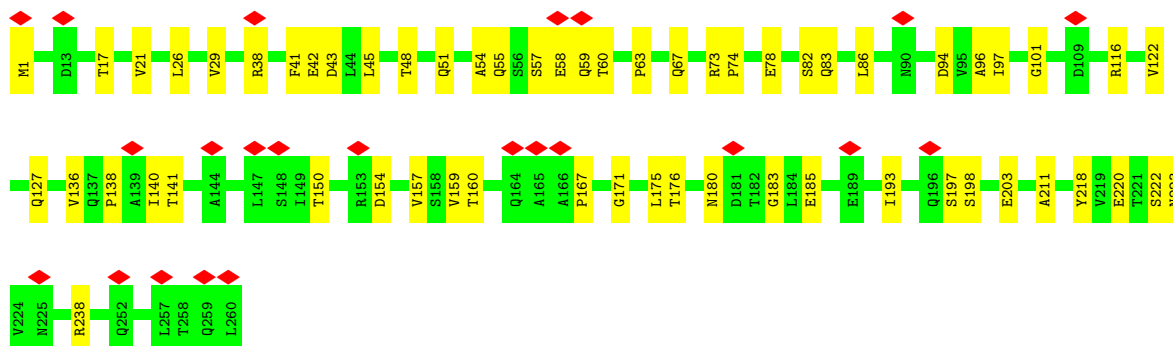
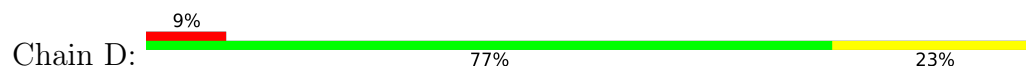


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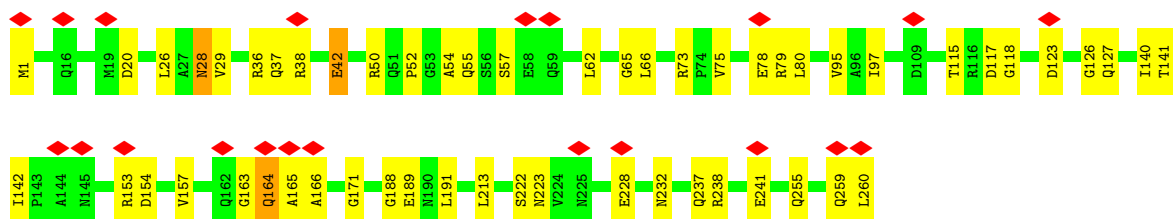
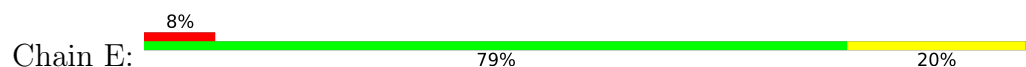




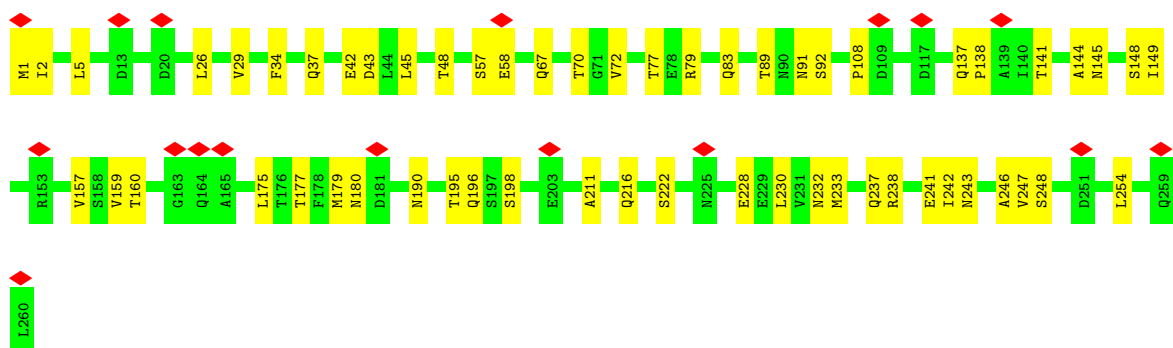
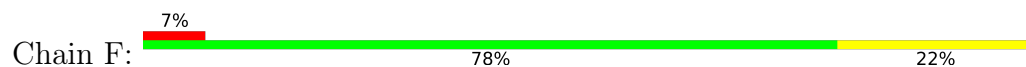
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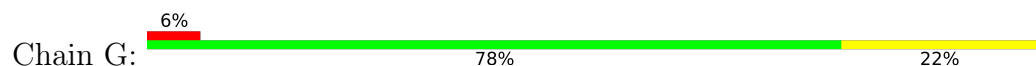
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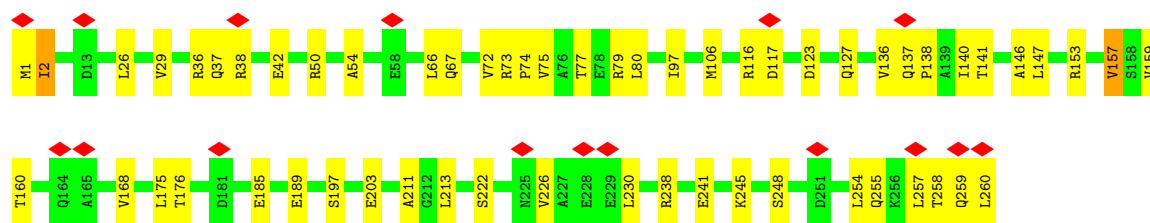


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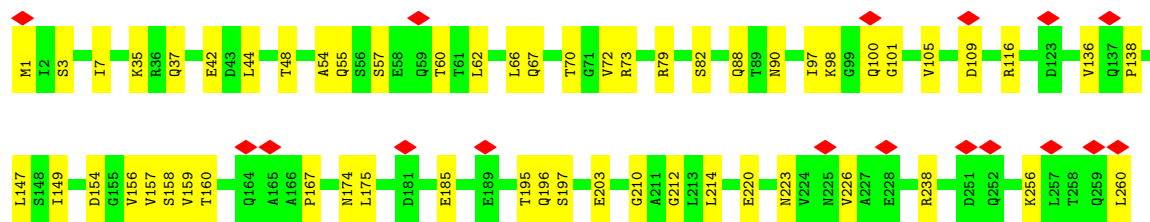
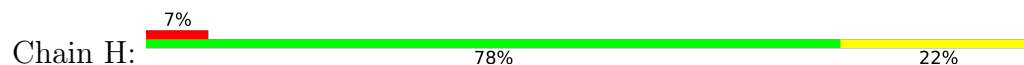


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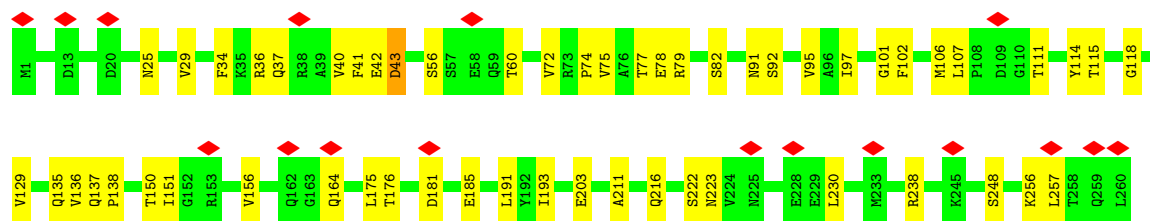
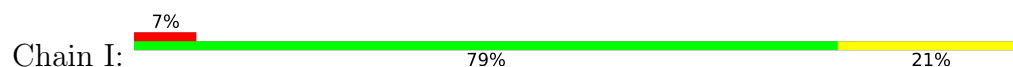




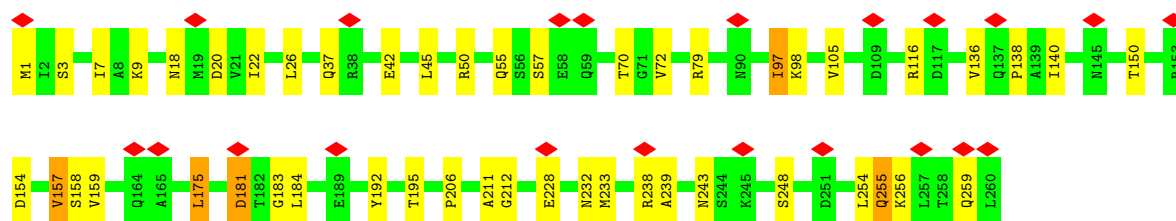
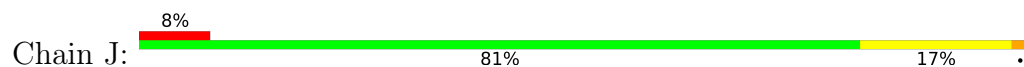
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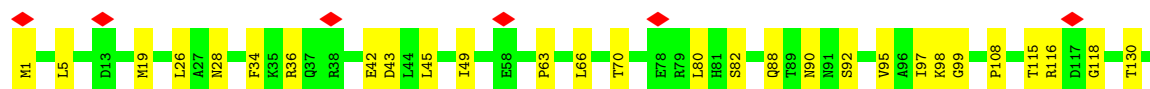
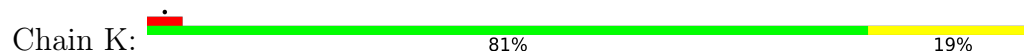
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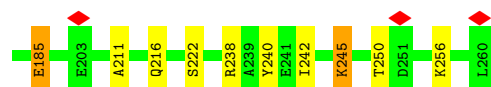
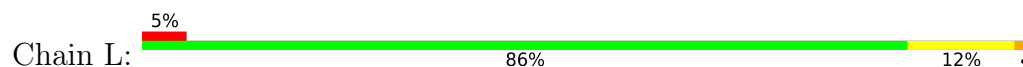


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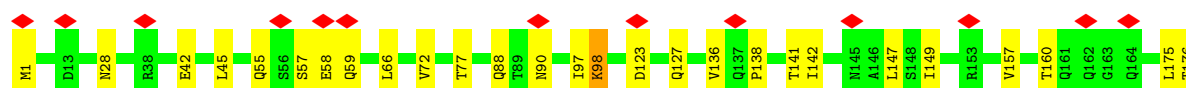
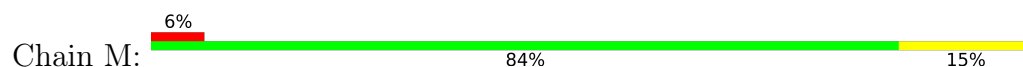




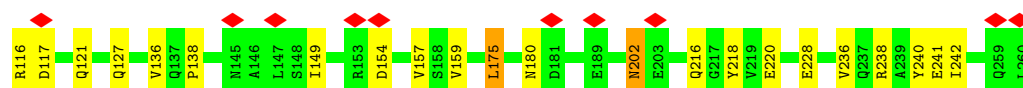
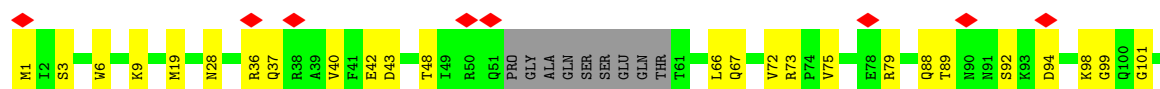
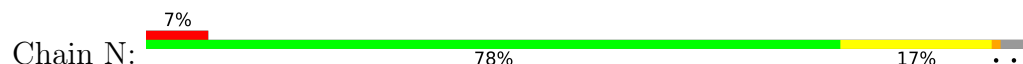
- Molecule 1: Flagellar basal-body rod protein FlgG



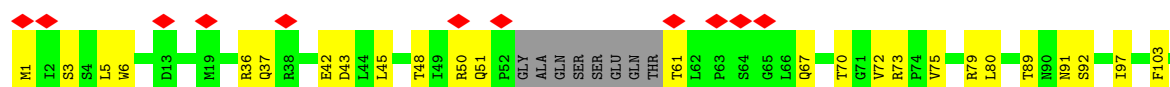
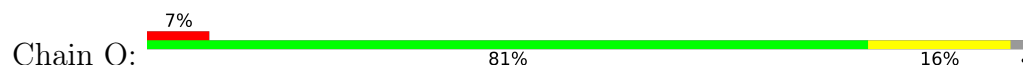
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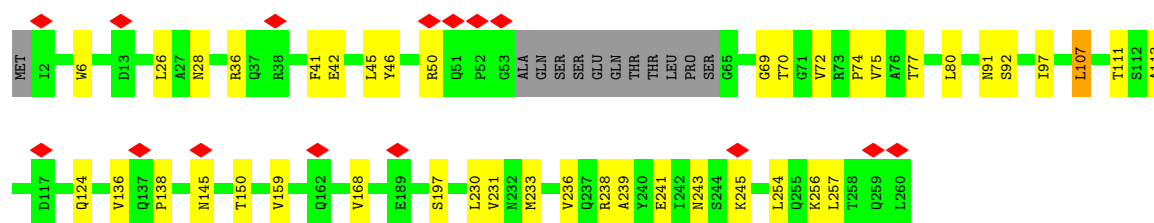
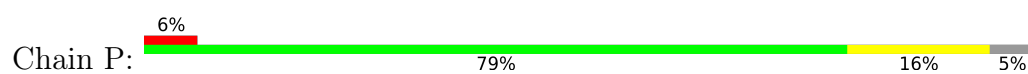
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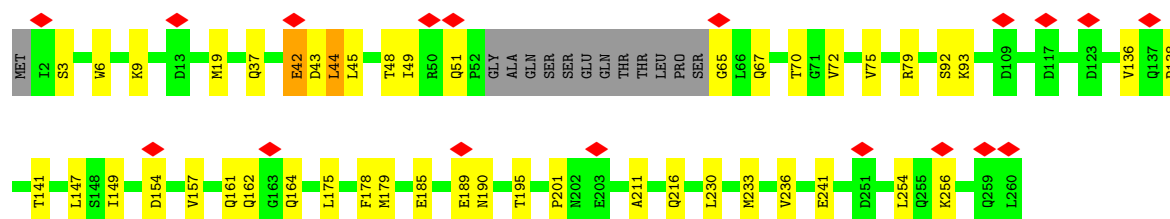
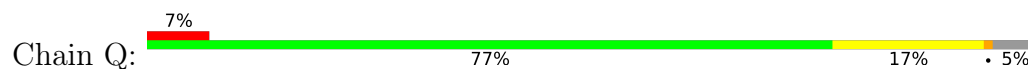
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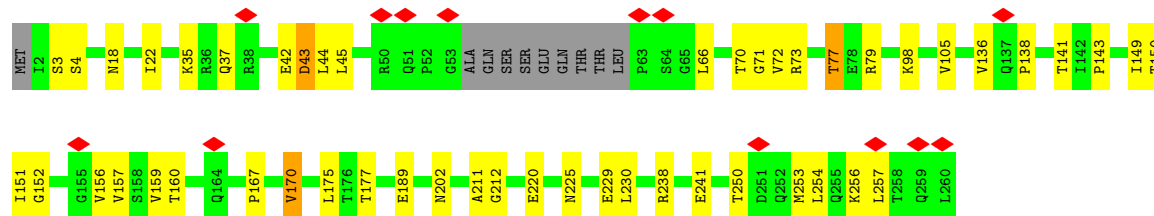
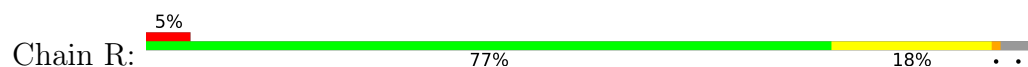
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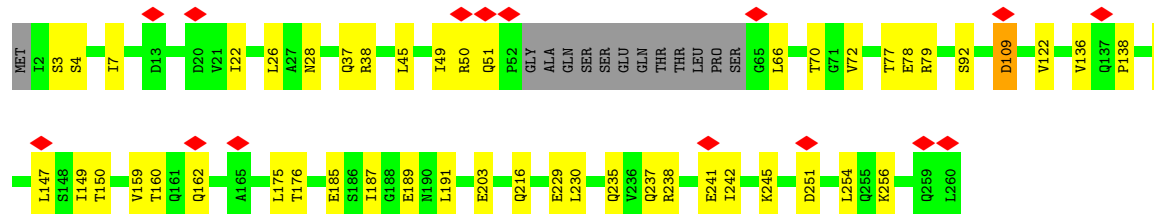
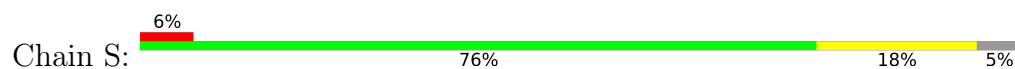
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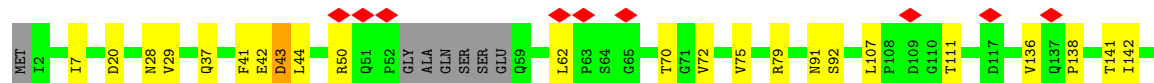
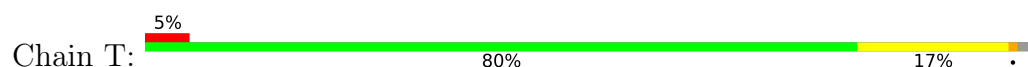
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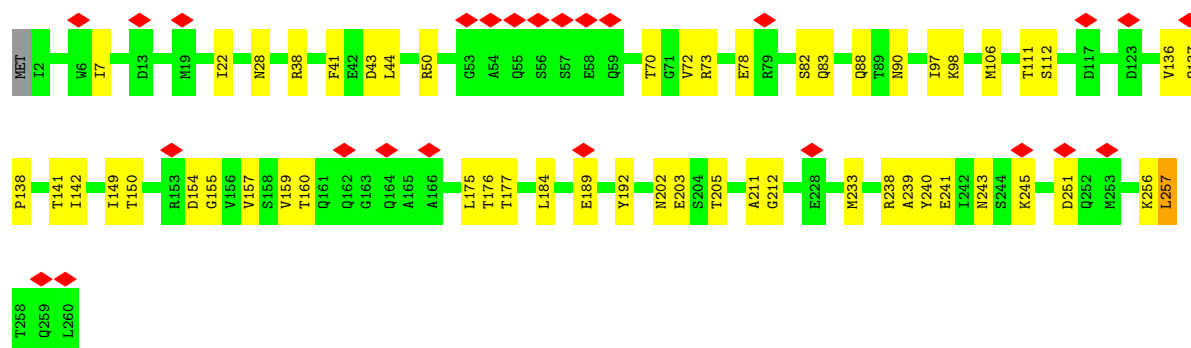
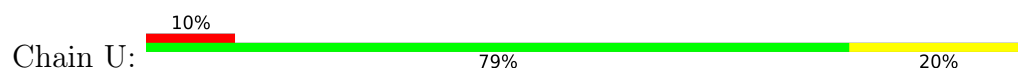


- Molecule 1: Flagellar basal-body rod protein FlgG

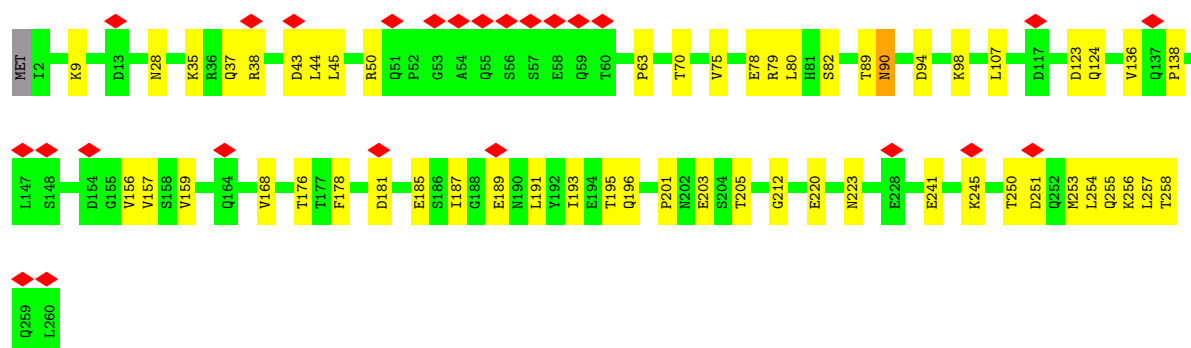
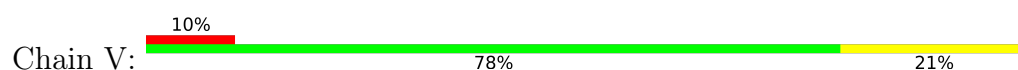




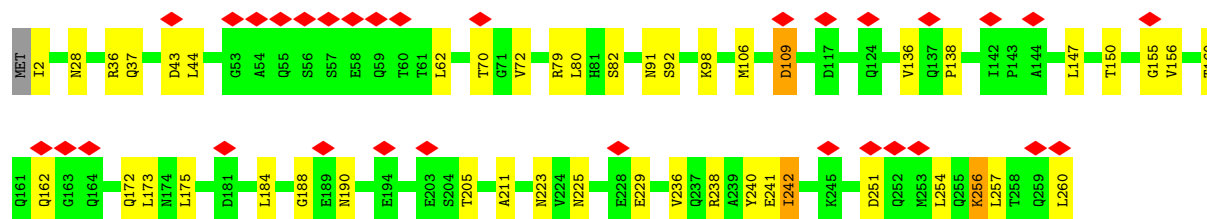
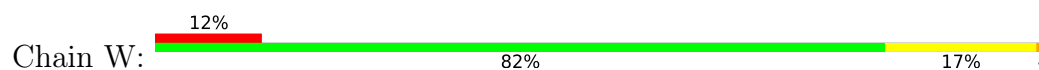
- Molecule 1: Flagellar basal-body rod protein FlgG



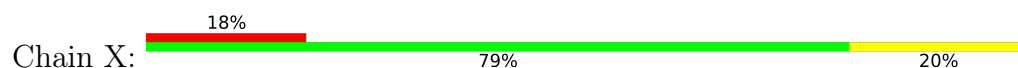
- Molecule 1: Flagellar basal-body rod protein FlgG

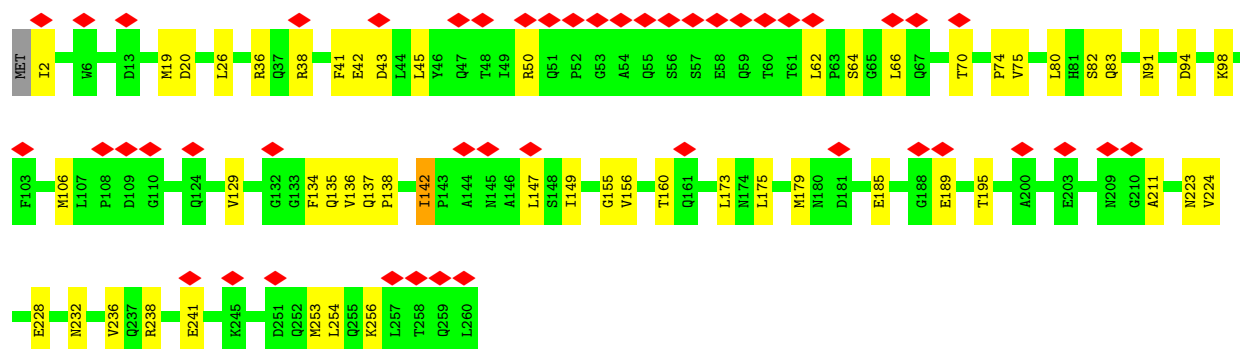


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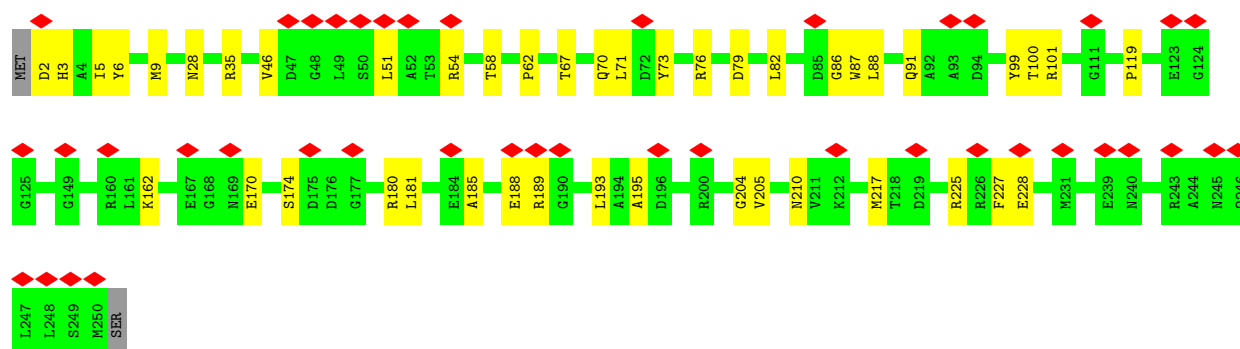
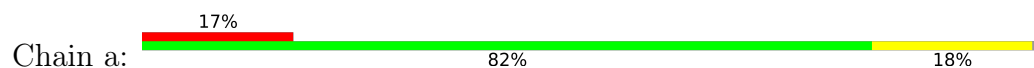


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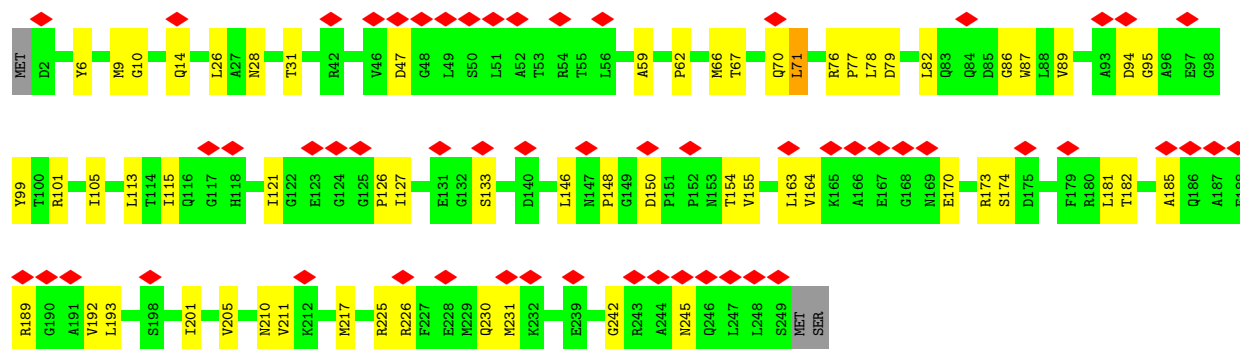
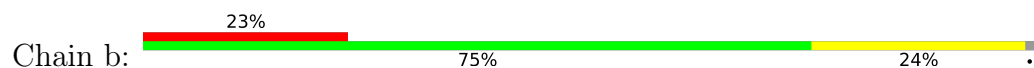




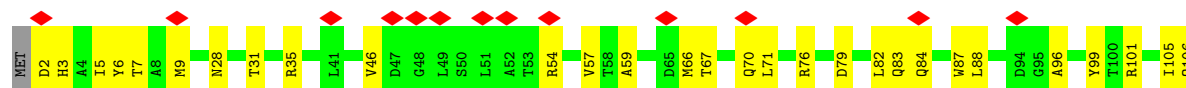
• Molecule 2: Flagellar basal-body rod protein FlgF

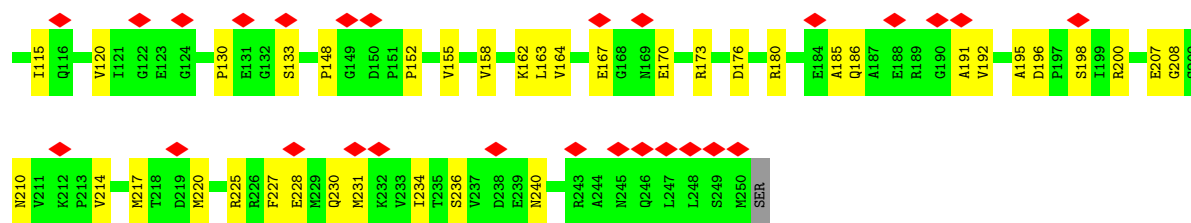


• Molecule 2: Flagellar basal-body rod protein FlgF

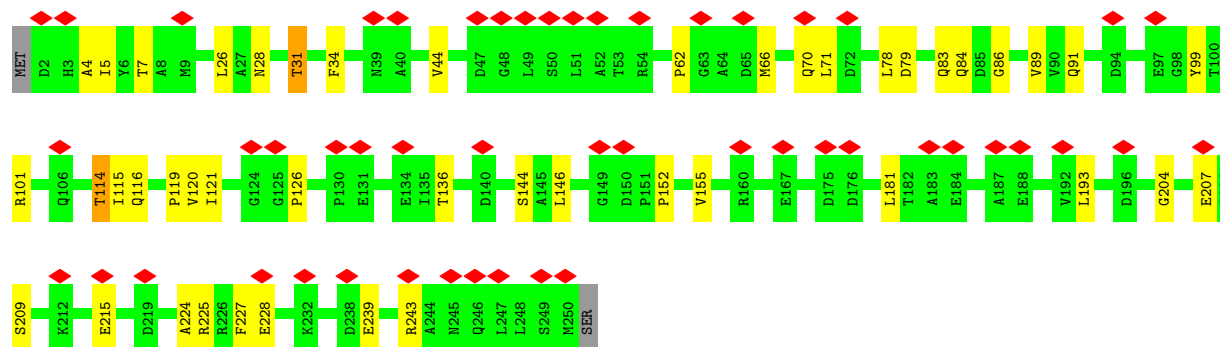
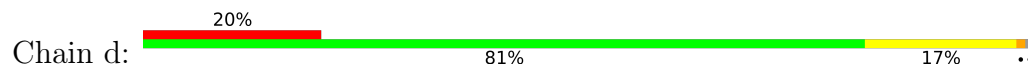


• Molecule 2: Flagellar basal-body rod protein FlgF

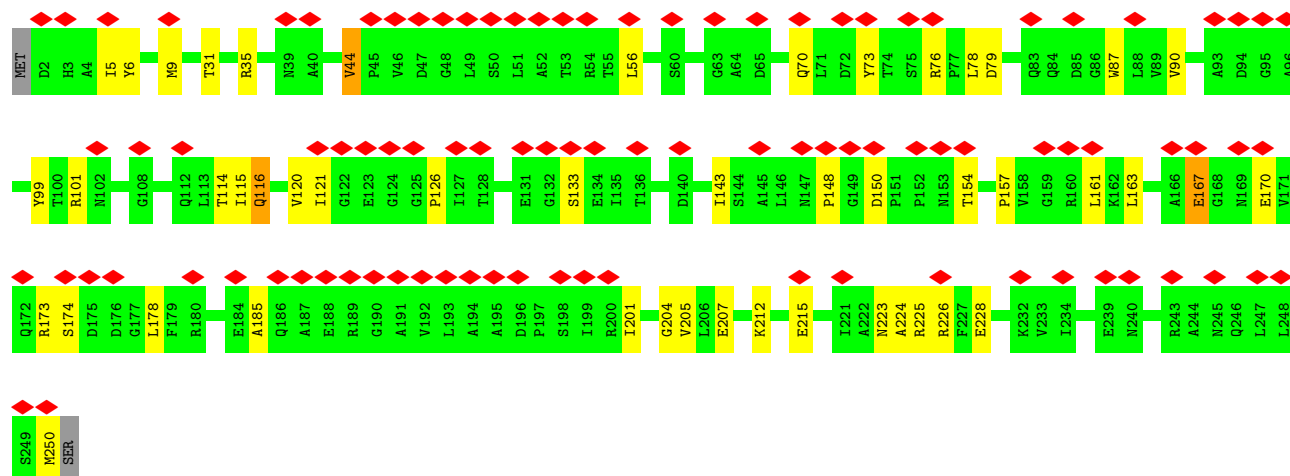
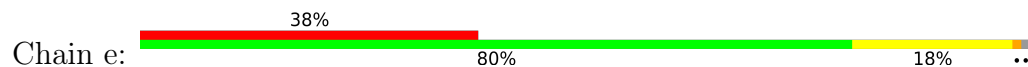




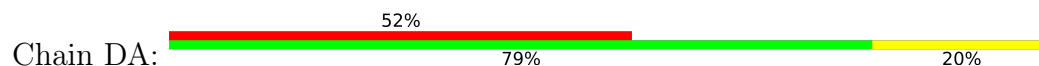
• Molecule 2: Flagellar basal-body rod protein FlgF

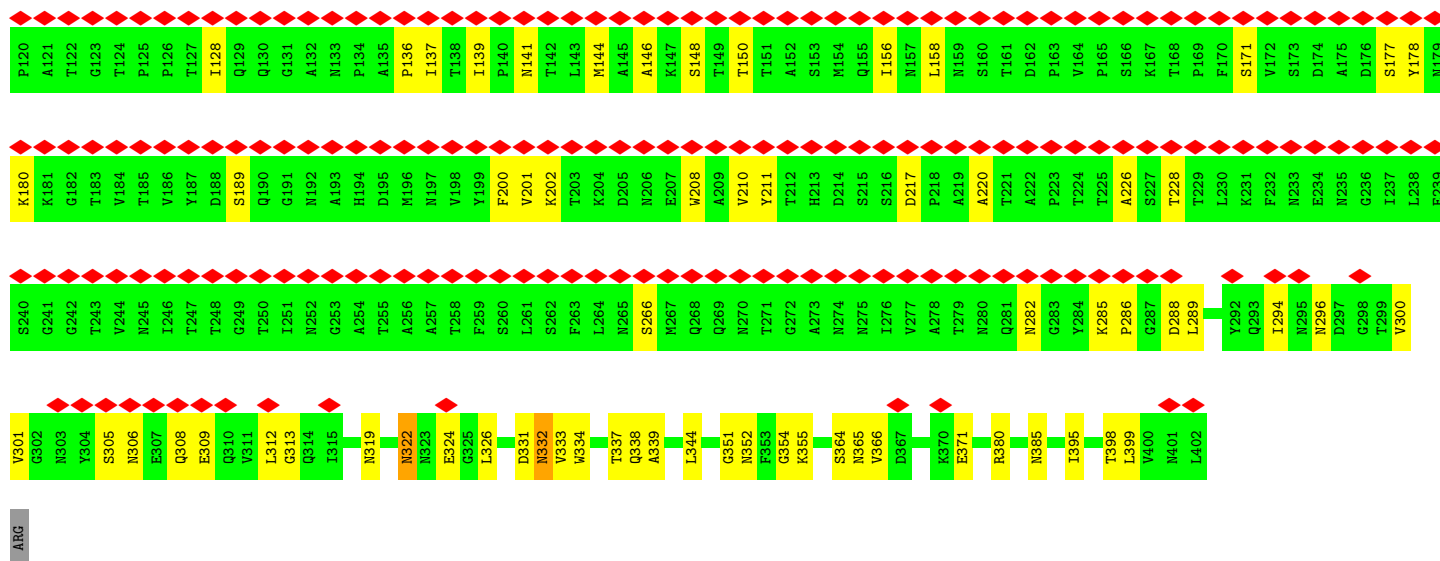


• Molecule 2: Flagellar basal-body rod protein FlgF

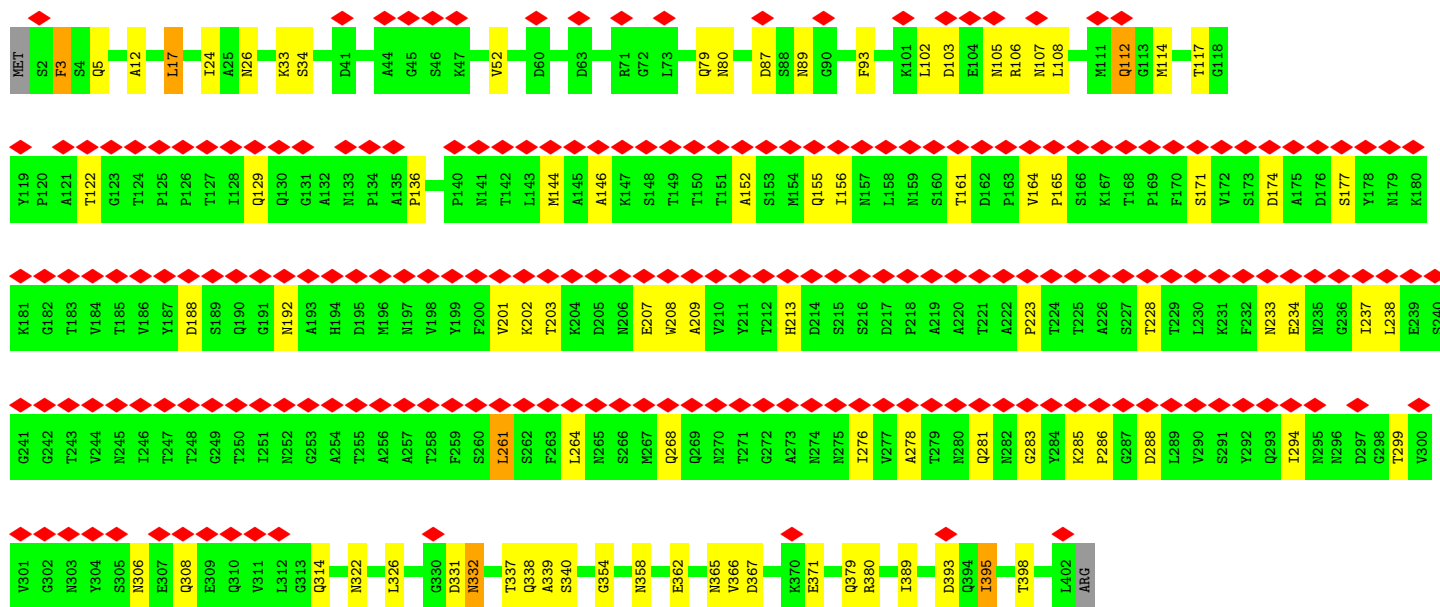
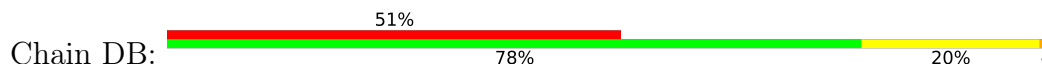


• Molecule 3: Flagellar hook protein FlgE

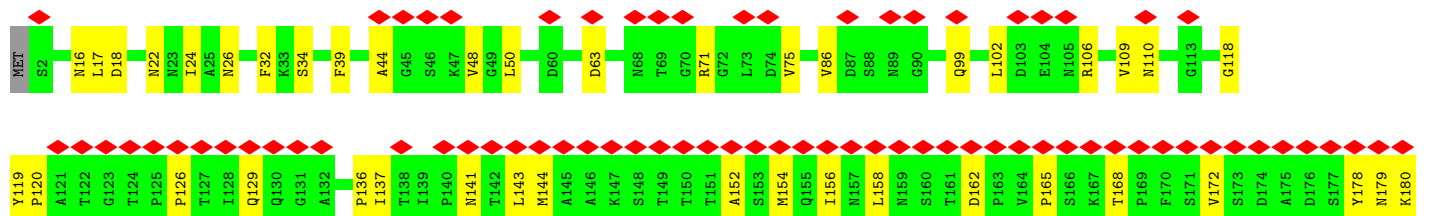
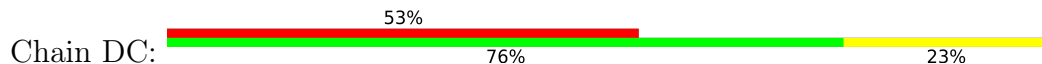


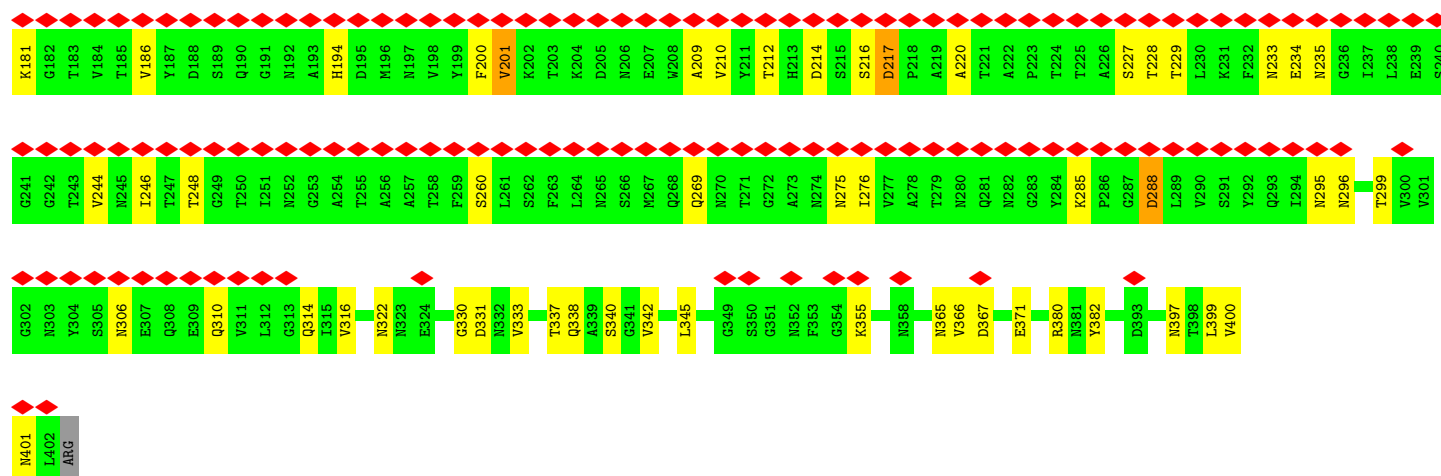


• Molecule 3: Flagellar hook protein FlgE

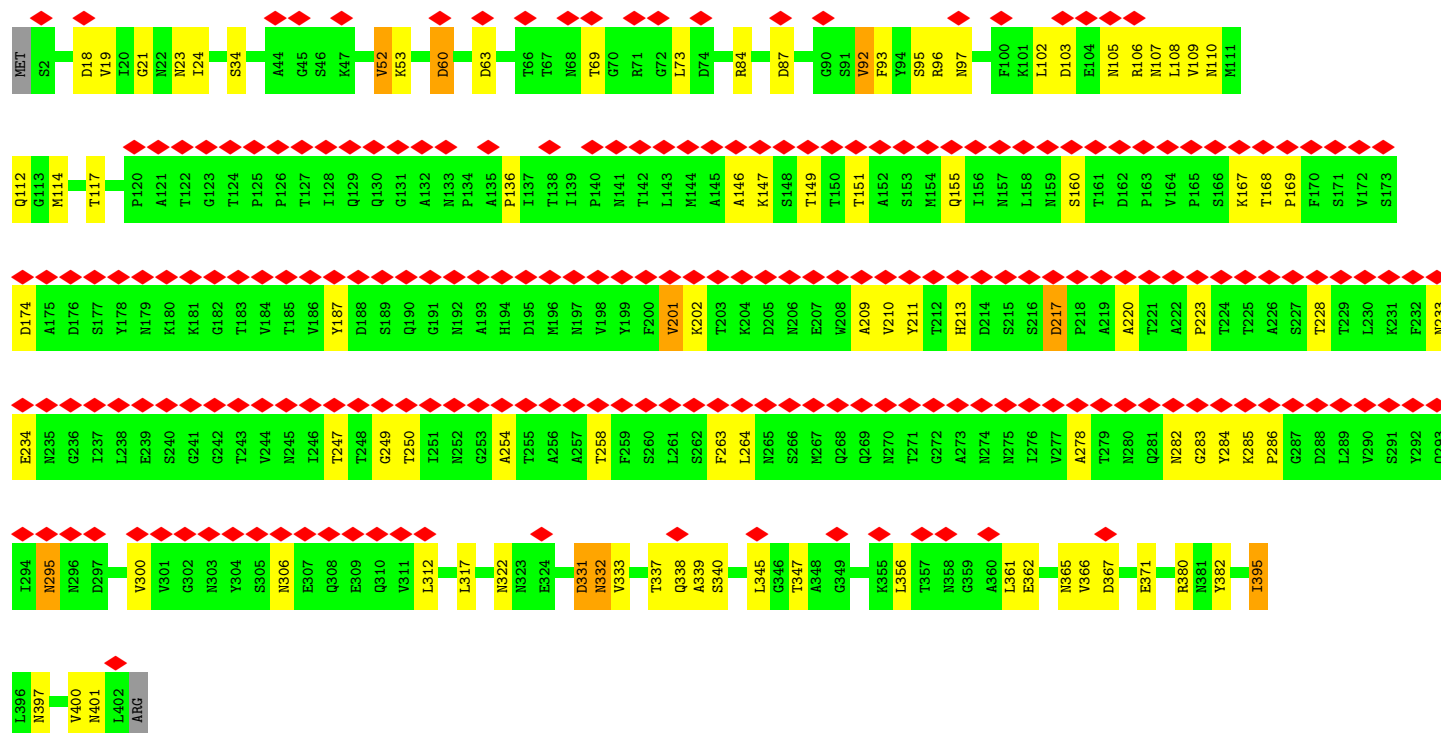
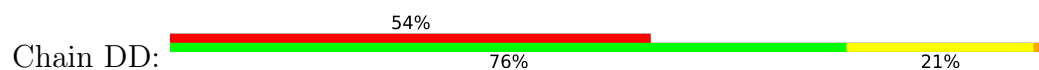


• Molecule 3: Flagellar hook protein FlgE

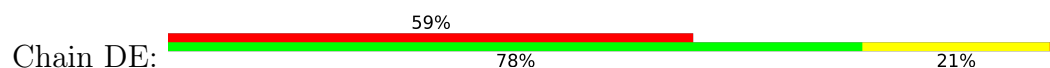


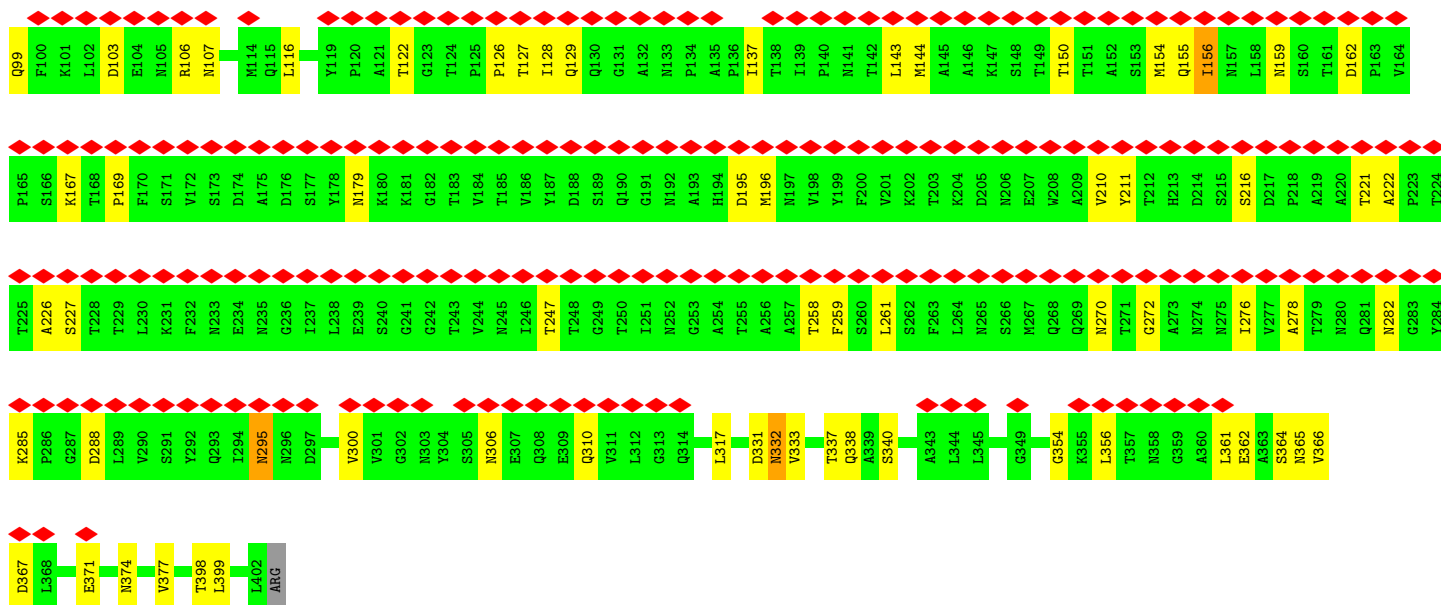


• Molecule 3: Flagellar hook protein FlgE

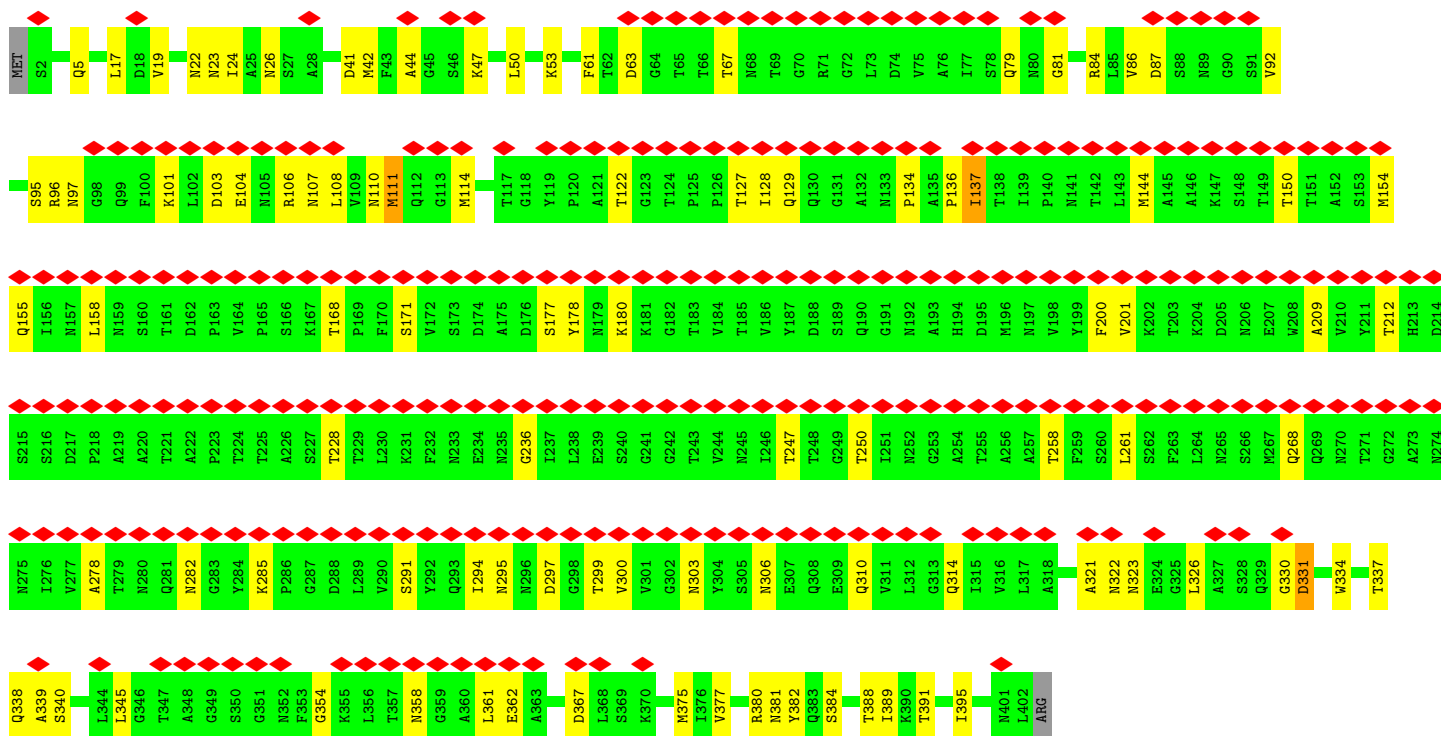
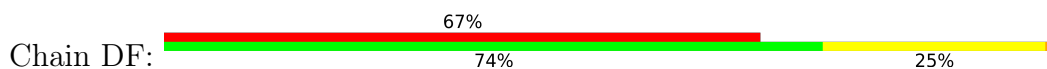


• Molecule 3: Flagellar hook protein FlgE

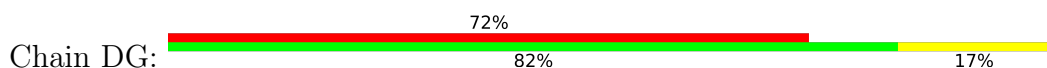


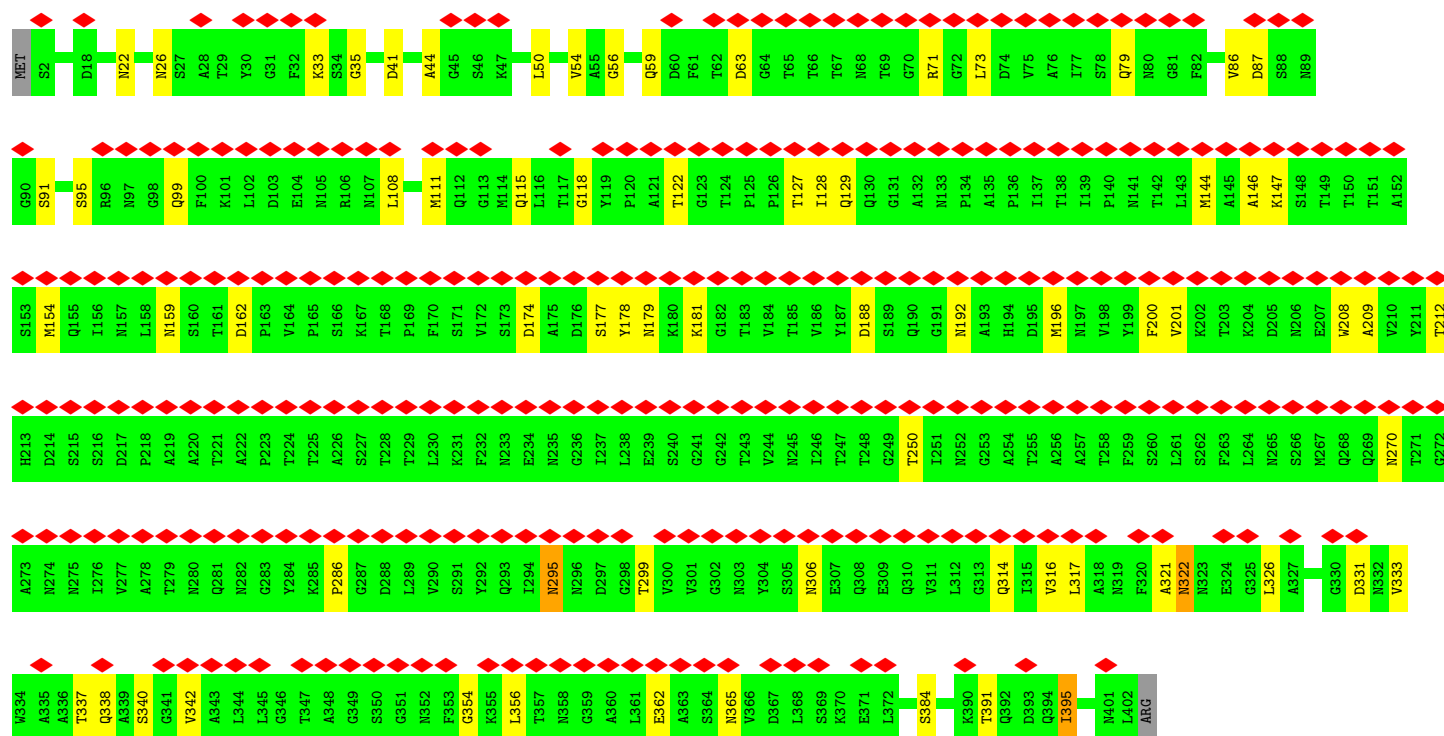


• Molecule 3: Flagellar hook protein FlgE

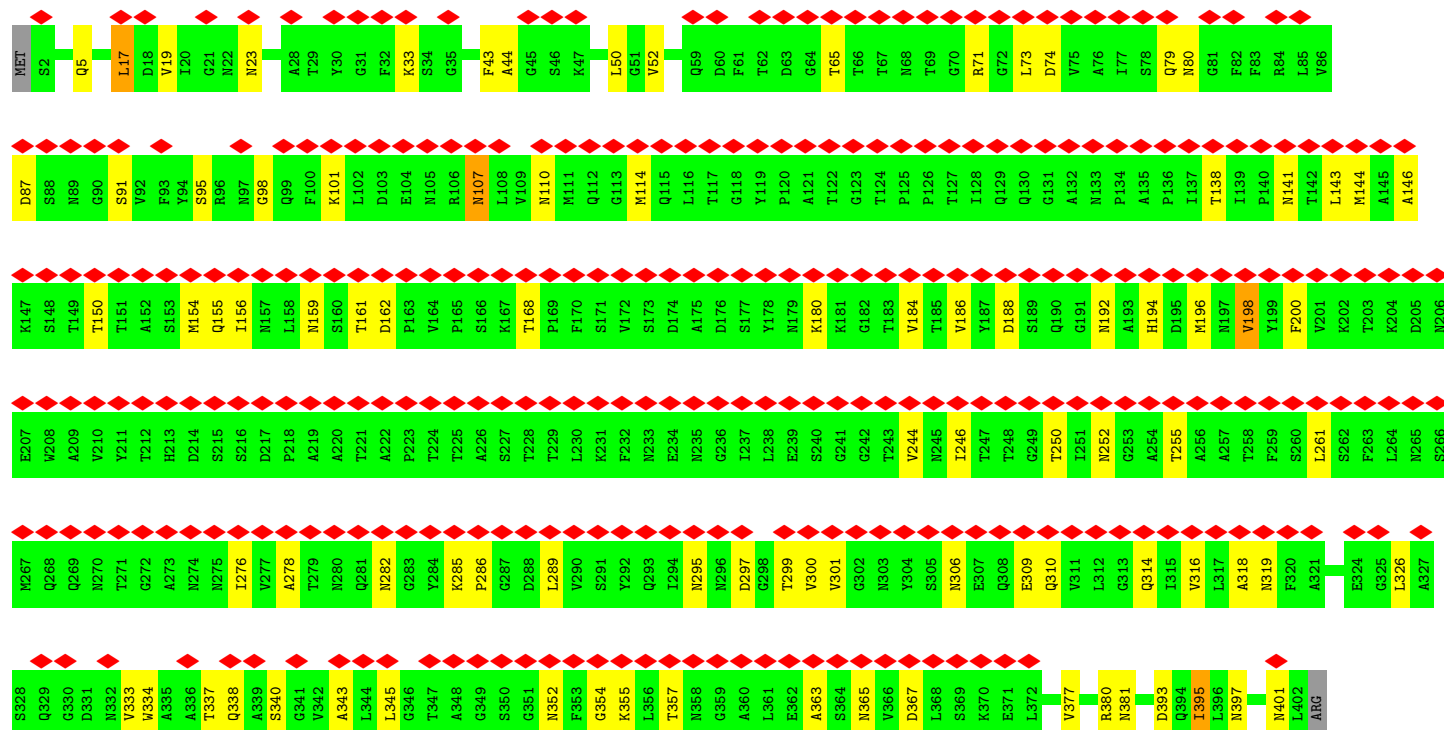
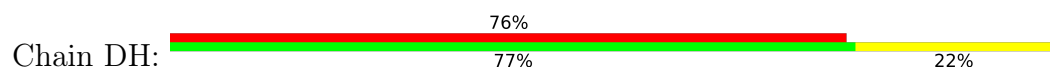


• Molecule 3: Flagellar hook protein FlgE

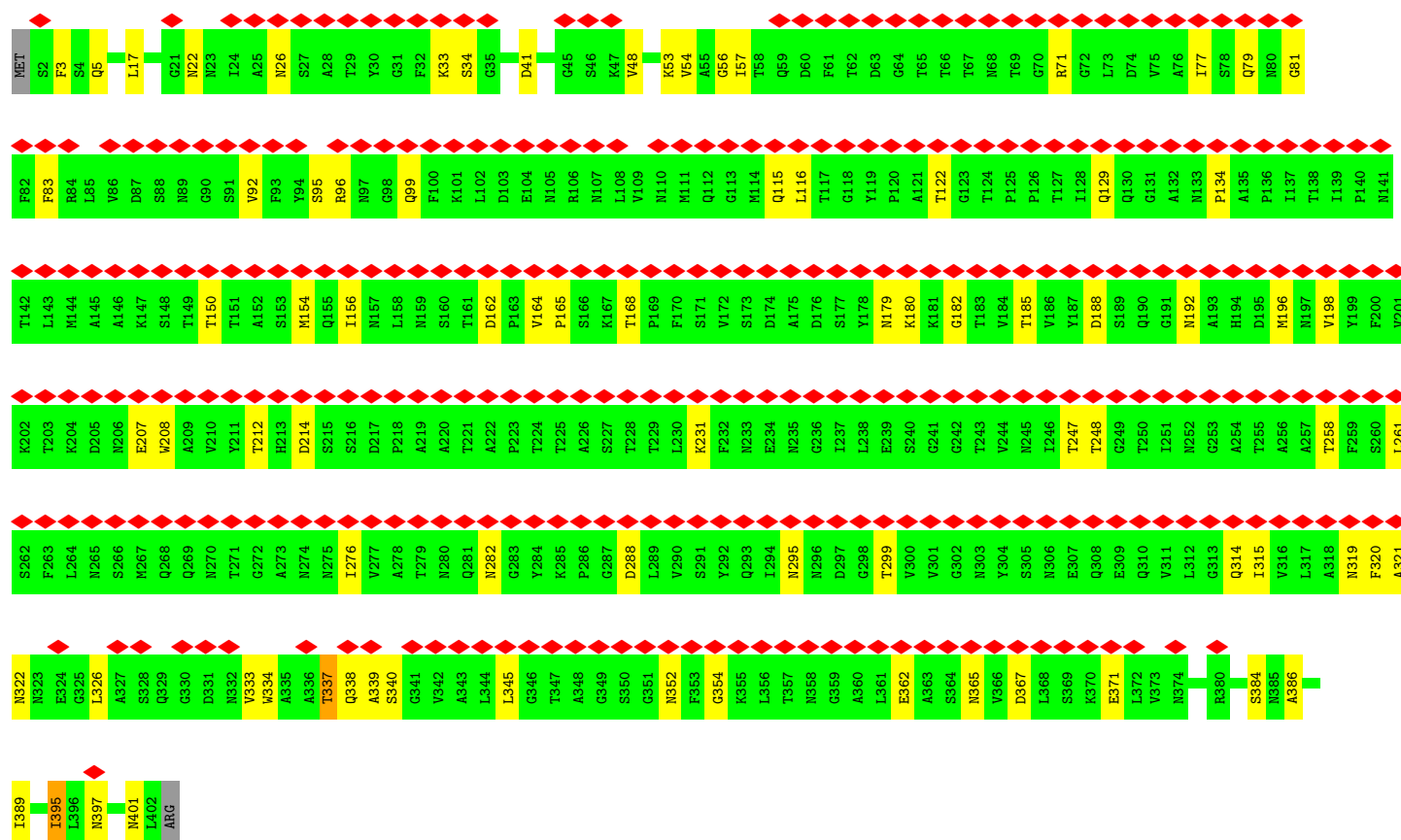
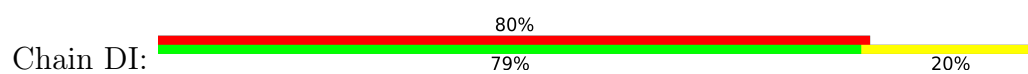




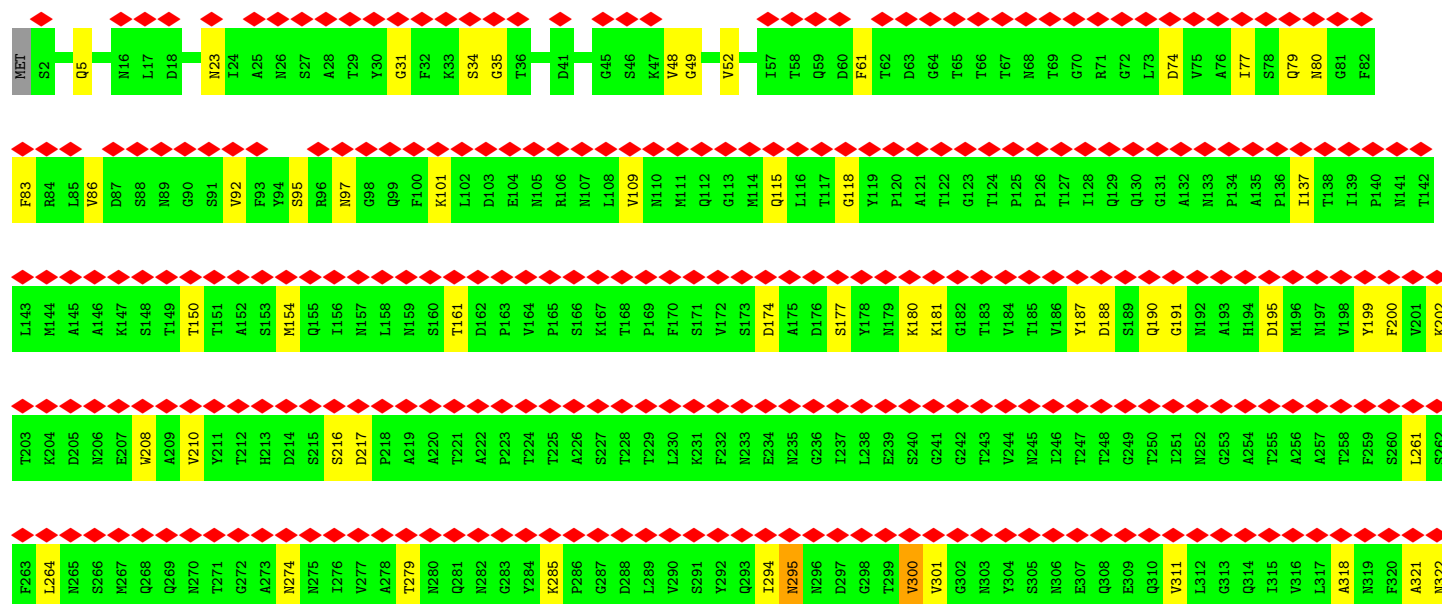
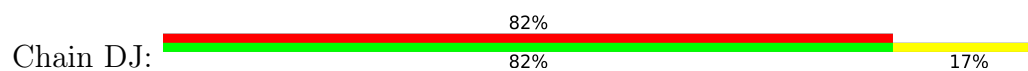
• Molecule 3: Flagellar hook protein FlgE

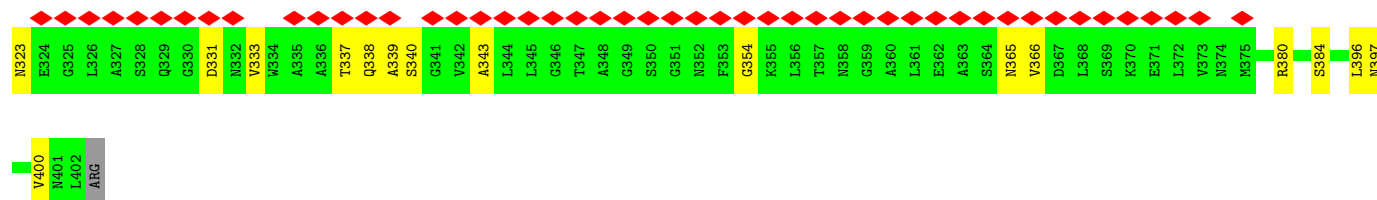


• Molecule 3: Flagellar hook protein FlgE

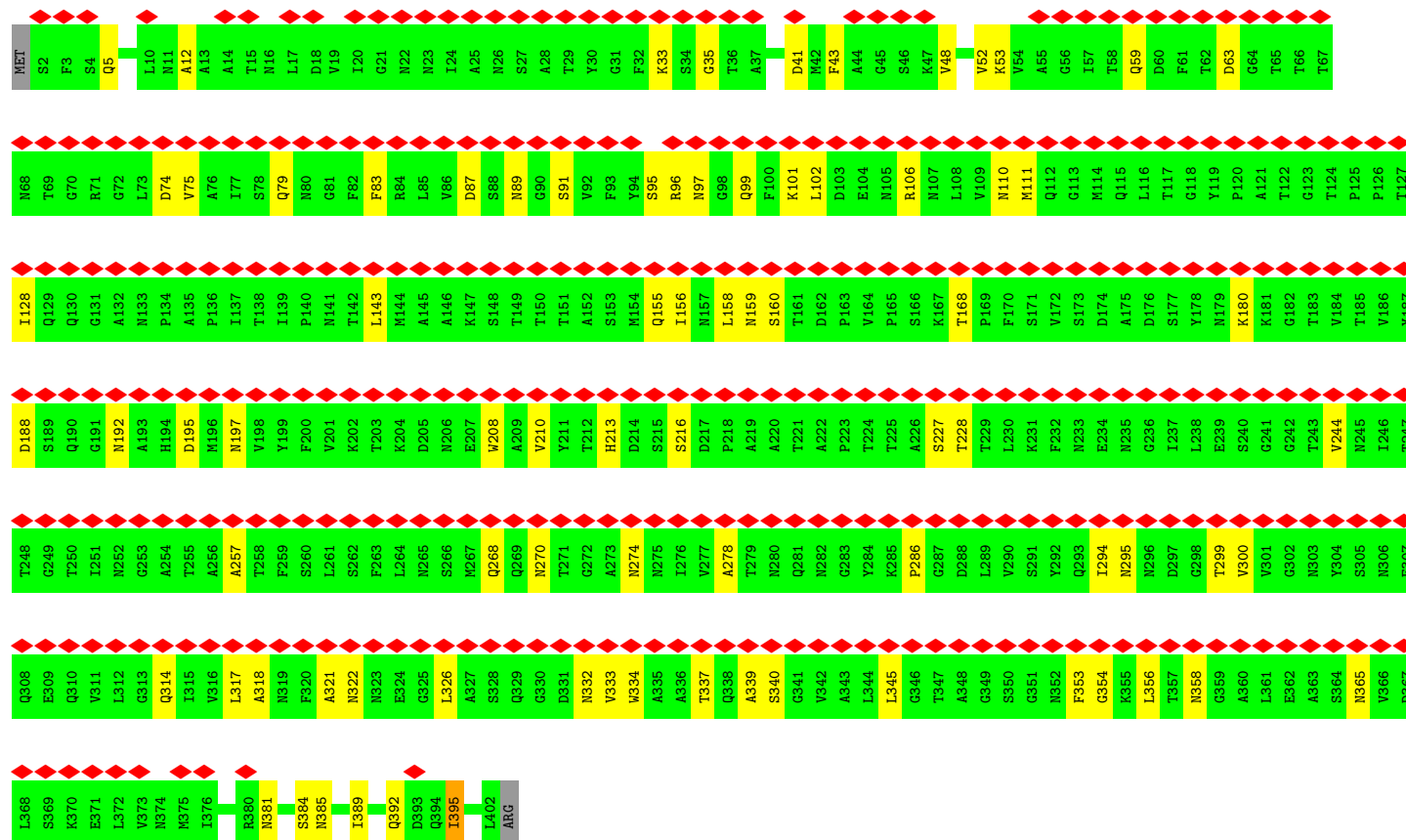
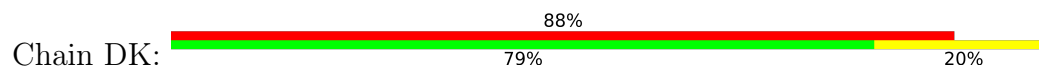


• Molecule 3: Flagellar hook protein FlgE





• Molecule 3: 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	118962	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	2.880	Depositor
Minimum map value	-1.506	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.592	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	0.17	0/1973	0.30	0/2682
1	B	0.16	0/1973	0.30	0/2682
1	C	0.16	0/1973	0.26	0/2682
1	D	0.16	0/1973	0.30	0/2682
1	E	0.16	0/1973	0.29	0/2682
1	F	0.18	0/1973	0.30	0/2682
1	G	0.17	0/1973	0.29	0/2682
1	H	0.17	0/1973	0.29	0/2682
1	I	0.17	0/1973	0.30	0/2682
1	J	0.17	0/1973	0.28	0/2682
1	K	0.18	0/1973	0.29	0/2682
1	L	0.17	0/1965	0.30	0/2672
1	M	0.19	0/1973	0.29	0/2682
1	N	0.16	0/1909	0.27	0/2593
1	O	0.17	0/1917	0.30	0/2605
1	P	0.17	0/1884	0.30	0/2559
1	Q	0.17	0/1880	0.29	0/2554
1	R	0.18	0/1898	0.30	0/2578
1	S	0.17	0/1880	0.29	0/2554
1	T	0.16	0/1925	0.28	0/2617
1	U	0.16	0/1965	0.28	0/2672
1	V	0.16	0/1965	0.29	0/2672
1	W	0.16	0/1965	0.32	0/2672
1	X	0.16	0/1965	0.34	0/2672
2	a	0.14	0/1836	0.30	0/2502
2	b	0.14	0/1828	0.28	0/2492
2	c	0.15	0/1836	0.29	0/2502
2	d	0.15	0/1836	0.31	0/2502
2	e	0.14	0/1836	0.31	0/2502
3	DA	0.13	0/2991	0.28	0/4076
3	DB	0.13	0/2991	0.27	0/4076
3	DC	0.13	0/2991	0.27	0/4076
3	DD	0.13	0/2991	0.27	0/4076
3	DE	0.12	0/2991	0.26	0/4076

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	DF	0.11	0/2991	0.25	0/4076
3	DG	0.11	0/2991	0.25	0/4076
3	DH	0.11	0/2991	0.27	0/4076
3	DI	0.11	0/2991	0.27	0/4076
3	DJ	0.11	0/2991	0.26	0/4076
3	DK	0.10	0/2991	0.25	0/4076
All	All	0.15	0/88867	0.28	0/120940

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1949	0	1926	31	0
1	B	1949	0	1926	45	0
1	C	1949	0	1926	41	0
1	D	1949	0	1926	41	0
1	E	1949	0	1926	37	0
1	F	1949	0	1926	39	0
1	G	1949	0	1926	42	0
1	H	1949	0	1926	36	0
1	I	1949	0	1926	35	0
1	J	1949	0	1926	34	0
1	K	1949	0	1926	31	0
1	L	1941	0	1914	27	0
1	M	1949	0	1926	32	0
1	N	1887	0	1871	36	0
1	O	1894	0	1878	30	0
1	P	1862	0	1839	26	0
1	Q	1858	0	1836	30	0
1	R	1875	0	1852	35	0
1	S	1858	0	1836	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	1902	0	1881	32	0
1	U	1941	0	1914	38	0
1	V	1941	0	1914	37	0
1	W	1941	0	1914	38	0
1	X	1941	0	1914	30	0
2	a	1812	0	1800	26	0
2	b	1804	0	1791	43	0
2	c	1812	0	1800	44	0
2	d	1812	0	1800	34	0
2	e	1812	0	1800	28	0
3	DA	2947	0	2839	49	0
3	DB	2947	0	2839	59	0
3	DC	2947	0	2839	56	0
3	DD	2947	0	2839	68	0
3	DE	2947	0	2839	58	0
3	DF	2947	0	2839	65	0
3	DG	2947	0	2839	48	0
3	DH	2947	0	2839	55	0
3	DI	2947	0	2839	45	0
3	DJ	2947	0	2839	39	0
3	DK	2947	0	2839	59	0
All	All	87698	0	85895	1383	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1383) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:136:VAL:HG12	1:X:138:PRO:HD2	1.60	0.83
1:M:98:LYS:O	1:M:212:GLY:HA3	1.79	0.81
1:C:136:VAL:HG12	1:C:138:PRO:HD2	1.63	0.81
1:C:256:LYS:HD3	1:G:241:GLU:HG2	1.63	0.78
3:DD:147:LYS:HB3	3:DD:283:GLY:HA2	1.66	0.77
1:M:136:VAL:HG12	1:M:138:PRO:HD2	1.66	0.77
3:DF:24:ILE:HD11	3:DK:384:SER:HB3	1.67	0.77
1:P:136:VAL:HG12	1:P:138:PRO:HD2	1.67	0.76
1:V:185:GLU:HG3	1:V:193:ILE:HG13	1.66	0.76
3:DA:210:VAL:HB	3:DA:228:THR:HB	1.67	0.76
1:V:136:VAL:HG12	1:V:138:PRO:HD2	1.69	0.75
1:Q:72:VAL:HB	1:V:28:ASN:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:136:VAL:HG12	1:W:138:PRO:HD2	1.69	0.75
1:S:136:VAL:HG12	1:S:138:PRO:HD2	1.69	0.74
1:J:136:VAL:HG12	1:J:138:PRO:HD2	1.70	0.74
1:O:136:VAL:HG12	1:O:138:PRO:HD2	1.69	0.74
1:U:176:THR:HG22	1:U:203:GLU:HG3	1.70	0.74
3:DA:285:LYS:O	3:DA:306:ASN:ND2	2.21	0.74
1:M:256:LYS:HG2	1:R:241:GLU:HG3	1.71	0.73
1:H:136:VAL:HG12	1:H:138:PRO:HD2	1.71	0.72
3:DH:295:ASN:ND2	3:DH:297:ASP:OD1	2.22	0.72
1:H:97:ILE:HD11	1:H:116:ARG:HG3	1.72	0.72
1:R:136:VAL:HG12	1:R:138:PRO:HD2	1.71	0.72
1:K:136:VAL:HG12	1:K:138:PRO:HD2	1.72	0.72
1:C:215:TYR:HB3	1:C:218:TYR:HD2	1.54	0.72
1:L:136:VAL:HG12	1:L:138:PRO:HD2	1.72	0.71
1:T:37:GLN:HG2	1:T:79:ARG:HG2	1.72	0.71
1:A:136:VAL:HG12	1:A:138:PRO:HD2	1.71	0.71
3:DB:146:ALA:HB2	3:DB:286:PRO:HD3	1.73	0.70
1:B:45:LEU:HB3	1:L:98:LYS:HD2	1.73	0.70
3:DA:351:GLY:O	3:DA:352:ASN:ND2	2.25	0.70
1:C:82:SER:HB3	1:C:223:ASN:HD22	1.57	0.70
1:I:43:ASP:N	1:I:43:ASP:OD1	2.23	0.70
1:G:38:ARG:HH12	1:G:80:LEU:HD21	1.57	0.69
1:Q:136:VAL:HG12	1:Q:138:PRO:HD2	1.74	0.69
1:X:134:PHE:HE2	1:X:189:GLU:HG3	1.57	0.69
3:DD:146:ALA:HB2	3:DD:286:PRO:HD3	1.74	0.69
2:c:170:GLU:HB2	2:c:185:ALA:HB2	1.74	0.69
1:J:37:GLN:HG2	1:J:79:ARG:HG2	1.74	0.69
1:N:116:ARG:NH1	1:N:220:GLU:OE1	2.26	0.69
3:DC:217:ASP:HB2	3:DC:220:ALA:HB2	1.75	0.68
3:DH:107:ASN:HB3	3:DH:138:THR:HG22	1.74	0.68
1:E:54:ALA:HB1	1:T:150:THR:HG21	1.73	0.68
3:DG:144:MET:SD	3:DG:306:ASN:ND2	2.66	0.68
1:R:256:LYS:HG2	1:W:241:GLU:HG2	1.74	0.68
3:DB:24:ILE:HD11	3:DG:384:SER:HB2	1.76	0.68
2:a:188:GLU:HG3	2:a:189:ARG:HG3	1.73	0.68
1:L:42:GLU:OE1	1:Q:190:ASN:ND2	2.27	0.68
1:U:98:LYS:O	1:U:212:GLY:HA3	1.94	0.68
1:G:72:VAL:HB	1:L:28:ASN:HB3	1.75	0.67
1:R:42:GLU:OE2	1:R:73:ARG:NH1	2.27	0.67
3:DF:326:LEU:HB3	3:DF:334:TRP:HB3	1.77	0.67
1:Q:51:GLN:NE2	1:V:75:VAL:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:170:GLU:HB2	2:a:185:ALA:HB2	1.76	0.67
3:DE:79:GLN:HB2	3:DE:354:GLY:HA3	1.75	0.67
3:DE:159:ASN:ND2	3:DE:270:ASN:OD1	2.27	0.67
3:DF:154:MET:HB2	3:DF:261:LEU:HD11	1.74	0.67
3:DB:322:ASN:ND2	3:DB:339:ALA:O	2.26	0.67
3:DB:285:LYS:O	3:DB:306:ASN:ND2	2.27	0.67
1:F:180:ASN:HB3	1:F:198:SER:HA	1.75	0.67
1:U:136:VAL:HG12	1:U:138:PRO:HD2	1.76	0.67
3:DF:285:LYS:O	3:DF:306:ASN:ND2	2.28	0.67
3:DK:102:LEU:HD23	3:DK:106:ARG:HE	1.60	0.67
1:X:38:ARG:HE	1:X:80:LEU:HD21	1.60	0.67
1:V:98:LYS:O	1:V:212:GLY:HA3	1.95	0.67
3:DD:210:VAL:HB	3:DD:228:THR:HB	1.77	0.66
2:e:35:ARG:O	2:e:173:ARG:NH2	2.28	0.66
3:DD:151:THR:OG1	3:DD:282:ASN:ND2	2.27	0.66
1:B:241:GLU:HG3	3:DE:398:THR:HG21	1.78	0.66
1:G:67:GLN:NE2	1:L:185:GLU:OE1	2.23	0.66
3:DA:322:ASN:ND2	3:DA:339:ALA:O	2.29	0.66
1:A:98:LYS:O	1:A:212:GLY:HA3	1.96	0.66
1:O:256:LYS:HG2	1:T:241:GLU:HG2	1.78	0.66
3:DH:154:MET:HE1	3:DH:198:VAL:HG11	1.77	0.65
1:G:136:VAL:HG12	1:G:138:PRO:HD2	1.77	0.65
3:DF:144:MET:SD	3:DF:310:GLN:NE2	2.70	0.65
3:DD:18:ASP:OD1	3:DI:5:GLN:NE2	2.25	0.65
1:U:106:MET:SD	1:U:137:GLN:NE2	2.69	0.65
1:U:239:ALA:O	1:U:243:ASN:ND2	2.28	0.65
1:E:164:GLN:NE2	1:E:166:ALA:O	2.30	0.64
1:T:251:ASP:OD1	2:c:225:ARG:NH1	2.30	0.64
3:DD:19:VAL:O	3:DD:23:ASN:ND2	2.30	0.64
1:D:127:GLN:HA	1:D:141:THR:HA	1.78	0.64
3:DG:79:GLN:HB2	3:DG:354:GLY:HA3	1.79	0.64
1:A:177:THR:OG1	1:A:202:ASN:OD1	2.13	0.64
3:DA:106:ARG:HD3	3:DF:321:ALA:HB1	1.78	0.64
1:J:45:LEU:HD13	1:U:98:LYS:HG2	1.80	0.64
1:R:37:GLN:HG2	1:R:79:ARG:HG2	1.79	0.64
1:B:83:GLN:NE2	1:B:84:GLY:O	2.31	0.64
3:DG:196:MET:SD	3:DG:212:THR:OG1	2.55	0.64
3:DJ:95:SER:HB3	3:DJ:333:VAL:HG23	1.80	0.64
1:D:82:SER:HB3	1:D:223:ASN:HD22	1.63	0.64
1:I:136:VAL:HG12	1:I:138:PRO:HD2	1.80	0.64
2:d:83:GLN:HG3	2:d:84:GLN:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DD:160:SER:O	3:DD:202:LYS:NZ	2.30	0.64
1:E:241:GLU:HG3	3:DB:398:THR:HG21	1.80	0.64
1:N:136:VAL:HG12	1:N:138:PRO:HD2	1.78	0.64
2:a:76:ARG:NH1	2:a:79:ASP:OD1	2.29	0.64
3:DD:234:GLU:O	3:DJ:190:GLN:NE2	2.25	0.64
3:DE:19:VAL:O	3:DE:23:ASN:ND2	2.31	0.64
1:M:181:ASP:OD1	1:M:181:ASP:N	2.32	0.63
1:H:37:GLN:HG2	1:H:79:ARG:HG2	1.80	0.63
1:N:19:MET:HB2	1:N:236:VAL:HG11	1.80	0.63
1:N:99:GLY:O	1:N:116:ARG:NH2	2.31	0.63
3:DE:16:ASN:HB2	3:DE:39:PHE:HZ	1.63	0.63
3:DG:200:PHE:HB3	3:DG:208:TRP:HE1	1.64	0.63
3:DH:144:MET:SD	3:DH:310:GLN:NE2	2.72	0.63
3:DD:155:GLN:HB2	3:DD:278:ALA:HB3	1.81	0.63
1:E:37:GLN:HB3	1:E:79:ARG:HD3	1.78	0.63
1:M:176:THR:HG22	1:M:203:GLU:HG2	1.80	0.63
1:B:28:ASN:HB3	3:DE:52:VAL:HB	1.81	0.63
1:Q:92:SER:O	1:Q:216:GLN:NE2	2.31	0.63
1:U:38:ARG:NH2	1:U:78:GLU:OE2	2.32	0.63
1:C:36:ARG:NH2	1:C:228:GLU:OE2	2.32	0.63
3:DH:33:LYS:HA	3:DH:365:ASN:HD21	1.64	0.63
1:K:228:GLU:OE1	1:K:232:ASN:ND2	2.32	0.63
3:DC:330:GLY:HA2	3:DH:43:PHE:H	1.64	0.62
1:I:78:GLU:OE1	1:N:121:GLN:NE2	2.31	0.62
2:c:76:ARG:NH1	2:c:79:ASP:OD1	2.30	0.62
2:e:223:ASN:OD1	2:e:226:ARG:NH2	2.32	0.62
1:V:38:ARG:NH2	1:V:78:GLU:OE2	2.32	0.62
1:N:36:ARG:NH1	1:N:228:GLU:OE2	2.33	0.62
3:DA:146:ALA:HB2	3:DA:286:PRO:HD3	1.82	0.62
3:DA:156:ILE:O	3:DA:266:SER:OG	2.13	0.62
1:C:242:ILE:HD12	1:G:230:LEU:HD21	1.82	0.62
2:a:91:GLN:HB3	2:a:119:PRO:HG2	1.80	0.62
3:DA:24:ILE:HD11	3:DF:384:SER:HB3	1.81	0.62
3:DC:32:PHE:O	3:DC:365:ASN:ND2	2.32	0.62
3:DH:299:THR:HG22	3:DH:314:GLN:HB3	1.82	0.62
3:DH:159:ASN:HB3	3:DH:162:ASP:HB2	1.81	0.62
1:A:123:ASP:OD1	1:A:127:GLN:N	2.31	0.62
1:B:136:VAL:HG12	1:B:138:PRO:HD2	1.82	0.62
1:G:1:MET:SD	1:G:1:MET:N	2.73	0.62
1:O:89:THR:HG23	1:O:91:ASN:H	1.65	0.62
3:DI:319:ASN:ND2	3:DI:352:ASN:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DK:35:GLY:HA2	3:DK:59:GLN:HA	1.82	0.62
1:A:145:ASN:OD1	1:A:161:GLN:NE2	2.33	0.61
1:X:228:GLU:O	1:X:232:ASN:ND2	2.31	0.61
1:C:1:MET:SD	1:C:1:MET:N	2.72	0.61
1:D:54:ALA:HB1	1:S:150:THR:HG21	1.82	0.61
3:DK:294:ILE:HG12	3:DK:300:VAL:HG12	1.80	0.61
1:I:175:LEU:HD11	1:I:211:ALA:HB1	1.83	0.61
2:a:28:ASN:HD22	1:V:43:ASP:HB3	1.65	0.61
1:C:42:GLU:HB2	1:G:189:GLU:HA	1.82	0.61
1:D:122:VAL:O	3:DC:322:ASN:ND2	2.32	0.61
1:G:176:THR:HB	1:G:203:GLU:HG3	1.81	0.61
1:U:154:ASP:OD1	1:U:155:GLY:N	2.31	0.61
3:DF:150:THR:OG1	3:DF:282:ASN:ND2	2.33	0.61
3:DI:122:THR:OG1	3:DI:129:GLN:NE2	2.33	0.61
1:V:38:ARG:HH12	1:V:80:LEU:HD21	1.66	0.61
1:G:66:LEU:HA	1:L:77:THR:HG22	1.83	0.61
3:DH:377:VAL:O	3:DH:381:ASN:ND2	2.27	0.61
1:H:174:ASN:ND2	1:H:203:GLU:OE2	2.34	0.61
1:J:1:MET:SD	1:J:1:MET:N	2.73	0.61
1:U:142:ILE:HD13	1:U:149:ILE:HG12	1.83	0.61
3:DC:126:PRO:HG2	3:DC:310:GLN:HE22	1.65	0.60
1:T:91:ASN:OD1	1:T:92:SER:N	2.35	0.60
1:V:82:SER:OG	1:V:223:ASN:ND2	2.32	0.60
3:DD:73:LEU:HD11	3:DD:108:LEU:HD11	1.82	0.60
3:DF:22:ASN:OD1	3:DF:26:ASN:ND2	2.34	0.60
3:DK:295:ASN:ND2	3:DK:299:THR:OG1	2.31	0.60
3:DF:178:TYR:HA	3:DF:201:VAL:HG23	1.83	0.60
3:DH:65:THR:H	3:DH:363:ALA:H	1.48	0.60
2:c:82:LEU:HD11	2:c:163:LEU:HD22	1.84	0.60
3:DC:22:ASN:OD1	3:DC:26:ASN:ND2	2.35	0.60
1:E:228:GLU:OE1	1:E:232:ASN:ND2	2.35	0.60
1:P:107:LEU:HD23	1:P:111:THR:HG23	1.84	0.60
3:DE:24:ILE:HD11	3:DJ:384:SER:HB3	1.83	0.60
1:K:19:MET:HB2	1:K:236:VAL:HG11	1.84	0.60
2:a:228:GLU:HG2	1:V:256:LYS:HG2	1.84	0.60
1:H:82:SER:OG	1:H:223:ASN:ND2	2.34	0.60
1:Q:37:GLN:HG2	1:Q:79:ARG:HG2	1.83	0.60
1:Q:161:GLN:OE1	1:Q:164:GLN:NE2	2.34	0.60
1:V:37:GLN:OE1	1:V:79:ARG:NH2	2.35	0.60
3:DG:71:ARG:NH2	3:DG:73:LEU:O	2.35	0.60
3:DE:150:THR:OG1	3:DE:282:ASN:ND2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:ASN:HB3	3:DB:52:VAL:HG12	1.84	0.59
1:Q:3:SER:HA	2:d:70:GLN:HG3	1.83	0.59
2:c:130:PRO:HD3	2:c:158:VAL:HG21	1.83	0.59
3:DE:122:THR:OG1	3:DE:129:GLN:NE2	2.35	0.59
1:L:175:LEU:HD11	1:L:211:ALA:HB1	1.84	0.59
3:DG:118:GLY:HA2	3:DG:316:VAL:HG13	1.84	0.59
1:A:38:ARG:NH1	1:A:78:GLU:OE2	2.36	0.59
1:B:258:THR:O	1:G:245:LYS:NZ	2.35	0.59
1:K:116:ARG:NH1	1:K:220:GLU:OE1	2.35	0.59
1:I:37:GLN:HG2	1:I:79:ARG:HG2	1.84	0.59
3:DC:144:MET:SD	3:DC:306:ASN:ND2	2.72	0.59
1:D:136:VAL:HG12	1:D:138:PRO:HD2	1.83	0.59
1:J:175:LEU:HD11	1:J:211:ALA:HB1	1.83	0.59
1:T:136:VAL:HG12	1:T:138:PRO:HD2	1.85	0.59
1:T:154:ASP:OD1	1:T:155:GLY:N	2.32	0.59
1:R:4:SER:HG	1:R:250:THR:HG1	1.51	0.59
3:DF:101:LYS:NZ	3:DF:110:ASN:O	2.36	0.59
1:L:56:SER:H	1:L:61:THR:HA	1.68	0.59
1:U:256:LYS:HG2	2:c:228:GLU:HG2	1.85	0.59
2:b:170:GLU:OE2	2:b:189:ARG:NH1	2.30	0.59
3:DD:217:ASP:HB2	3:DD:220:ALA:HB2	1.85	0.59
3:DK:159:ASN:ND2	3:DK:270:ASN:OD1	2.36	0.59
1:Q:175:LEU:HD11	1:Q:211:ALA:HB1	1.83	0.59
1:U:44:LEU:HB2	1:U:70:THR:HB	1.85	0.59
3:DB:33:LYS:NZ	3:DB:362:GLU:OE2	2.36	0.59
3:DB:106:ARG:HD3	3:DG:321:ALA:HB1	1.85	0.59
1:E:38:ARG:NH2	1:E:78:GLU:OE2	2.36	0.58
1:E:66:LEU:HA	1:I:77:THR:HG22	1.85	0.58
3:DC:118:GLY:HA3	3:DC:137:ILE:HD11	1.84	0.58
3:DC:201:VAL:HG22	3:DC:209:ALA:HB3	1.85	0.58
3:DG:162:ASP:OD2	3:DG:179:ASN:ND2	2.36	0.58
3:DC:34:SER:HB3	3:DC:366:VAL:HG22	1.85	0.58
3:DJ:180:LYS:HD3	3:DJ:274:ASN:HB3	1.85	0.58
1:P:72:VAL:HB	1:U:28:ASN:HB3	1.85	0.58
2:d:146:LEU:HB2	2:d:155:VAL:HG12	1.84	0.58
1:W:2:ILE:HG13	1:W:254:LEU:HD11	1.85	0.58
3:DD:24:ILE:HD11	3:DI:384:SER:HB2	1.86	0.58
3:DE:295:ASN:OD1	3:DE:295:ASN:N	2.33	0.58
1:N:67:GLN:HE22	1:S:185:GLU:HG3	1.68	0.58
1:S:109:ASP:OD1	1:S:109:ASP:N	2.36	0.58
3:DI:337:THR:O	3:DI:340:SER:OG	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DI:397:ASN:OD1	3:DI:401:ASN:ND2	2.37	0.58
1:W:175:LEU:HD11	1:W:211:ALA:HB1	1.85	0.58
3:DG:295:ASN:OD1	3:DG:295:ASN:N	2.36	0.58
1:V:176:THR:HG22	1:V:203:GLU:HG2	1.84	0.58
3:DF:331:ASP:N	3:DF:331:ASP:OD1	2.32	0.58
3:DG:22:ASN:OD1	3:DG:26:ASN:ND2	2.36	0.58
3:DH:319:ASN:HD22	3:DH:352:ASN:HB3	1.69	0.58
3:DC:295:ASN:ND2	3:DC:299:THR:OG1	2.27	0.58
3:DF:295:ASN:ND2	3:DF:299:THR:OG1	2.37	0.58
2:c:6:TYR:O	2:c:9:MET:HG3	2.03	0.58
3:DH:285:LYS:O	3:DH:306:ASN:ND2	2.29	0.58
3:DJ:322:ASN:ND2	3:DJ:339:ALA:O	2.37	0.58
1:S:92:SER:O	1:S:216:GLN:NE2	2.34	0.57
1:S:237:GLN:O	1:S:241:GLU:HG2	2.04	0.57
1:A:241:GLU:HG3	3:DA:398:THR:HG21	1.85	0.57
1:C:120:PHE:HB3	1:C:128:LEU:HD11	1.86	0.57
1:I:256:LYS:HG3	1:N:241:GLU:HG2	1.85	0.57
1:R:35:LYS:NZ	1:R:220:GLU:OE2	2.37	0.57
2:b:82:LEU:HD11	2:b:163:LEU:HD22	1.85	0.57
2:d:136:THR:OG1	2:d:144:SER:OG	2.21	0.57
3:DE:106:ARG:HD3	3:DJ:321:ALA:HB1	1.84	0.57
3:DG:73:LEU:HD11	3:DG:108:LEU:HD11	1.87	0.57
3:DI:295:ASN:ND2	3:DI:299:THR:OG1	2.35	0.57
1:A:42:GLU:OE2	1:A:73:ARG:NH1	2.36	0.57
1:L:92:SER:O	1:L:216:GLN:NE2	2.38	0.57
1:O:91:ASN:OD1	1:O:92:SER:N	2.36	0.57
3:DG:122:THR:OG1	3:DG:129:GLN:NE2	2.37	0.57
3:DI:299:THR:HG22	3:DI:314:GLN:HB3	1.85	0.57
3:DK:33:LYS:HG2	3:DK:59:GLN:HB3	1.86	0.57
1:B:175:LEU:HD11	1:B:211:ALA:HB1	1.86	0.57
1:C:148:SER:HG	1:C:160:THR:HG1	1.51	0.57
1:N:9:LYS:NZ	1:T:228:GLU:OE2	2.37	0.57
1:S:176:THR:HG22	1:S:203:GLU:HG2	1.86	0.57
3:DB:122:THR:OG1	3:DB:129:GLN:NE2	2.37	0.57
3:DE:167:LYS:HE2	3:DE:169:PRO:HG2	1.86	0.57
3:DF:42:MET:HE2	3:DF:53:LYS:HG3	1.87	0.57
1:F:1:MET:SD	1:F:1:MET:N	2.77	0.57
1:N:48:THR:HG22	1:N:67:GLN:HG2	1.87	0.57
2:c:236:SER:O	2:c:240:ASN:ND2	2.34	0.57
3:DK:210:VAL:O	3:DK:227:SER:N	2.37	0.57
1:D:42:GLU:OE2	1:D:73:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:92:SER:O	1:I:216:GLN:NE2	2.37	0.57
1:O:48:THR:HG22	1:O:67:GLN:HG2	1.85	0.57
2:d:215:GLU:OE1	1:V:9:LYS:NZ	2.38	0.57
3:DD:322:ASN:ND2	3:DD:339:ALA:O	2.37	0.57
1:D:38:ARG:NH2	1:D:78:GLU:OE2	2.37	0.57
3:DA:217:ASP:HB2	3:DA:220:ALA:HB2	1.86	0.57
3:DF:180:LYS:HB3	3:DF:200:PHE:HB2	1.86	0.57
1:N:42:GLU:HB2	1:S:189:GLU:HA	1.86	0.57
1:U:98:LYS:O	1:U:212:GLY:CA	2.52	0.57
3:DE:143:LEU:HD22	3:DE:288:ASP:HA	1.87	0.57
1:C:66:LEU:HD11	1:G:74:PRO:HB2	1.87	0.57
1:J:239:ALA:O	1:J:243:ASN:ND2	2.35	0.57
2:e:143:ILE:HD11	2:e:161:LEU:HG	1.87	0.57
1:V:98:LYS:O	1:V:212:GLY:CA	2.53	0.57
3:DF:236:GLY:HA2	3:DF:268:GLN:HE21	1.69	0.57
3:DG:178:TYR:HA	3:DG:201:VAL:HG23	1.85	0.57
1:M:1:MET:HE2	1:S:235:GLN:HG2	1.87	0.56
2:b:170:GLU:HB2	2:b:185:ALA:HB2	1.87	0.56
3:DH:146:ALA:HB2	3:DH:286:PRO:HD3	1.86	0.56
1:H:72:VAL:HB	1:M:28:ASN:HB3	1.87	0.56
3:DD:201:VAL:HG13	3:DD:209:ALA:HB3	1.85	0.56
3:DH:397:ASN:OD1	3:DH:401:ASN:ND2	2.37	0.56
3:DI:337:THR:OG1	3:DI:338:GLN:N	2.38	0.56
1:G:36:ARG:HH11	1:G:80:LEU:HD12	1.71	0.56
3:DA:332:ASN:OD1	3:DA:332:ASN:N	2.32	0.56
3:DB:365:ASN:O	3:DB:365:ASN:ND2	2.39	0.56
3:DE:337:THR:O	3:DE:340:SER:OG	2.24	0.56
3:DF:79:GLN:HB2	3:DF:354:GLY:HA3	1.85	0.56
3:DF:158:LEU:HB2	3:DF:268:GLN:HA	1.85	0.56
3:DJ:174:ASP:HB2	3:DJ:177:SER:HB2	1.85	0.56
1:G:2:ILE:HD11	1:G:254:LEU:HD13	1.88	0.56
1:T:260:LEU:HD12	2:b:231:MET:HB3	1.86	0.56
3:DD:105:ASN:OD1	3:DD:107:ASN:ND2	2.38	0.56
1:A:238:ARG:NH1	3:DB:393:ASP:OD1	2.38	0.56
1:D:101:GLY:HA3	1:D:175:LEU:HD13	1.87	0.56
1:R:44:LEU:HB2	1:R:70:THR:HG23	1.86	0.56
1:X:82:SER:HB3	1:X:223:ASN:HD22	1.70	0.56
3:DJ:79:GLN:HB3	3:DJ:354:GLY:HA3	1.87	0.56
3:DK:75:VAL:HG12	3:DK:358:ASN:HA	1.86	0.56
1:F:2:ILE:HD11	1:F:254:LEU:HD13	1.88	0.56
1:K:99:GLY:O	1:K:116:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:254:LEU:HD23	1:W:238:ARG:HG3	1.87	0.56
3:DH:154:MET:HE2	3:DH:261:LEU:HD21	1.87	0.56
1:K:1:MET:SD	1:K:1:MET:N	2.78	0.56
1:N:42:GLU:OE2	1:N:73:ARG:NE	2.37	0.56
1:E:55:GLN:NE2	1:E:57:SER:O	2.35	0.56
1:K:256:LYS:HG2	1:P:241:GLU:HG3	1.88	0.56
2:e:90:VAL:HG12	2:e:120:VAL:HA	1.88	0.56
3:DD:149:THR:HA	3:DD:283:GLY:HA3	1.88	0.56
3:DH:44:ALA:H	3:DH:50:LEU:HD23	1.70	0.56
1:B:231:VAL:O	1:B:235:GLN:HG2	2.06	0.56
1:G:255:GLN:OE1	1:G:259:GLN:NE2	2.38	0.56
3:DA:144:MET:HE3	3:DA:306:ASN:HD21	1.71	0.56
3:DB:174:ASP:HB3	3:DB:177:SER:HB2	1.88	0.56
3:DC:143:LEU:HD22	3:DC:288:ASP:HA	1.88	0.56
3:DG:33:LYS:NZ	3:DG:362:GLU:OE2	2.38	0.56
3:DJ:101:LYS:N	3:DJ:109:VAL:O	2.37	0.56
1:B:40:VAL:HG23	1:B:75:VAL:HG13	1.88	0.56
1:B:150:THR:OG1	1:B:158:SER:OG	2.22	0.56
1:H:98:LYS:O	1:H:212:GLY:HA3	2.06	0.56
1:I:230:LEU:HD12	3:DC:399:LEU:HG	1.87	0.56
2:b:89:VAL:HG12	2:b:121:ILE:HB	1.88	0.56
2:d:62:PRO:HG3	1:W:62:LEU:HD12	1.88	0.56
1:W:91:ASN:OD1	1:W:92:SER:N	2.39	0.56
1:A:258:THR:O	1:K:245:LYS:NZ	2.38	0.55
1:P:45:LEU:O	1:P:70:THR:OG1	2.17	0.55
1:R:43:ASP:OD1	1:R:43:ASP:N	2.30	0.55
3:DA:87:ASP:OD2	3:DA:91:SER:OG	2.24	0.55
3:DB:203:THR:OG1	3:DB:207:GLU:OE2	2.25	0.55
1:C:260:LEU:HD22	1:G:248:SER:HB2	1.87	0.55
1:S:256:LYS:HG2	1:X:241:GLU:HG2	1.87	0.55
1:D:55:GLN:NE2	1:D:57:SER:O	2.40	0.55
1:D:175:LEU:HD11	1:D:211:ALA:HB1	1.88	0.55
1:F:228:GLU:OE1	1:F:232:ASN:ND2	2.38	0.55
2:b:76:ARG:NH1	2:b:79:ASP:OD1	2.40	0.55
2:c:35:ARG:NH1	2:c:67:THR:O	2.39	0.55
3:DD:106:ARG:HE	3:DI:321:ALA:HB1	1.72	0.55
1:D:29:VAL:O	1:D:222:SER:OG	2.24	0.55
1:G:258:THR:O	1:M:245:LYS:NZ	2.38	0.55
1:G:123:ASP:OD1	1:G:127:GLN:N	2.39	0.55
1:Q:19:MET:HB2	1:Q:236:VAL:HG11	1.88	0.55
1:Q:48:THR:HG22	1:Q:67:GLN:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DD:362:GLU:N	3:DD:362:GLU:OE1	2.40	0.55
3:DH:150:THR:OG1	3:DH:282:ASN:ND2	2.39	0.55
3:DI:116:LEU:HD21	3:DI:315:ILE:HG12	1.89	0.55
3:DK:83:PHE:HB2	3:DK:95:SER:O	2.07	0.55
3:DK:99:GLN:HG3	3:DK:111:MET:HE3	1.87	0.55
1:C:28:ASN:HB3	3:DD:52:VAL:HB	1.88	0.55
1:H:147:LEU:HB2	1:H:160:THR:HG23	1.89	0.55
1:L:42:GLU:HB2	1:L:75:VAL:HB	1.89	0.55
2:d:89:VAL:HG23	2:d:121:ILE:HG13	1.89	0.55
3:DK:180:LYS:HD3	3:DK:274:ASN:HB3	1.88	0.55
2:c:105:ILE:HG12	2:c:115:ILE:HD11	1.87	0.55
3:DH:318:ALA:HB1	3:DH:343:ALA:HB1	1.89	0.55
1:B:153:ARG:HD2	1:B:213:LEU:HD13	1.89	0.55
1:D:180:ASN:O	1:D:183:GLY:N	2.33	0.55
2:b:105:ILE:HG12	2:b:115:ILE:HD11	1.87	0.55
1:M:55:GLN:HG3	2:e:157:PRO:HG3	1.88	0.54
3:DK:101:LYS:HB3	3:DK:111:MET:HE1	1.90	0.54
1:B:252:GLN:OE1	1:F:237:GLN:NE2	2.39	0.54
1:U:257:LEU:HB2	2:c:227:PHE:HE2	1.72	0.54
2:a:6:TYR:O	2:a:9:MET:HG3	2.06	0.54
3:DB:105:ASN:OD1	3:DB:107:ASN:ND2	2.41	0.54
3:DE:155:GLN:HB3	3:DE:278:ALA:HB3	1.88	0.54
1:B:153:ARG:HG3	1:B:213:LEU:HD22	1.88	0.54
1:O:195:THR:HG22	2:c:152:PRO:HB2	1.89	0.54
1:S:4:SER:OG	1:X:20:ASP:OD1	2.23	0.54
2:b:133:SER:OG	2:b:146:LEU:N	2.41	0.54
2:d:207:GLU:OE1	2:d:207:GLU:N	2.34	0.54
1:B:57:SER:HG	1:B:60:THR:HG1	1.55	0.54
1:B:55:GLN:NE2	1:B:57:SER:O	2.40	0.54
3:DB:208:TRP:HE1	3:DB:268:GLN:HG3	1.72	0.54
3:DC:44:ALA:HB2	3:DC:50:LEU:HD11	1.88	0.54
3:DJ:154:MET:HE2	3:DJ:261:LEU:HD21	1.89	0.54
3:DK:318:ALA:HB2	3:DK:345:LEU:HD13	1.89	0.54
1:H:88:GLN:NE2	1:H:90:ASN:OD1	2.36	0.54
1:L:256:LYS:HG2	1:Q:241:GLU:HG2	1.89	0.54
1:X:62:LEU:HD23	1:X:62:LEU:H	1.71	0.54
1:D:57:SER:HB3	1:D:60:THR:HG22	1.89	0.54
1:G:50:ARG:NH1	1:L:75:VAL:O	2.41	0.54
3:DB:171:SER:N	3:DB:177:SER:OG	2.35	0.54
3:DC:288:ASP:OD1	3:DC:288:ASP:N	2.40	0.54
1:K:92:SER:O	1:K:216:GLN:NE2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:146:LEU:HB2	2:b:155:VAL:HG12	1.89	0.54
1:W:155:GLY:O	1:W:173:LEU:N	2.35	0.54
3:DB:379:GLN:HA	3:DG:395:ILE:HD11	1.89	0.54
3:DD:151:THR:HG1	3:DD:282:ASN:HD21	1.52	0.54
1:E:52:PRO:HB3	1:E:65:GLY:H	1.72	0.54
1:J:42:GLU:OE1	1:O:190:ASN:ND2	2.40	0.54
1:D:1:MET:SD	1:D:1:MET:N	2.78	0.54
1:J:255:GLN:OE1	1:J:259:GLN:NE2	2.40	0.54
2:e:6:TYR:O	2:e:9:MET:HG3	2.08	0.54
3:DE:44:ALA:HB2	3:DE:50:LEU:HD11	1.90	0.54
3:DG:63:ASP:N	3:DG:63:ASP:OD1	2.41	0.54
1:K:82:SER:OG	1:K:223:ASN:ND2	2.38	0.53
3:DD:103:ASP:OD1	3:DD:107:ASN:N	2.37	0.53
3:DI:81:GLY:O	3:DI:96:ARG:NH1	2.41	0.53
3:DK:317:LEU:HD11	3:DK:356:LEU:HD21	1.90	0.53
1:G:54:ALA:HB1	1:W:150:THR:HG21	1.90	0.53
1:H:66:LEU:HA	1:M:77:THR:HG22	1.90	0.53
2:d:34:PHE:HB3	2:d:209:SER:HB3	1.90	0.53
2:e:44:VAL:HG23	2:e:56:LEU:HB2	1.90	0.53
3:DF:294:ILE:HG12	3:DF:300:VAL:HG12	1.91	0.53
1:H:100:GLN:NE2	1:H:210:GLY:O	2.42	0.53
3:DC:233:ASN:OD1	3:DC:234:GLU:N	2.41	0.53
3:DD:117:THR:HA	3:DD:136:PRO:HA	1.90	0.53
3:DH:155:GLN:HB2	3:DH:278:ALA:HB3	1.90	0.53
3:DK:195:ASP:H	3:DK:216:SER:HB3	1.73	0.53
1:E:260:LEU:HD22	1:I:248:SER:HB2	1.90	0.53
1:I:42:GLU:HG2	1:I:75:VAL:HB	1.90	0.53
1:I:56:SER:OG	1:I:60:THR:OG1	2.25	0.53
1:B:29:VAL:O	1:B:222:SER:OG	2.24	0.53
1:G:147:LEU:HB2	1:G:160:THR:HG23	1.91	0.53
2:a:174:SER:OG	2:a:180:ARG:NH1	2.41	0.53
2:e:170:GLU:N	2:e:170:GLU:OE1	2.41	0.53
3:DF:297:ASP:O	3:DF:314:GLN:NE2	2.36	0.53
3:DF:322:ASN:ND2	3:DF:339:ALA:O	2.40	0.53
3:DI:54:VAL:HG12	3:DI:56:GLY:H	1.73	0.53
3:DK:158:LEU:HD13	3:DK:208:TRP:CD2	2.44	0.53
1:I:29:VAL:O	1:I:222:SER:OG	2.26	0.53
3:DB:34:SER:HB3	3:DB:366:VAL:HG22	1.89	0.53
3:DF:44:ALA:H	3:DF:50:LEU:HD13	1.72	0.53
1:E:115:THR:HB	1:E:191:LEU:HD23	1.90	0.53
1:I:257:LEU:HB2	1:N:240:TYR:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:242:ILE:HD12	1:R:230:LEU:HD21	1.89	0.53
1:P:233:MET:HA	1:P:236:VAL:HG22	1.90	0.53
2:a:82:LEU:HD21	2:a:88:LEU:HG	1.89	0.53
1:W:147:LEU:HB2	1:W:160:THR:HG23	1.90	0.53
3:DJ:180:LYS:HB3	3:DJ:200:PHE:HB2	1.90	0.53
1:M:58:GLU:HG3	1:M:59:GLN:HG3	1.91	0.53
3:DD:87:ASP:HB3	3:DD:114:MET:HE3	1.91	0.53
1:C:48:THR:HG22	1:C:67:GLN:HG2	1.91	0.53
1:O:45:LEU:O	1:O:70:THR:OG1	2.23	0.53
3:DD:284:TYR:HB2	3:DD:306:ASN:HD22	1.74	0.53
3:DH:355:LYS:NZ	3:DH:357:THR:OG1	2.36	0.53
3:DK:188:ASP:OD1	3:DK:192:ASN:N	2.41	0.53
1:B:80:LEU:HD13	1:F:91:ASN:HD21	1.73	0.53
1:K:98:LYS:O	1:K:212:GLY:HA3	2.09	0.53
1:T:43:ASP:OD1	1:T:43:ASP:N	2.42	0.53
1:D:180:ASN:HB3	1:D:198:SER:HA	1.91	0.52
1:P:36:ARG:HH21	1:P:80:LEU:HD22	1.74	0.52
1:F:149:ILE:HG13	1:F:159:VAL:HG22	1.91	0.52
1:K:88:GLN:NE2	1:K:90:ASN:OD1	2.42	0.52
1:R:45:LEU:HD23	1:W:188:GLY:HA3	1.91	0.52
1:U:251:ASP:OD1	2:a:225:ARG:NH1	2.42	0.52
2:d:89:VAL:HG12	2:d:99:TYR:HD1	1.74	0.52
3:DH:184:VAL:HB	3:DH:196:MET:HB2	1.91	0.52
2:e:31:THR:HG22	1:X:41:PHE:HB2	1.91	0.52
3:DD:69:THR:HG21	3:DD:361:LEU:HD12	1.91	0.52
3:DD:337:THR:O	3:DD:340:SER:OG	2.25	0.52
1:A:82:SER:HB2	1:A:223:ASN:HD22	1.74	0.52
1:F:148:SER:HG	1:F:160:THR:HG1	1.54	0.52
1:H:55:GLN:NE2	1:H:57:SER:O	2.42	0.52
1:W:79:ARG:NH2	1:W:184:LEU:O	2.43	0.52
3:DC:120:PRO:O	3:DC:129:GLN:NE2	2.43	0.52
3:DD:102:LEU:HD23	3:DD:106:ARG:HD2	1.92	0.52
3:DF:382:TYR:CD2	3:DK:395:ILE:HD11	2.44	0.52
1:B:162:GLN:OE1	3:DK:89:ASN:ND2	2.42	0.52
2:e:115:ILE:HG13	2:e:120:VAL:HG22	1.92	0.52
3:DG:299:THR:HA	3:DG:314:GLN:HA	1.92	0.52
3:DI:22:ASN:OD1	3:DI:26:ASN:ND2	2.42	0.52
1:B:245:LYS:HB3	1:F:233:MET:HE1	1.92	0.52
1:C:55:GLN:NE2	1:C:57:SER:O	2.43	0.52
3:DA:18:ASP:OD1	3:DF:5:GLN:NE2	2.36	0.52
3:DB:79:GLN:HB2	3:DB:354:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DG:299:THR:HG22	3:DG:314:GLN:HB3	1.91	0.52
1:B:43:ASP:N	1:B:43:ASP:OD1	2.42	0.52
1:B:155:GLY:O	1:B:173:LEU:N	2.38	0.52
1:H:98:LYS:O	1:H:212:GLY:CA	2.57	0.52
1:N:149:ILE:HG13	1:N:159:VAL:HG12	1.91	0.52
1:O:150:THR:OG1	1:O:158:SER:OG	2.27	0.52
2:d:228:GLU:HG2	1:W:256:LYS:HD3	1.90	0.52
3:DE:162:ASP:OD2	3:DE:179:ASN:ND2	2.43	0.52
3:DE:116:LEU:HD23	3:DE:137:ILE:HG21	1.90	0.52
1:J:50:ARG:HH12	1:O:75:VAL:HG23	1.75	0.52
1:J:228:GLU:HG2	1:J:232:ASN:HD21	1.74	0.52
2:b:121:ILE:HA	2:b:126:PRO:HA	1.92	0.52
3:DC:102:LEU:HD21	3:DC:106:ARG:HE	1.74	0.52
3:DD:397:ASN:OD1	3:DD:401:ASN:ND2	2.43	0.52
3:DF:144:MET:HE3	3:DF:306:ASN:HD21	1.75	0.52
3:DJ:337:THR:O	3:DJ:340:SER:OG	2.23	0.52
1:D:140:ILE:HD12	1:D:171:GLY:HA3	1.91	0.51
3:DD:95:SER:HB2	3:DD:333:VAL:HG12	1.92	0.51
3:DK:337:THR:O	3:DK:340:SER:OG	2.28	0.51
1:C:66:LEU:HG	1:G:77:THR:HG23	1.92	0.51
1:I:129:VAL:HA	1:I:135:GLN:HA	1.92	0.51
1:K:154:ASP:OD1	1:K:154:ASP:N	2.38	0.51
1:L:21:VAL:O	1:L:25:ASN:ND2	2.41	0.51
1:M:98:LYS:O	1:M:212:GLY:CA	2.54	0.51
1:O:1:MET:SD	2:c:70:GLN:NE2	2.80	0.51
2:b:173:ARG:HG2	2:b:174:SER:H	1.76	0.51
1:X:129:VAL:HG12	1:X:135:GLN:HB3	1.91	0.51
3:DC:156:ILE:HD11	3:DC:158:LEU:HD21	1.90	0.51
1:H:149:ILE:HG13	1:H:159:VAL:HG22	1.93	0.51
1:K:45:LEU:O	1:K:70:THR:OG1	2.24	0.51
1:N:67:GLN:NE2	1:S:185:GLU:HG3	2.26	0.51
2:b:181:LEU:HD21	2:b:193:LEU:HD11	1.92	0.51
3:DE:34:SER:HB3	3:DE:366:VAL:HG22	1.93	0.51
3:DF:345:LEU:HD23	3:DF:345:LEU:H	1.74	0.51
1:B:106:MET:HE3	1:B:135:GLN:HE21	1.75	0.51
1:G:175:LEU:HD11	1:G:211:ALA:HB1	1.92	0.51
1:N:37:GLN:HB3	1:N:79:ARG:HG2	1.91	0.51
1:T:147:LEU:HB2	1:T:160:THR:HG23	1.93	0.51
3:DH:367:ASP:OD1	3:DH:367:ASP:N	2.43	0.51
1:E:42:GLU:OE2	1:E:73:ARG:NE	2.44	0.51
1:J:150:THR:OG1	1:J:158:SER:OG	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:147:LEU:HB2	1:S:160:THR:HG23	1.93	0.51
3:DH:19:VAL:O	3:DH:23:ASN:ND2	2.32	0.51
3:DK:156:ILE:HD11	3:DK:180:LYS:HG2	1.92	0.51
1:A:151:ILE:HG12	1:A:157:VAL:HG12	1.93	0.51
1:E:29:VAL:O	1:E:222:SER:OG	2.29	0.51
1:L:41:PHE:HA	1:L:74:PRO:HA	1.91	0.51
1:U:78:GLU:OE1	2:c:106:GLN:NE2	2.40	0.51
3:DG:365:ASN:O	3:DG:365:ASN:ND2	2.43	0.51
1:R:160:THR:HG22	1:R:167:PRO:HB3	1.93	0.51
2:c:133:SER:HA	2:c:148:PRO:HD3	1.92	0.51
2:c:176:ASP:OD1	2:c:176:ASP:N	2.42	0.51
2:d:79:ASP:O	2:d:204:GLY:N	2.43	0.51
3:DA:294:ILE:HG12	3:DA:300:VAL:HG12	1.92	0.51
3:DC:180:LYS:HB3	3:DC:200:PHE:HB2	1.91	0.51
3:DH:319:ASN:ND2	3:DH:352:ASN:O	2.44	0.51
1:U:245:LYS:HG2	2:c:217:MET:HE1	1.93	0.51
3:DB:213:HIS:HB2	3:DB:223:PRO:HG3	1.93	0.51
3:DC:18:ASP:OD1	3:DH:5:GLN:NE2	2.43	0.51
3:DD:365:ASN:O	3:DD:365:ASN:ND2	2.44	0.51
3:DF:67:THR:N	3:DF:361:LEU:O	2.39	0.51
1:Q:161:GLN:HB2	1:Q:164:GLN:HE21	1.75	0.51
2:d:89:VAL:HG12	2:d:99:TYR:CD1	2.46	0.51
2:e:150:ASP:OD1	2:e:154:THR:OG1	2.22	0.51
3:DB:281:GLN:OE1	3:DB:283:GLY:N	2.42	0.51
3:DD:60:ASP:N	3:DD:60:ASP:OD1	2.43	0.51
1:A:98:LYS:O	1:A:212:GLY:CA	2.58	0.51
1:D:63:PRO:O	1:H:197:SER:OG	2.24	0.51
1:G:230:LEU:HD12	3:DE:399:LEU:HG	1.92	0.51
1:U:50:ARG:NH2	2:c:59:ALA:O	2.44	0.51
2:d:225:ARG:NH1	1:V:251:ASP:OD1	2.44	0.51
3:DF:122:THR:OG1	3:DF:129:GLN:NE2	2.44	0.51
2:c:167:GLU:N	2:c:170:GLU:OE2	2.44	0.50
3:DA:150:THR:OG1	3:DA:282:ASN:ND2	2.35	0.50
3:DD:295:ASN:OD1	3:DD:295:ASN:N	2.43	0.50
1:I:151:ILE:N	1:I:216:GLN:OE1	2.44	0.50
1:S:66:LEU:HD11	1:X:74:PRO:HB2	1.92	0.50
2:d:114:THR:HA	2:d:120:VAL:HG23	1.92	0.50
1:V:195:THR:OG1	1:V:196:GLN:N	2.44	0.50
3:DB:87:ASP:HB3	3:DB:114:MET:HE3	1.93	0.50
3:DD:250:THR:HA	3:DD:254:ALA:HB3	1.92	0.50
3:DF:104:GLU:HB3	3:DK:339:ALA:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DG:331:ASP:OD1	3:DG:331:ASP:N	2.43	0.50
1:P:256:LYS:HG2	1:U:241:GLU:HG3	1.93	0.50
3:DF:337:THR:OG1	3:DF:338:GLN:N	2.44	0.50
1:B:260:LEU:HD22	1:F:248:SER:HB3	1.93	0.50
1:C:185:GLU:HB3	1:C:193:ILE:HG13	1.94	0.50
2:b:77:PRO:HG2	2:b:78:LEU:HD23	1.92	0.50
3:DB:288:ASP:OD1	3:DB:288:ASP:N	2.45	0.50
1:B:126:GLY:O	1:B:142:ILE:N	2.44	0.50
1:D:45:LEU:HB3	1:N:98:LYS:HD2	1.94	0.50
3:DC:71:ARG:NH1	3:DC:99:GLN:OE1	2.44	0.50
3:DI:214:ASP:OD2	3:DI:248:THR:OG1	2.29	0.50
3:DI:322:ASN:ND2	3:DI:339:ALA:O	2.45	0.50
2:c:87:TRP:HB2	2:c:164:VAL:HG23	1.93	0.50
2:d:91:GLN:HB3	2:d:119:PRO:HG2	1.93	0.50
3:DE:365:ASN:ND2	3:DE:365:ASN:O	2.45	0.50
3:DF:87:ASP:HB2	3:DF:114:MET:HE1	1.93	0.50
3:DI:165:PRO:HD3	3:DI:179:ASN:HD21	1.76	0.50
1:C:237:GLN:HA	3:DD:395:ILE:HD11	1.94	0.50
3:DJ:195:ASP:H	3:DJ:216:SER:HB3	1.76	0.50
3:DJ:301:VAL:HG22	3:DJ:311:VAL:HG12	1.93	0.50
3:DK:381:ASN:O	3:DK:385:ASN:ND2	2.41	0.50
1:B:42:GLU:OE2	1:F:190:ASN:ND2	2.32	0.50
1:D:160:THR:HG22	1:D:167:PRO:HB3	1.92	0.50
1:I:106:MET:HE2	1:I:137:GLN:HA	1.94	0.50
1:J:228:GLU:O	1:J:232:ASN:ND2	2.28	0.50
3:DF:84:ARG:HH21	3:DF:134:PRO:HB2	1.76	0.50
3:DG:159:ASN:ND2	3:DG:270:ASN:OD1	2.44	0.50
3:DI:154:MET:HB2	3:DI:261:LEU:HD11	1.93	0.50
1:C:127:GLN:HA	1:C:141:THR:HA	1.92	0.49
1:D:51:GLN:NE2	1:H:185:GLU:OE1	2.45	0.49
1:E:123:ASP:OD1	1:E:127:GLN:N	2.36	0.49
1:H:154:ASP:OD1	1:H:154:ASP:N	2.42	0.49
1:P:124:GLN:H	1:P:124:GLN:CD	2.20	0.49
1:X:50:ARG:NH2	1:X:64:SER:O	2.43	0.49
3:DA:22:ASN:OD1	3:DA:26:ASN:ND2	2.45	0.49
3:DB:188:ASP:OD1	3:DB:192:ASN:N	2.45	0.49
1:F:42:GLU:OE1	1:K:190:ASN:ND2	2.45	0.49
1:R:175:LEU:HD11	1:R:211:ALA:HB1	1.92	0.49
3:DC:337:THR:OG1	3:DC:338:GLN:N	2.45	0.49
3:DG:95:SER:HB2	3:DG:333:VAL:HG12	1.94	0.49
3:DI:79:GLN:HB2	3:DI:354:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DK:143:LEU:HD12	3:DK:286:PRO:HB2	1.94	0.49
1:C:24:ASN:OD1	1:C:37:GLN:NE2	2.45	0.49
1:M:147:LEU:HB2	1:M:160:THR:HG23	1.94	0.49
1:O:251:ASP:OD1	1:U:238:ARG:NH2	2.44	0.49
1:P:6:TRP:CE3	2:a:70:GLN:HG2	2.47	0.49
1:R:70:THR:OG1	1:R:71:GLY:N	2.44	0.49
1:T:42:GLU:HB2	1:T:75:VAL:HG21	1.94	0.49
2:b:86:GLY:O	2:b:101:ARG:NH1	2.45	0.49
2:e:170:GLU:HB2	2:e:185:ALA:HB2	1.93	0.49
1:W:109:ASP:N	1:W:109:ASP:OD1	2.42	0.49
3:DB:201:VAL:HG13	3:DB:209:ALA:HB3	1.92	0.49
3:DC:152:ALA:N	3:DC:260:SER:O	2.44	0.49
3:DE:362:GLU:OE1	3:DE:362:GLU:N	2.35	0.49
1:J:55:GLN:HG3	1:J:57:SER:O	2.12	0.49
1:J:154:ASP:HA	1:J:206:PRO:HB2	1.94	0.49
1:L:42:GLU:HG3	1:Q:189:GLU:HA	1.92	0.49
1:M:66:LEU:HA	1:R:77:THR:HG22	1.94	0.49
1:T:176:THR:HG22	1:T:203:GLU:HB3	1.94	0.49
1:U:41:PHE:HB2	2:c:31:THR:HG22	1.94	0.49
1:X:82:SER:OG	1:X:83:GLN:N	2.45	0.49
3:DC:285:LYS:O	3:DC:306:ASN:ND2	2.38	0.49
3:DE:156:ILE:HB	3:DE:276:ILE:HG13	1.94	0.49
3:DF:291:SER:O	3:DF:303:ASN:N	2.42	0.49
1:B:181:ASP:N	1:B:181:ASP:OD1	2.46	0.49
1:D:176:THR:HG22	1:D:203:GLU:HB3	1.95	0.49
1:G:260:LEU:O	1:M:245:LYS:NZ	2.32	0.49
1:I:72:VAL:HB	1:N:28:ASN:HB3	1.95	0.49
1:L:5:LEU:HG	1:L:250:THR:HG21	1.95	0.49
1:L:48:THR:HG22	1:L:67:GLN:HG2	1.94	0.49
1:Q:195:THR:HG22	2:d:152:PRO:HB2	1.95	0.49
1:S:251:ASP:OD1	2:b:225:ARG:NH1	2.45	0.49
2:d:239:GLU:OE1	2:d:243:ARG:NH1	2.45	0.49
2:e:115:ILE:HG22	2:e:116:GLN:HG3	1.94	0.49
2:e:133:SER:HA	2:e:148:PRO:HD3	1.93	0.49
1:Q:6:TRP:HZ3	1:Q:9:LYS:HZ1	1.59	0.49
2:a:35:ARG:HH11	2:a:101:ARG:HD3	1.78	0.49
2:c:83:GLN:HG2	2:c:84:GLN:H	1.78	0.49
3:DA:365:ASN:ND2	3:DA:365:ASN:O	2.45	0.49
3:DC:154:MET:HE1	3:DC:156:ILE:HB	1.95	0.49
1:E:126:GLY:O	1:E:142:ILE:N	2.39	0.49
1:I:115:THR:HB	1:I:191:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:44:LEU:HD21	1:R:73:ARG:HB3	1.94	0.49
1:B:37:GLN:HG2	1:B:79:ARG:HG2	1.94	0.49
1:E:237:GLN:HA	3:DB:395:ILE:HD11	1.94	0.49
1:F:242:ILE:HD12	1:K:230:LEU:HD11	1.95	0.49
1:L:29:VAL:O	1:L:222:SER:OG	2.31	0.49
2:c:2:ASP:O	2:c:5:ILE:HG22	2.12	0.49
2:c:162:LYS:HG3	2:c:195:ALA:HB2	1.95	0.49
2:e:212:LYS:HB2	2:e:215:GLU:HB3	1.94	0.49
3:DF:155:GLN:HB2	3:DF:278:ALA:HB3	1.94	0.49
3:DH:194:HIS:HB3	3:DH:196:MET:HE3	1.94	0.49
3:DK:63:ASP:OD1	3:DK:96:ARG:NH2	2.45	0.49
3:DK:317:LEU:HD12	3:DK:353:PHE:HB3	1.94	0.49
1:I:82:SER:HB3	1:I:223:ASN:HD22	1.78	0.49
3:DF:337:THR:O	3:DF:340:SER:OG	2.30	0.49
1:O:43:ASP:OD1	1:O:43:ASP:N	2.40	0.49
1:U:175:LEU:HD21	1:U:211:ALA:HB1	1.94	0.49
3:DE:285:LYS:O	3:DE:306:ASN:ND2	2.34	0.49
3:DE:317:LEU:HD11	3:DE:356:LEU:HD21	1.94	0.49
1:E:140:ILE:HD12	1:E:171:GLY:HA3	1.95	0.48
3:DJ:79:GLN:HG3	3:DJ:80:ASN:H	1.78	0.48
1:A:52:PRO:HB3	1:A:65:GLY:H	1.78	0.48
1:D:185:GLU:HG3	1:D:193:ILE:HG13	1.94	0.48
1:M:123:ASP:OD1	1:M:127:GLN:N	2.46	0.48
1:Q:45:LEU:O	1:Q:70:THR:OG1	2.24	0.48
1:U:72:VAL:HB	2:c:28:ASN:HB3	1.95	0.48
2:d:228:GLU:HA	1:W:256:LYS:HD2	1.95	0.48
3:DA:148:SER:HG	3:DA:189:SER:HG	1.60	0.48
3:DF:19:VAL:O	3:DF:23:ASN:ND2	2.35	0.48
3:DG:87:ASP:OD1	3:DG:91:SER:N	2.45	0.48
1:B:242:ILE:HD12	1:F:230:LEU:HD21	1.94	0.48
1:G:257:LEU:HB2	1:L:240:TYR:HE1	1.78	0.48
1:R:177:THR:OG1	1:R:202:ASN:OD1	2.30	0.48
2:d:86:GLY:O	2:d:101:ARG:NH1	2.46	0.48
3:DA:211:TYR:CE1	3:DA:226:ALA:HA	2.48	0.48
3:DC:210:VAL:O	3:DC:227:SER:OG	2.29	0.48
3:DD:63:ASP:OD1	3:DD:63:ASP:N	2.46	0.48
3:DG:41:ASP:OD1	3:DG:41:ASP:N	2.43	0.48
1:A:83:GLN:HG2	3:DG:44:ALA:HB1	1.94	0.48
1:O:36:ARG:HD3	1:O:80:LEU:HD12	1.95	0.48
3:DB:165:PRO:HG2	3:DB:201:VAL:HG23	1.95	0.48
3:DC:119:TYR:HD2	3:DC:314:GLN:HE21	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DD:174:ASP:OD1	3:DD:174:ASP:N	2.46	0.48
3:DK:197:ASN:HB2	3:DK:213:HIS:HB3	1.95	0.48
2:a:58:THR:OG1	1:V:50:ARG:NH1	2.47	0.48
1:X:42:GLU:HB2	1:X:75:VAL:HB	1.95	0.48
3:DI:150:THR:HB	3:DI:282:ASN:HD21	1.78	0.48
3:DK:326:LEU:HB3	3:DK:334:TRP:HB3	1.94	0.48
1:B:35:LYS:NZ	1:B:82:SER:O	2.37	0.48
1:B:256:LYS:HG2	1:F:241:GLU:HG2	1.96	0.48
1:C:53:GLY:HA2	1:G:197:SER:HB3	1.96	0.48
1:F:45:LEU:O	1:F:70:THR:OG1	2.23	0.48
1:N:242:ILE:HD12	1:S:230:LEU:HD21	1.96	0.48
2:b:6:TYR:O	2:b:9:MET:HG3	2.14	0.48
3:DF:247:THR:HG22	3:DF:258:THR:HG22	1.93	0.48
3:DH:186:VAL:HG13	3:DH:194:HIS:HB2	1.95	0.48
3:DH:316:VAL:HG21	3:DH:345:LEU:HD23	1.96	0.48
3:DK:87:ASP:OD1	3:DK:91:SER:N	2.46	0.48
1:L:154:ASP:HB3	1:L:156:VAL:HG12	1.95	0.48
1:M:127:GLN:HG2	1:M:141:THR:HG22	1.95	0.48
2:d:224:ALA:O	2:d:228:GLU:HG3	2.13	0.48
3:DD:300:VAL:HG23	3:DD:312:LEU:H	1.78	0.48
3:DG:317:LEU:HD11	3:DG:356:LEU:HD21	1.95	0.48
3:DJ:188:ASP:OD1	3:DJ:191:GLY:N	2.47	0.48
1:I:107:LEU:HD12	1:I:111:THR:HG23	1.96	0.48
1:N:88:GLN:HB3	1:N:218:TYR:CE2	2.49	0.48
1:T:142:ILE:HD13	1:T:149:ILE:HD13	1.95	0.48
1:T:189:GLU:OE1	2:c:200:ARG:NH2	2.47	0.48
2:b:150:ASP:OD1	2:b:154:THR:OG1	2.19	0.48
2:e:224:ALA:HB1	1:X:253:MET:HE3	1.96	0.48
3:DB:238:LEU:HD23	3:DB:264:LEU:HA	1.94	0.48
1:B:157:VAL:O	1:B:170:VAL:N	2.43	0.48
1:M:66:LEU:HD12	1:R:77:THR:HG22	1.96	0.48
1:N:92:SER:O	1:N:216:GLN:NE2	2.37	0.48
1:R:98:LYS:O	1:R:212:GLY:HA3	2.14	0.48
1:T:175:LEU:HD22	1:T:206:PRO:HG3	1.95	0.48
3:DH:73:LEU:HD13	3:DH:101:LYS:HA	1.96	0.48
3:DI:247:THR:HG22	3:DI:258:THR:HA	1.96	0.48
1:E:117:ASP:OD1	1:E:118:GLY:N	2.47	0.48
1:J:9:LYS:HG2	1:P:231:VAL:HG21	1.96	0.48
2:a:87:TRP:HB3	2:a:99:TYR:HB3	1.96	0.48
3:DC:235:ASN:O	3:DC:269:GLN:NE2	2.45	0.48
3:DC:299:THR:HG22	3:DC:314:GLN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DD:382:TYR:CD2	3:DI:395:ILE:HD11	2.48	0.48
3:DE:331:ASP:OD1	3:DE:331:ASP:N	2.43	0.48
3:DE:332:ASN:OD1	3:DE:332:ASN:N	2.46	0.48
3:DG:201:VAL:HG12	3:DG:209:ALA:HB3	1.96	0.48
3:DH:144:MET:HE3	3:DH:306:ASN:HD21	1.78	0.48
1:F:175:LEU:HD11	1:F:211:ALA:HB1	1.96	0.47
1:G:153:ARG:HD3	1:G:213:LEU:HD13	1.94	0.47
1:H:35:LYS:NZ	1:H:220:GLU:OE2	2.39	0.47
1:H:57:SER:OG	1:H:60:THR:OG1	2.20	0.47
1:Q:256:LYS:HE2	1:V:241:GLU:HG3	1.95	0.47
1:S:22:ILE:HG23	1:S:229:GLU:HG3	1.96	0.47
3:DC:212:THR:HG21	3:DC:246:ILE:HD12	1.96	0.47
3:DD:167:LYS:HG3	3:DD:169:PRO:HD2	1.94	0.47
3:DE:74:ASP:OD1	3:DE:74:ASP:N	2.47	0.47
3:DH:180:LYS:HB3	3:DH:200:PHE:HB2	1.95	0.47
1:R:43:ASP:HB3	1:W:28:ASN:HD22	1.79	0.47
2:a:73:TYR:HA	2:a:205:VAL:HG12	1.96	0.47
3:DA:79:GLN:HB2	3:DA:354:GLY:HA2	1.95	0.47
3:DI:95:SER:HB3	3:DI:333:VAL:HG12	1.95	0.47
3:DJ:5:GLN:OE1	3:DJ:5:GLN:N	2.42	0.47
3:DJ:187:TYR:HB3	3:DJ:191:GLY:HA2	1.95	0.47
1:E:255:GLN:OE1	1:E:259:GLN:NE2	2.40	0.47
1:J:98:LYS:O	1:J:212:GLY:HA3	2.15	0.47
1:M:258:THR:O	1:S:245:LYS:NZ	2.30	0.47
2:b:71:LEU:HD12	2:b:205:VAL:HG11	1.95	0.47
1:W:36:ARG:HD3	1:W:80:LEU:HD12	1.96	0.47
3:DA:288:ASP:OD1	3:DA:305:SER:OG	2.26	0.47
3:DC:214:ASP:OD2	3:DC:248:THR:OG1	2.25	0.47
3:DF:95:SER:OG	3:DF:97:ASN:OD1	2.30	0.47
3:DG:35:GLY:HA2	3:DG:59:GLN:HA	1.97	0.47
1:B:59:GLN:HE21	1:K:108:PRO:HB3	1.80	0.47
1:P:50:ARG:H	1:P:50:ARG:HD3	1.78	0.47
1:U:184:LEU:HB3	1:U:192:TYR:HB3	1.96	0.47
3:DB:294:ILE:O	3:DB:358:ASN:ND2	2.46	0.47
3:DD:247:THR:HG22	3:DD:258:THR:HB	1.96	0.47
3:DI:326:LEU:HB3	3:DI:334:TRP:HB3	1.95	0.47
1:L:245:LYS:HG2	1:Q:233:MET:HE1	1.96	0.47
2:e:228:GLU:HG2	1:X:256:LYS:HG2	1.97	0.47
3:DC:86:VAL:HG11	3:DC:136:PRO:HG3	1.95	0.47
3:DG:54:VAL:HG12	3:DG:56:GLY:H	1.78	0.47
3:DH:188:ASP:OD1	3:DH:192:ASN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:ARG:HA	1:F:238:ARG:HD3	1.68	0.47
1:O:42:GLU:O	1:O:73:ARG:N	2.41	0.47
2:d:28:ASN:HB3	1:W:72:VAL:HB	1.96	0.47
2:e:76:ARG:NH1	2:e:79:ASP:OD1	2.47	0.47
1:V:90:ASN:O	1:V:90:ASN:ND2	2.45	0.47
3:DB:332:ASN:OD1	3:DB:332:ASN:N	2.45	0.47
1:A:94:ASP:N	1:A:94:ASP:OD1	2.45	0.47
1:M:42:GLU:HB2	1:R:189:GLU:HA	1.97	0.47
3:DD:110:ASN:ND2	3:DD:112:GLN:OE1	2.48	0.47
3:DE:195:ASP:OD2	3:DE:216:SER:OG	2.32	0.47
3:DG:146:ALA:HB2	3:DG:286:PRO:HD3	1.97	0.47
3:DG:337:THR:OG1	3:DG:338:GLN:N	2.48	0.47
3:DH:110:ASN:OD1	3:DH:114:MET:N	2.41	0.47
3:DH:337:THR:O	3:DH:340:SER:OG	2.25	0.47
3:DI:156:ILE:HD11	3:DI:180:LYS:HG2	1.97	0.47
3:DK:160:SER:HA	3:DK:268:GLN:HE21	1.80	0.47
3:DK:208:TRP:NE1	3:DK:268:GLN:OE1	2.42	0.47
1:U:88:GLN:NE2	1:U:90:ASN:OD1	2.34	0.47
1:X:175:LEU:HD11	1:X:211:ALA:HB1	1.97	0.47
3:DC:194:HIS:HA	3:DC:216:SER:OG	2.15	0.47
3:DE:196:MET:HG3	3:DE:259:PHE:HZ	1.79	0.47
3:DI:365:ASN:ND2	3:DI:365:ASN:O	2.48	0.47
1:H:109:ASP:OD2	1:S:162:GLN:NE2	2.47	0.47
3:DC:367:ASP:O	3:DC:371:GLU:HG2	2.15	0.47
3:DD:211:TYR:HB3	3:DD:213:HIS:HE1	1.79	0.47
3:DG:188:ASP:OD1	3:DG:192:ASN:N	2.48	0.47
1:D:57:SER:OG	1:D:58:GLU:N	2.48	0.46
1:G:146:ALA:HB1	1:G:159:VAL:HG21	1.97	0.46
3:DA:211:TYR:HE1	3:DA:226:ALA:HA	1.81	0.46
1:F:144:ALA:O	1:F:145:ASN:ND2	2.48	0.46
1:K:36:ARG:HH22	1:K:225:ASN:HB3	1.80	0.46
1:N:66:LEU:HA	1:S:77:THR:HG22	1.96	0.46
1:Q:43:ASP:OD1	1:Q:44:LEU:N	2.49	0.46
1:X:142:ILE:HD12	1:X:149:ILE:HG12	1.97	0.46
1:F:83:GLN:HG2	3:DF:44:ALA:HB1	1.96	0.46
1:L:42:GLU:O	1:L:73:ARG:N	2.41	0.46
2:a:62:PRO:HA	1:V:63:PRO:HG2	1.97	0.46
2:b:10:GLY:O	2:b:14:GLN:HG2	2.15	0.46
3:DA:202:LYS:HB2	3:DA:208:TRP:CZ3	2.50	0.46
3:DE:54:VAL:HG12	3:DE:56:GLY:H	1.79	0.46
3:DE:129:GLN:OE1	3:DE:129:GLN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DJ:181:LYS:HG3	3:DJ:199:TYR:HE1	1.81	0.46
3:DK:155:GLN:HB3	3:DK:278:ALA:HB3	1.97	0.46
1:D:82:SER:HB3	1:D:223:ASN:ND2	2.30	0.46
1:E:1:MET:HE1	1:J:239:ALA:N	2.31	0.46
1:F:89:THR:OG1	1:F:91:ASN:OD1	2.24	0.46
2:d:4:ALA:O	2:d:7:THR:HB	2.15	0.46
3:DA:178:TYR:HA	3:DA:201:VAL:HG22	1.98	0.46
3:DJ:365:ASN:O	3:DJ:365:ASN:ND2	2.49	0.46
1:F:37:GLN:HG2	1:F:79:ARG:HG2	1.98	0.46
1:R:143:PRO:HD3	1:R:170:VAL:HG21	1.97	0.46
1:R:225:ASN:O	1:R:229:GLU:HG2	2.16	0.46
2:b:99:TYR:HE2	2:b:181:LEU:HG	1.81	0.46
3:DD:337:THR:OG1	3:DD:338:GLN:N	2.48	0.46
3:DI:71:ARG:NH1	3:DI:99:GLN:OE1	2.48	0.46
1:A:257:LEU:HG	1:P:230:LEU:HD12	1.97	0.46
1:J:238:ARG:HA	1:J:238:ARG:HD3	1.75	0.46
1:K:43:ASP:OD1	1:K:43:ASP:N	2.47	0.46
1:U:177:THR:OG1	1:U:202:ASN:OD1	2.24	0.46
2:b:67:THR:O	2:b:210:ASN:ND2	2.49	0.46
3:DC:296:ASN:HB3	3:DC:355:LYS:HE3	1.96	0.46
1:A:167:PRO:HG3	3:DG:338:GLN:HB2	1.96	0.46
1:H:97:ILE:HG22	1:H:214:LEU:HD23	1.97	0.46
1:M:88:GLN:NE2	1:M:90:ASN:OD1	2.49	0.46
1:U:257:LEU:HA	2:c:231:MET:HE3	1.96	0.46
1:V:89:THR:OG1	1:V:94:ASP:OD2	2.24	0.46
3:DA:56:GLY:HA2	3:DF:47:LYS:NZ	2.30	0.46
3:DE:337:THR:OG1	3:DE:338:GLN:N	2.49	0.46
2:b:87:TRP:HB2	2:b:164:VAL:HG22	1.97	0.46
2:c:96:ALA:HB3	2:c:180:ARG:HH21	1.80	0.46
3:DI:320:PHE:HB3	3:DI:340:SER:O	2.16	0.46
3:DJ:31:GLY:HA3	3:DJ:97:ASN:HB2	1.98	0.46
3:DK:79:GLN:HE21	3:DK:354:GLY:HA3	1.80	0.46
3:DK:143:LEU:HD23	3:DK:143:LEU:H	1.80	0.46
3:DK:392:GLN:HA	3:DK:395:ILE:HG22	1.98	0.46
1:A:19:MET:HB2	1:A:236:VAL:HG11	1.97	0.46
1:D:41:PHE:HA	1:D:74:PRO:HA	1.96	0.46
1:D:116:ARG:NH1	1:D:220:GLU:OE1	2.49	0.46
1:N:101:GLY:HA3	1:N:175:LEU:HD13	1.98	0.46
1:R:4:SER:OG	1:R:250:THR:OG1	2.23	0.46
2:a:217:MET:HE1	1:V:245:LYS:HG2	1.98	0.46
2:d:227:PHE:HE2	1:W:257:LEU:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:250:THR:HA	1:V:253:MET:HG2	1.97	0.46
3:DG:174:ASP:HB3	3:DG:177:SER:HB2	1.98	0.46
3:DG:326:LEU:HD23	3:DG:340:SER:HB2	1.96	0.46
1:B:66:LEU:HD12	1:F:77:THR:HG23	1.97	0.46
1:C:238:ARG:NH1	1:C:241:GLU:OE1	2.49	0.46
1:N:72:VAL:HB	1:S:28:ASN:HB3	1.97	0.46
1:X:43:ASP:N	1:X:43:ASP:OD1	2.46	0.46
3:DD:317:LEU:HD11	3:DD:356:LEU:HD21	1.98	0.46
3:DG:178:TYR:HE1	3:DG:181:LYS:HB2	1.81	0.46
3:DJ:337:THR:OG1	3:DJ:338:GLN:N	2.48	0.46
3:DK:97:ASN:OD1	3:DK:332:ASN:ND2	2.49	0.46
1:B:39:ALA:HA	1:B:77:THR:HA	1.98	0.45
1:F:57:SER:OG	1:F:58:GLU:N	2.49	0.45
1:L:242:ILE:HD12	1:Q:230:LEU:HD21	1.99	0.45
1:O:72:VAL:HB	1:T:28:ASN:HB3	1.97	0.45
1:T:72:VAL:HB	2:b:28:ASN:HB3	1.98	0.45
2:d:225:ARG:HG3	1:V:254:LEU:HD23	1.97	0.45
3:DJ:77:ILE:HD11	3:DJ:83:PHE:CE1	2.51	0.45
1:C:115:THR:OG1	1:C:117:ASP:OD1	2.32	0.45
1:D:17:THR:O	1:D:21:VAL:HG13	2.16	0.45
1:J:184:LEU:HB3	1:J:192:TYR:HB3	1.97	0.45
1:N:180:ASN:ND2	1:S:122:VAL:O	2.49	0.45
1:O:43:ASP:HA	1:O:72:VAL:HA	1.98	0.45
3:DE:137:ILE:HD11	3:DE:300:VAL:HG11	1.97	0.45
1:G:1:MET:HE1	1:M:238:ARG:HB2	1.98	0.45
1:R:254:LEU:HD23	1:X:238:ARG:HG3	1.99	0.45
3:DA:337:THR:OG1	3:DA:338:GLN:N	2.50	0.45
3:DC:345:LEU:HD12	3:DC:345:LEU:H	1.81	0.45
3:DH:192:ASN:OD1	3:DH:252:ASN:ND2	2.43	0.45
3:DJ:318:ALA:HB1	3:DJ:343:ALA:HB1	1.97	0.45
1:A:45:LEU:O	1:A:70:THR:HG22	2.16	0.45
1:A:164:GLN:HG3	1:A:166:ALA:HB3	1.99	0.45
1:B:49:ILE:HB	1:B:66:LEU:HD23	1.99	0.45
1:H:3:SER:O	1:H:7:ILE:HG13	2.16	0.45
1:H:44:LEU:HD21	1:H:73:ARG:HD3	1.98	0.45
1:J:228:GLU:HG2	1:J:232:ASN:ND2	2.31	0.45
2:c:230:GLN:O	2:c:234:ILE:HG12	2.17	0.45
2:d:115:ILE:HG22	2:d:116:GLN:HG3	1.99	0.45
1:V:35:LYS:NZ	1:V:220:GLU:OE2	2.44	0.45
1:W:37:GLN:HG2	1:W:79:ARG:HG3	1.98	0.45
3:DC:118:GLY:HA2	3:DC:316:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DD:380:ARG:HA	3:DD:380:ARG:HD3	1.70	0.45
3:DF:41:ASP:OD1	3:DF:41:ASP:N	2.50	0.45
3:DK:160:SER:HB3	3:DK:270:ASN:HB2	1.99	0.45
1:D:45:LEU:HD22	1:N:98:LYS:HG3	1.99	0.45
1:P:107:LEU:HD21	1:P:113:ALA:HB2	1.98	0.45
1:T:62:LEU:HD13	2:b:62:PRO:HG3	1.98	0.45
3:DD:95:SER:OG	3:DD:97:ASN:OD1	2.35	0.45
3:DI:41:ASP:OD1	3:DI:41:ASP:N	2.40	0.45
3:DK:128:ILE:HD13	3:DK:314:GLN:HB3	1.99	0.45
1:C:22:ILE:HG21	1:C:233:MET:HG3	1.98	0.45
1:C:164:GLN:HG3	1:C:166:ALA:HB3	1.99	0.45
1:D:59:GLN:N	1:D:59:GLN:OE1	2.50	0.45
1:F:29:VAL:O	1:F:222:SER:OG	2.34	0.45
1:W:82:SER:HB3	1:W:223:ASN:HD22	1.81	0.45
3:DB:3:PHE:HE1	3:DB:389:ILE:HG23	1.81	0.45
3:DB:144:MET:HE1	3:DB:308:GLN:HB2	1.97	0.45
3:DH:107:ASN:OD1	3:DH:107:ASN:N	2.45	0.45
3:DI:134:PRO:HG2	3:DI:345:LEU:HD13	1.97	0.45
1:J:97:ILE:HD12	1:J:175:LEU:HD22	1.98	0.45
1:K:227:ALA:HA	3:DA:399:LEU:HD21	1.99	0.45
1:O:5:LEU:HD23	1:O:5:LEU:HA	1.81	0.45
1:Q:42:GLU:HG3	1:V:189:GLU:HA	1.99	0.45
1:R:151:ILE:HG12	1:R:157:VAL:HG22	1.98	0.45
2:e:225:ARG:NH1	1:W:251:ASP:OD1	2.50	0.45
1:V:181:ASP:OD1	1:V:181:ASP:N	2.47	0.45
3:DH:95:SER:HB2	3:DH:333:VAL:HG12	1.97	0.45
1:D:183:GLY:O	1:D:197:SER:OG	2.35	0.45
3:DH:326:LEU:HB3	3:DH:334:TRP:HB3	1.99	0.45
1:C:127:GLN:HG2	1:C:141:THR:HB	1.99	0.45
1:H:256:LYS:HG2	1:M:241:GLU:HG2	1.99	0.45
1:K:238:ARG:HA	1:K:238:ARG:HD3	1.71	0.45
2:a:86:GLY:O	2:a:101:ARG:NH1	2.49	0.45
3:DB:155:GLN:HB2	3:DB:278:ALA:HB3	1.97	0.45
3:DD:103:ASP:OD2	3:DD:107:ASN:ND2	2.50	0.45
3:DF:201:VAL:HG12	3:DF:209:ALA:HB3	1.98	0.45
3:DF:330:GLY:HA2	3:DK:43:PHE:H	1.82	0.45
3:DJ:397:ASN:HA	3:DJ:400:VAL:HG12	1.98	0.45
1:R:72:VAL:HB	1:W:28:ASN:HB3	1.98	0.45
1:T:41:PHE:HB2	2:b:31:THR:HG22	1.99	0.45
3:DB:102:LEU:HB2	3:DG:322:ASN:HB2	1.99	0.45
3:DB:112:GLN:HG2	3:DB:331:ASP:CG	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DC:331:ASP:N	3:DC:331:ASP:OD1	2.49	0.45
3:DB:337:THR:O	3:DB:340:SER:OG	2.29	0.44
3:DE:29:THR:O	3:DE:364:SER:HB3	2.17	0.44
3:DJ:295:ASN:OD1	3:DJ:295:ASN:N	2.33	0.44
3:DK:101:LYS:NZ	3:DK:110:ASN:O	2.51	0.44
1:D:82:SER:OG	1:D:83:GLN:N	2.50	0.44
1:S:254:LEU:HD23	2:b:225:ARG:HG3	1.98	0.44
2:a:3:HIS:C	2:a:54:ARG:HH12	2.25	0.44
2:b:105:ILE:HA	2:b:115:ILE:HG12	1.99	0.44
2:c:196:ASP:OD2	2:c:198:SER:OG	2.34	0.44
3:DG:127:THR:OG1	3:DG:128:ILE:N	2.50	0.44
3:DH:244:VAL:HG12	3:DH:246:ILE:HG12	1.99	0.44
1:E:255:GLN:HE21	1:E:255:GLN:HB3	1.63	0.44
1:G:38:ARG:NH1	1:G:80:LEU:HD21	2.27	0.44
1:H:101:GLY:O	1:H:116:ARG:NH1	2.51	0.44
3:DC:16:ASN:HB2	3:DC:39:PHE:HZ	1.83	0.44
3:DK:210:VAL:HB	3:DK:228:THR:HG22	2.00	0.44
1:I:181:ASP:N	1:I:181:ASP:OD1	2.50	0.44
1:K:63:PRO:O	1:P:197:SER:OG	2.31	0.44
2:d:114:THR:OG1	2:d:115:ILE:O	2.35	0.44
2:e:101:ARG:HH21	2:e:207:GLU:CD	2.26	0.44
1:X:2:ILE:HG13	1:X:254:LEU:HD21	1.99	0.44
3:DA:141:ASN:HA	3:DA:289:LEU:HD22	1.99	0.44
3:DC:106:ARG:HH12	3:DC:141:ASN:HB3	1.82	0.44
3:DC:109:VAL:HG12	3:DC:110:ASN:O	2.17	0.44
3:DE:247:THR:HG22	3:DE:258:THR:HB	1.98	0.44
3:DH:143:LEU:HD11	3:DH:286:PRO:HB2	2.00	0.44
1:B:85:ASN:OD1	1:B:221:THR:OG1	2.35	0.44
1:G:36:ARG:HD2	1:G:80:LEU:HD12	2.00	0.44
1:G:42:GLU:OE2	1:G:73:ARG:NH2	2.50	0.44
1:L:45:LEU:HB2	1:W:98:LYS:HE2	1.99	0.44
1:U:43:ASP:HB3	2:c:28:ASN:HD22	1.81	0.44
2:d:31:THR:HG23	2:d:34:PHE:HB2	2.00	0.44
1:X:147:LEU:HB2	1:X:160:THR:HG23	1.99	0.44
3:DB:233:ASN:N	3:DB:237:ILE:O	2.38	0.44
3:DB:234:GLU:OE1	3:DH:255:THR:N	2.50	0.44
3:DC:165:PRO:HG3	3:DC:179:ASN:HD21	1.83	0.44
3:DE:22:ASN:OD1	3:DE:26:ASN:ND2	2.49	0.44
3:DF:81:GLY:O	3:DF:96:ARG:NH1	2.49	0.44
3:DH:156:ILE:HG12	3:DH:276:ILE:HG12	2.00	0.44
3:DI:188:ASP:OD1	3:DI:192:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:GLU:HG2	3:DC:400:VAL:HG11	2.00	0.44
1:I:34:PHE:HB3	1:I:222:SER:HB3	1.99	0.44
1:I:238:ARG:HA	1:I:238:ARG:HD3	1.73	0.44
1:O:79:ARG:NH2	1:O:184:LEU:O	2.50	0.44
1:R:18:ASN:O	1:R:22:ILE:HG12	2.16	0.44
1:R:253:MET:HE1	1:W:236:VAL:HG12	1.99	0.44
3:DF:377:VAL:O	3:DF:381:ASN:ND2	2.49	0.44
3:DG:99:GLN:HG3	3:DG:111:MET:HE3	2.00	0.44
3:DG:200:PHE:HB3	3:DG:208:TRP:NE1	2.30	0.44
1:I:135:GLN:OE1	1:I:135:GLN:N	2.44	0.44
1:T:107:LEU:HD12	1:T:111:THR:HG23	1.99	0.44
1:T:245:LYS:HG2	2:b:217:MET:HE1	2.00	0.44
1:W:172:GLN:HE21	1:W:205:THR:HG23	1.82	0.44
3:DD:285:LYS:O	3:DD:306:ASN:ND2	2.51	0.44
3:DE:156:ILE:HB	3:DE:276:ILE:HA	2.00	0.44
3:DI:386:ALA:O	3:DI:389:ILE:HG22	2.17	0.44
3:DK:74:ASP:OD1	3:DK:74:ASP:N	2.49	0.44
3:DK:322:ASN:ND2	3:DK:339:ALA:O	2.50	0.44
1:C:205:THR:HG23	1:C:208:LEU:HD13	1.99	0.44
1:E:164:GLN:HE21	1:E:164:GLN:HB3	1.56	0.44
1:F:26:LEU:HD23	1:F:26:LEU:HA	1.86	0.44
1:L:2:ILE:HD12	1:L:2:ILE:HA	1.91	0.44
1:O:3:SER:OG	1:T:20:ASP:OD2	2.26	0.44
1:P:42:GLU:CG	1:U:189:GLU:HA	2.48	0.44
1:U:245:LYS:HG3	2:c:220:MET:HE1	2.00	0.44
3:DB:380:ARG:NE	3:DH:393:ASP:OD1	2.50	0.44
3:DF:171:SER:N	3:DF:177:SER:OG	2.51	0.44
3:DF:375:MET:HE3	3:DF:375:MET:HB2	1.89	0.44
3:DJ:34:SER:HB3	3:DJ:366:VAL:HG12	2.00	0.44
3:DK:41:ASP:OD1	3:DK:41:ASP:N	2.51	0.44
3:DK:365:ASN:O	3:DK:365:ASN:ND2	2.50	0.44
1:E:50:ARG:HH21	1:E:62:LEU:HD21	1.83	0.44
1:P:239:ALA:O	1:P:243:ASN:ND2	2.41	0.44
2:d:228:GLU:HG2	1:W:256:LYS:NZ	2.32	0.44
3:DI:207:GLU:HG3	3:DI:231:LYS:HG2	1.98	0.44
1:N:89:THR:OG1	1:N:94:ASP:OD2	2.31	0.43
1:P:245:LYS:HE3	1:P:245:LYS:HB2	1.78	0.43
1:Q:178:PHE:CE2	1:Q:201:PRO:HB3	2.53	0.43
3:DF:380:ARG:HA	3:DF:380:ARG:HD3	1.76	0.43
1:E:237:GLN:HG3	3:DB:395:ILE:HG13	1.99	0.43
1:P:41:PHE:HA	1:P:74:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:35:ARG:O	2:c:173:ARG:NH2	2.44	0.43
2:c:82:LEU:HD21	2:c:88:LEU:HG	1.99	0.43
2:d:121:ILE:HA	2:d:126:PRO:HA	2.00	0.43
1:V:123:ASP:OD1	1:V:124:GLN:N	2.44	0.43
1:W:106:MET:HE3	1:W:106:MET:HB3	1.93	0.43
3:DB:326:LEU:HD12	3:DB:326:LEU:H	1.83	0.43
3:DB:337:THR:OG1	3:DB:338:GLN:N	2.50	0.43
1:D:154:ASP:N	1:D:154:ASP:OD1	2.40	0.43
1:J:7:ILE:HG12	1:J:70:THR:O	2.19	0.43
1:S:38:ARG:NE	1:S:78:GLU:OE2	2.49	0.43
1:B:238:ARG:HA	1:B:238:ARG:HD3	1.71	0.43
1:D:94:ASP:OD1	1:D:94:ASP:N	2.47	0.43
1:E:36:ARG:NH1	1:E:223:ASN:O	2.51	0.43
1:F:243:ASN:O	1:F:247:VAL:HG23	2.18	0.43
1:G:106:MET:HE1	1:G:137:GLN:HA	2.00	0.43
1:P:46:TYR:CD1	1:P:69:GLY:HA2	2.53	0.43
1:S:49:ILE:HB	1:S:66:LEU:HD22	2.00	0.43
2:e:87:TRP:HB3	2:e:99:TYR:HB3	2.00	0.43
2:e:116:GLN:HG3	2:e:116:GLN:H	1.63	0.43
1:W:147:LEU:HD11	1:W:162:GLN:HA	2.00	0.43
3:DE:39:PHE:HD1	3:DE:54:VAL:HG22	1.82	0.43
3:DE:159:ASN:ND2	3:DE:272:GLY:O	2.52	0.43
3:DH:337:THR:OG1	3:DH:338:GLN:N	2.50	0.43
1:G:140:ILE:HD13	1:G:157:VAL:HG11	2.01	0.43
1:K:115:THR:HB	1:K:191:LEU:HD23	2.00	0.43
1:P:42:GLU:HB2	1:P:75:VAL:HB	2.00	0.43
2:c:3:HIS:HB2	2:c:54:ARG:HH12	1.83	0.43
1:W:188:GLY:O	1:W:190:ASN:N	2.44	0.43
3:DC:63:ASP:N	3:DC:63:ASP:OD1	2.51	0.43
3:DD:73:LEU:HD12	3:DD:73:LEU:HA	1.85	0.43
3:DD:233:ASN:OD1	3:DD:234:GLU:N	2.42	0.43
3:DD:367:ASP:O	3:DD:371:GLU:HG2	2.18	0.43
3:DI:3:PHE:HD1	3:DI:389:ILE:HD11	1.84	0.43
3:DI:34:SER:H	3:DI:365:ASN:HD21	1.65	0.43
3:DI:162:ASP:HB3	3:DI:208:TRP:HH2	1.83	0.43
3:DJ:86:VAL:O	3:DJ:115:GLN:N	2.50	0.43
1:A:147:LEU:HD11	1:A:162:GLN:HA	2.01	0.43
1:F:42:GLU:OE2	1:K:190:ASN:N	2.52	0.43
1:P:257:LEU:HB2	1:U:240:TYR:HE2	1.84	0.43
1:R:238:ARG:HA	1:R:238:ARG:HD3	1.77	0.43
1:T:175:LEU:HD21	1:T:211:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:79:ASP:O	2:a:204:GLY:N	2.47	0.43
1:X:91:ASN:ND2	1:X:94:ASP:OD1	2.52	0.43
1:X:155:GLY:O	1:X:173:LEU:N	2.46	0.43
3:DA:144:MET:HE1	3:DA:308:GLN:HB2	2.00	0.43
3:DA:331:ASP:HA	3:DF:41:ASP:O	2.19	0.43
3:DC:380:ARG:HA	3:DC:380:ARG:HD3	1.76	0.43
3:DF:108:LEU:HB2	3:DF:137:ILE:HG23	2.00	0.43
1:O:37:GLN:HG2	1:O:79:ARG:HG2	2.00	0.43
1:O:67:GLN:HE22	1:T:186:SER:H	1.66	0.43
1:S:45:LEU:O	1:S:70:THR:OG1	2.28	0.43
2:b:181:LEU:HB3	2:b:185:ALA:HB3	2.01	0.43
2:c:186:GLN:HG3	2:c:191:ALA:HA	2.01	0.43
3:DB:12:ALA:HB2	3:DB:52:VAL:HG21	2.00	0.43
1:Q:42:GLU:OE1	1:Q:75:VAL:HB	2.19	0.43
2:d:227:PHE:HD2	1:W:256:LYS:HZ1	1.67	0.43
3:DA:139:ILE:HA	3:DA:312:LEU:HD13	1.99	0.43
3:DE:87:ASP:OD1	3:DE:91:SER:N	2.52	0.43
3:DF:382:TYR:CG	3:DK:395:ILE:HD11	2.53	0.43
3:DI:367:ASP:O	3:DI:371:GLU:HG2	2.18	0.43
1:E:238:ARG:NH2	3:DC:397:ASN:HB2	2.34	0.43
1:T:154:ASP:HB3	1:T:156:VAL:HG12	2.01	0.43
2:b:113:LEU:HD12	2:b:127:ILE:HG12	2.01	0.43
3:DA:380:ARG:HD3	3:DA:380:ARG:HA	1.72	0.43
3:DE:211:TYR:CE1	3:DE:226:ALA:HA	2.54	0.43
3:DH:380:ARG:HD3	3:DH:380:ARG:HA	1.81	0.43
1:E:80:LEU:HD22	1:I:91:ASN:HD21	1.83	0.43
1:F:108:PRO:HG2	1:L:153:ARG:NH1	2.34	0.43
1:G:29:VAL:O	1:G:222:SER:OG	2.35	0.43
1:I:25:ASN:ND2	1:I:36:ARG:HB2	2.34	0.43
1:I:137:GLN:HB3	1:I:138:PRO:HD3	2.01	0.43
1:I:256:LYS:HD3	1:I:256:LYS:O	2.18	0.43
1:J:97:ILE:HG23	1:J:116:ARG:HE	1.84	0.43
1:J:254:LEU:HD23	1:P:238:ARG:HG3	2.01	0.43
1:R:3:SER:O	2:e:70:GLN:NE2	2.52	0.43
1:T:29:VAL:O	1:T:222:SER:OG	2.37	0.43
2:c:87:TRP:HB3	2:c:99:TYR:HB3	2.01	0.43
1:V:45:LEU:HD23	1:V:45:LEU:H	1.83	0.43
3:DD:53:LYS:HE3	3:DD:53:LYS:HB2	1.85	0.43
3:DF:367:ASP:OD1	3:DF:367:ASP:N	2.47	0.43
3:DK:392:GLN:O	3:DK:395:ILE:HG22	2.18	0.43
1:C:115:THR:OG1	1:C:116:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:7:ILE:HG12	1:S:70:THR:O	2.19	0.42
1:U:82:SER:OG	1:U:83:GLN:N	2.52	0.42
3:DD:331:ASP:O	3:DD:333:VAL:N	2.46	0.42
3:DG:108:LEU:HD13	3:DG:108:LEU:HA	1.84	0.42
3:DH:79:GLN:HB3	3:DH:354:GLY:HA3	2.00	0.42
3:DH:301:VAL:HG13	3:DH:309:GLU:HG2	2.01	0.42
3:DJ:154:MET:HB2	3:DJ:279:THR:HG22	2.01	0.42
1:C:46:TYR:CD1	1:C:69:GLY:HA2	2.55	0.42
1:C:57:SER:OG	1:C:58:GLU:N	2.52	0.42
1:D:218:TYR:OH	3:DI:53:LYS:HD2	2.19	0.42
1:I:41:PHE:HA	1:I:74:PRO:HA	2.01	0.42
1:N:1:MET:N	2:b:211:VAL:H	2.17	0.42
1:O:97:ILE:HD11	1:O:103:PHE:CE2	2.54	0.42
1:X:19:MET:HB2	1:X:236:VAL:HG11	2.02	0.42
3:DA:331:ASP:O	3:DA:333:VAL:N	2.44	0.42
3:DC:397:ASN:OD1	3:DC:401:ASN:ND2	2.52	0.42
3:DD:332:ASN:OD1	3:DD:332:ASN:N	2.49	0.42
3:DJ:202:LYS:HB2	3:DJ:208:TRP:CZ3	2.54	0.42
1:A:137:GLN:HB3	1:A:138:PRO:HD3	2.01	0.42
1:D:57:SER:HB3	1:D:60:THR:CG2	2.49	0.42
1:F:195:THR:OG1	1:F:196:GLN:N	2.51	0.42
1:H:54:ALA:HB3	1:H:62:LEU:HD13	2.00	0.42
2:a:227:PHE:CE1	1:V:257:LEU:HB2	2.55	0.42
2:b:66:MET:SD	2:b:66:MET:N	2.91	0.42
3:DD:217:ASP:CG	3:DD:249:GLY:HA3	2.44	0.42
3:DE:144:MET:SD	3:DE:306:ASN:ND2	2.74	0.42
3:DF:388:THR:O	3:DF:391:THR:HG22	2.18	0.42
3:DH:17:LEU:HD13	3:DH:17:LEU:HA	1.89	0.42
3:DI:83:PHE:HB2	3:DI:95:SER:O	2.20	0.42
1:F:92:SER:O	1:F:216:GLN:NE2	2.53	0.42
1:J:26:LEU:HD23	1:J:26:LEU:HA	1.87	0.42
1:J:140:ILE:HD13	1:J:157:VAL:HG11	2.00	0.42
1:J:181:ASP:OD1	1:J:181:ASP:N	2.52	0.42
1:K:130:THR:HG22	1:K:134:PHE:O	2.20	0.42
1:L:238:ARG:HD3	1:L:238:ARG:HA	1.78	0.42
1:M:45:LEU:HD13	1:X:98:LYS:HG2	2.01	0.42
1:S:37:GLN:HG2	1:S:79:ARG:HG2	2.01	0.42
1:W:256:LYS:HE2	1:W:256:LYS:HB3	1.47	0.42
3:DE:154:MET:HB2	3:DE:261:LEU:HD11	2.00	0.42
3:DI:33:LYS:NZ	3:DI:362:GLU:OE2	2.51	0.42
3:DJ:74:ASP:N	3:DJ:74:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ARG:HA	1:C:238:ARG:HD3	1.72	0.42
1:E:95:VAL:O	1:E:118:GLY:HA3	2.19	0.42
1:E:255:GLN:O	1:E:259:GLN:HG2	2.19	0.42
1:N:43:ASP:N	1:N:43:ASP:OD1	2.43	0.42
1:Q:93:LYS:HE3	1:Q:93:LYS:HB2	1.92	0.42
2:a:162:LYS:HG3	2:a:195:ALA:HB2	2.01	0.42
2:d:181:LEU:HD11	2:d:193:LEU:HG	2.01	0.42
3:DD:34:SER:HB3	3:DD:366:VAL:HG22	2.02	0.42
3:DD:108:LEU:HD13	3:DD:108:LEU:HA	1.83	0.42
3:DF:106:ARG:HE	3:DK:321:ALA:HB1	1.84	0.42
3:DG:178:TYR:CE1	3:DG:181:LYS:HB2	2.54	0.42
1:B:59:GLN:HG2	1:B:60:THR:HG23	2.00	0.42
1:C:36:ARG:HD2	1:C:223:ASN:O	2.20	0.42
2:b:82:LEU:HA	2:b:201:ILE:HG22	2.02	0.42
1:V:178:PHE:CE1	1:V:201:PRO:HB3	2.55	0.42
3:DA:296:ASN:HB2	3:DA:355:LYS:HE3	2.02	0.42
3:DB:108:LEU:HD13	3:DB:108:LEU:HA	1.91	0.42
3:DD:247:THR:HA	3:DD:258:THR:HA	2.02	0.42
3:DF:61:PHE:CE2	3:DF:323:ASN:HB3	2.55	0.42
3:DF:362:GLU:OE1	3:DF:362:GLU:N	2.52	0.42
3:DG:86:VAL:HG23	3:DG:115:GLN:HB2	2.02	0.42
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.89	0.42
1:A:260:LEU:HD22	1:J:248:SER:HB2	2.01	0.42
1:M:254:LEU:HA	1:M:254:LEU:HD23	1.82	0.42
1:N:202:ASN:OD1	1:N:202:ASN:N	2.52	0.42
3:DA:34:SER:HB3	3:DA:366:VAL:HG22	2.02	0.42
3:DA:119:TYR:HB2	3:DA:128:ILE:HD11	2.00	0.42
3:DC:382:TYR:CD2	3:DH:395:ILE:HD11	2.55	0.42
3:DH:74:ASP:OD1	3:DH:74:ASP:N	2.51	0.42
3:DK:95:SER:HB2	3:DK:97:ASN:HD22	1.85	0.42
1:B:48:THR:HG22	1:B:67:GLN:HG2	2.02	0.42
1:E:154:ASP:OD1	1:E:154:ASP:N	2.53	0.42
1:G:26:LEU:HD23	1:G:26:LEU:HA	1.89	0.42
1:J:18:ASN:O	1:J:22:ILE:HG12	2.19	0.42
1:N:154:ASP:OD1	1:N:154:ASP:N	2.38	0.42
1:S:238:ARG:HA	1:S:238:ARG:HD3	1.83	0.42
1:T:44:LEU:HB2	1:T:70:THR:HB	2.02	0.42
2:a:181:LEU:HD11	2:a:193:LEU:HG	2.02	0.42
2:d:66:MET:SD	2:d:66:MET:N	2.92	0.42
3:DA:117:THR:HA	3:DA:136:PRO:HA	2.02	0.42
3:DA:326:LEU:HB3	3:DA:334:TRP:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DB:93:PHE:CD2	3:DB:114:MET:HE1	2.55	0.42
3:DC:228:THR:HG21	3:DC:244:VAL:HG21	2.01	0.42
3:DG:147:LYS:HB3	3:DG:147:LYS:HE3	1.83	0.42
3:DI:182:GLY:HA3	3:DI:276:ILE:HD11	2.00	0.42
3:DK:188:ASP:HA	3:DK:257:ALA:HB2	2.02	0.42
1:A:109:ASP:OD1	1:A:110:GLY:N	2.53	0.42
1:C:187:ILE:HG13	1:C:191:LEU:HB2	2.02	0.42
1:I:185:GLU:HB3	1:I:193:ILE:HG13	2.02	0.42
1:K:5:LEU:HD23	1:K:5:LEU:HA	1.94	0.42
1:Q:147:LEU:HD11	1:Q:162:GLN:HB2	2.02	0.42
1:S:3:SER:O	1:S:7:ILE:HG13	2.19	0.42
1:S:50:ARG:HE	1:S:51:GLN:H	1.68	0.42
1:U:7:ILE:HG12	1:U:70:THR:O	2.19	0.42
3:DB:117:THR:HA	3:DB:136:PRO:HA	2.01	0.42
3:DB:152:ALA:HB3	3:DB:261:LEU:HG	2.02	0.42
3:DD:21:GLY:HA2	3:DD:24:ILE:HG22	2.01	0.42
1:C:77:THR:O	1:C:77:THR:OG1	2.36	0.42
1:H:158:SER:OG	1:H:167:PRO:HB2	2.20	0.42
1:H:238:ARG:HD3	1:H:238:ARG:HA	1.84	0.42
1:K:49:ILE:HB	1:K:66:LEU:HB3	2.01	0.42
1:N:6:TRP:CD1	2:b:70:GLN:HB2	2.54	0.42
1:O:254:LEU:HD23	1:U:238:ARG:HG3	2.02	0.42
1:R:43:ASP:HB3	1:W:28:ASN:ND2	2.35	0.42
1:S:187:ILE:HG13	1:S:191:LEU:HB2	2.01	0.42
2:e:73:TYR:HD1	2:e:205:VAL:HG12	1.85	0.42
2:e:174:SER:OG	2:e:178:LEU:O	2.38	0.42
3:DD:210:VAL:HG11	3:DD:263:PHE:CZ	2.55	0.42
3:DE:127:THR:OG1	3:DE:128:ILE:N	2.52	0.42
3:DE:367:ASP:O	3:DE:371:GLU:HG2	2.19	0.42
3:DG:154:MET:HE2	3:DG:154:MET:HB2	1.95	0.42
1:C:254:LEU:HD23	1:H:238:ARG:HG2	2.01	0.41
1:F:137:GLN:HB3	1:F:138:PRO:HD3	2.01	0.41
1:T:7:ILE:HG12	1:T:70:THR:O	2.20	0.41
1:U:22:ILE:HG21	1:U:233:MET:HG3	2.02	0.41
2:b:226:ARG:O	2:b:230:GLN:HG2	2.20	0.41
3:DC:178:TYR:CE1	3:DC:181:LYS:HB2	2.55	0.41
3:DD:93:PHE:CD2	3:DD:114:MET:HE1	2.55	0.41
3:DE:39:PHE:CD1	3:DE:54:VAL:HG22	2.55	0.41
3:DF:103:ASP:N	3:DF:107:ASN:O	2.52	0.41
3:DF:127:THR:OG1	3:DF:128:ILE:N	2.53	0.41
3:DH:79:GLN:HG3	3:DH:80:ASN:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DJ:118:GLY:HA3	3:DJ:137:ILE:HD11	2.02	0.41
1:C:38:ARG:NH1	1:C:78:GLU:OE2	2.53	0.41
1:D:26:LEU:HD23	1:D:26:LEU:HA	1.93	0.41
1:I:95:VAL:O	1:I:118:GLY:HA3	2.20	0.41
3:DB:299:THR:HG22	3:DB:314:GLN:HB3	2.01	0.41
3:DC:186:VAL:HG23	3:DC:194:HIS:HB2	2.02	0.41
3:DG:73:LEU:HD12	3:DG:73:LEU:HA	1.89	0.41
3:DJ:380:ARG:HD3	3:DJ:380:ARG:HA	1.78	0.41
1:G:97:ILE:HG23	1:G:116:ARG:HE	1.86	0.41
1:G:238:ARG:HA	1:G:238:ARG:HD3	1.78	0.41
1:H:195:THR:OG1	1:H:196:GLN:N	2.49	0.41
1:J:42:GLU:HB3	1:O:189:GLU:HA	2.01	0.41
1:N:40:VAL:HG23	1:N:75:VAL:HG13	2.02	0.41
1:S:242:ILE:HG21	1:X:26:LEU:HD22	2.03	0.41
2:e:76:ARG:O	2:e:204:GLY:HA2	2.20	0.41
3:DE:22:ASN:ND2	3:DJ:49:GLY:HA3	2.35	0.41
1:C:67:GLN:HE22	1:G:185:GLU:HG3	1.86	0.41
1:C:254:LEU:HD12	1:C:254:LEU:HA	1.83	0.41
1:F:34:PHE:HB3	1:F:222:SER:HB3	2.02	0.41
1:H:48:THR:HG22	1:H:67:GLN:HG2	2.01	0.41
1:J:3:SER:O	1:J:7:ILE:HG13	2.20	0.41
2:c:101:ARG:HH21	2:c:207:GLU:CD	2.29	0.41
1:V:43:ASP:OD1	1:V:43:ASP:N	2.51	0.41
1:V:255:GLN:HA	1:V:258:THR:HG22	2.02	0.41
3:DA:103:ASP:OD1	3:DA:103:ASP:N	2.54	0.41
3:DA:301:VAL:HG13	3:DA:309:GLU:HB3	2.02	0.41
3:DB:156:ILE:HD13	3:DB:276:ILE:HG12	2.02	0.41
3:DE:126:PRO:HG2	3:DE:310:GLN:NE2	2.35	0.41
3:DE:331:ASP:O	3:DE:333:VAL:N	2.50	0.41
3:DF:17:LEU:HA	3:DF:17:LEU:HD23	1.80	0.41
3:DI:115:GLN:H	3:DI:115:GLN:CD	2.29	0.41
3:DJ:23:ASN:HD21	3:DJ:35:GLY:H	1.69	0.41
3:DK:12:ALA:HB2	3:DK:52:VAL:HG21	2.02	0.41
1:F:43:ASP:HA	1:F:72:VAL:HA	2.02	0.41
1:F:148:SER:OG	1:F:160:THR:OG1	2.26	0.41
1:G:37:GLN:HG2	1:G:79:ARG:HG2	2.02	0.41
1:G:176:THR:HA	1:G:203:GLU:HA	2.01	0.41
1:O:6:TRP:HZ3	2:c:208:GLY:HA3	1.85	0.41
1:Q:49:ILE:O	1:Q:65:GLY:HA3	2.21	0.41
1:T:50:ARG:NH2	2:b:59:ALA:O	2.53	0.41
1:U:44:LEU:HD21	1:U:73:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:2:ASP:O	2:a:5:ILE:HG22	2.20	0.41
2:e:121:ILE:HA	2:e:126:PRO:HA	2.01	0.41
3:DB:80:ASN:OD1	3:DB:80:ASN:N	2.54	0.41
3:DB:202:LYS:HB2	3:DB:208:TRP:CZ3	2.55	0.41
3:DD:345:LEU:H	3:DD:345:LEU:HD22	1.85	0.41
3:DF:26:ASN:OD1	3:DK:52:VAL:HG12	2.20	0.41
3:DH:156:ILE:HG13	3:DH:276:ILE:HG23	2.02	0.41
1:B:38:ARG:HD3	1:B:80:LEU:HD21	2.03	0.41
1:C:145:ASN:O	1:C:145:ASN:ND2	2.53	0.41
1:D:176:THR:HA	1:D:203:GLU:HA	2.03	0.41
1:J:256:LYS:HD2	1:J:256:LYS:HA	1.90	0.41
1:P:91:ASN:OD1	1:P:92:SER:N	2.53	0.41
2:a:67:THR:O	2:a:210:ASN:ND2	2.54	0.41
2:c:66:MET:SD	2:c:66:MET:N	2.93	0.41
2:c:101:ARG:NH2	2:c:207:GLU:OE1	2.52	0.41
1:W:225:ASN:O	1:W:229:GLU:HG2	2.20	0.41
3:DE:103:ASP:OD1	3:DE:107:ASN:N	2.42	0.41
3:DE:221:THR:OG1	3:DE:222:ALA:N	2.53	0.41
3:DJ:61:PHE:CE2	3:DJ:323:ASN:HB3	2.56	0.41
1:B:2:ILE:HD11	1:B:254:LEU:HD21	2.02	0.41
1:B:218:TYR:CE2	3:DK:53:LYS:HG2	2.56	0.41
1:H:260:LEU:HD22	1:M:248:SER:HB2	2.02	0.41
1:J:183:GLY:O	1:J:195:THR:OG1	2.34	0.41
1:N:3:SER:HA	2:b:70:GLN:HG3	2.03	0.41
3:DA:319:ASN:O	3:DA:344:LEU:HB3	2.20	0.41
3:DB:103:ASP:OD1	3:DB:107:ASN:N	2.49	0.41
3:DG:44:ALA:H	3:DG:50:LEU:HD13	1.85	0.41
3:DI:288:ASP:OD1	3:DI:288:ASP:N	2.50	0.41
3:DJ:187:TYR:CE2	3:DJ:285:LYS:HB3	2.55	0.41
1:F:72:VAL:HB	1:K:28:ASN:HB3	2.03	0.41
1:H:62:LEU:O	1:M:197:SER:OG	2.39	0.41
1:K:95:VAL:O	1:K:118:GLY:HA3	2.21	0.41
1:O:50:ARG:HA	1:O:50:ARG:NE	2.35	0.41
1:P:145:ASN:O	1:P:145:ASN:ND2	2.54	0.41
1:R:257:LEU:HB2	1:W:240:TYR:HE1	1.85	0.41
2:b:71:LEU:HB2	2:b:205:VAL:HG12	2.03	0.41
3:DA:29:THR:O	3:DA:364:SER:HB3	2.21	0.41
3:DA:158:LEU:HD13	3:DA:208:TRP:CD2	2.55	0.41
3:DC:275:ASN:OD1	3:DC:276:ILE:N	2.54	0.41
3:DF:17:LEU:HD12	3:DK:395:ILE:HD12	2.02	0.41
3:DI:196:MET:HE2	3:DI:196:MET:HB2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DK:95:SER:HB3	3:DK:333:VAL:HG12	2.02	0.41
3:DK:295:ASN:HD21	3:DK:299:THR:HG1	1.59	0.41
1:A:237:GLN:HG3	3:DA:395:ILE:HG22	2.03	0.41
1:B:57:SER:HA	1:Q:154:ASP:CG	2.46	0.41
1:C:56:SER:O	1:R:152:GLY:HA3	2.20	0.41
1:D:238:ARG:HD3	1:D:238:ARG:HA	1.79	0.41
1:I:101:GLY:HA3	1:I:175:LEU:HD13	2.02	0.41
1:O:1:MET:HE2	2:c:210:ASN:HA	2.03	0.41
1:S:26:LEU:HD23	1:S:26:LEU:HA	1.91	0.41
1:S:149:ILE:HG13	1:S:159:VAL:HG12	2.02	0.41
1:T:155:GLY:C	1:T:172:GLN:HG3	2.46	0.41
1:U:111:THR:OG1	1:U:112:SER:N	2.54	0.41
2:a:100:THR:OG1	2:a:101:ARG:N	2.54	0.41
1:W:44:LEU:HB2	1:W:70:THR:HB	2.03	0.41
3:DA:128:ILE:HD13	3:DA:313:GLY:HA2	2.02	0.41
3:DB:17:LEU:HD23	3:DB:17:LEU:HA	1.75	0.41
3:DC:162:ASP:OD1	3:DC:162:ASP:N	2.53	0.41
3:DD:95:SER:OG	3:DD:96:ARG:N	2.54	0.41
3:DE:99:GLN:NE2	3:DE:361:LEU:HD11	2.36	0.41
3:DE:159:ASN:OD1	3:DE:162:ASP:N	2.54	0.41
3:DE:210:VAL:O	3:DE:227:SER:HB3	2.21	0.41
3:DE:374:ASN:HA	3:DE:377:VAL:HG22	2.03	0.41
3:DF:63:ASP:N	3:DF:63:ASP:OD1	2.54	0.41
3:DF:86:VAL:HG11	3:DF:136:PRO:HG3	2.03	0.41
3:DH:87:ASP:OD1	3:DH:91:SER:N	2.54	0.41
3:DK:228:THR:HG21	3:DK:244:VAL:HG21	2.03	0.41
1:A:208:LEU:HD21	3:DB:89:ASN:HD21	1.86	0.41
1:E:42:GLU:HG3	1:E:75:VAL:HB	2.02	0.41
1:F:5:LEU:HD12	1:F:5:LEU:HA	1.81	0.41
2:b:94:ASP:OD1	2:b:95:GLY:N	2.54	0.41
2:b:133:SER:HA	2:b:148:PRO:HD3	2.03	0.41
3:DB:380:ARG:HD3	3:DB:380:ARG:HA	1.78	0.41
3:DD:84:ARG:NH1	3:DD:92:VAL:HG21	2.36	0.41
3:DD:397:ASN:HA	3:DD:400:VAL:HG12	2.02	0.41
3:DH:141:ASN:OD1	3:DH:289:LEU:HB3	2.21	0.41
3:DI:198:VAL:HG22	3:DI:212:THR:HG22	2.02	0.41
3:DJ:217:ASP:OD1	3:DJ:217:ASP:N	2.53	0.41
1:B:85:ASN:O	1:B:221:THR:OG1	2.39	0.40
1:D:48:THR:HG22	1:D:67:GLN:HG2	2.03	0.40
1:E:188:GLY:C	1:E:189:GLU:HG2	2.46	0.40
1:F:48:THR:HG22	1:F:67:GLN:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:ALA:HB2	1:K:26:LEU:HD23	2.02	0.40
1:H:1:MET:HE1	1:N:238:ARG:HB2	2.04	0.40
1:H:42:GLU:HB3	1:M:189:GLU:HA	2.02	0.40
1:I:176:THR:HG22	1:I:203:GLU:HB3	2.02	0.40
1:O:51:GLN:NE2	1:T:75:VAL:O	2.53	0.40
1:Q:185:GLU:HB2	1:Q:195:THR:HG21	2.02	0.40
2:b:26:LEU:HD23	2:b:26:LEU:HA	1.93	0.40
2:c:170:GLU:N	2:c:170:GLU:OE1	2.54	0.40
2:d:26:LEU:HD13	1:W:242:ILE:HG23	2.03	0.40
1:V:38:ARG:NH1	1:V:80:LEU:HD21	2.34	0.40
1:V:187:ILE:HG13	1:V:191:LEU:HB2	2.02	0.40
1:W:43:ASP:N	1:W:43:ASP:OD1	2.54	0.40
1:X:36:ARG:HB3	1:X:224:VAL:HG22	2.03	0.40
3:DA:171:SER:N	3:DA:177:SER:OG	2.41	0.40
3:DB:102:LEU:HD12	3:DB:106:ARG:HA	2.03	0.40
1:D:43:ASP:OD1	1:D:43:ASP:N	2.55	0.40
1:K:34:PHE:HB3	1:K:222:SER:HB3	2.02	0.40
1:O:6:TRP:CZ3	2:c:208:GLY:HA3	2.56	0.40
2:e:167:GLU:CD	2:e:167:GLU:H	2.29	0.40
1:V:44:LEU:HB2	1:V:70:THR:HB	2.03	0.40
1:X:45:LEU:O	1:X:70:THR:OG1	2.27	0.40
1:X:106:MET:HE2	1:X:137:GLN:OE1	2.21	0.40
3:DC:337:THR:O	3:DC:340:SER:OG	2.24	0.40
1:A:140:ILE:HD12	1:A:171:GLY:HA3	2.03	0.40
1:A:245:LYS:HG3	1:J:233:MET:HE1	2.03	0.40
1:B:1:MET:HE2	1:B:1:MET:HA	2.03	0.40
1:D:86:LEU:HD22	1:D:96:ALA:HB1	2.04	0.40
1:I:102:PHE:HB3	1:I:114:TYR:HB3	2.03	0.40
1:M:142:ILE:HD13	1:M:149:ILE:HD13	2.02	0.40
1:R:238:ARG:NH1	1:R:241:GLU:OE1	2.54	0.40
1:U:43:ASP:OD1	1:U:43:ASP:N	2.50	0.40
1:V:107:LEU:HD23	1:V:107:LEU:HA	1.92	0.40
3:DB:367:ASP:O	3:DB:371:GLU:HG2	2.21	0.40
3:DC:331:ASP:O	3:DC:333:VAL:N	2.50	0.40
3:DD:109:VAL:HG12	3:DD:110:ASN:O	2.22	0.40
3:DE:99:GLN:HE22	3:DE:361:LEU:HD11	1.86	0.40
3:DH:74:ASP:HA	3:DH:98:GLY:O	2.21	0.40
3:DJ:294:ILE:HG12	3:DJ:300:VAL:HG12	2.03	0.40
1:E:20:ASP:OD1	3:DB:5:GLN:NE2	2.54	0.40
1:E:163:GLY:C	1:E:165:ALA:H	2.29	0.40
1:H:7:ILE:HG12	1:H:70:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:57:SER:OG	1:M:58:GLU:N	2.55	0.40
1:P:26:LEU:HA	1:P:26:LEU:HD23	1.88	0.40
2:b:47:ASP:OD1	2:b:47:ASP:N	2.54	0.40
3:DA:9:GLY:C	3:DA:385:ASN:HD22	2.30	0.40
3:DE:21:GLY:HA2	3:DE:24:ILE:HG22	2.04	0.40
3:DF:294:ILE:O	3:DF:358:ASN:ND2	2.55	0.40
1:A:36:ARG:HE	1:A:80:LEU:HD12	1.86	0.40
1:C:178:PHE:CE1	1:C:201:PRO:HB3	2.56	0.40
1:E:153:ARG:HG2	1:E:213:LEU:HD22	2.04	0.40
1:M:88:GLN:HB2	1:M:218:TYR:CE2	2.57	0.40
1:N:127:GLN:OE1	1:N:127:GLN:N	2.53	0.40
2:b:242:GLY:HA2	2:b:245:ASN:ND2	2.37	0.40
3:DA:180:LYS:HB3	3:DA:200:PHE:HB2	2.03	0.40
3:DB:164:VAL:HG22	3:DB:202:LYS:HG3	2.02	0.40
3:DD:187:TYR:CD2	3:DD:285:LYS:HB3	2.56	0.40
3:DD:213:HIS:CD2	3:DD:223:PRO:HD2	2.57	0.40
3:DF:101:LYS:HD3	3:DF:111:MET:HE3	2.04	0.40
3:DK:5:GLN:H	3:DK:5:GLN:HG2	1.68	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%)	247 (96%)	11 (4%)	0	100	100
1	B	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	C	258/260 (99%)	246 (95%)	12 (5%)	0	100	100
1	D	258/260 (99%)	244 (95%)	14 (5%)	0	100	100
1	E	258/260 (99%)	246 (95%)	12 (5%)	0	100	100
1	F	258/260 (99%)	250 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	258/260 (99%)	250 (97%)	8 (3%)	0	100	100
1	H	258/260 (99%)	244 (95%)	14 (5%)	0	100	100
1	I	258/260 (99%)	249 (96%)	9 (4%)	0	100	100
1	J	258/260 (99%)	246 (95%)	12 (5%)	0	100	100
1	K	258/260 (99%)	246 (95%)	12 (5%)	0	100	100
1	L	257/260 (99%)	249 (97%)	8 (3%)	0	100	100
1	M	258/260 (99%)	243 (94%)	15 (6%)	0	100	100
1	N	247/260 (95%)	240 (97%)	7 (3%)	0	100	100
1	O	248/260 (95%)	242 (98%)	6 (2%)	0	100	100
1	P	244/260 (94%)	233 (96%)	11 (4%)	0	100	100
1	Q	243/260 (94%)	237 (98%)	6 (2%)	0	100	100
1	R	246/260 (95%)	232 (94%)	14 (6%)	0	100	100
1	S	243/260 (94%)	234 (96%)	9 (4%)	0	100	100
1	T	249/260 (96%)	242 (97%)	7 (3%)	0	100	100
1	U	257/260 (99%)	243 (95%)	14 (5%)	0	100	100
1	V	257/260 (99%)	247 (96%)	10 (4%)	0	100	100
1	W	257/260 (99%)	245 (95%)	12 (5%)	0	100	100
1	X	257/260 (99%)	244 (95%)	13 (5%)	0	100	100
2	a	247/251 (98%)	240 (97%)	7 (3%)	0	100	100
2	b	246/251 (98%)	236 (96%)	10 (4%)	0	100	100
2	c	247/251 (98%)	240 (97%)	7 (3%)	0	100	100
2	d	247/251 (98%)	230 (93%)	17 (7%)	0	100	100
2	e	247/251 (98%)	235 (95%)	12 (5%)	0	100	100
3	DA	399/403 (99%)	377 (94%)	22 (6%)	0	100	100
3	DB	399/403 (99%)	376 (94%)	23 (6%)	0	100	100
3	DC	399/403 (99%)	378 (95%)	21 (5%)	0	100	100
3	DD	399/403 (99%)	370 (93%)	29 (7%)	0	100	100
3	DE	399/403 (99%)	381 (96%)	18 (4%)	0	100	100
3	DF	399/403 (99%)	383 (96%)	16 (4%)	0	100	100
3	DG	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
3	DH	399/403 (99%)	384 (96%)	14 (4%)	1 (0%)	36	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	DI	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
3	DJ	399/403 (99%)	379 (95%)	20 (5%)	0	100	100
3	DK	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
All	All	11724/11928 (98%)	11213 (96%)	510 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	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%)	208 (97%)	7 (3%)	33	65
1	B	215/215 (100%)	209 (97%)	6 (3%)	38	68
1	C	215/215 (100%)	209 (97%)	6 (3%)	38	68
1	D	215/215 (100%)	211 (98%)	4 (2%)	50	73
1	E	215/215 (100%)	208 (97%)	7 (3%)	33	65
1	F	215/215 (100%)	211 (98%)	4 (2%)	50	73
1	G	215/215 (100%)	208 (97%)	7 (3%)	33	65
1	H	215/215 (100%)	210 (98%)	5 (2%)	44	70
1	I	215/215 (100%)	209 (97%)	6 (3%)	38	68
1	J	215/215 (100%)	206 (96%)	9 (4%)	26	60
1	K	215/215 (100%)	211 (98%)	4 (2%)	50	73
1	L	214/215 (100%)	210 (98%)	4 (2%)	50	73
1	M	215/215 (100%)	207 (96%)	8 (4%)	30	63
1	N	208/215 (97%)	204 (98%)	4 (2%)	50	73
1	O	209/215 (97%)	203 (97%)	6 (3%)	37	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	204/215 (95%)	196 (96%)	8 (4%)	28	62
1	Q	204/215 (95%)	198 (97%)	6 (3%)	37	67
1	R	206/215 (96%)	196 (95%)	10 (5%)	22	55
1	S	204/215 (95%)	200 (98%)	4 (2%)	48	72
1	T	210/215 (98%)	206 (98%)	4 (2%)	50	73
1	U	214/215 (100%)	206 (96%)	8 (4%)	30	63
1	V	214/215 (100%)	208 (97%)	6 (3%)	38	68
1	W	214/215 (100%)	209 (98%)	5 (2%)	44	70
1	X	214/215 (100%)	208 (97%)	6 (3%)	38	68
2	a	191/193 (99%)	188 (98%)	3 (2%)	55	75
2	b	190/193 (98%)	187 (98%)	3 (2%)	55	75
2	c	191/193 (99%)	183 (96%)	8 (4%)	26	60
2	d	191/193 (99%)	185 (97%)	6 (3%)	35	66
2	e	191/193 (99%)	182 (95%)	9 (5%)	23	57
3	DA	321/323 (99%)	314 (98%)	7 (2%)	45	71
3	DB	321/323 (99%)	312 (97%)	9 (3%)	38	68
3	DC	321/323 (99%)	310 (97%)	11 (3%)	32	64
3	DD	321/323 (99%)	309 (96%)	12 (4%)	30	63
3	DE	321/323 (99%)	317 (99%)	4 (1%)	63	79
3	DF	321/323 (99%)	311 (97%)	10 (3%)	35	66
3	DG	321/323 (99%)	315 (98%)	6 (2%)	50	73
3	DH	321/323 (99%)	312 (97%)	9 (3%)	38	68
3	DI	321/323 (99%)	311 (97%)	10 (3%)	35	66
3	DJ	321/323 (99%)	310 (97%)	11 (3%)	32	64
3	DK	321/323 (99%)	317 (99%)	4 (1%)	63	79
All	All	9580/9678 (99%)	9314 (97%)	266 (3%)	38	68

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	97	ILE
1	A	105	VAL

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Mol	Chain	Res	Type
1	A	115	THR
1	A	164	GLN
1	A	205	THR
1	A	256	LYS
1	B	42	GLU
1	B	75	VAL
1	B	77	THR
1	B	97	ILE
1	B	185	GLU
1	B	258	THR
1	C	26	LEU
1	C	45	LEU
1	C	77	THR
1	C	97	ILE
1	C	105	VAL
1	C	159	VAL
1	D	97	ILE
1	D	150	THR
1	D	157	VAL
1	D	159	VAL
1	E	26	LEU
1	E	28	ASN
1	E	42	GLU
1	E	97	ILE
1	E	141	THR
1	E	157	VAL
1	E	164	GLN
1	F	141	THR
1	F	157	VAL
1	F	177	THR
1	F	179	MET
1	G	2	ILE
1	G	75	VAL
1	G	117	ASP
1	G	141	THR
1	G	157	VAL
1	G	168	VAL
1	G	226	VAL
1	H	105	VAL
1	H	156	VAL
1	H	157	VAL
1	H	175	LEU

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Mol	Chain	Res	Type
1	H	226	VAL
1	I	40	VAL
1	I	43	ASP
1	I	97	ILE
1	I	150	THR
1	I	156	VAL
1	I	164	GLN
1	J	20	ASP
1	J	72	VAL
1	J	97	ILE
1	J	105	VAL
1	J	157	VAL
1	J	159	VAL
1	J	175	LEU
1	J	181	ASP
1	J	255	GLN
1	K	42	GLU
1	K	80	LEU
1	K	97	ILE
1	K	156	VAL
1	L	42	GLU
1	L	156	VAL
1	L	185	GLU
1	L	245	LYS
1	M	72	VAL
1	M	97	ILE
1	M	98	LYS
1	M	157	VAL
1	M	175	LEU
1	M	181	ASP
1	M	195	THR
1	M	258	THR
1	N	117	ASP
1	N	157	VAL
1	N	175	LEU
1	N	202	ASN
1	O	61	THR
1	O	156	VAL
1	O	157	VAL
1	O	168	VAL
1	O	179	MET
1	O	241	GLU

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Mol	Chain	Res	Type
1	P	28	ASN
1	P	77	THR
1	P	97	ILE
1	P	107	LEU
1	P	150	THR
1	P	159	VAL
1	P	168	VAL
1	P	254	LEU
1	Q	42	GLU
1	Q	44	LEU
1	Q	141	THR
1	Q	149	ILE
1	Q	157	VAL
1	Q	179	MET
1	R	43	ASP
1	R	66	LEU
1	R	77	THR
1	R	105	VAL
1	R	141	THR
1	R	149	ILE
1	R	150	THR
1	R	156	VAL
1	R	159	VAL
1	R	170	VAL
1	S	72	VAL
1	S	109	ASP
1	S	141	THR
1	S	175	LEU
1	T	43	ASP
1	T	141	THR
1	T	156	VAL
1	T	157	VAL
1	U	97	ILE
1	U	141	THR
1	U	150	THR
1	U	157	VAL
1	U	159	VAL
1	U	160	THR
1	U	205	THR
1	U	257	LEU
2	a	46	VAL
2	a	51	LEU

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Mol	Chain	Res	Type
2	a	71	LEU
2	b	71	LEU
2	b	182	THR
2	b	192	VAL
2	c	7	THR
2	c	46	VAL
2	c	57	VAL
2	c	71	LEU
2	c	120	VAL
2	c	155	VAL
2	c	192	VAL
2	c	214	VAL
2	d	5	ILE
2	d	31	THR
2	d	44	VAL
2	d	71	LEU
2	d	78	LEU
2	d	114	THR
2	e	5	ILE
2	e	44	VAL
2	e	78	LEU
2	e	114	THR
2	e	116	GLN
2	e	163	LEU
2	e	167	GLU
2	e	201	ILE
2	e	250	MET
1	V	90	ASN
1	V	156	VAL
1	V	157	VAL
1	V	159	VAL
1	V	168	VAL
1	V	205	THR
1	W	109	ASP
1	W	156	VAL
1	W	242	ILE
1	W	256	LYS
1	W	260	LEU
1	X	66	LEU
1	X	142	ILE
1	X	156	VAL
1	X	179	MET

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Mol	Chain	Res	Type
1	X	185	GLU
1	X	195	THR
3	DA	48	VAL
3	DA	52	VAL
3	DA	137	ILE
3	DA	322	ASN
3	DA	324	GLU
3	DA	332	ASN
3	DA	371	GLU
3	DB	3	PHE
3	DB	17	LEU
3	DB	26	ASN
3	DB	112	GLN
3	DB	161	THR
3	DB	228	THR
3	DB	261	LEU
3	DB	332	ASN
3	DB	395	ILE
3	DC	17	LEU
3	DC	24	ILE
3	DC	48	VAL
3	DC	75	VAL
3	DC	168	THR
3	DC	172	VAL
3	DC	201	VAL
3	DC	217	ASP
3	DC	229	THR
3	DC	288	ASP
3	DC	342	VAL
3	DD	52	VAL
3	DD	60	ASP
3	DD	92	VAL
3	DD	168	THR
3	DD	201	VAL
3	DD	217	ASP
3	DD	264	LEU
3	DD	295	ASN
3	DD	331	ASP
3	DD	332	ASN
3	DD	347	THR
3	DD	395	ILE
3	DE	17	LEU

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Mol	Chain	Res	Type
3	DE	156	ILE
3	DE	295	ASN
3	DE	332	ASN
3	DF	92	VAL
3	DF	111	MET
3	DF	137	ILE
3	DF	168	THR
3	DF	212	THR
3	DF	228	THR
3	DF	250	THR
3	DF	331	ASP
3	DF	389	ILE
3	DF	395	ILE
3	DG	250	THR
3	DG	295	ASN
3	DG	322	ASN
3	DG	342	VAL
3	DG	391	THR
3	DG	395	ILE
3	DH	17	LEU
3	DH	52	VAL
3	DH	107	ASN
3	DH	161	THR
3	DH	168	THR
3	DH	198	VAL
3	DH	250	THR
3	DH	300	VAL
3	DH	395	ILE
3	DI	17	LEU
3	DI	48	VAL
3	DI	57	ILE
3	DI	77	ILE
3	DI	92	VAL
3	DI	164	VAL
3	DI	168	THR
3	DI	185	THR
3	DI	337	THR
3	DI	395	ILE
3	DJ	48	VAL
3	DJ	52	VAL
3	DJ	92	VAL
3	DJ	150	THR

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Mol	Chain	Res	Type
3	DJ	161	THR
3	DJ	210	VAL
3	DJ	264	LEU
3	DJ	295	ASN
3	DJ	300	VAL
3	DJ	331	ASP
3	DJ	396	LEU
3	DK	48	VAL
3	DK	168	THR
3	DK	389	ILE
3	DK	395	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	161	GLN
1	A	209	ASN
1	B	67	GLN
1	B	174	ASN
1	C	164	GLN
1	D	16	GLN
1	D	47	GLN
1	D	90	ASN
1	D	127	GLN
1	D	209	ASN
1	E	81	HIS
1	E	135	GLN
1	E	209	ASN
1	F	24	ASN
1	F	255	GLN
1	F	259	GLN
1	G	16	GLN
1	G	145	ASN
1	G	259	GLN
1	H	190	ASN
1	I	24	ASN
1	I	55	GLN
1	I	235	GLN
1	J	180	ASN
1	J	202	ASN
1	K	81	HIS

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Mol	Chain	Res	Type
1	K	88	GLN
1	K	90	ASN
1	M	15	GLN
1	M	88	GLN
1	N	16	GLN
1	N	81	HIS
1	N	85	ASN
1	N	196	GLN
1	O	15	GLN
1	O	16	GLN
1	O	24	ASN
1	O	104	GLN
1	O	259	GLN
1	P	15	GLN
1	P	180	ASN
1	Q	81	HIS
1	Q	164	GLN
1	Q	174	ASN
1	S	67	GLN
1	S	104	GLN
1	T	24	ASN
1	U	15	GLN
1	U	137	GLN
1	U	145	ASN
1	U	162	GLN
2	a	169	ASN
2	c	3	HIS
2	c	14	GLN
2	d	19	GLN
2	d	70	GLN
2	d	102	ASN
2	d	147	ASN
2	e	112	GLN
2	e	116	GLN
2	e	230	GLN
1	V	15	GLN
1	V	28	ASN
1	V	135	GLN
1	V	180	ASN
1	V	209	ASN
1	W	202	ASN
1	X	162	GLN

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Mol	Chain	Res	Type
1	X	172	GLN
3	DA	192	ASN
3	DB	89	ASN
3	DB	107	ASN
3	DB	115	GLN
3	DB	129	GLN
3	DB	192	ASN
3	DB	310	GLN
3	DC	107	ASN
3	DC	179	ASN
3	DC	274	ASN
3	DC	322	ASN
3	DC	365	ASN
3	DD	59	GLN
3	DD	303	ASN
3	DD	397	ASN
3	DD	401	ASN
3	DE	99	GLN
3	DE	107	ASN
3	DE	129	GLN
3	DE	197	ASN
3	DE	310	GLN
3	DE	385	ASN
3	DE	387	GLN
3	DF	129	GLN
3	DF	130	GLN
3	DF	206	ASN
3	DF	268	GLN
3	DF	310	GLN
3	DF	397	ASN
3	DF	401	ASN
3	DG	5	GLN
3	DG	129	GLN
3	DG	133	ASN
3	DG	190	GLN
3	DH	268	GLN
3	DH	310	GLN
3	DH	365	ASN
3	DI	129	GLN
3	DI	157	ASN
3	DI	303	ASN
3	DI	379	GLN

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Mol	Chain	Res	Type
3	DJ	23	ASN
3	DJ	133	ASN
3	DJ	268	GLN
3	DJ	392	GLN
3	DK	79	GLN
3	DK	89	ASN
3	DK	107	ASN

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

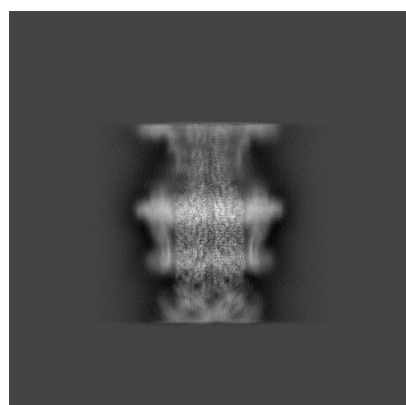
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30336. These allow visual inspection of the internal detail of the map and identification of artifacts.

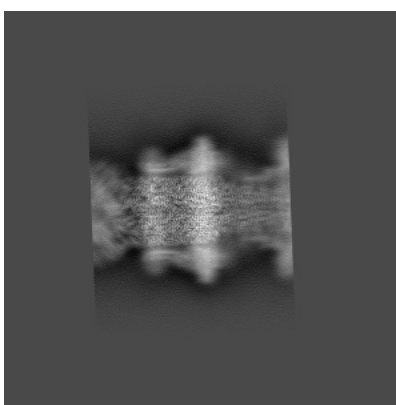
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

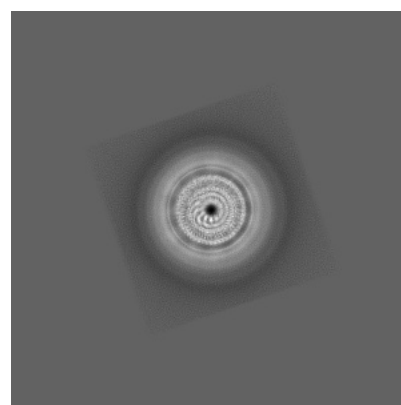
6.1.1 Primary map



X



Y

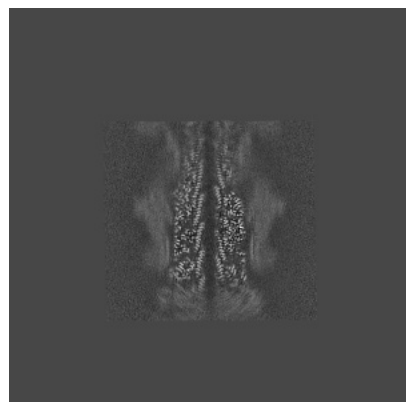


Z

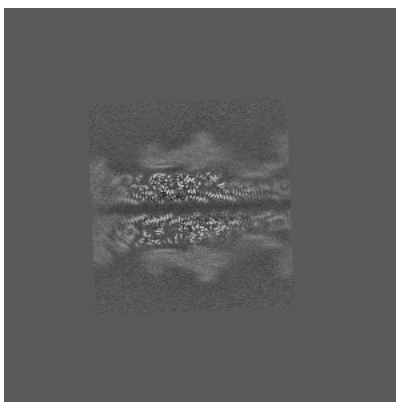
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

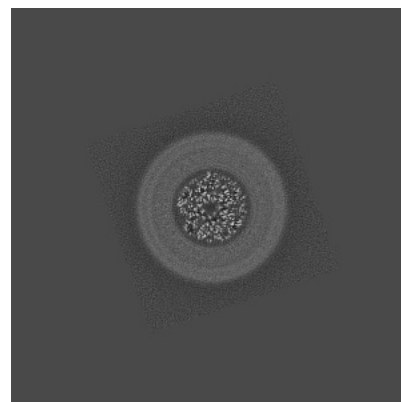
6.2.1 Primary map



X Index: 256



Y Index: 256

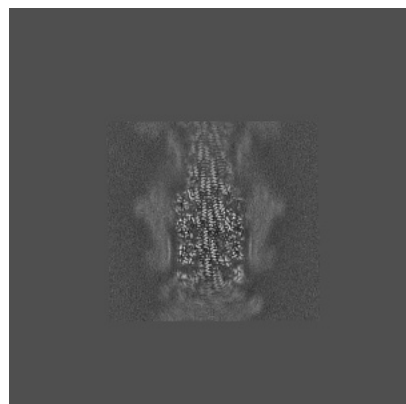


Z Index: 256

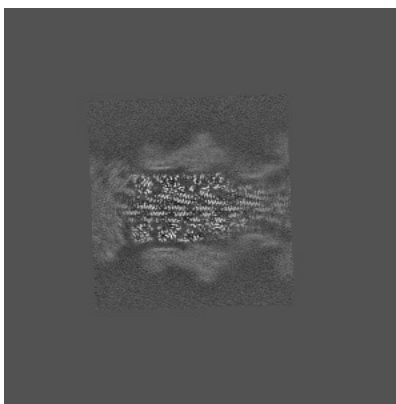
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

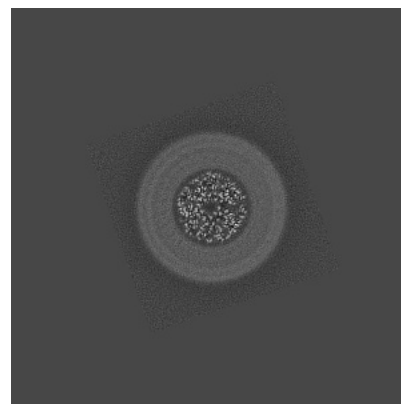
6.3.1 Primary map



X Index: 269



Y Index: 243

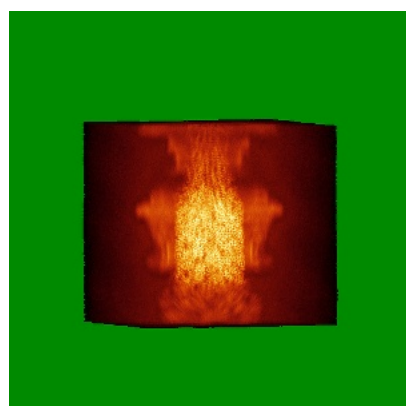


Z Index: 255

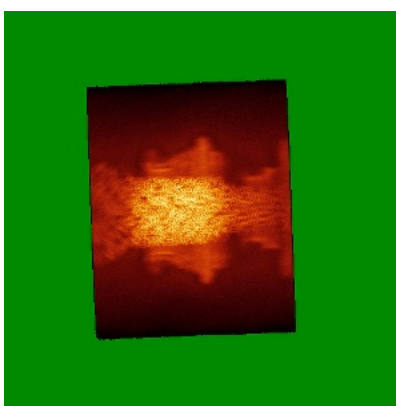
The images above show the largest variance slices of the map in three orthogonal directions.

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

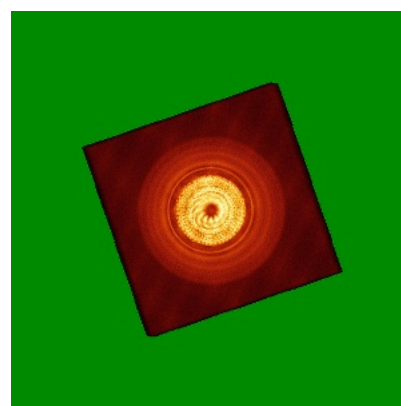
6.4.1 Primary map



X



Y

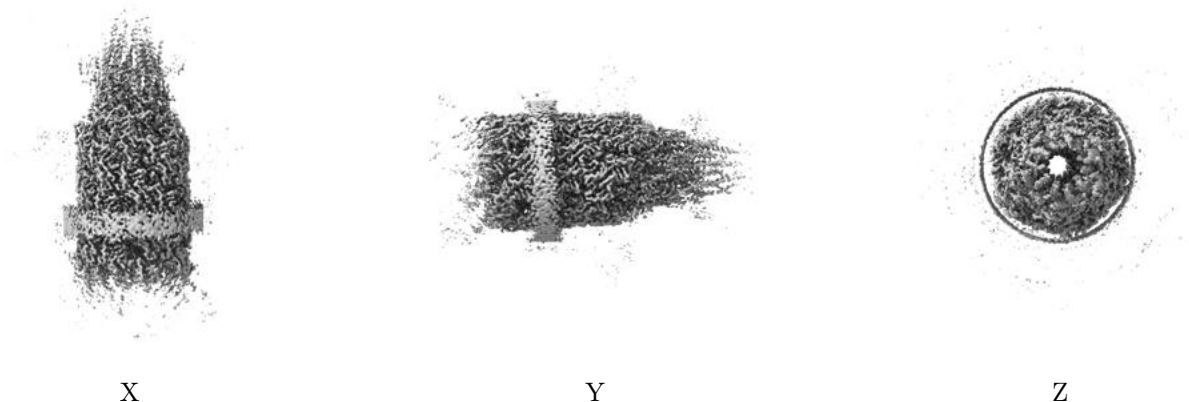


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.592. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

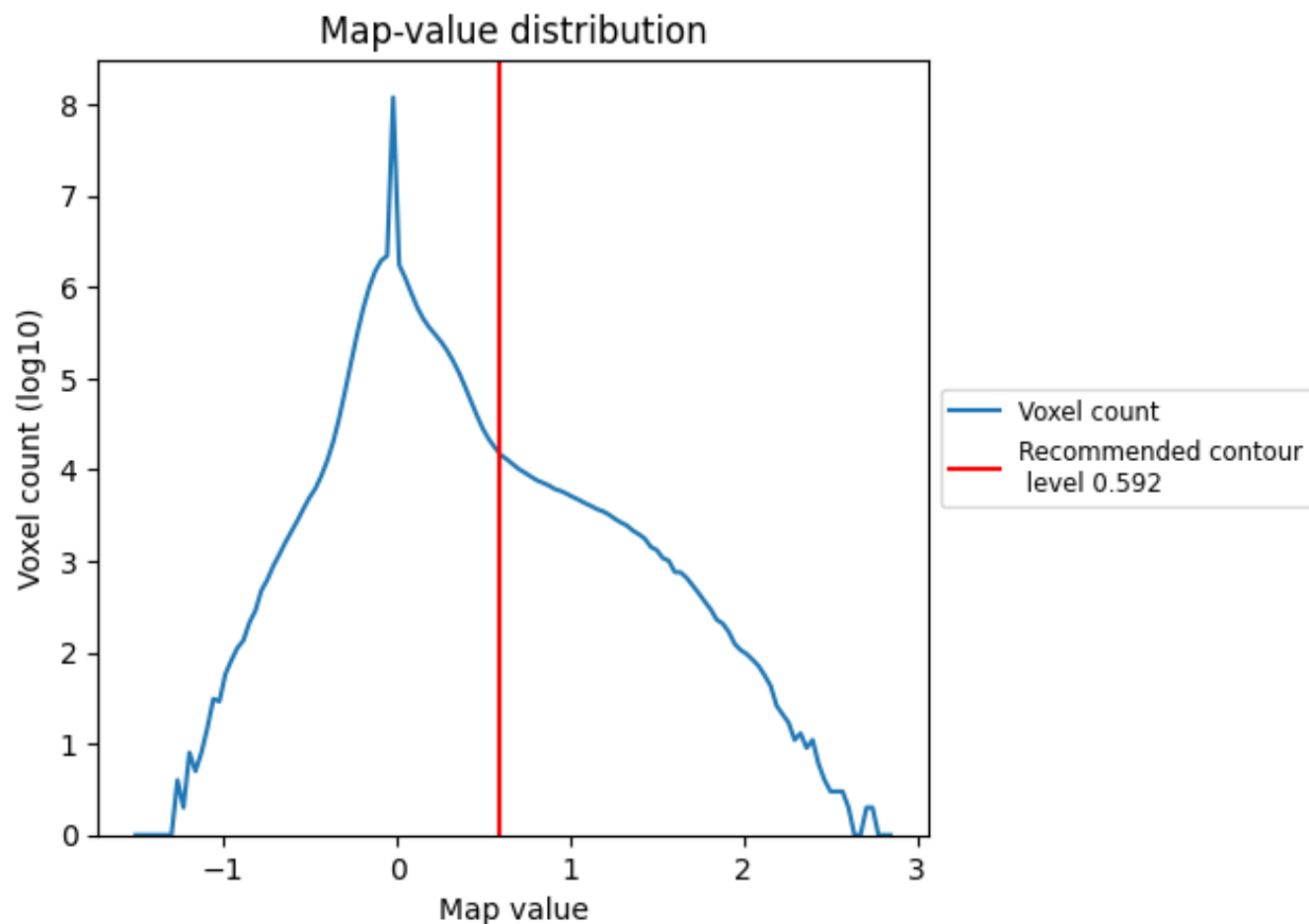
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

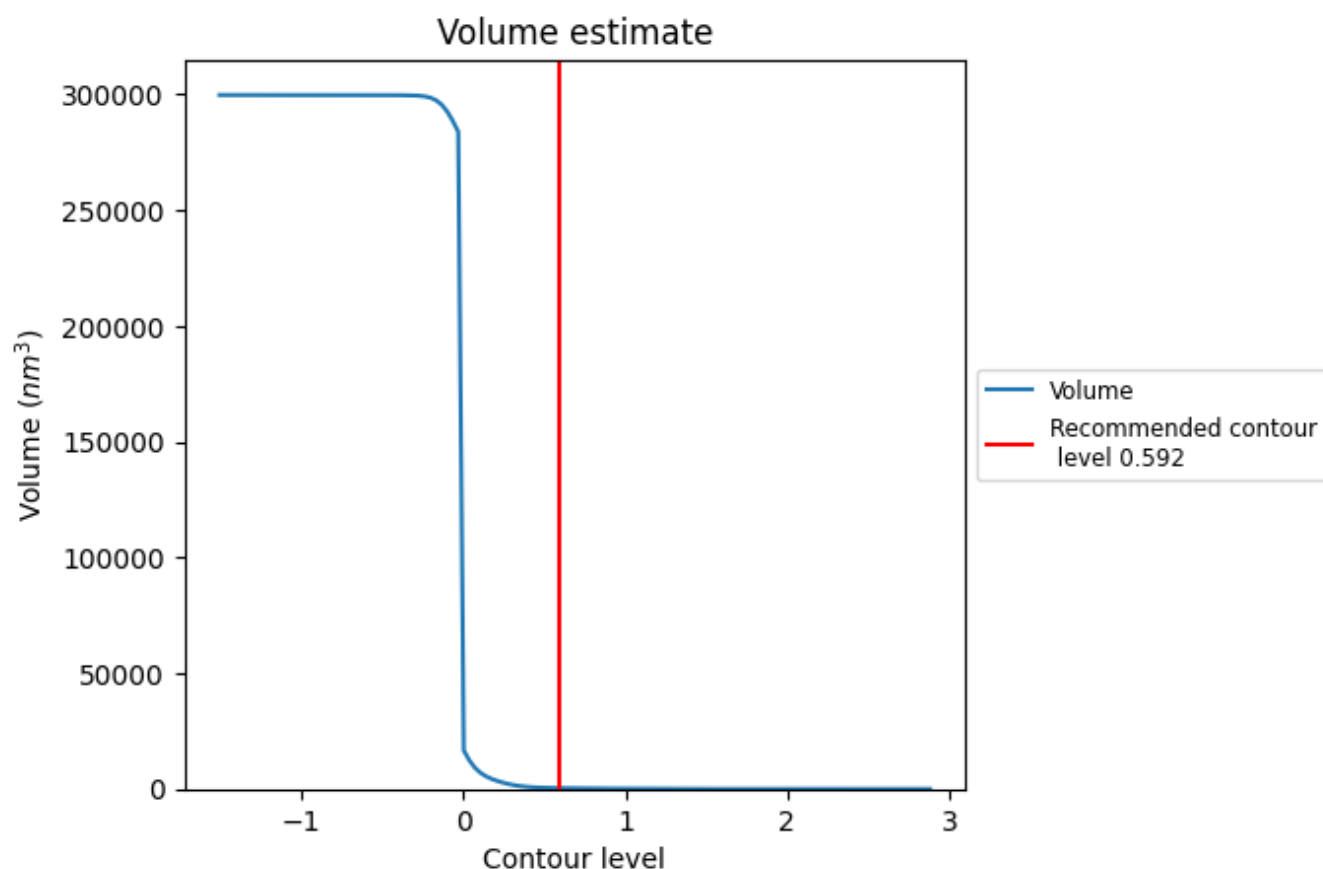
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

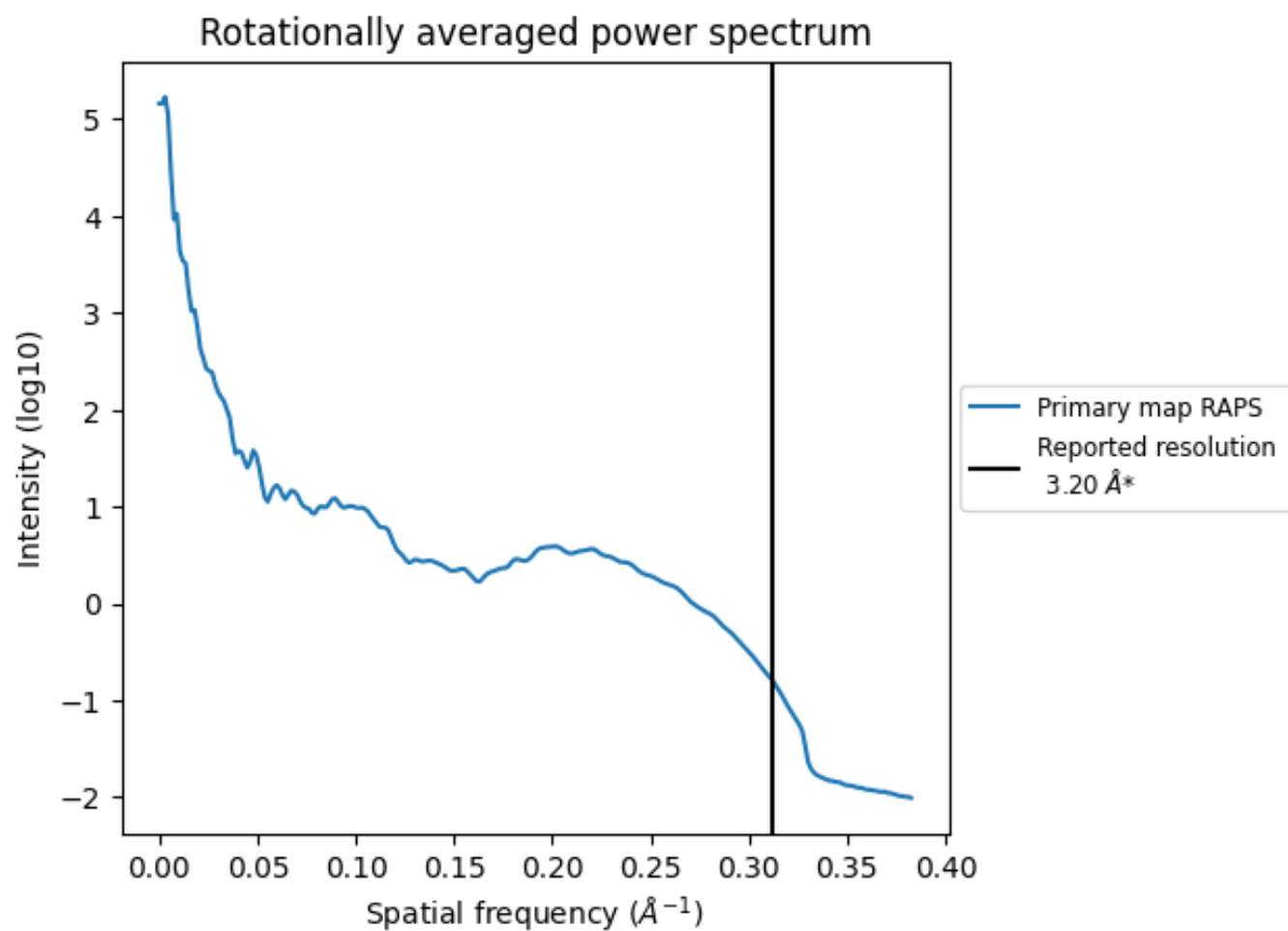
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 363 nm³; this corresponds to an approximate mass of 327 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 0.312 Å⁻¹

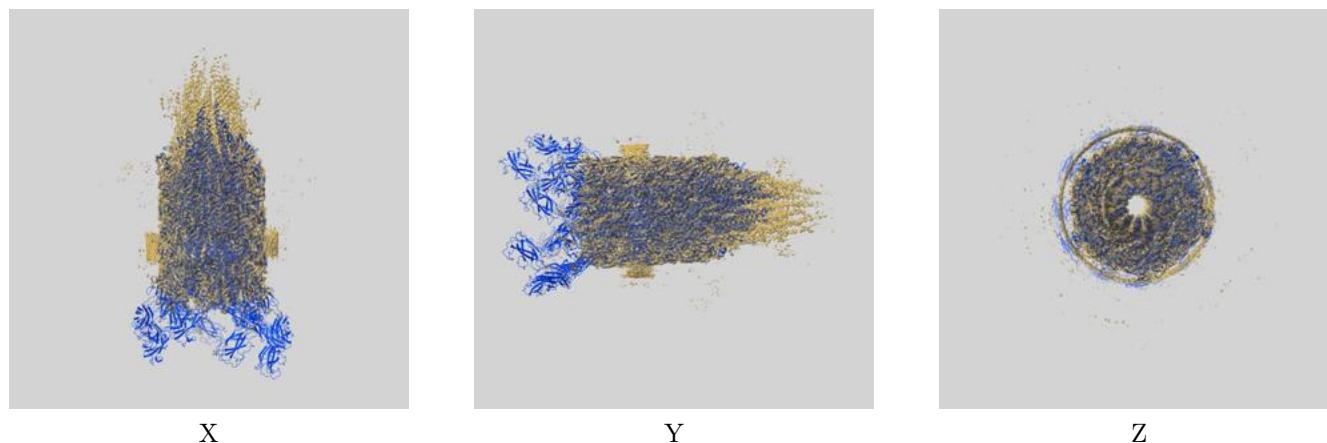
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

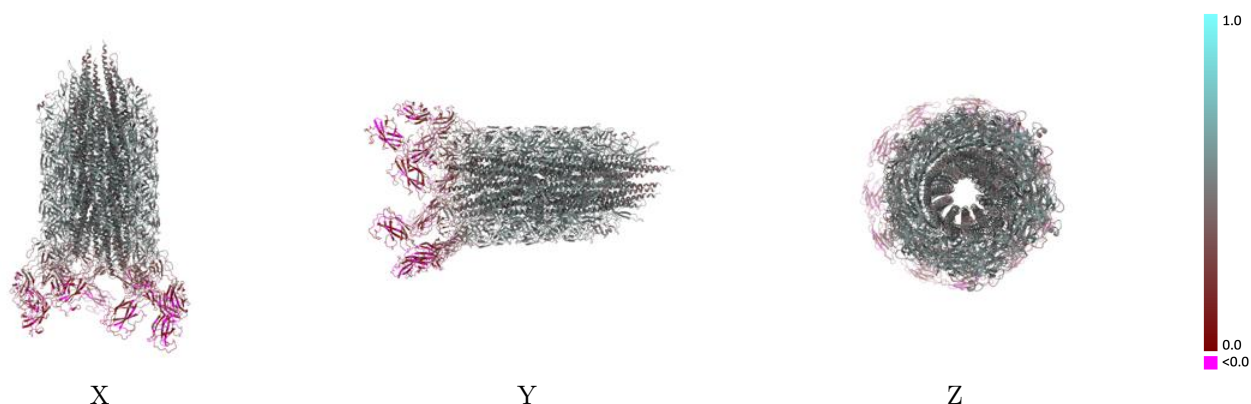
This section contains information regarding the fit between EMDB map EMD-30336 and PDB model 7CBM. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



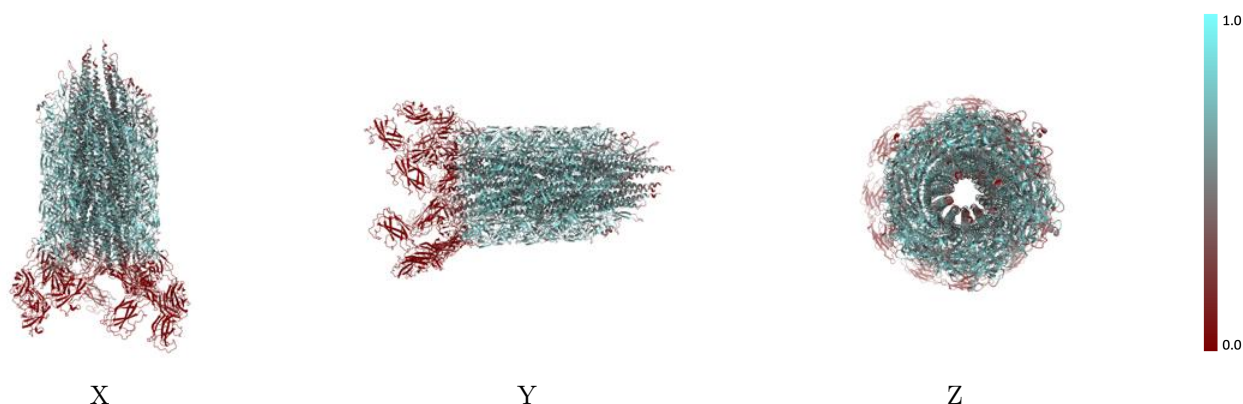
The images above show the 3D surface view of the map at the recommended contour level 0.592 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



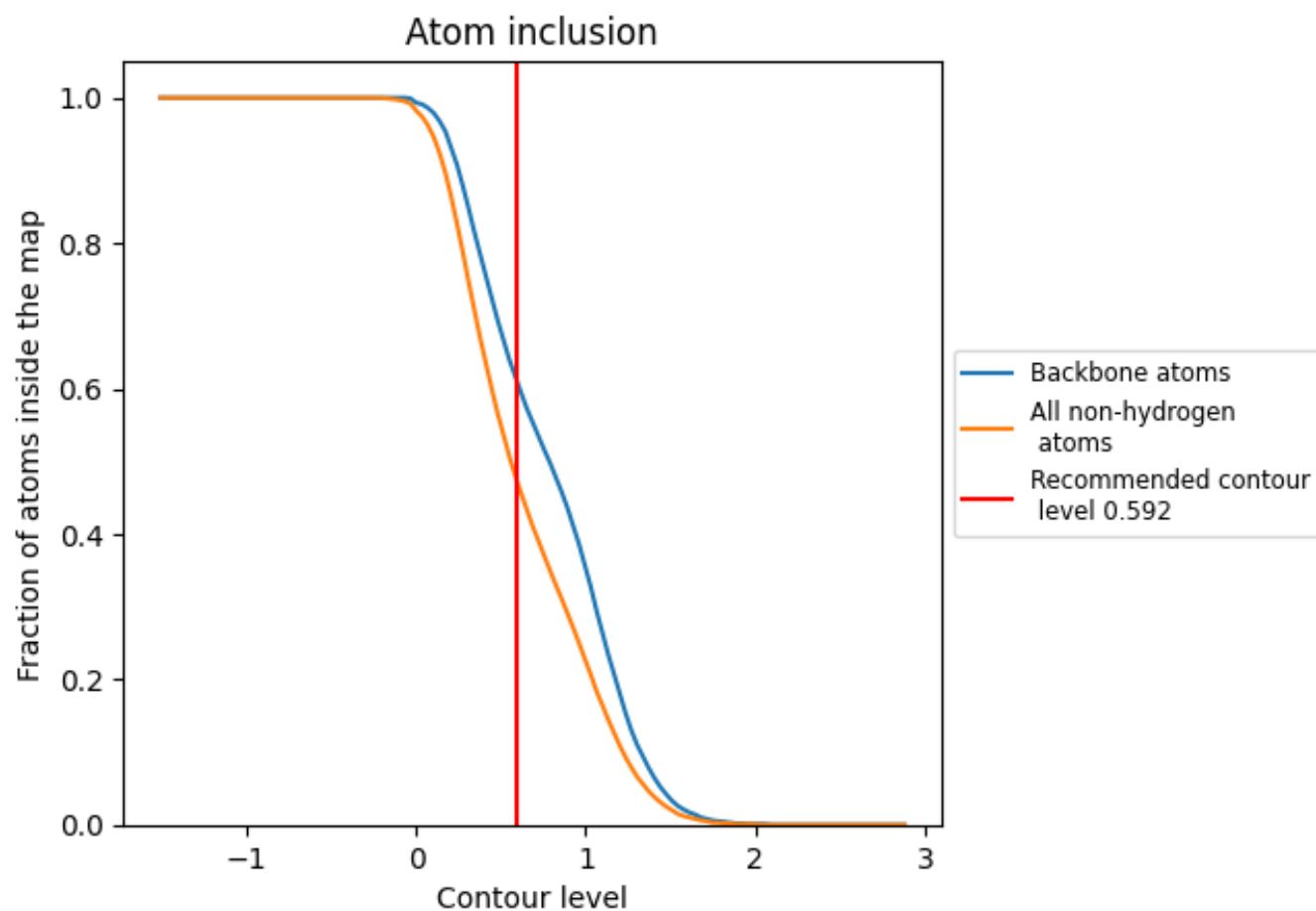
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.592).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 48% 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 (0.592) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4750	 0.4250
A	 0.6340	 0.5010
B	 0.5900	 0.4870
C	 0.6340	 0.4940
D	 0.6110	 0.4920
DA	 0.3370	 0.3380
DB	 0.3410	 0.3600
DC	 0.3260	 0.3530
DD	 0.3290	 0.3260
DE	 0.2990	 0.3280
DF	 0.2400	 0.3140
DG	 0.2120	 0.2970
DH	 0.1840	 0.2910
DI	 0.1510	 0.2550
DJ	 0.1410	 0.2460
DK	 0.0930	 0.2160
E	 0.6090	 0.4930
F	 0.6410	 0.5000
G	 0.6390	 0.5030
H	 0.6510	 0.5060
I	 0.6300	 0.5050
J	 0.6280	 0.5060
K	 0.6580	 0.5090
L	 0.6360	 0.5140
M	 0.6610	 0.5140
N	 0.6150	 0.5090
O	 0.6150	 0.5000
P	 0.6380	 0.5040
Q	 0.6340	 0.5080
R	 0.6520	 0.5100
S	 0.6600	 0.5070
T	 0.6310	 0.5090
U	 0.6080	 0.4970
V	 0.6140	 0.4960
W	 0.6080	 0.4980



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Chain	Atom inclusion	Q-score
X	 0.5640	 0.4770
a	 0.5640	 0.4810
b	 0.5460	 0.4600
c	 0.5810	 0.4830
d	 0.5570	 0.4870
e	 0.4510	 0.4710