Full wwPDB EM Validation Report

Oct 5, 2026 – 04:21 PM EDT

PDB ID	:	12EQ / pdb_000012eq
EMDB ID	:	EMD-76383
Title	:	Subtomogram average structure of flagellar export apparatus and MS-ring in Borrelia burgdorferi
Authors	:	Yue, J.; Liu, J.
Deposited on	:	2026-03-31
Resolution	:	16.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

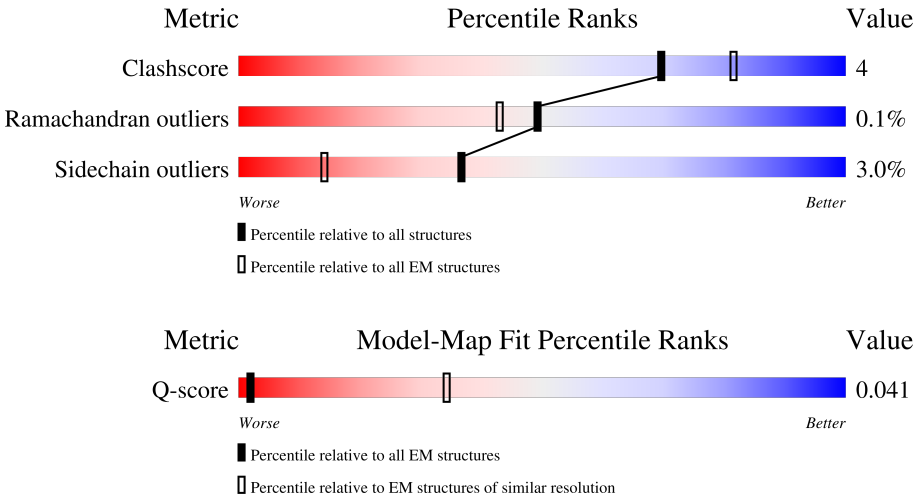
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 16.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	41 (15.50 - 16.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	0	569	8% 33% 63%
1	1	569	8% 32% 63%
1	2	569	8% 32% 64%
1	3	569	8% 33% 63%

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Mol	Chain	Length	Quality of chain
1	4	569	8% 32% 5% 63%
1	5	569	8% 33% 63%
1	6	569	7% 32% 64%
1	7	569	8% 32% 63%
1	8	569	8% 31% 5% 63%
1	9	569	8% 33% 63%
1	A	569	15% 41% 5% 54%
1	AA	569	7% 32% 63%
1	AB	569	7% 33% 63%
1	AC	569	16% 30% 5% 64%
1	AD	569	18% 30% 5% 64%
1	AE	569	16% 30% 6% 64%
1	AF	569	18% 30% 6% 64%
1	AG	569	15% 31% 5% 64%
1	AH	569	18% 30% 6% 64%
1	AI	569	15% 30% 5% 64%
1	AJ	569	18% 30% 5% 64%
1	AK	569	16% 30% 5% 64%
1	AL	569	18% 30% 5% 64%
1	AM	569	17% 30% 5% 64%
1	AN	569	18% 30% 5% 64%
1	AO	569	17% 30% 5% 64%
1	AP	569	18% 30% 5% 64%
1	AQ	569	17% 30% 5% 64%
1	AR	569	18% 30% 5% 64%

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Mol	Chain	Length	Quality of chain
1	AS	569	17% 30% 5% 64%
1	AT	569	18% 31% 64%
1	B	569	15% 40% 6% 54%
1	C	569	14% 40% 5% 54%
1	D	569	14% 40% 6% 54%
1	E	569	15% 40% 6% 54%
1	F	569	15% 41% 5% 54%
1	G	569	15% 40% 6% 54%
1	H	569	15% 41% 5% 54%
1	I	569	16% 41% 5% 54%
1	J	569	15% 41% 5% 54%
1	K	569	15% 41% 5% 54%
1	L	569	14% 41% 5% 54%
1	M	569	14% 41% 5% 54%
1	N	569	15% 38% 7% 54%
1	O	569	16% 40% 5% 54%
1	P	569	15% 41% 5% 54%
1	Q	569	16% 40% 6% 54%
1	R	569	15% 41% 5% 54%
1	S	569	16% 39% 7% 54%
1	T	569	15% 41% 5% 54%
1	U	569	14% 41% 5% 54%
1	V	569	15% 40% 5% 54%
1	W	569	15% 40% 6% 54%
1	X	569	15% 40% 7% 54%

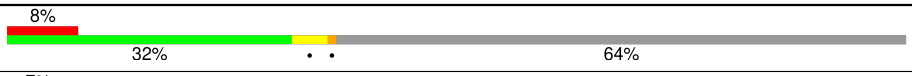
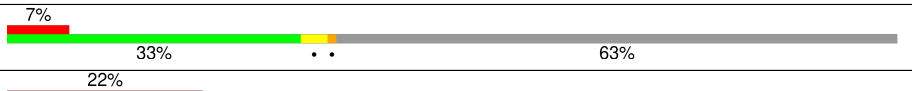
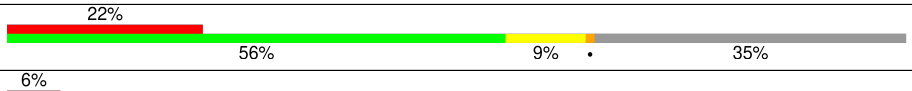
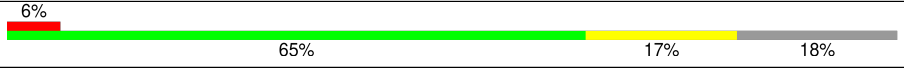
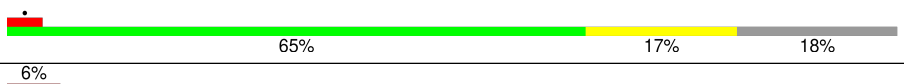
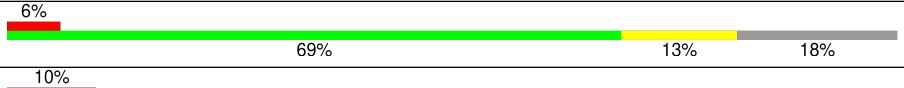
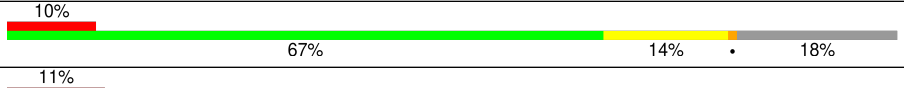
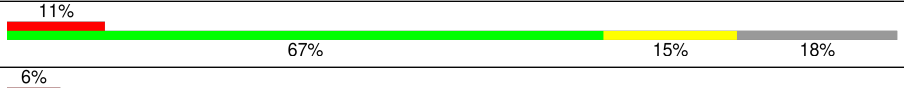
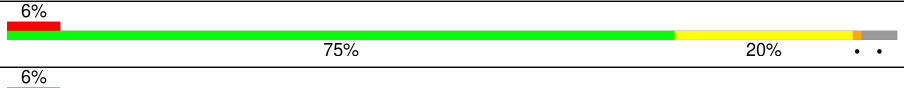
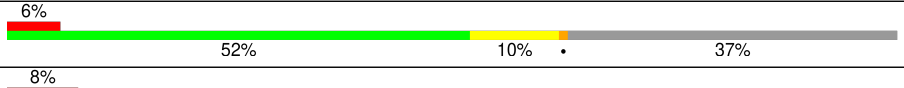
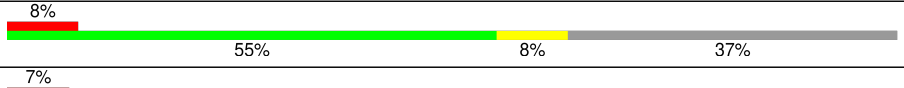
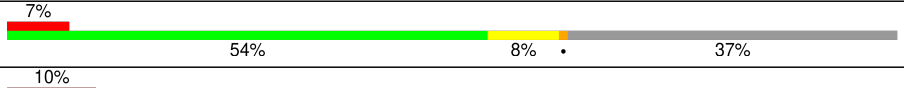
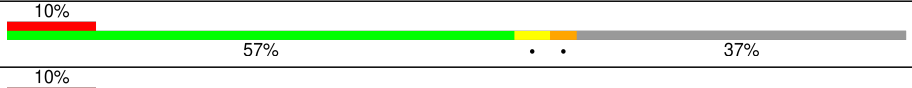
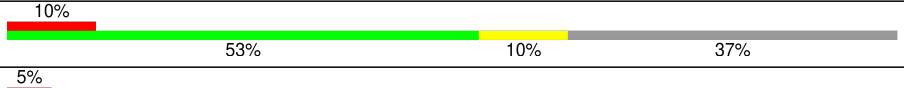
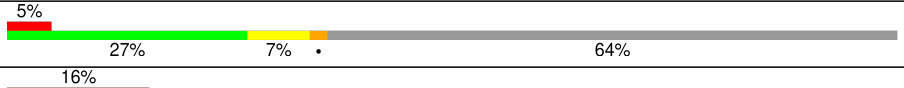
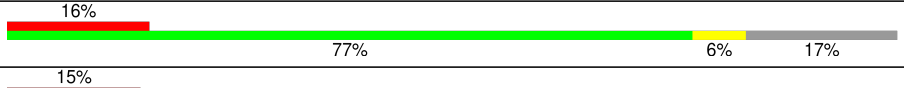
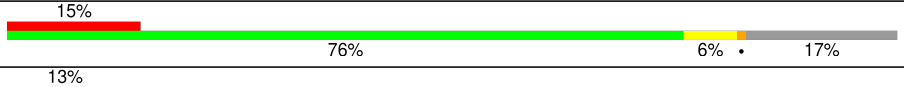
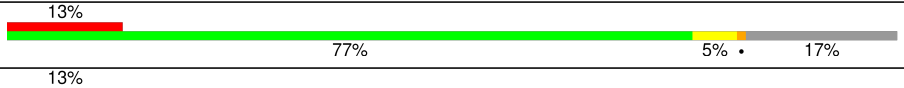
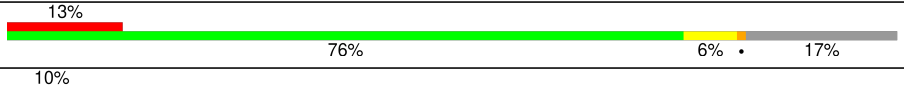
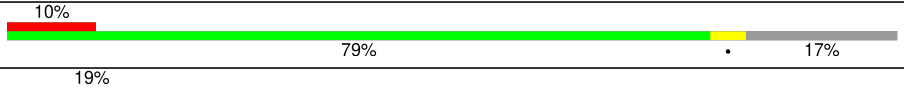
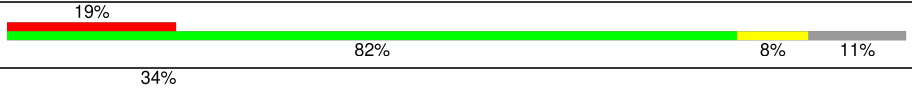
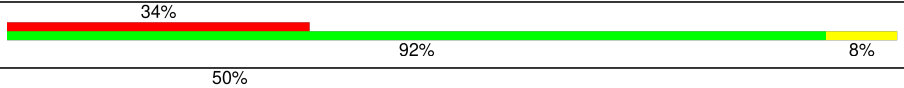
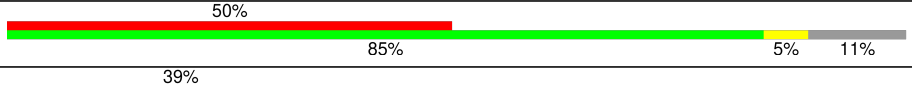
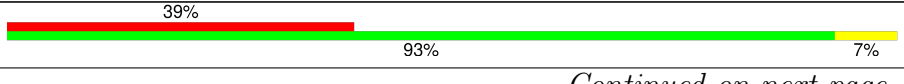
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Mol	Chain	Length	Quality of chain
1	Y	569	15% 42% 54%
1	Z	569	15% 42% 54%
1	a	569	15% 41% 5% 54%
1	b	569	15% 40% 6% 54%
1	c	569	15% 40% 6% 54%
1	d	569	14% 40% 6% 54%
1	e	569	15% 40% 5% 54%
1	f	569	15% 41% 5% 54%
1	g	569	14% 41% 5% 54%
1	h	569	15% 41% 5% 54%
1	i	569	15% 40% 6% 54%
1	j	569	15% 41% 5% 54%
1	k	569	15% 42% 54%
1	l	569	14% 41% 5% 54%
1	m	569	15% 39% 7% 54%
1	n	569	14% 42% 54%
1	o	569	15% 40% 5% 54%
1	p	569	7% 32% 63%
1	q	569	8% 33% 63%
1	r	569	8% 33% 63%
1	s	569	7% 33% 63%
1	t	569	6% 32% 64%
1	u	569	7% 32% 63%
1	v	569	7% 33% 63%
1	w	569	9% 33% 63%

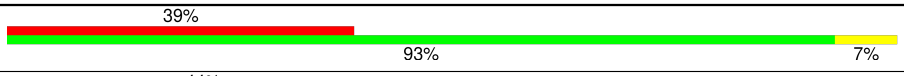
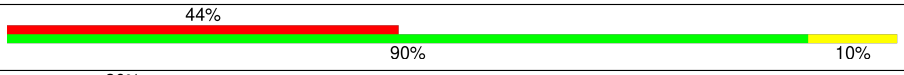
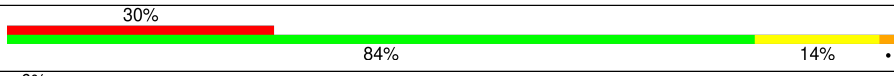
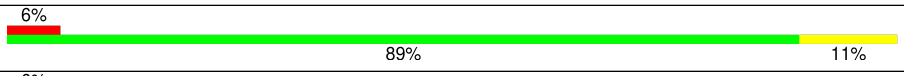
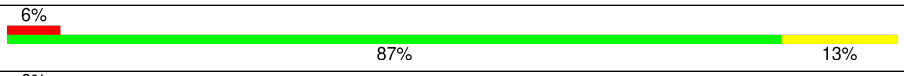
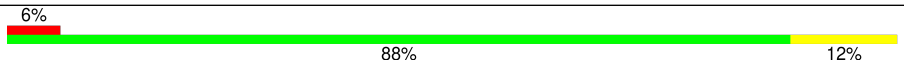
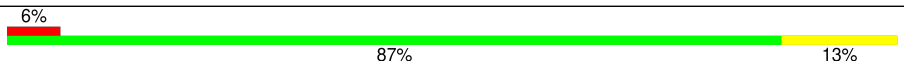
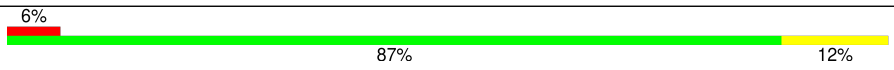
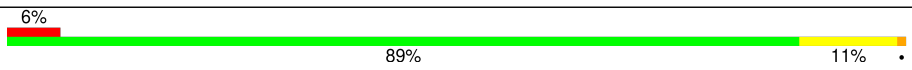
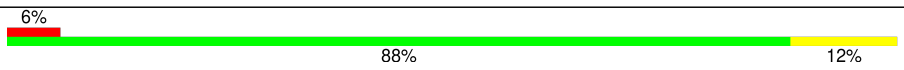
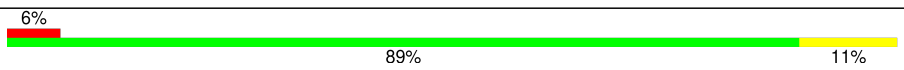
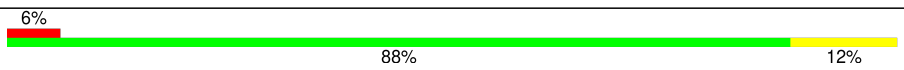
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Mol	Chain	Length	Quality of chain
1	x	569	
1	y	569	
1	z	569	
2	AX	372	
3	AY	254	
3	AZ	254	
3	Aa	254	
3	Ab	254	
3	Ac	254	
4	Ad	269	
5	Ae	111	
5	Af	111	
5	Ag	111	
5	Ah	111	
5	Ai	111	
5	Aj	111	
6	Ak	135	
6	Al	135	
6	Am	135	
6	An	135	
6	Ao	135	
7	Ap	152	
7	Aq	152	
7	Ar	152	
7	As	152	

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Mol	Chain	Length	Quality of chain
7	At	152	
7	Au	152	
8	AU	87	
8	AV	87	
8	AW	87	
8	Av	87	
9	A1	697	
9	A2	697	
9	A3	697	
9	A4	697	
9	A5	697	
9	Aw	697	
9	Ax	697	
9	Ay	697	
9	Az	697	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 231030 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 M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	B	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	C	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	D	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	E	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	F	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	G	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	H	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	I	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	J	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	K	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	L	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	M	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	N	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	O	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	P	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	Q	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	S	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	T	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	U	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	V	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	W	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	X	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	Y	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	Z	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	a	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	b	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	c	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	d	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	e	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	f	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	g	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	h	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	i	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	j	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	k	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	l	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	n	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	o	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	p	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	q	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	r	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	s	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	t	205	Total	C	N	O	S	0	0
			1595	1028	270	295	2		
1	u	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	v	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	w	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	x	205	Total	C	N	O	S	0	0
			1595	1028	270	295	2		
1	y	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	z	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	1	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	2	205	Total	C	N	O	S	0	0
			1595	1028	270	295	2		
1	3	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	4	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	5	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	6	205	Total	C	N	O	S	0	0
			1595	1028	270	295	2		
1	7	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	9	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	0	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	AA	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	AB	209	Total	C	N	O	S	0	0
			1632	1054	275	301	2		
1	AC	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AD	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AE	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AF	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AG	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AH	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AI	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AJ	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AK	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AL	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AM	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AN	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AO	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AP	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AQ	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AR	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AS	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		
1	AT	202	Total	C	N	O	S	0	0
			1614	1036	276	299	3		

- Molecule 2 is a protein called Flagellar biosynthetic protein FlhB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AX	242	Total	C	N	O	S	0	0
			1988	1325	311	342	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AY	209	Total	C	N	O	S	0	0
			1665	1118	255	277	15		
3	AZ	209	Total	C	N	O	S	0	0
			1656	1114	252	275	15		
3	Aa	209	Total	C	N	O	S	0	0
			1657	1116	252	274	15		
3	Ab	209	Total	C	N	O	S	0	0
			1666	1119	255	277	15		
3	Ac	209	Total	C	N	O	S	0	0
			1676	1128	256	277	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ad	259	Total	C	N	O	S	0	0
			2083	1434	304	340	5		

- Molecule 5 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ae	70	Total	C	N	O	S	0	0
			542	342	94	104	2		
5	Af	70	Total	C	N	O	S	0	0
			542	342	94	104	2		
5	Ag	70	Total	C	N	O	S	0	0
			542	342	94	104	2		
5	Ah	70	Total	C	N	O	S	0	0
			530	333	91	104	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ai	70	Total	C	N	O	S	0	0
			542	342	94	104	2		
5	Aj	40	Total	C	N	O	S	0	0
			308	193	55	58	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Ak	112	Total	C	N	O	S	0	0
			920	577	161	177	5		
6	Al	112	Total	C	N	O	S	0	0
			920	577	161	177	5		
6	Am	112	Total	C	N	O	S	0	0
			920	577	161	177	5		
6	An	112	Total	C	N	O	S	0	0
			920	577	161	177	5		
6	Ao	112	Total	C	N	O	S	0	0
			920	577	161	177	5		

- Molecule 7 is a protein called Flagellar basal-body rod protein FlgC.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ap	136	Total	C	N	O	S	0	0
			1030	639	187	200	4		
7	Aq	152	Total	C	N	O	S	0	0
			1153	724	201	224	4		
7	Ar	136	Total	C	N	O	S	0	0
			1034	641	188	201	4		
7	As	152	Total	C	N	O	S	0	0
			1169	732	208	225	4		
7	At	152	Total	C	N	O	S	0	0
			1169	732	208	225	4		
7	Au	152	Total	C	N	O	S	0	0
			1169	732	208	225	4		

- Molecule 8 is a protein called Flagellar biosynthetic protein FliQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Av	87	Total	C	N	O	S	0	0
			678	463	99	112	4		
8	AU	87	Total	C	N	O	S	0	0
			682	465	100	113	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	AV	87	Total	C	N	O	S	0	0
			692	471	104	113	4		
8	AW	87	Total	C	N	O	S	0	0
			692	471	104	113	4		

- Molecule 9 is a protein called Flagellar biosynthesis protein FlhA.

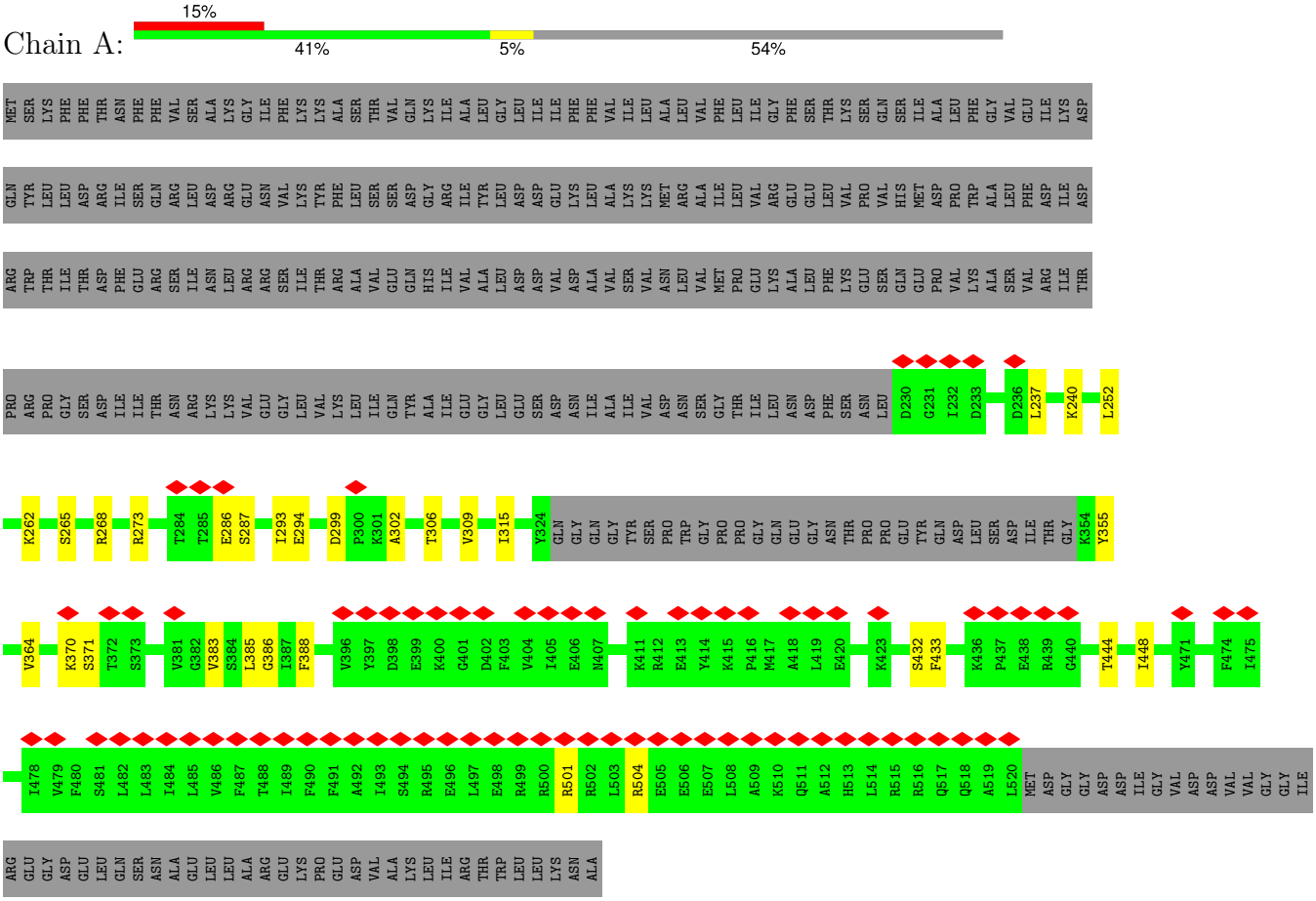
Mol	Chain	Residues	Atoms					AltConf	Trace
9	Aw	697	Total	C	N	O	S	0	0
			5429	3527	875	1015	12		
9	Ax	697	Total	C	N	O	S	0	0
			5429	3527	875	1015	12		
9	Ay	697	Total	C	N	O	S	0	0
			5429	3527	875	1015	12		
9	Az	697	Total	C	N	O	S	0	0
			5429	3527	875	1015	12		
9	A1	697	Total	C	N	O	S	0	0
			5429	3527	875	1015	12		
9	A2	697	Total	C	N	O	S	0	0
			5429	3527	875	1015	12		
9	A3	697	Total	C	N	O	S	0	0
			5429	3527	875	1015	12		
9	A4	697	Total	C	N	O	S	0	0
			5429	3527	875	1015	12		
9	A5	697	Total	C	N	O	S	0	0
			5429	3527	875	1015	12		

3 Residue-property plots (i)

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

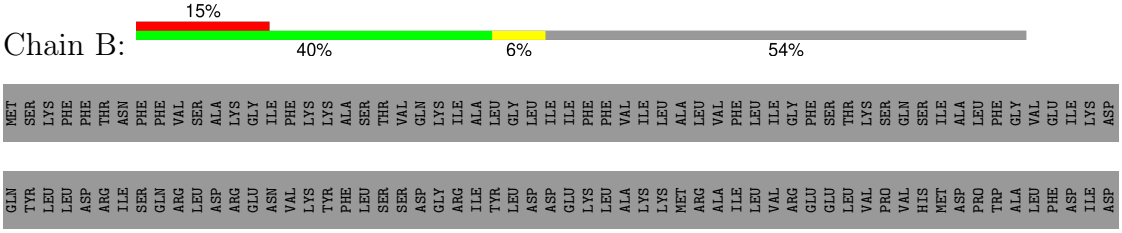
• Molecule 1: Flagellar M-ring protein

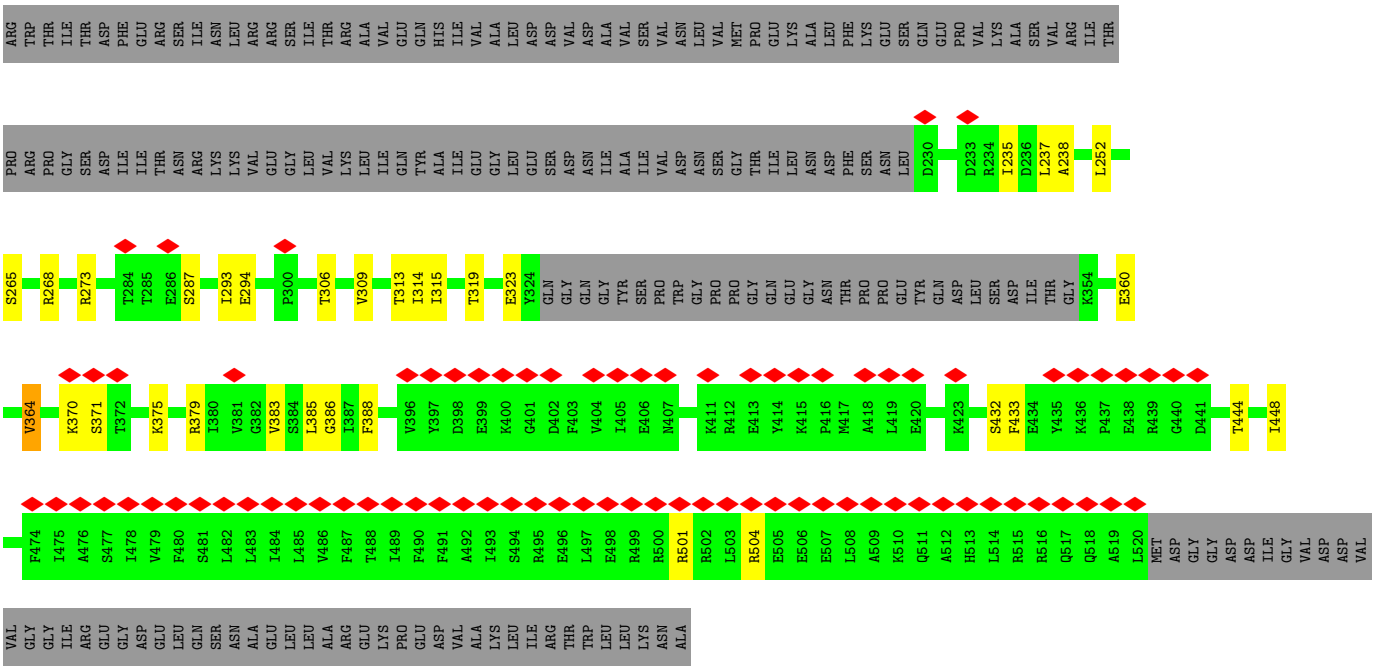
Chain A:



• Molecule 1: Flagellar M-ring protein

Chain B:

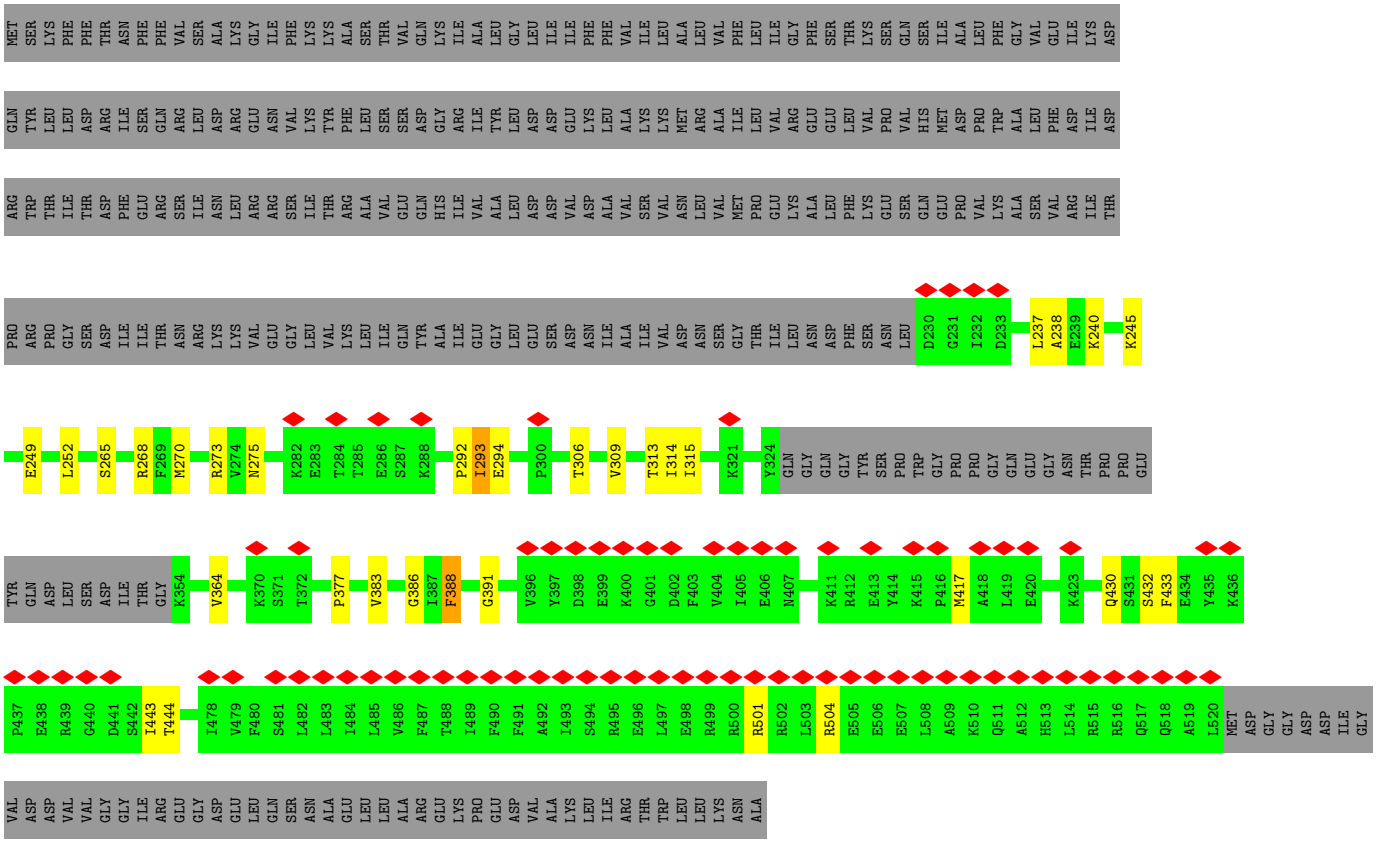




• Molecule 1: Flagellar M-ring protein

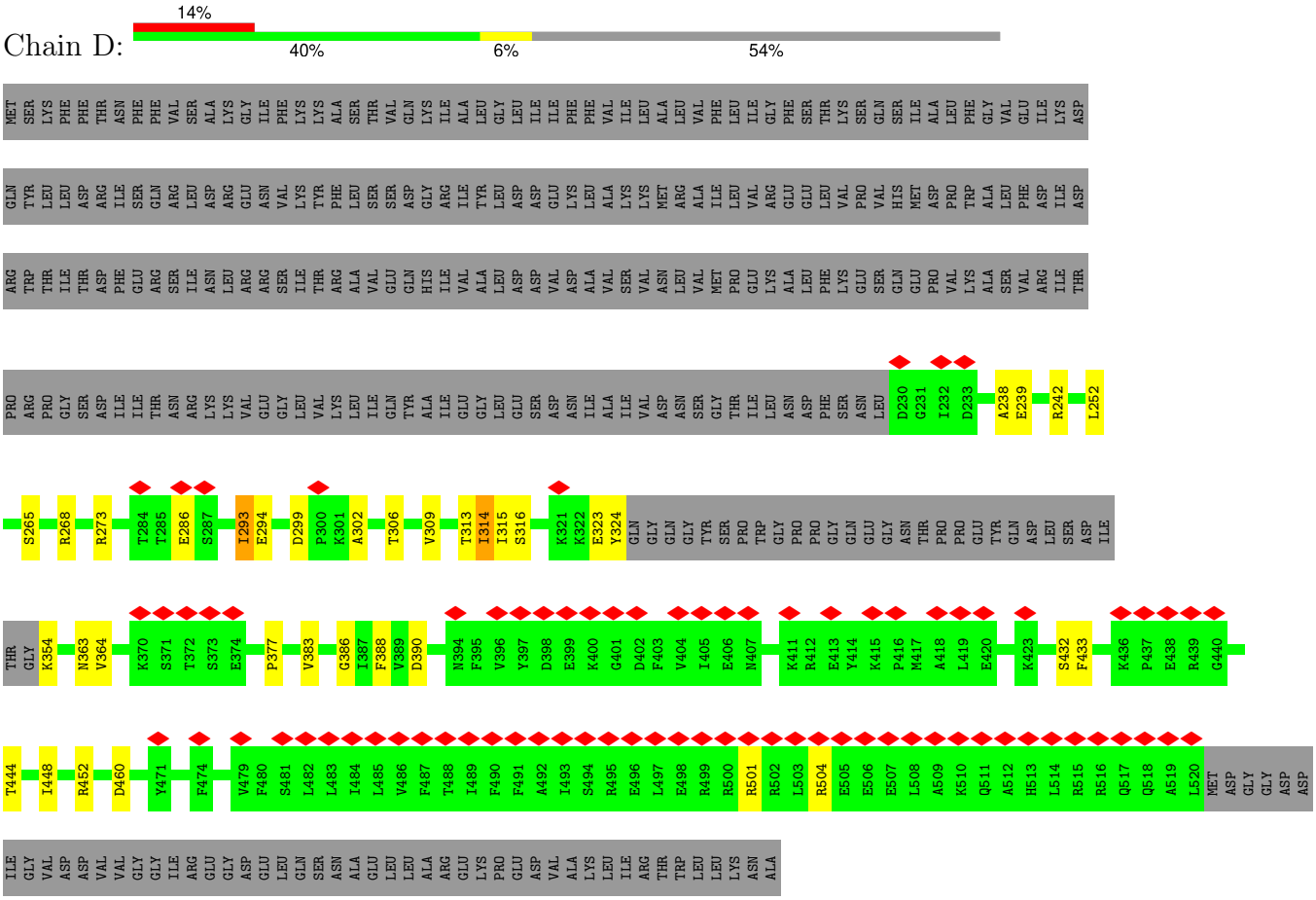
Chain C:





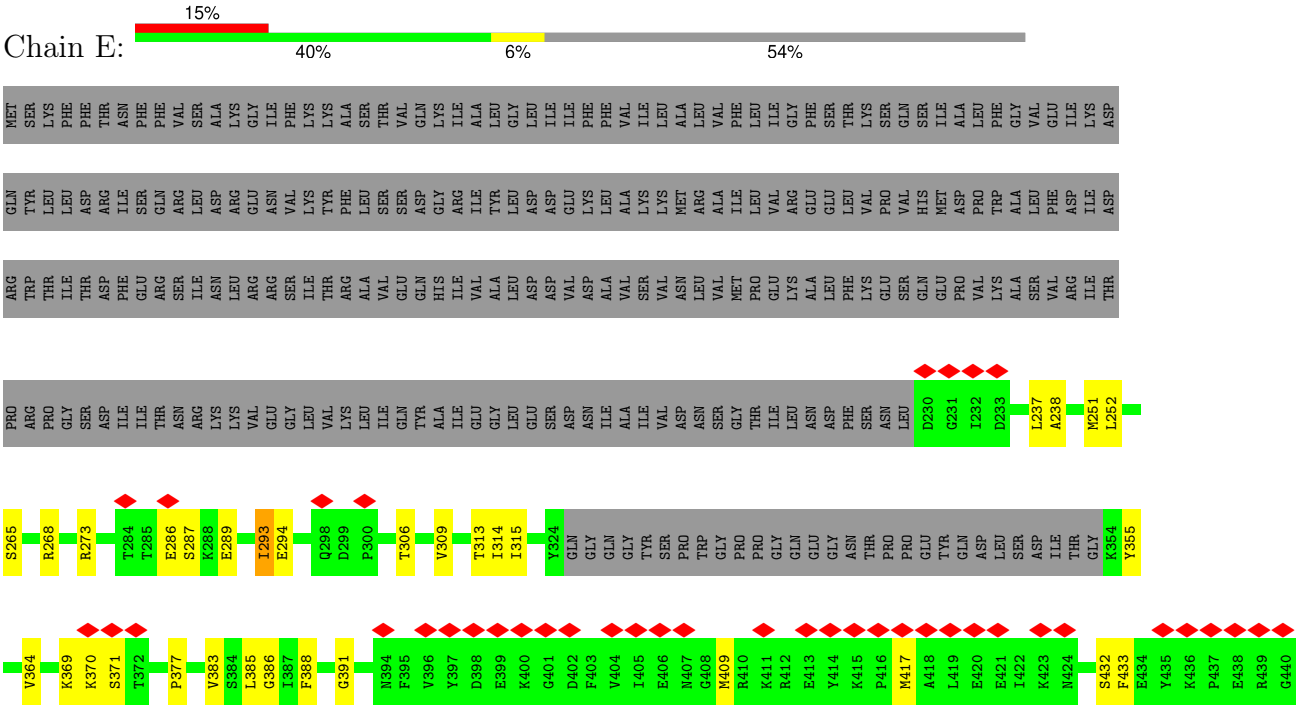
• Molecule 1: Flagellar M-ring protein

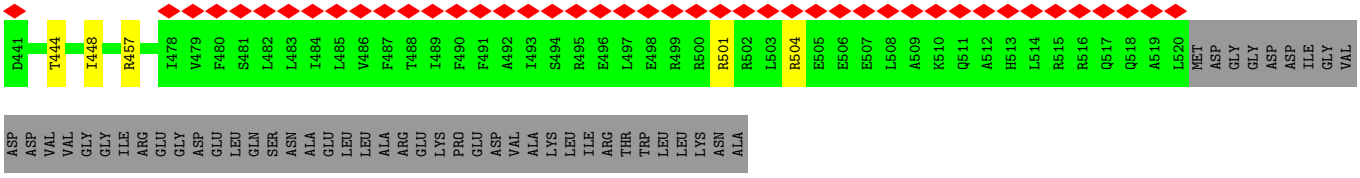
Chain D:



• Molecule 1: Flagellar M-ring protein

Chain E:

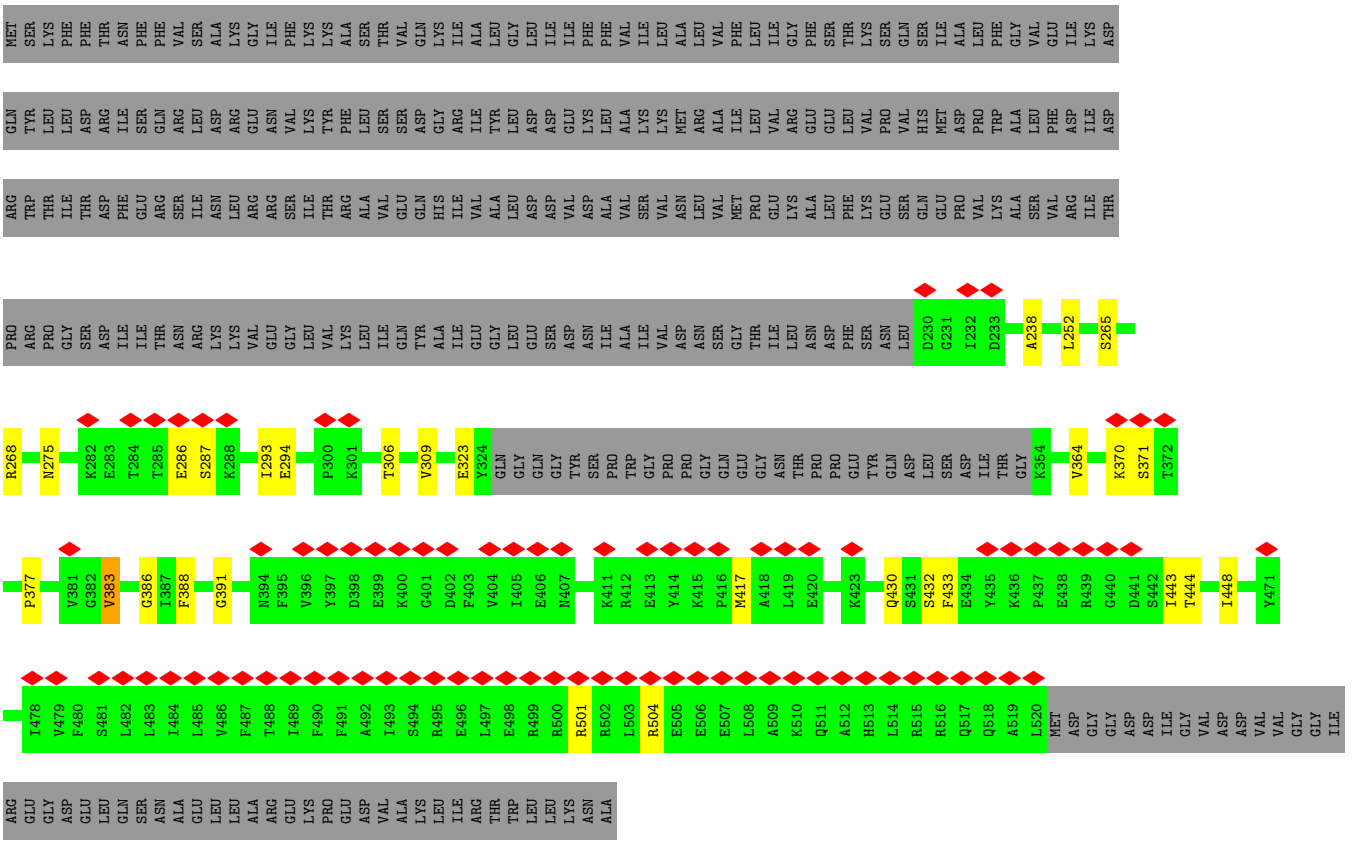




• Molecule 1: Flagellar M-ring protein

Chain F:

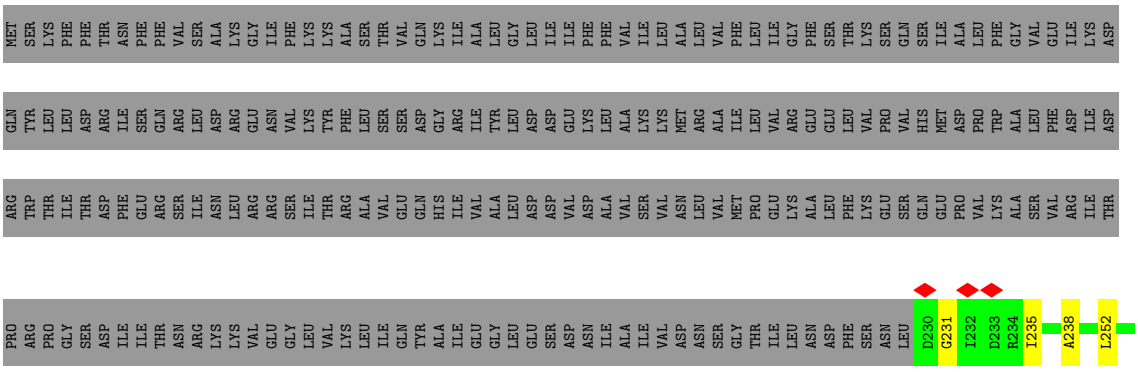


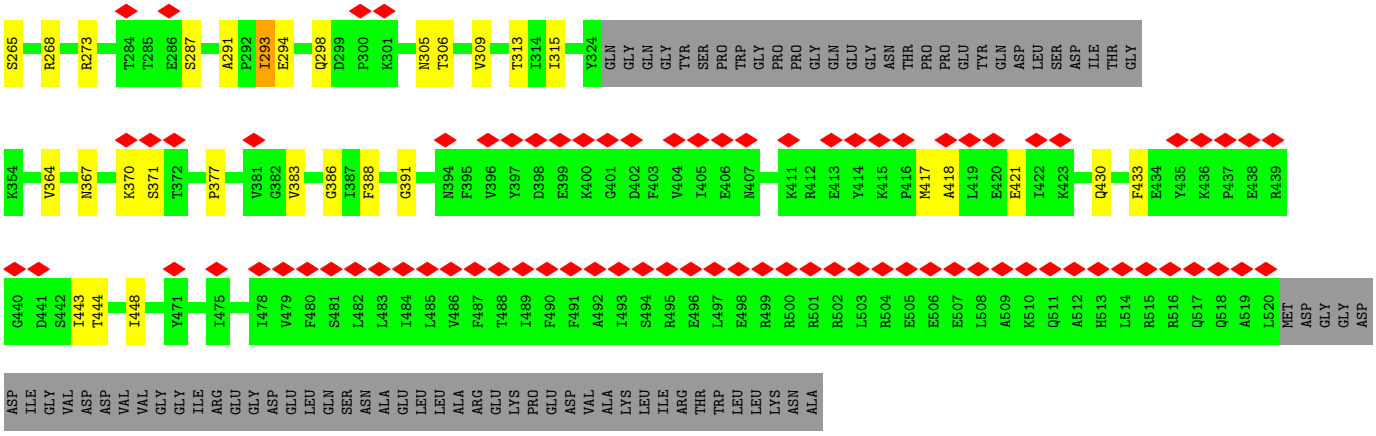


• Molecule 1: Flagellar M-ring protein

Chain G:



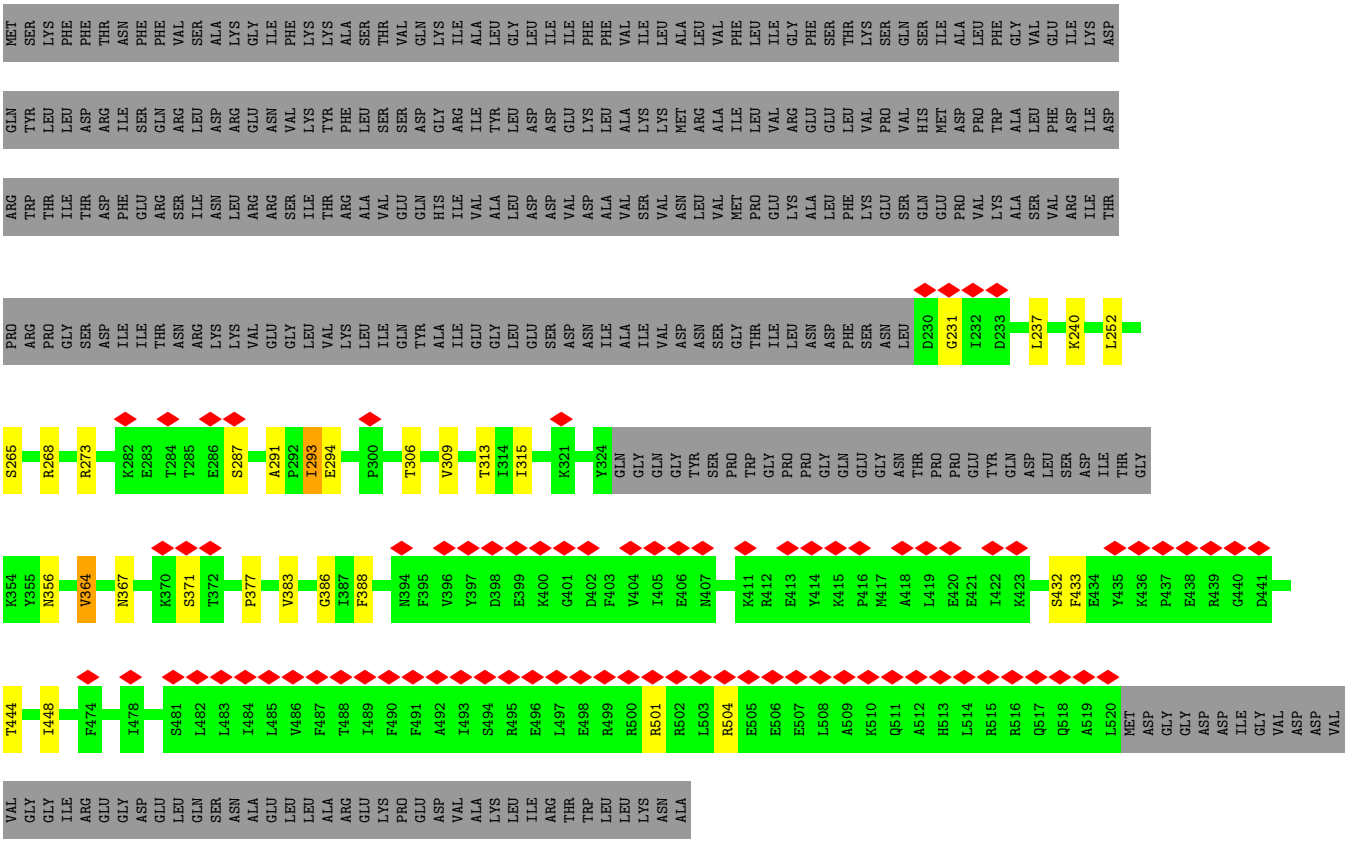




• Molecule 1: Flagellar M-ring protein

Chain H:

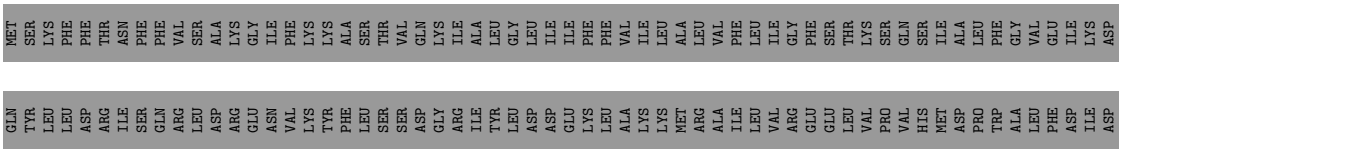


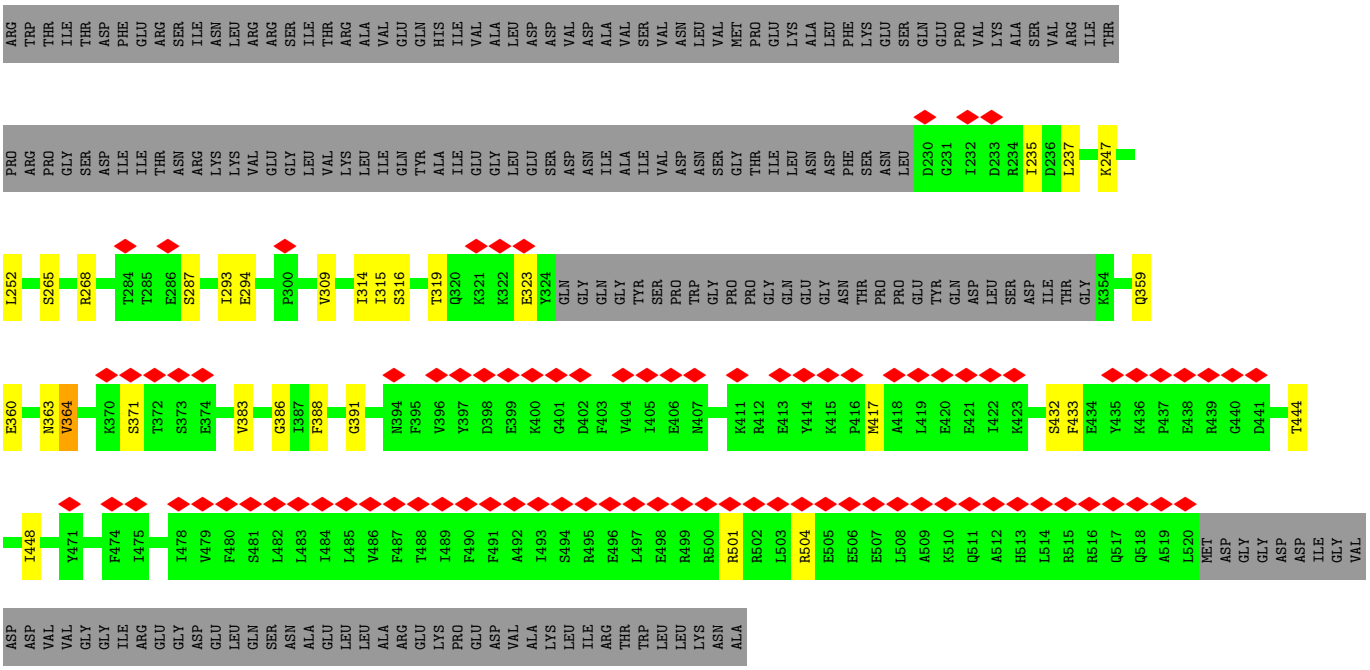


• Molecule 1: Flagellar M-ring protein

Chain I:



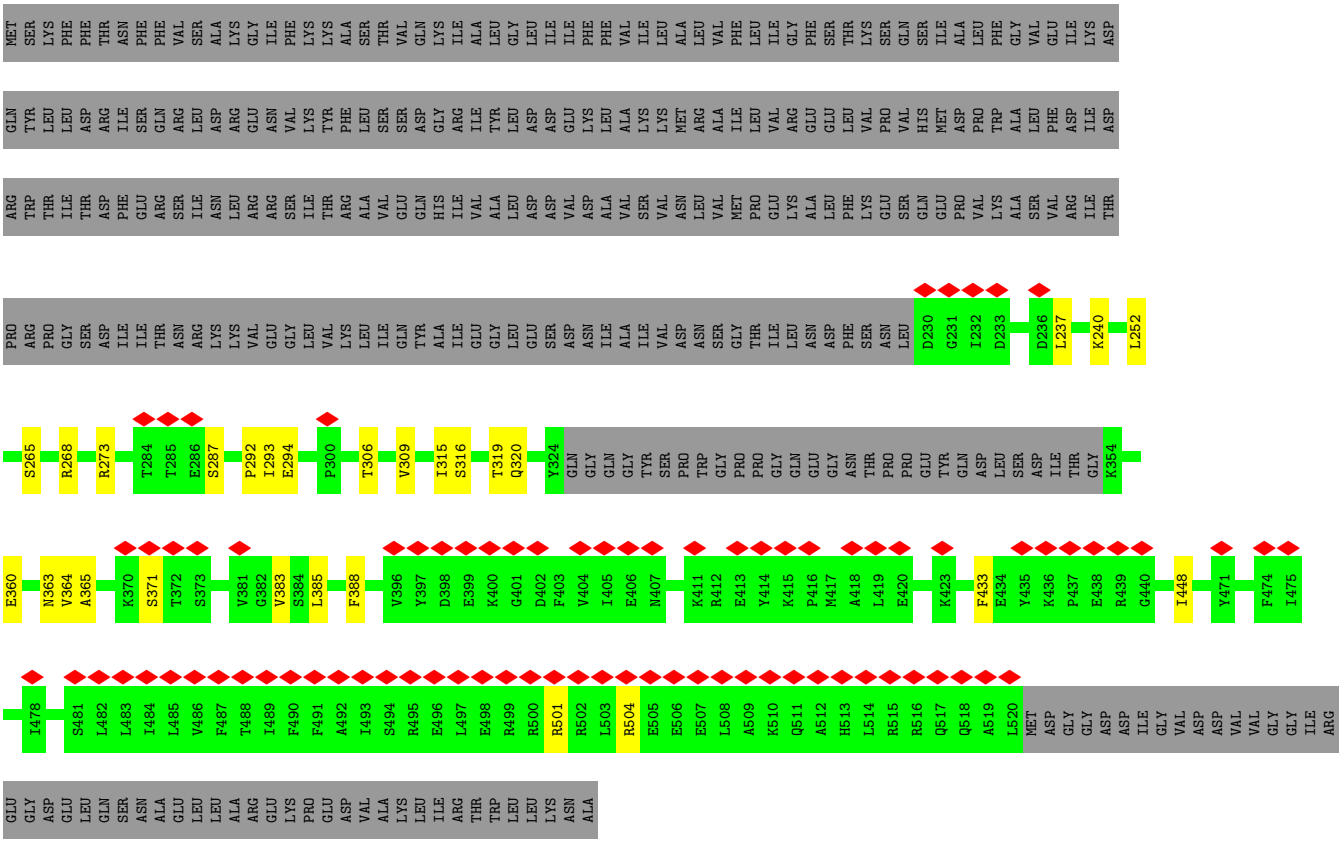




• Molecule 1: Flagellar M-ring protein

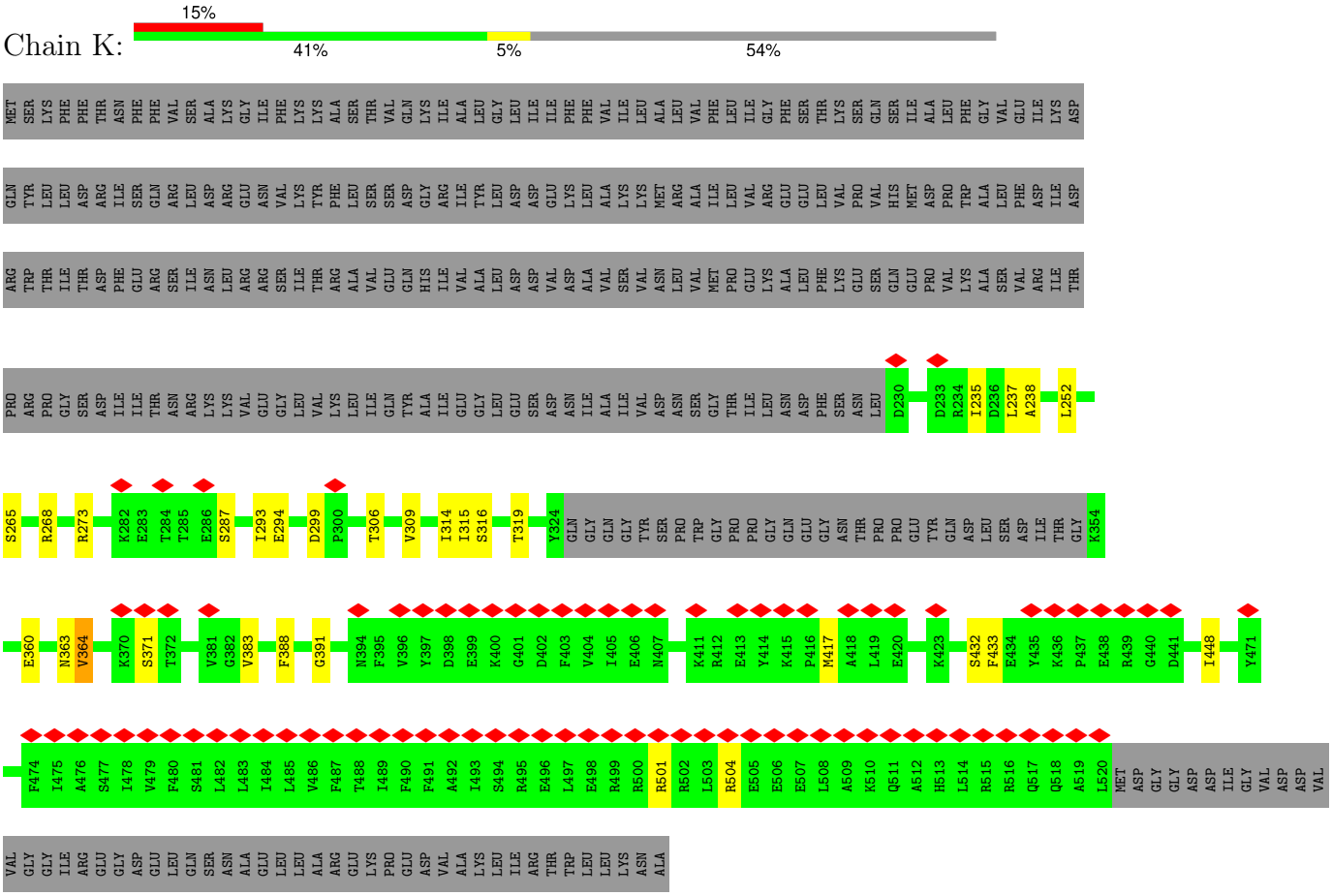
Chain J:





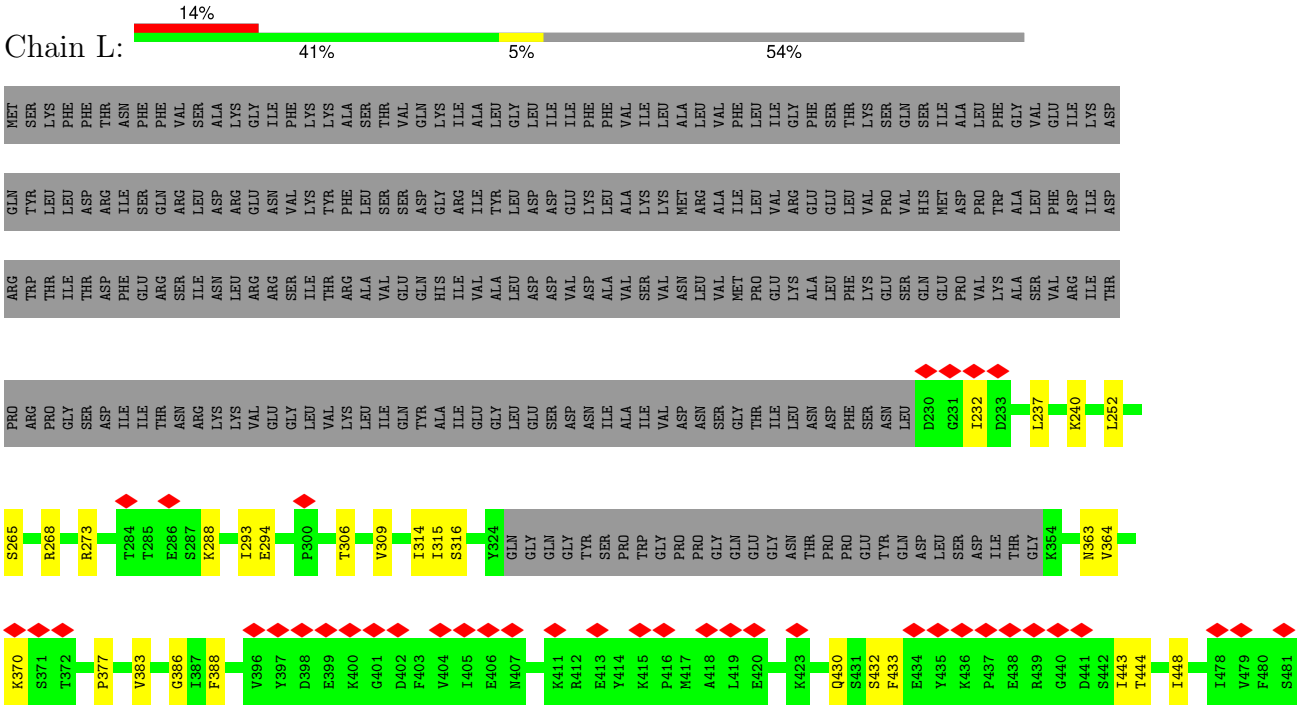
• Molecule 1: Flagellar M-ring protein

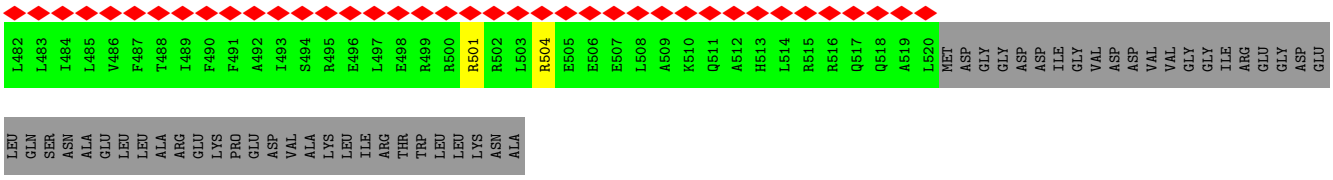
Chain K:



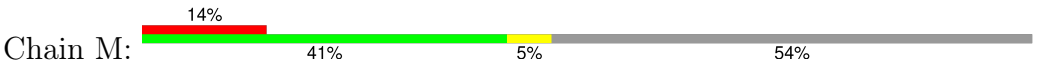
• Molecule 1: Flagellar M-ring protein

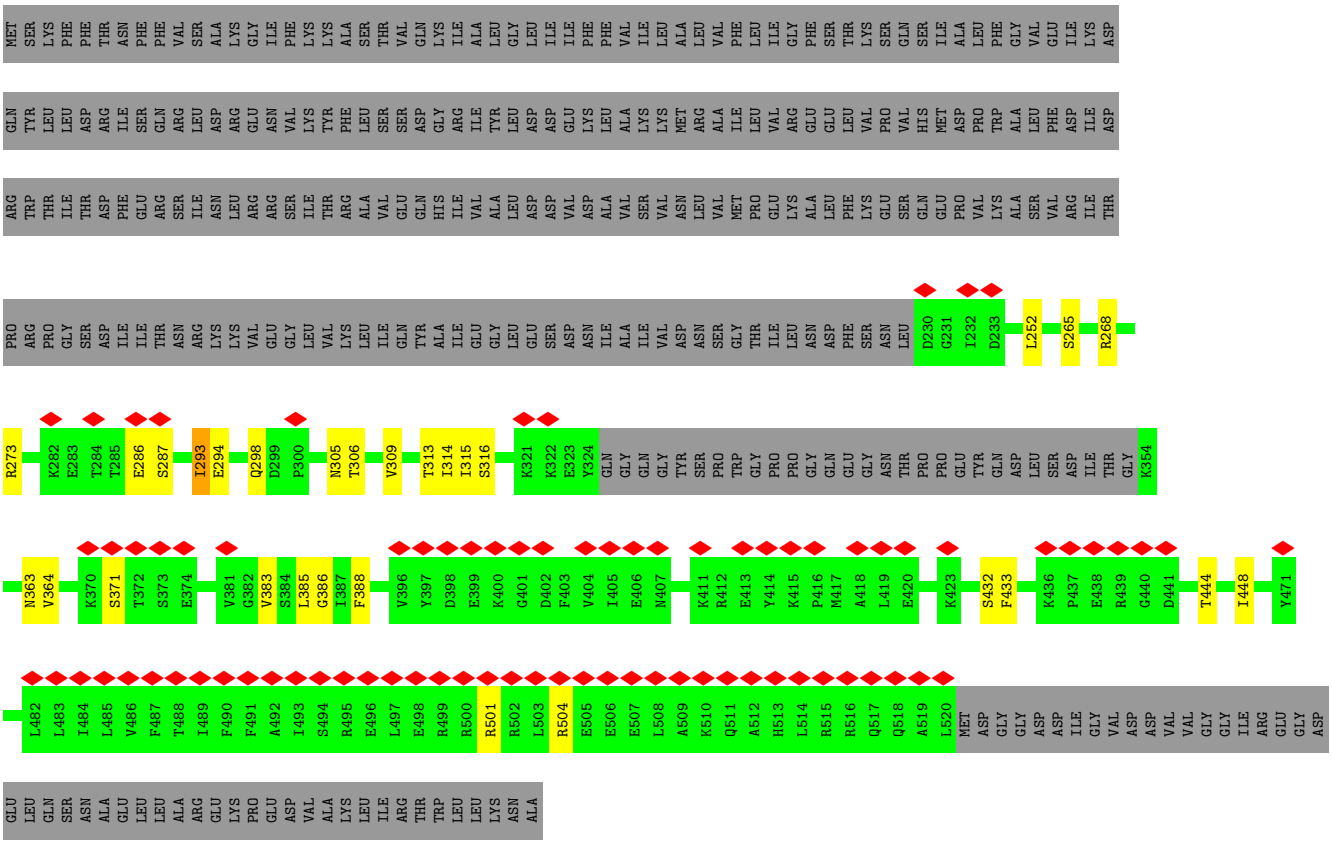
Chain L:



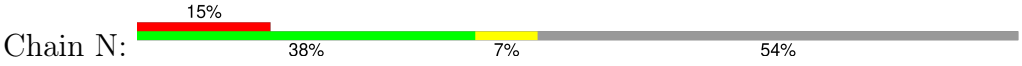


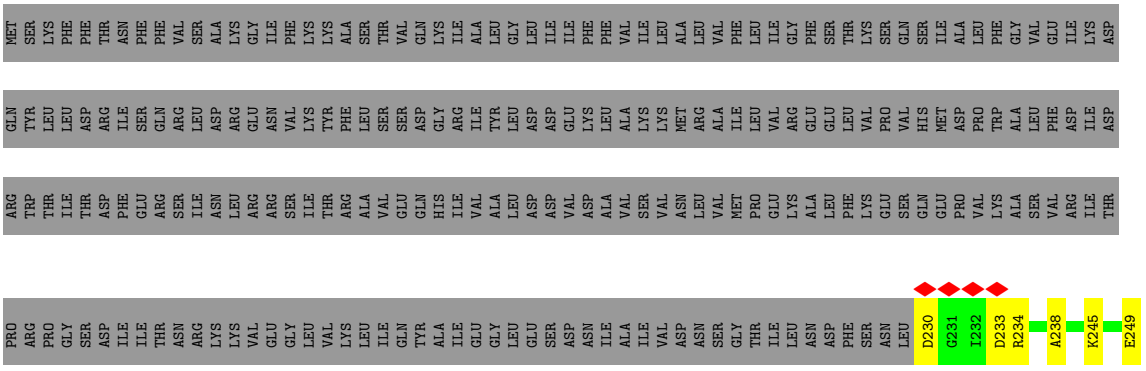
• Molecule 1: Flagellar M-ring protein

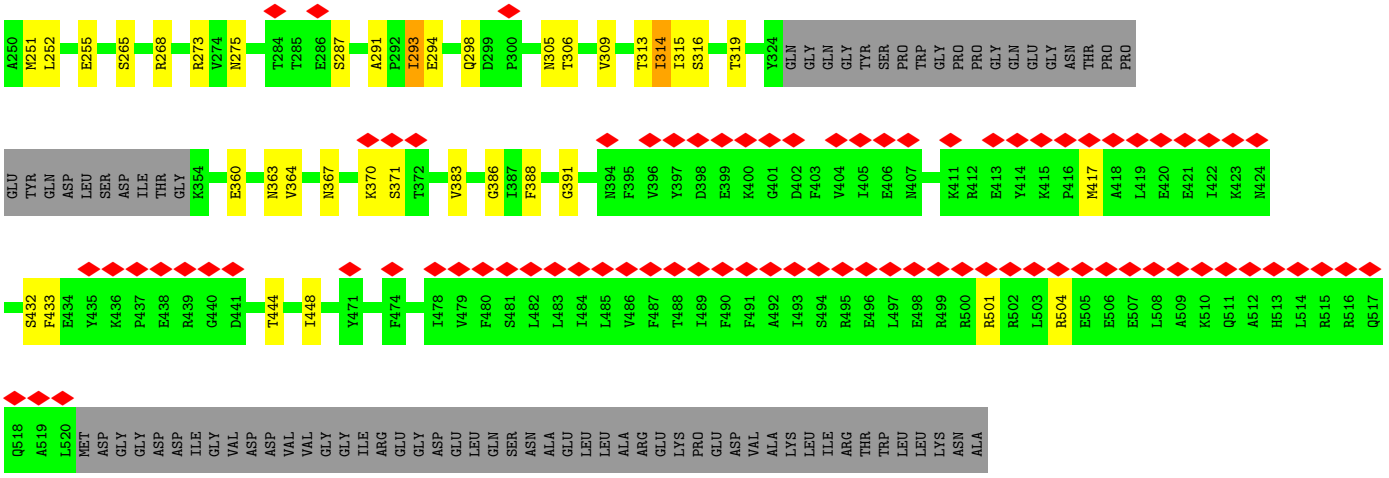




• Molecule 1: Flagellar M-ring protein



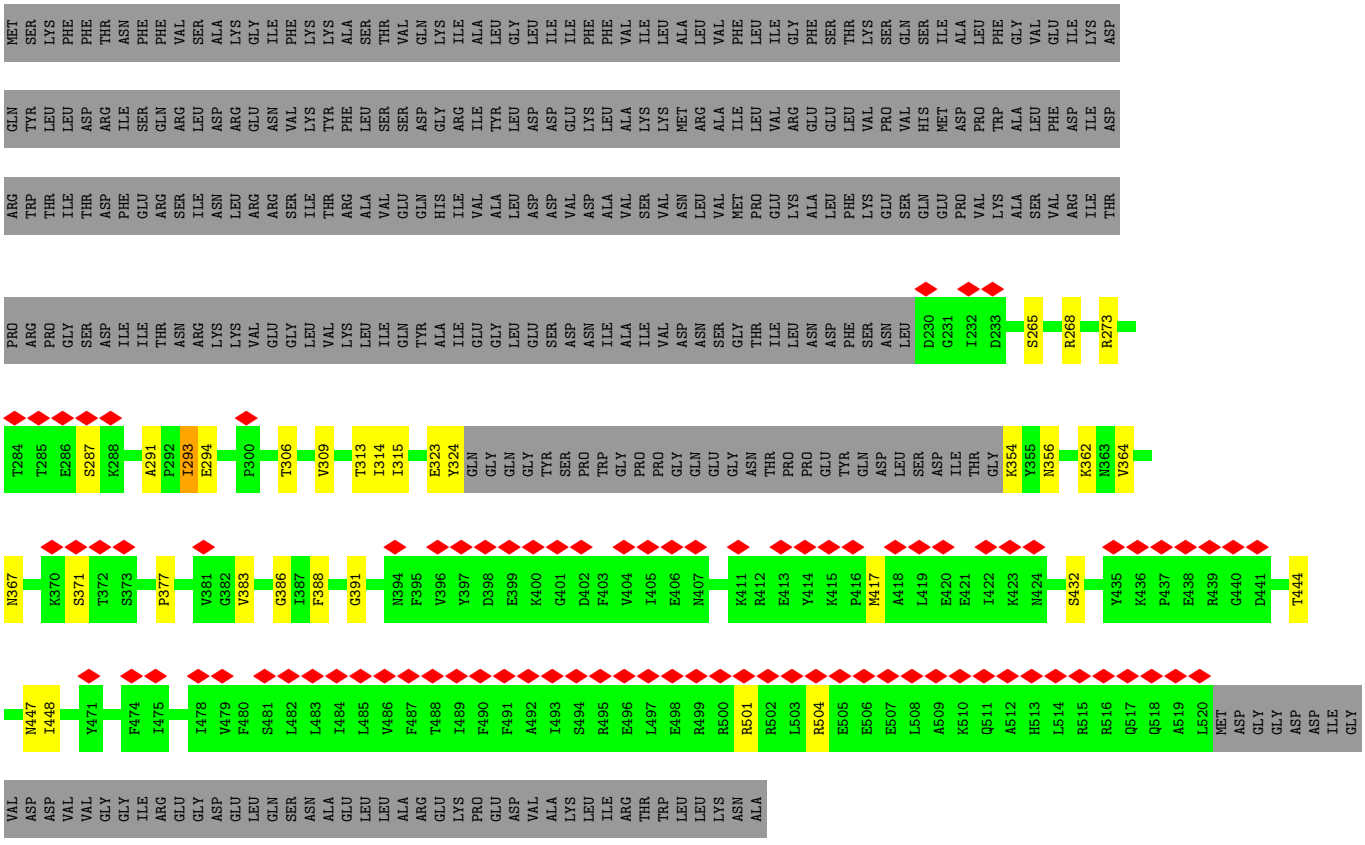




• Molecule 1: Flagellar M-ring protein

Chain O:



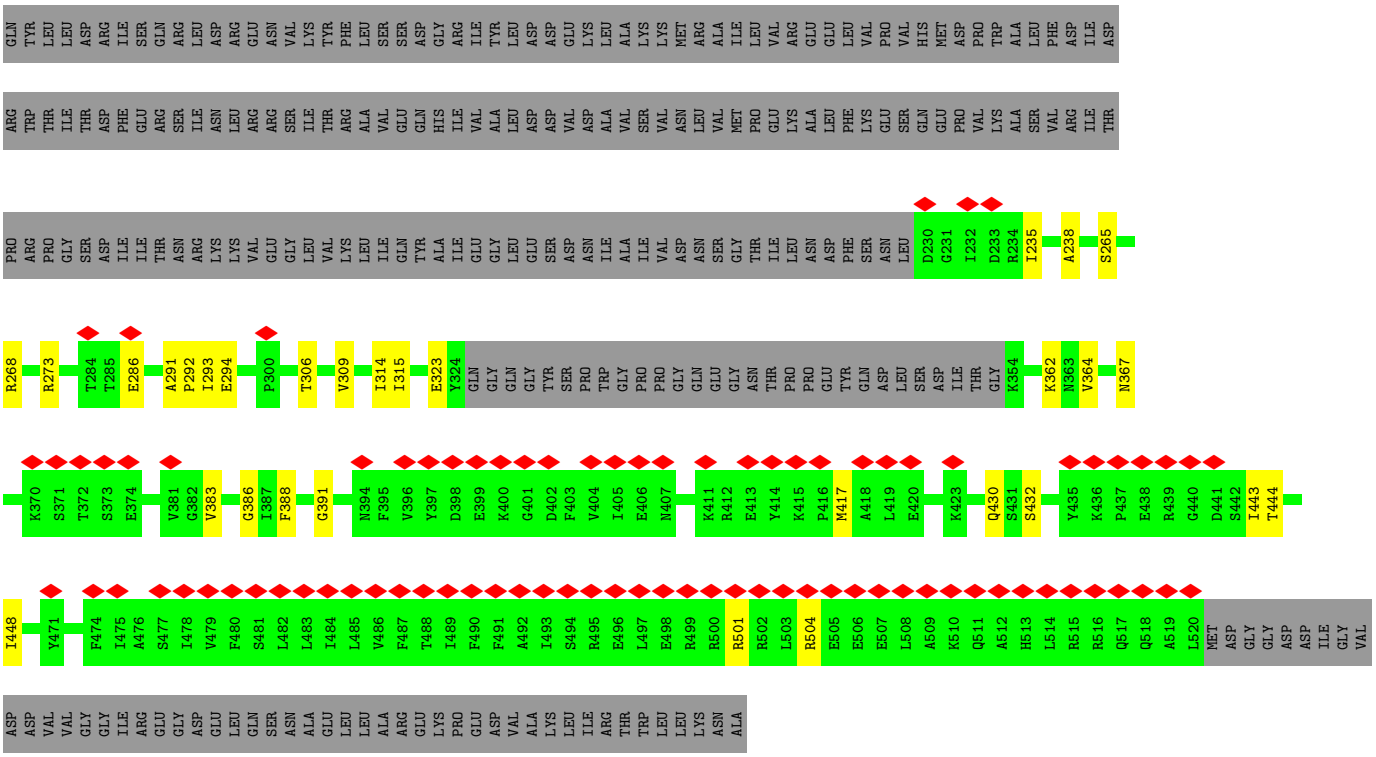


• Molecule 1: Flagellar M-ring protein

Chain P:



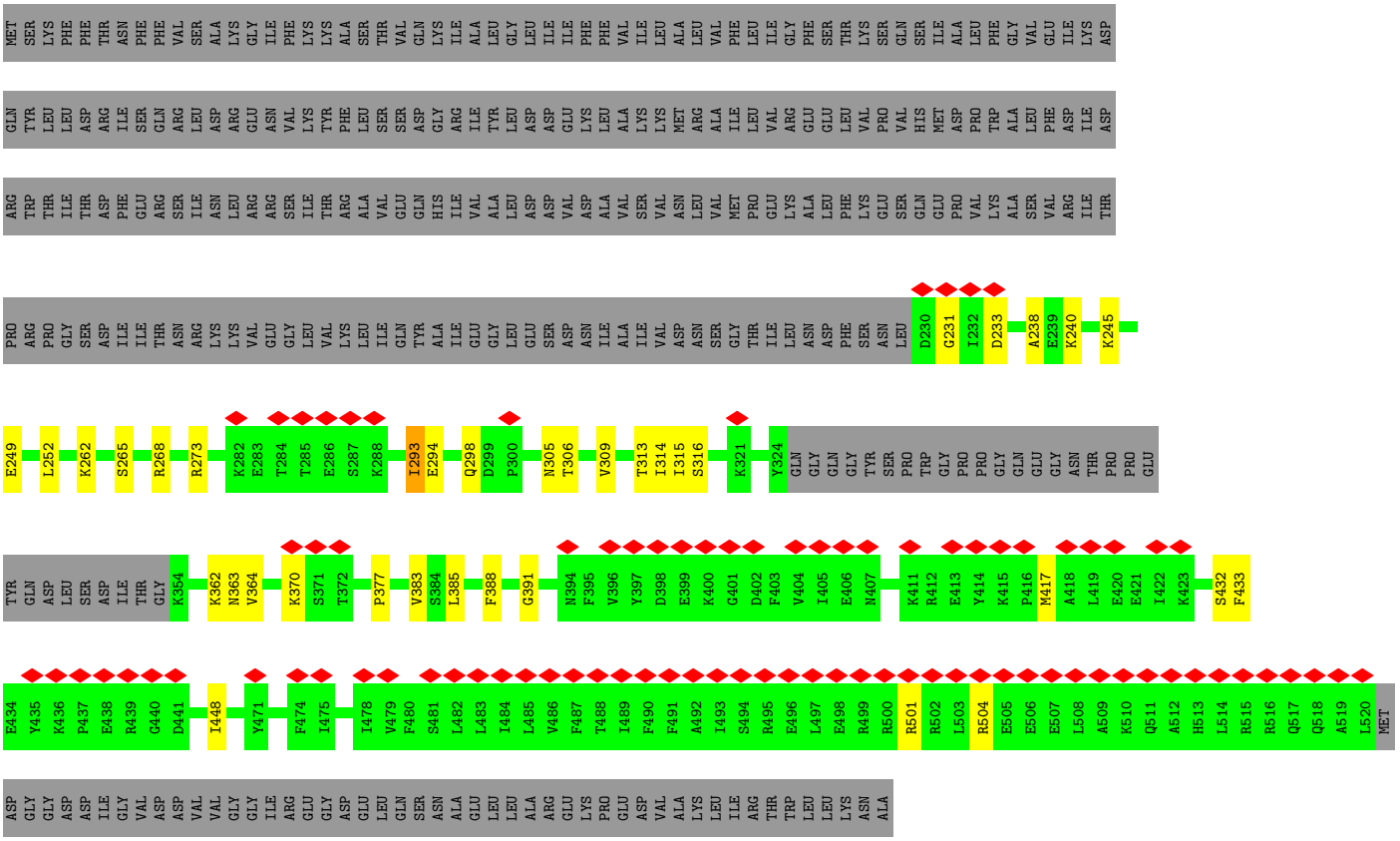




• Molecule 1: Flagellar M-ring protein

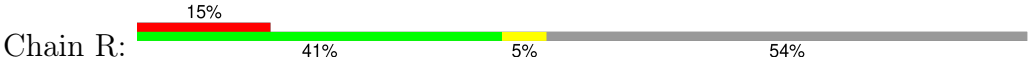
Chain Q:

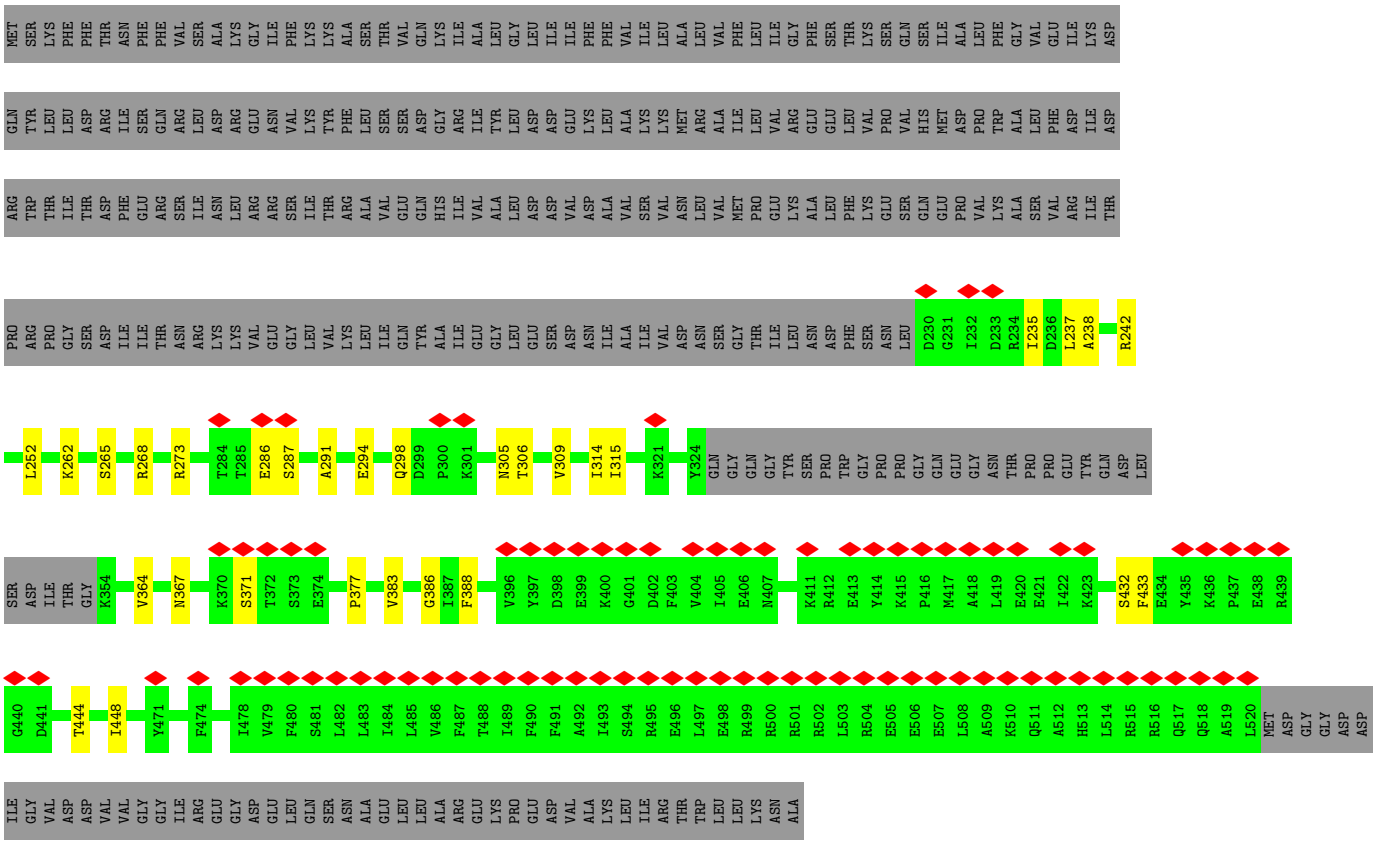




• Molecule 1: Flagellar M-ring protein

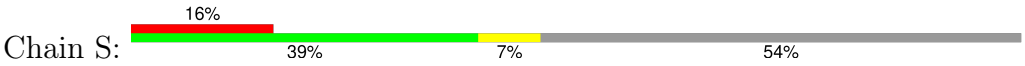
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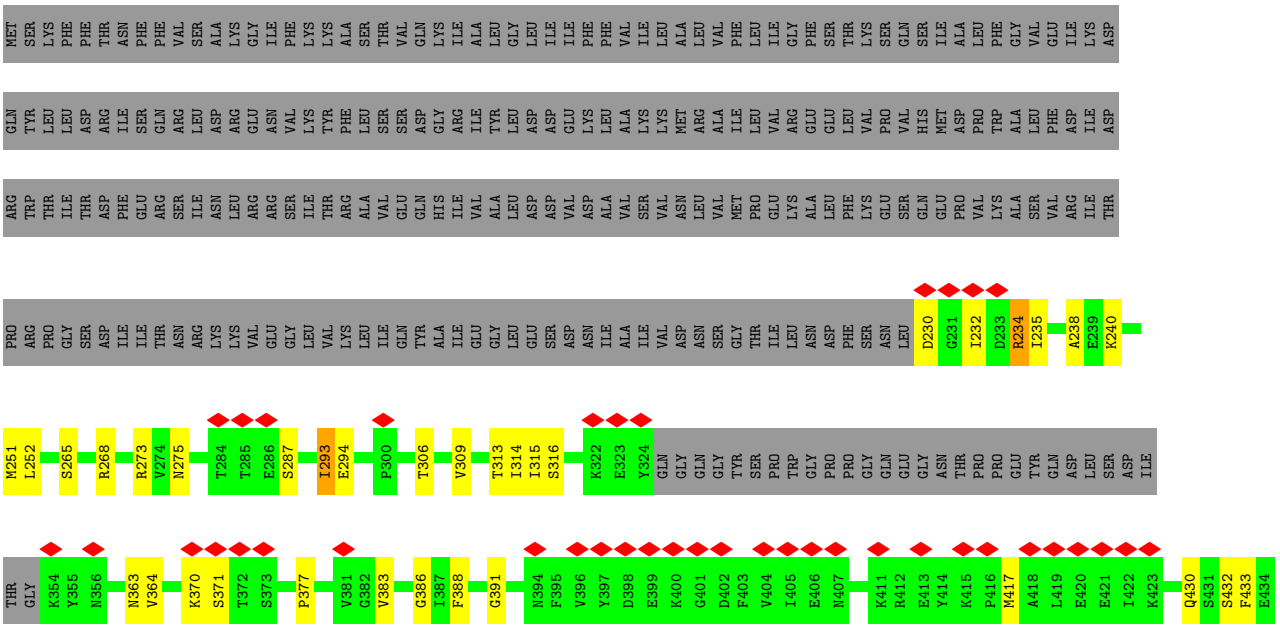


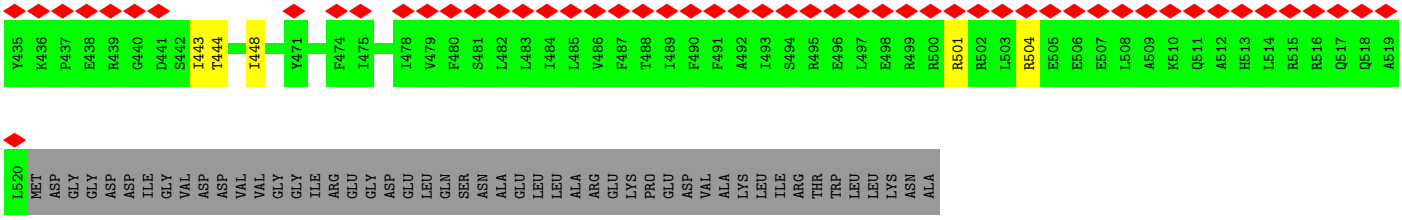


• Molecule 1: Flagellar M-ring protein

Chain S:



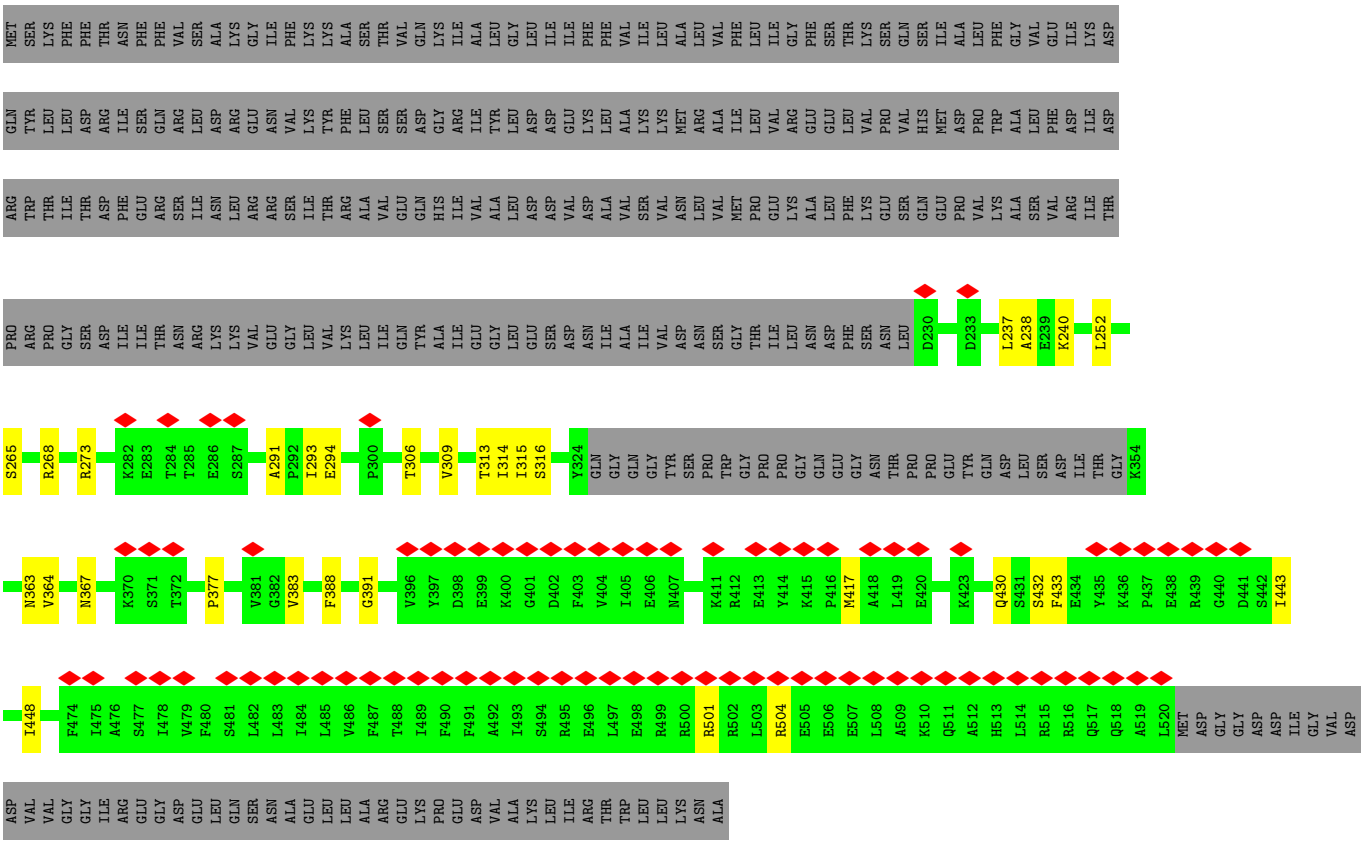




• Molecule 1: Flagellar M-ring protein

Chain T:

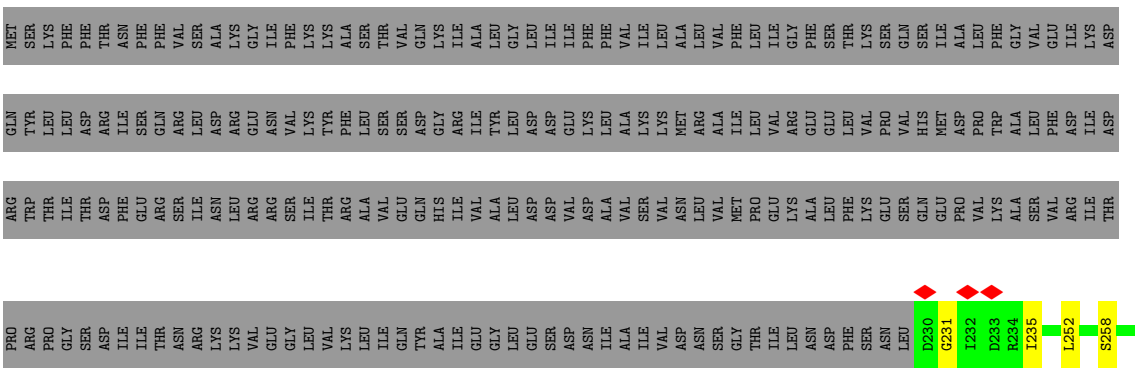


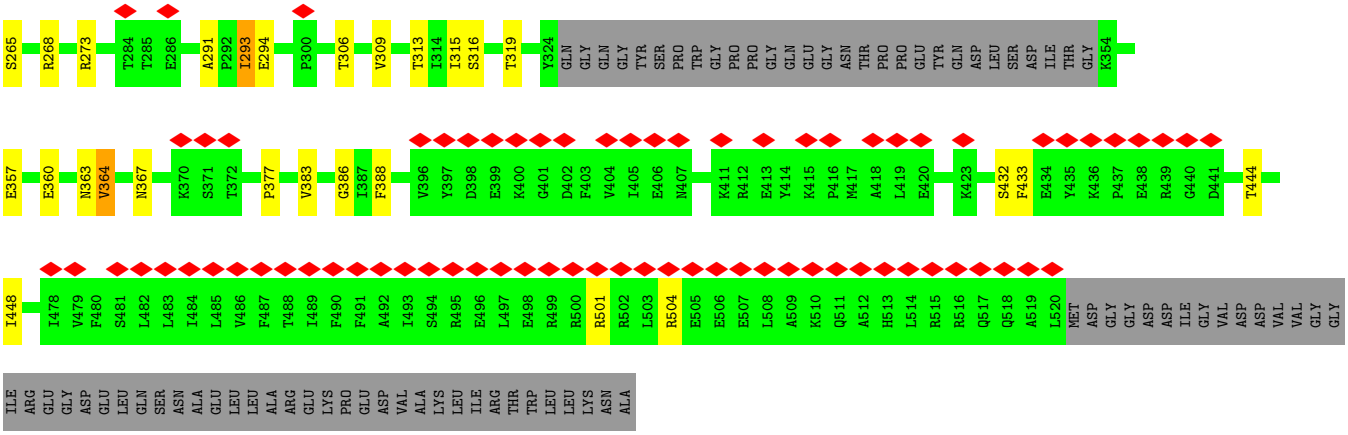


• Molecule 1: Flagellar M-ring protein

Chain U:



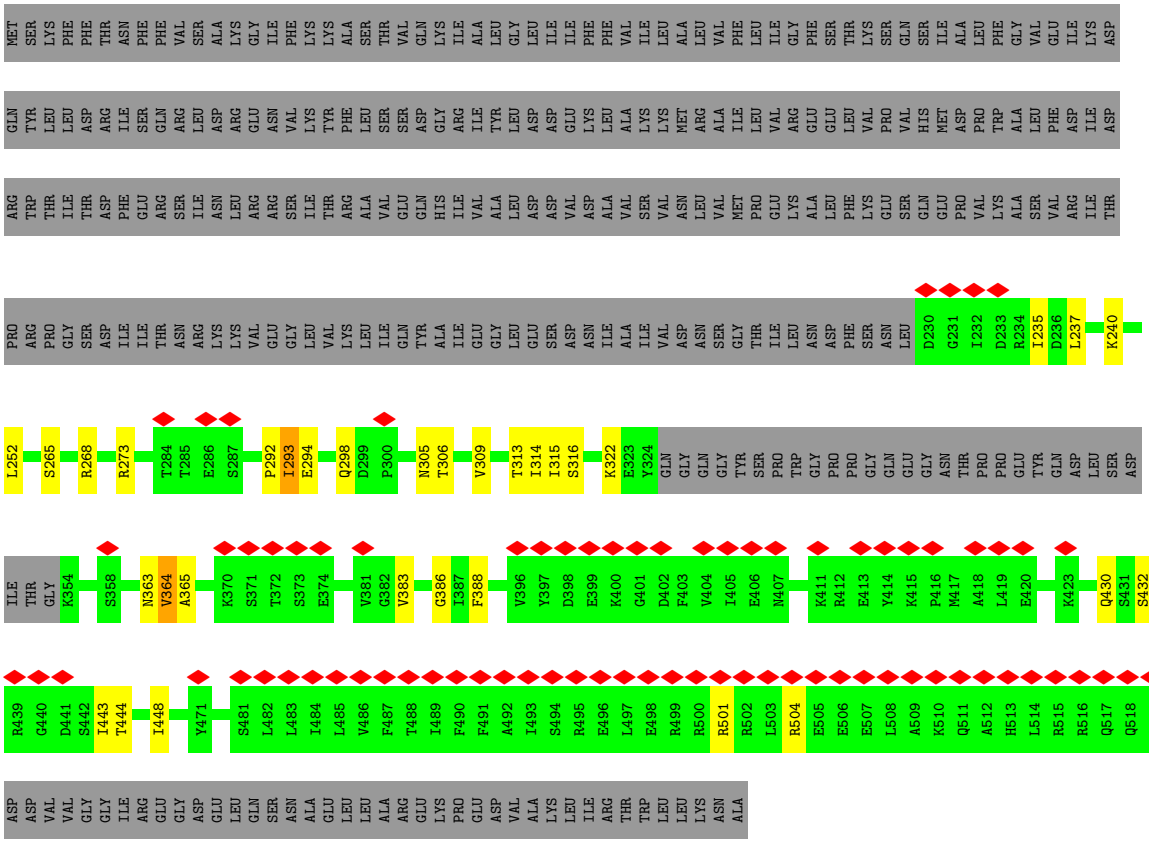




• Molecule 1: Flagellar M-ring protein

Chain V:

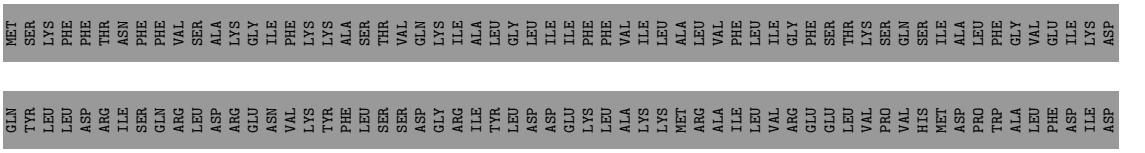


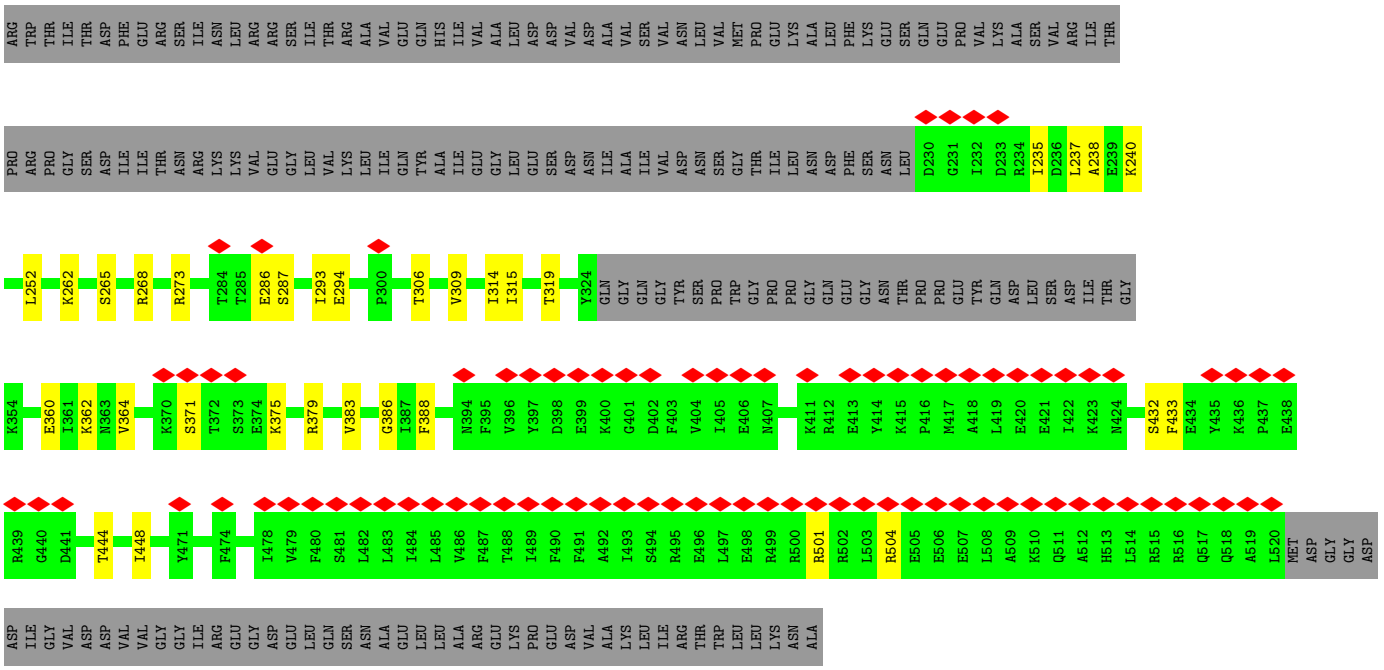


• Molecule 1: Flagellar M-ring protein

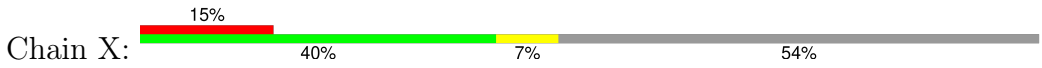
Chain W:

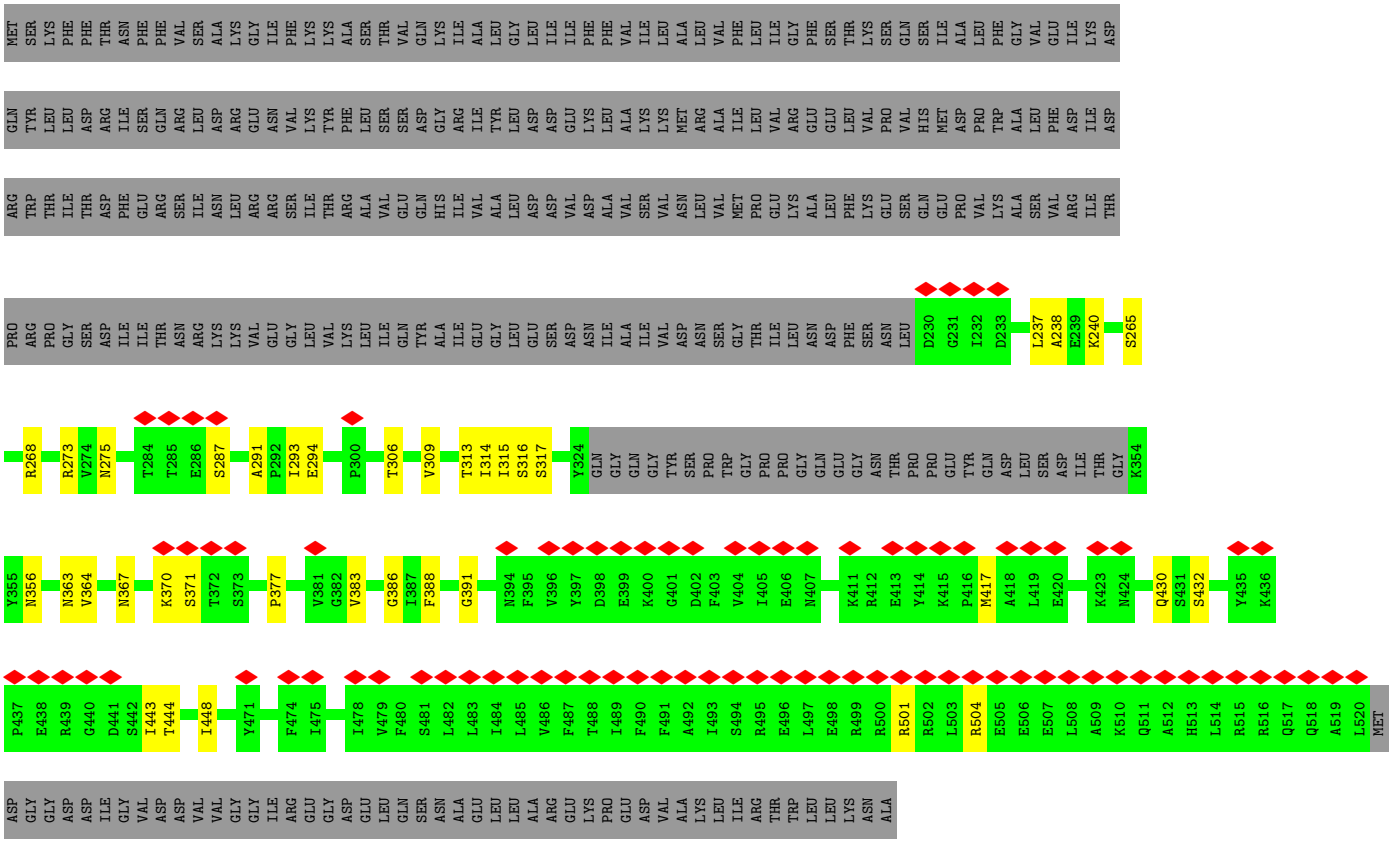






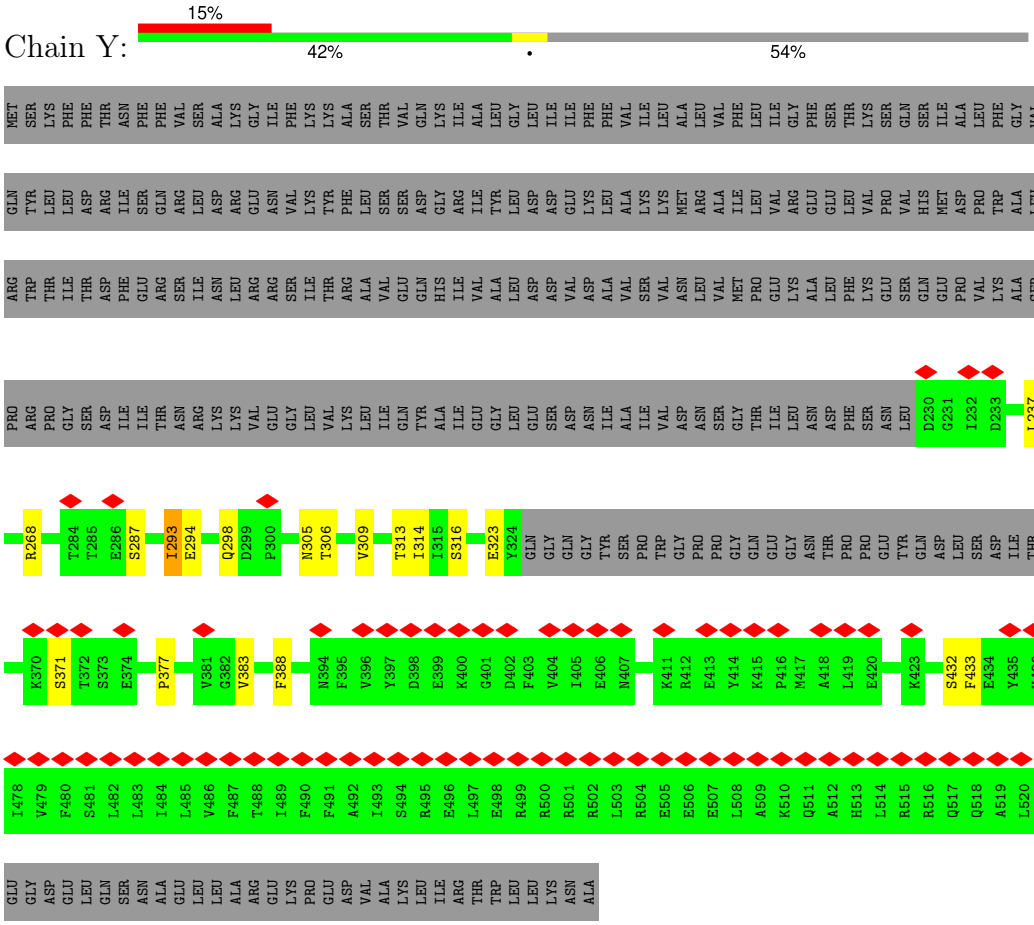
• Molecule 1: Flagellar M-ring protein





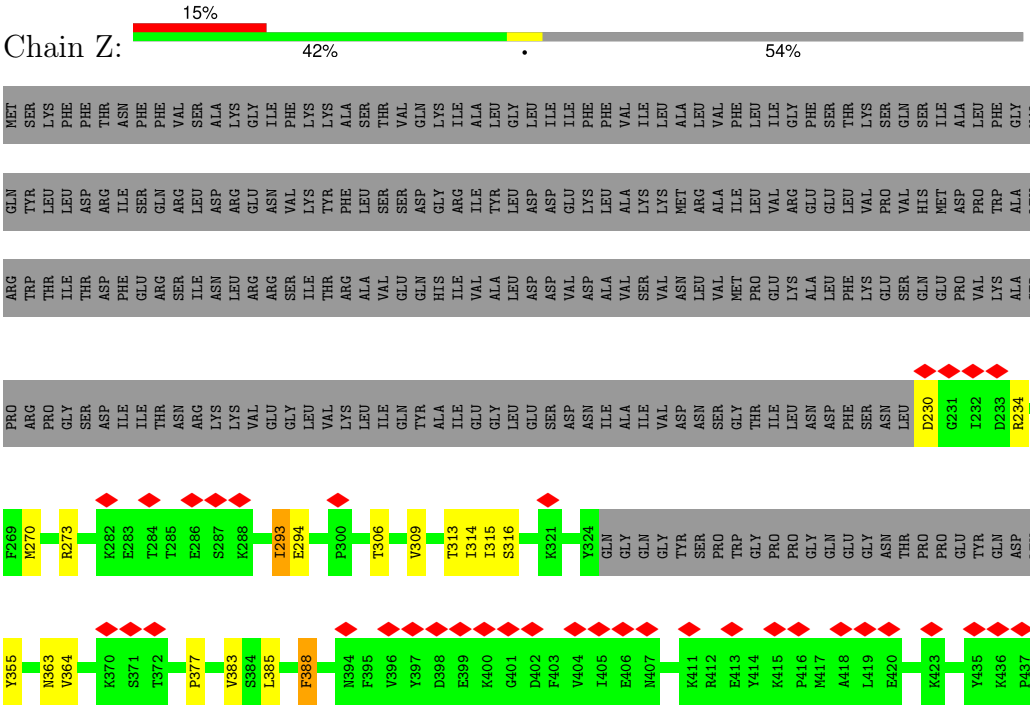
• Molecule 1: Flagellar M-ring protein

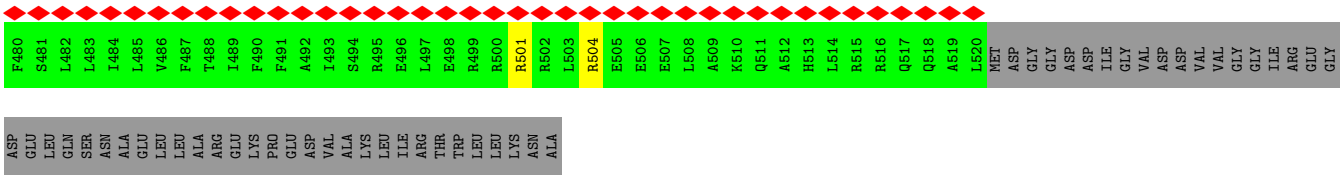
Chain Y:



• Molecule 1: Flagellar M-ring protein

Chain Z:

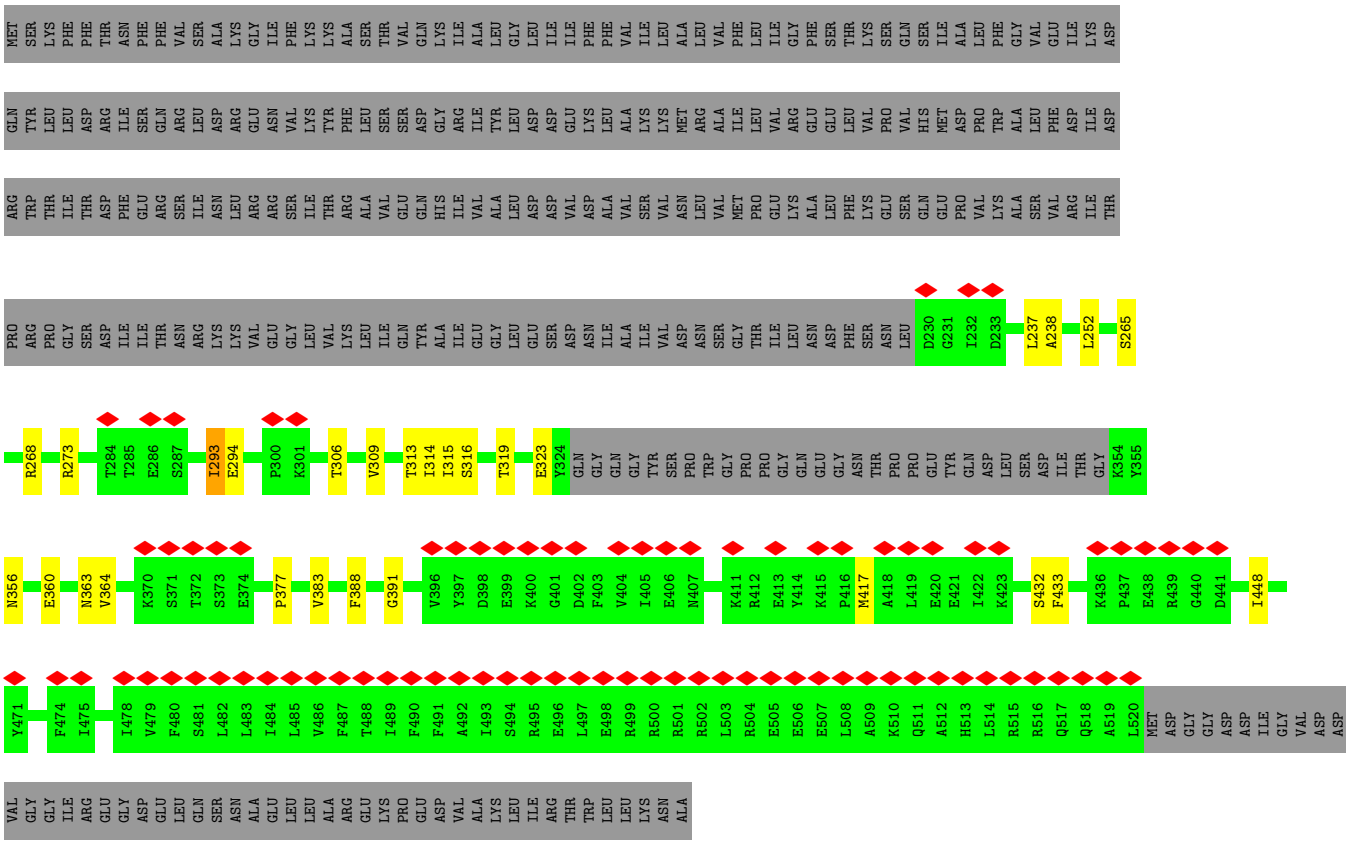




• Molecule 1: Flagellar M-ring protein

Chain a:

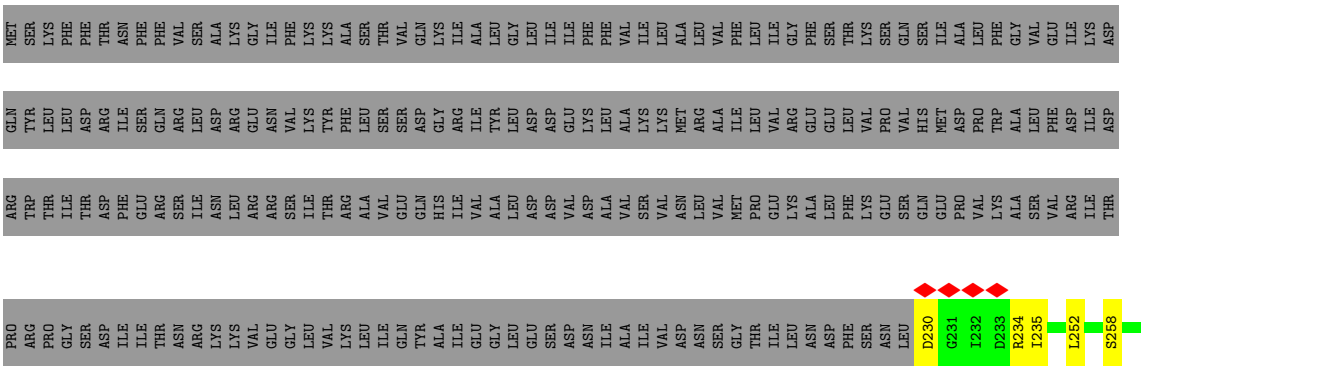


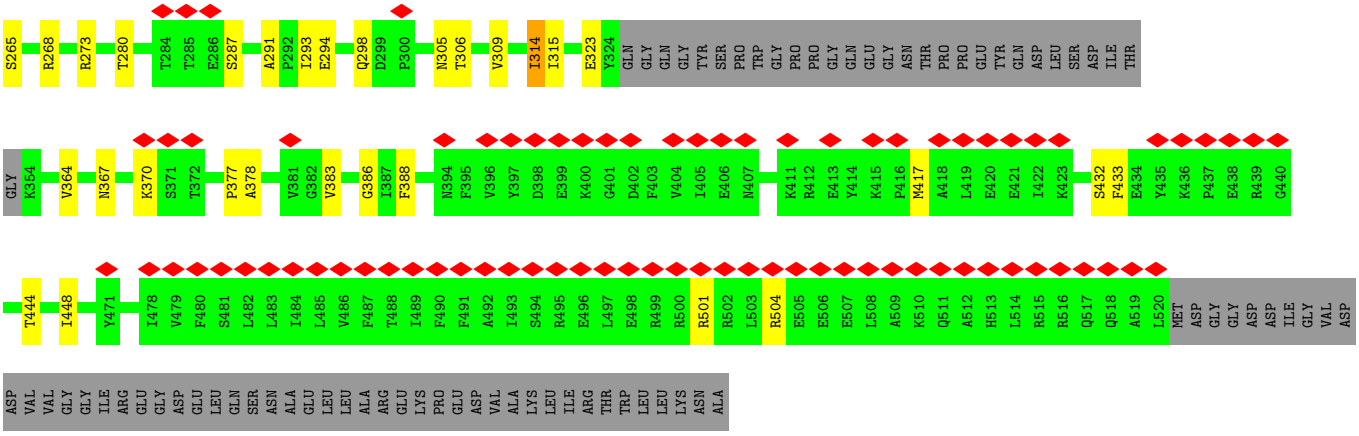


• Molecule 1: Flagellar M-ring protein

Chain b:



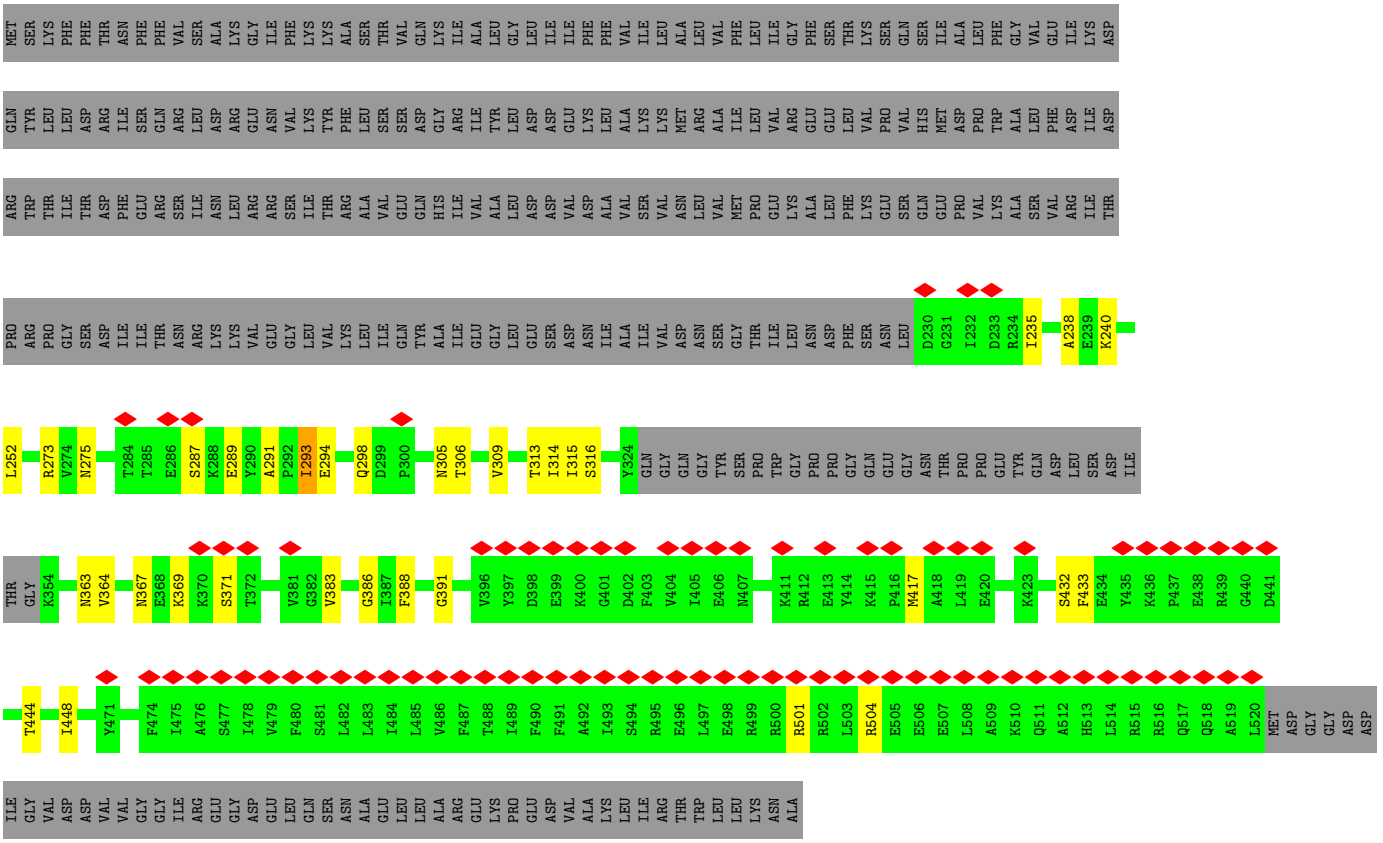




• Molecule 1: Flagellar M-ring protein

Chain c:

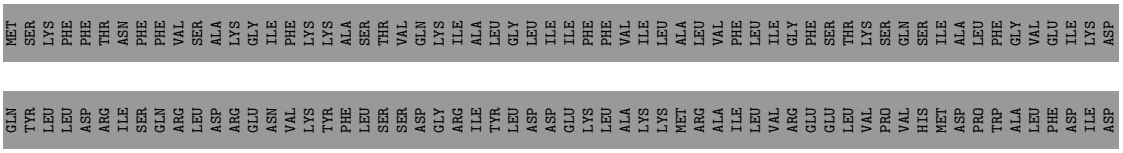


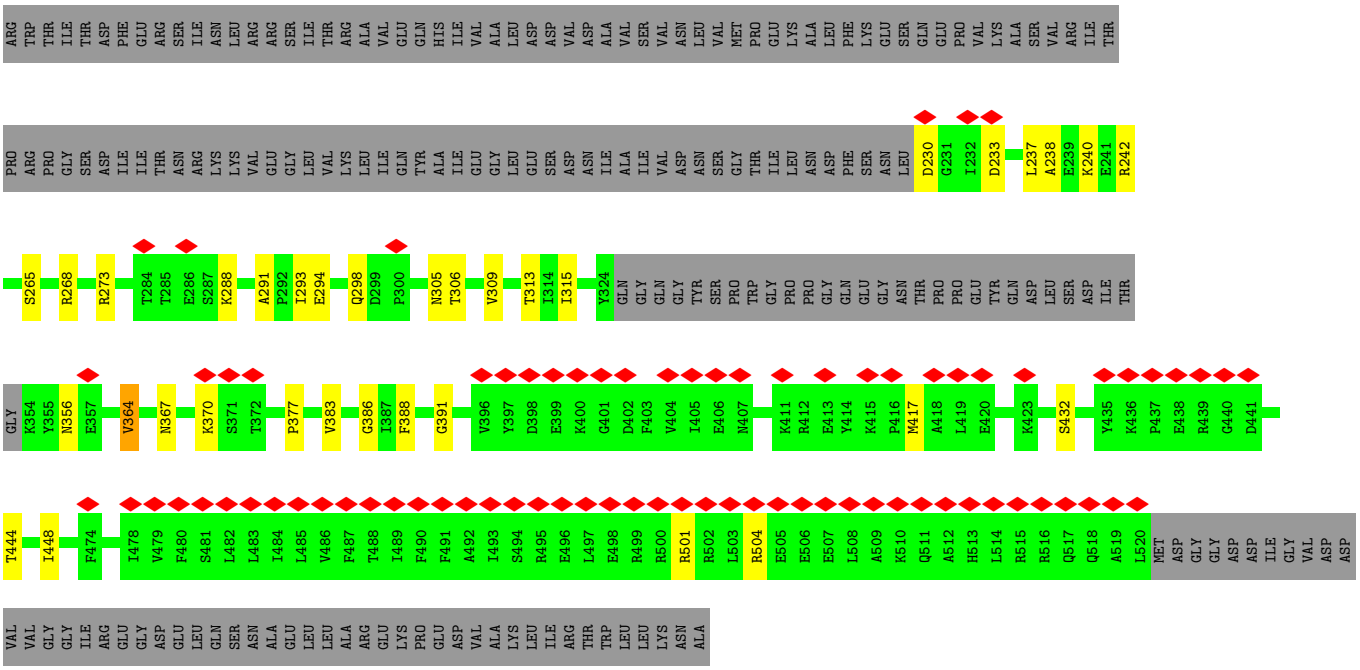


• Molecule 1: Flagellar M-ring protein

Chain d:



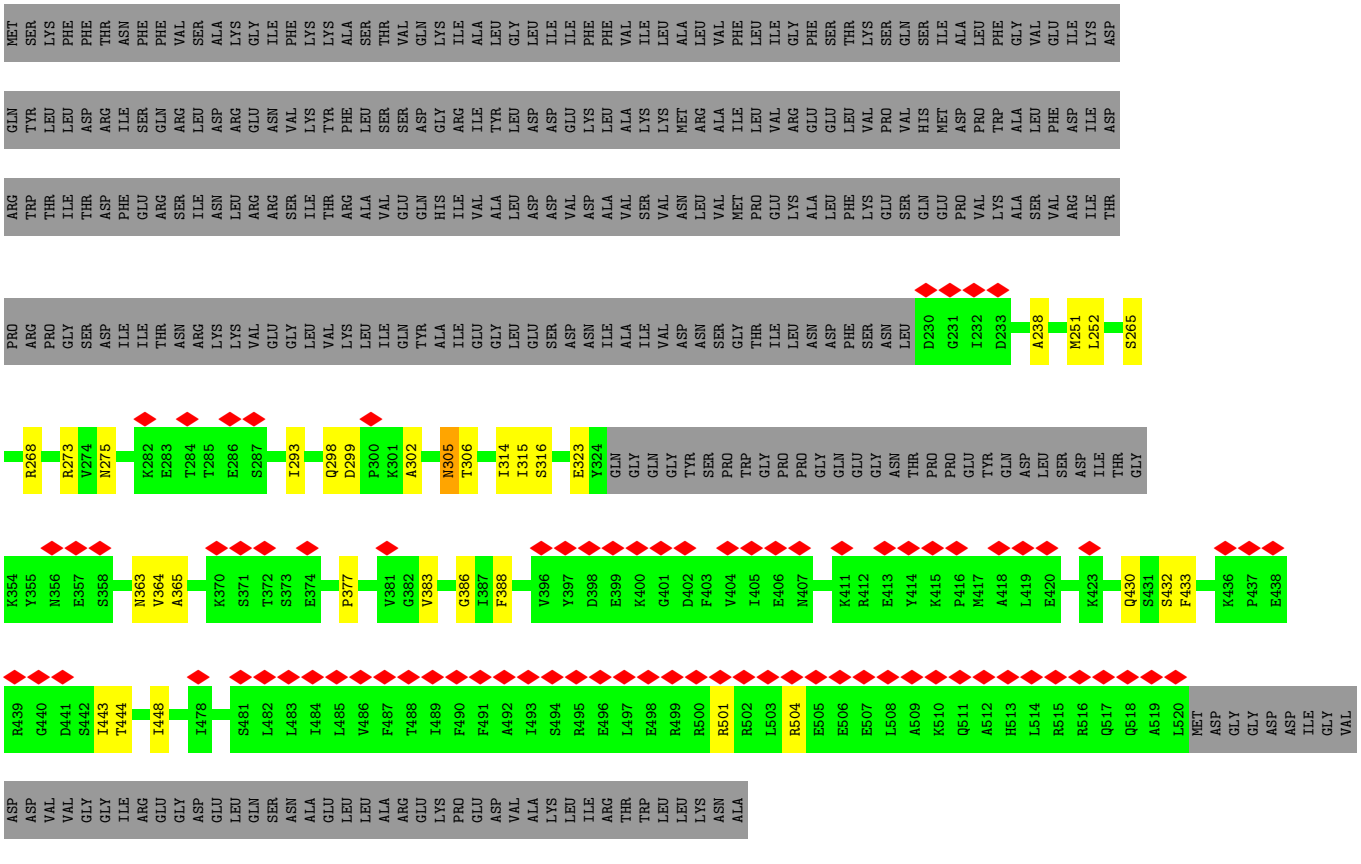




• Molecule 1: Flagellar M-ring protein

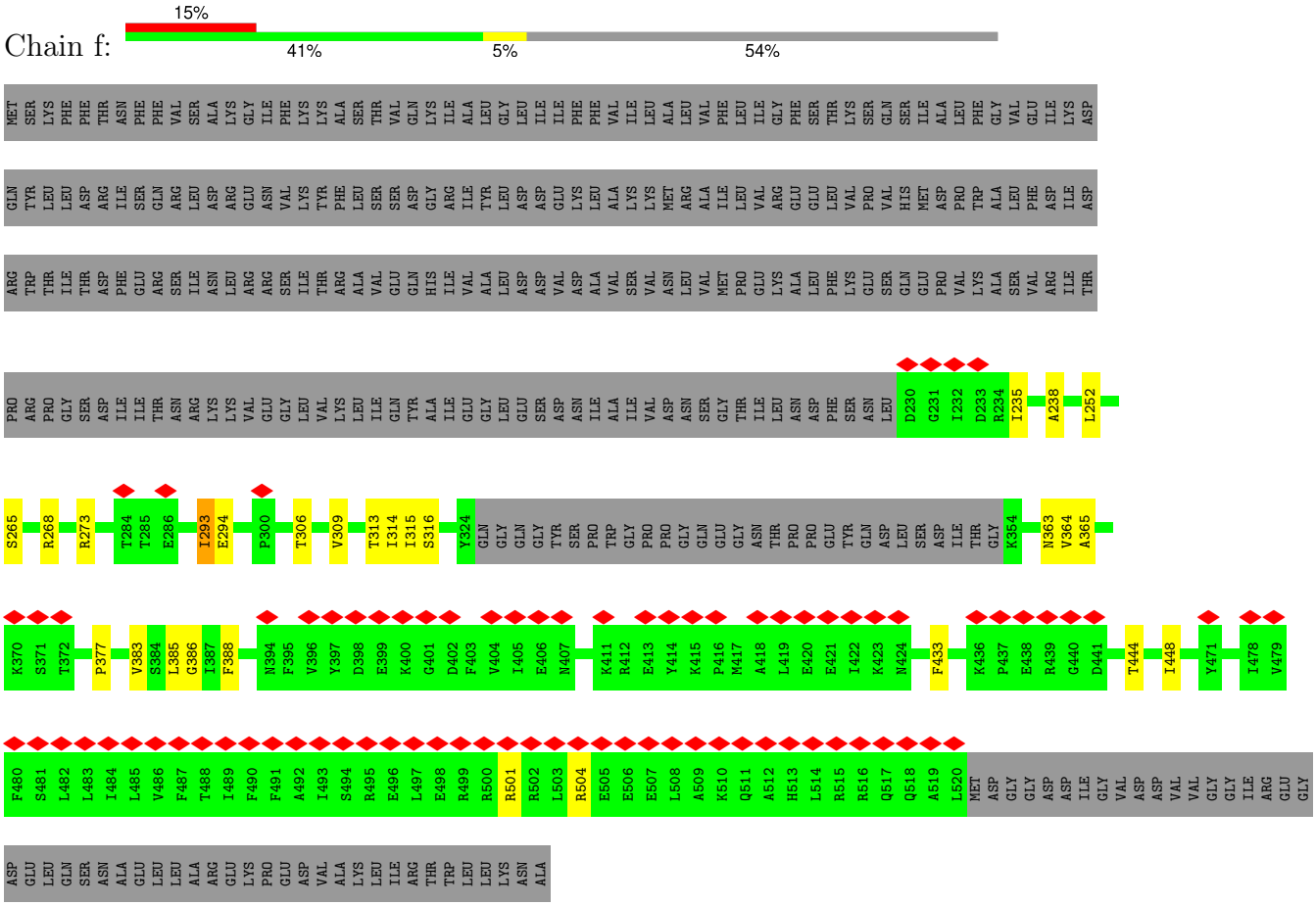
Chain e:





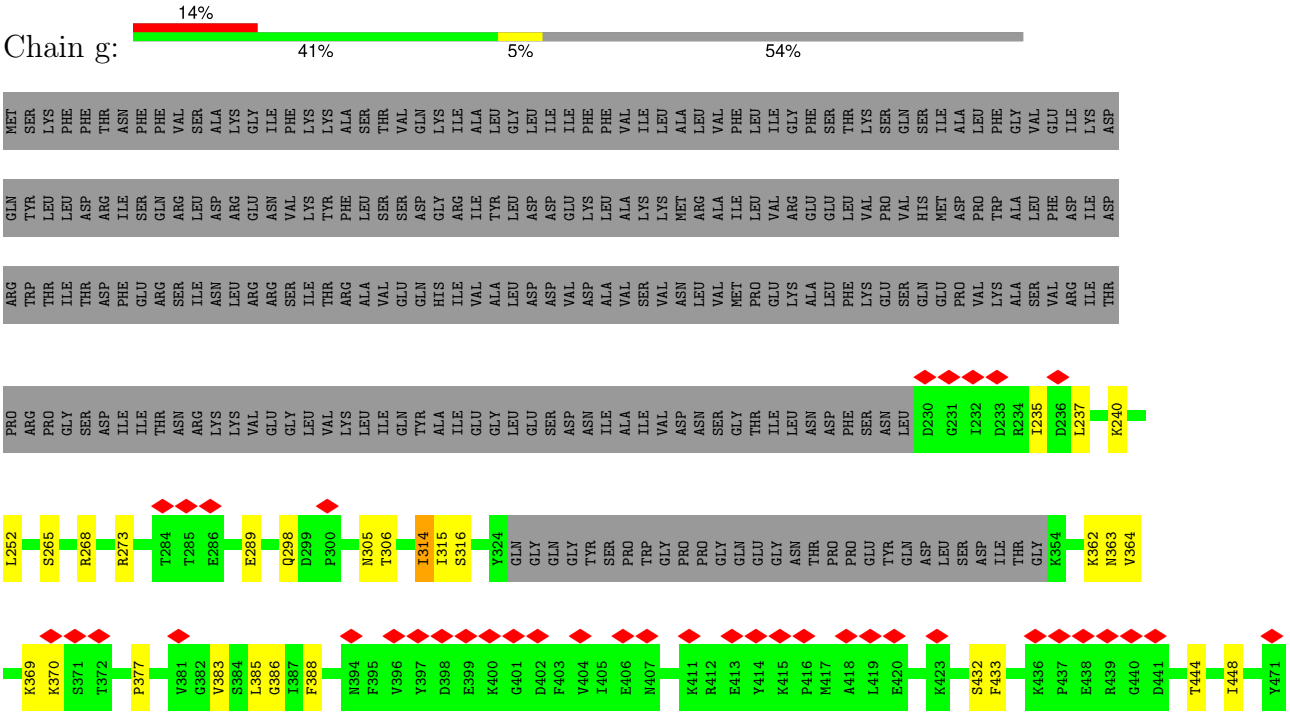
• Molecule 1: Flagellar M-ring protein

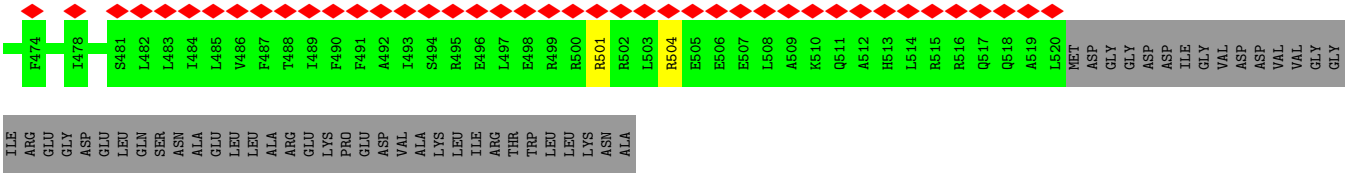
Chain f:



• Molecule 1: Flagellar M-ring protein

Chain g:

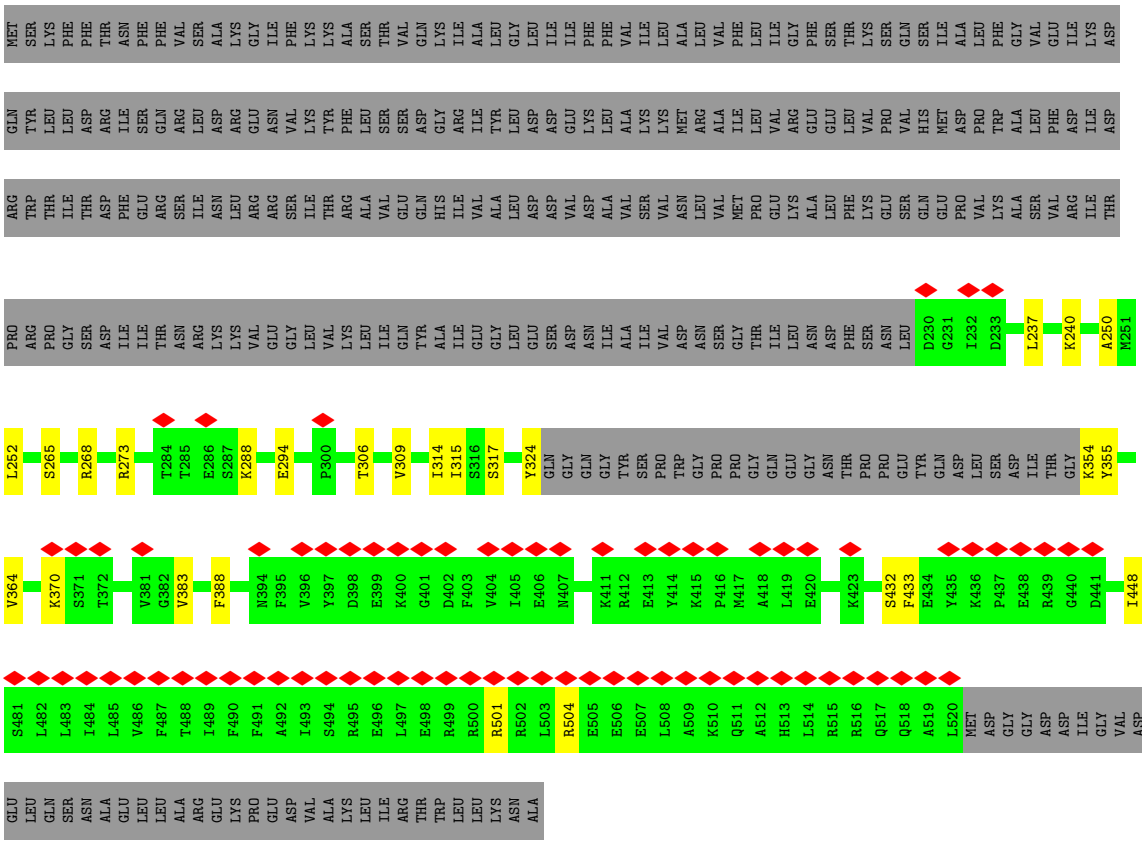




• Molecule 1: Flagellar M-ring protein

Chain h:

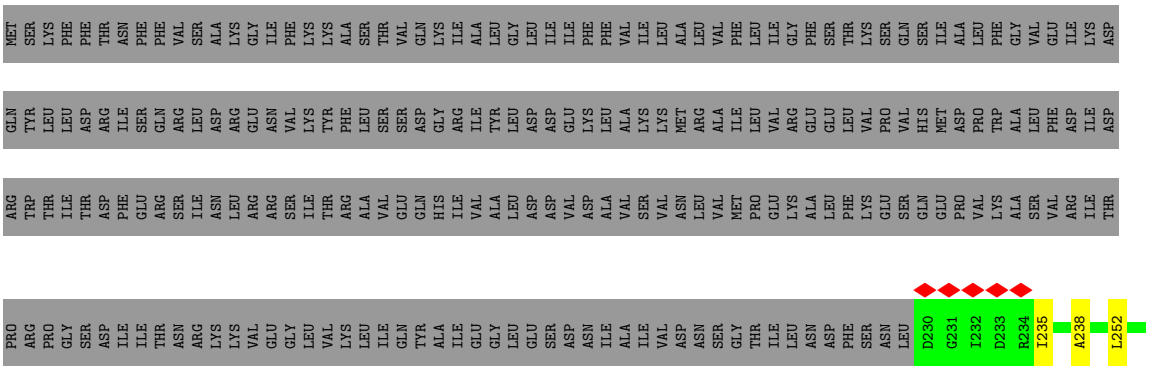


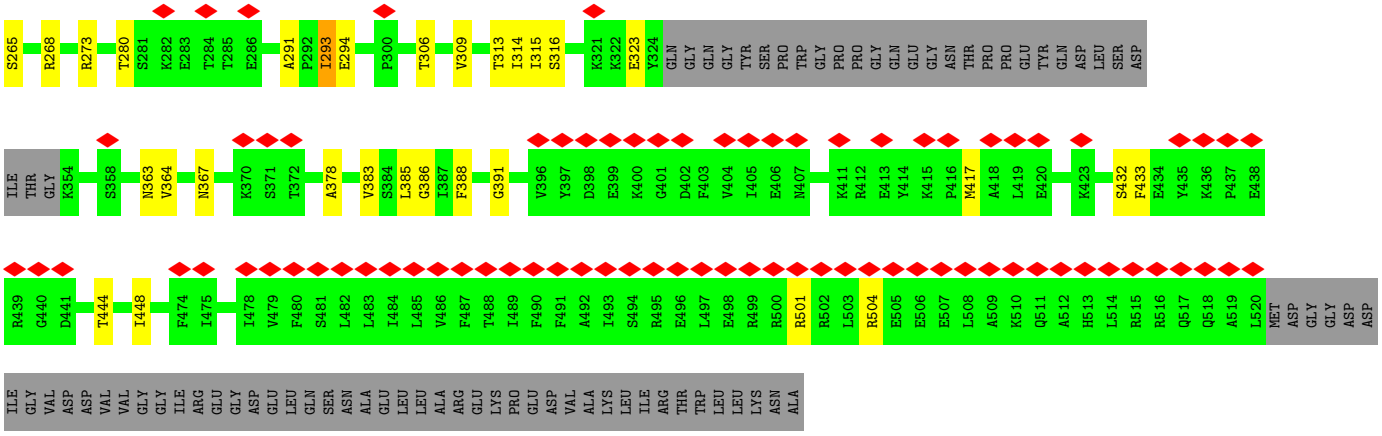


• Molecule 1: Flagellar M-ring protein

Chain i:



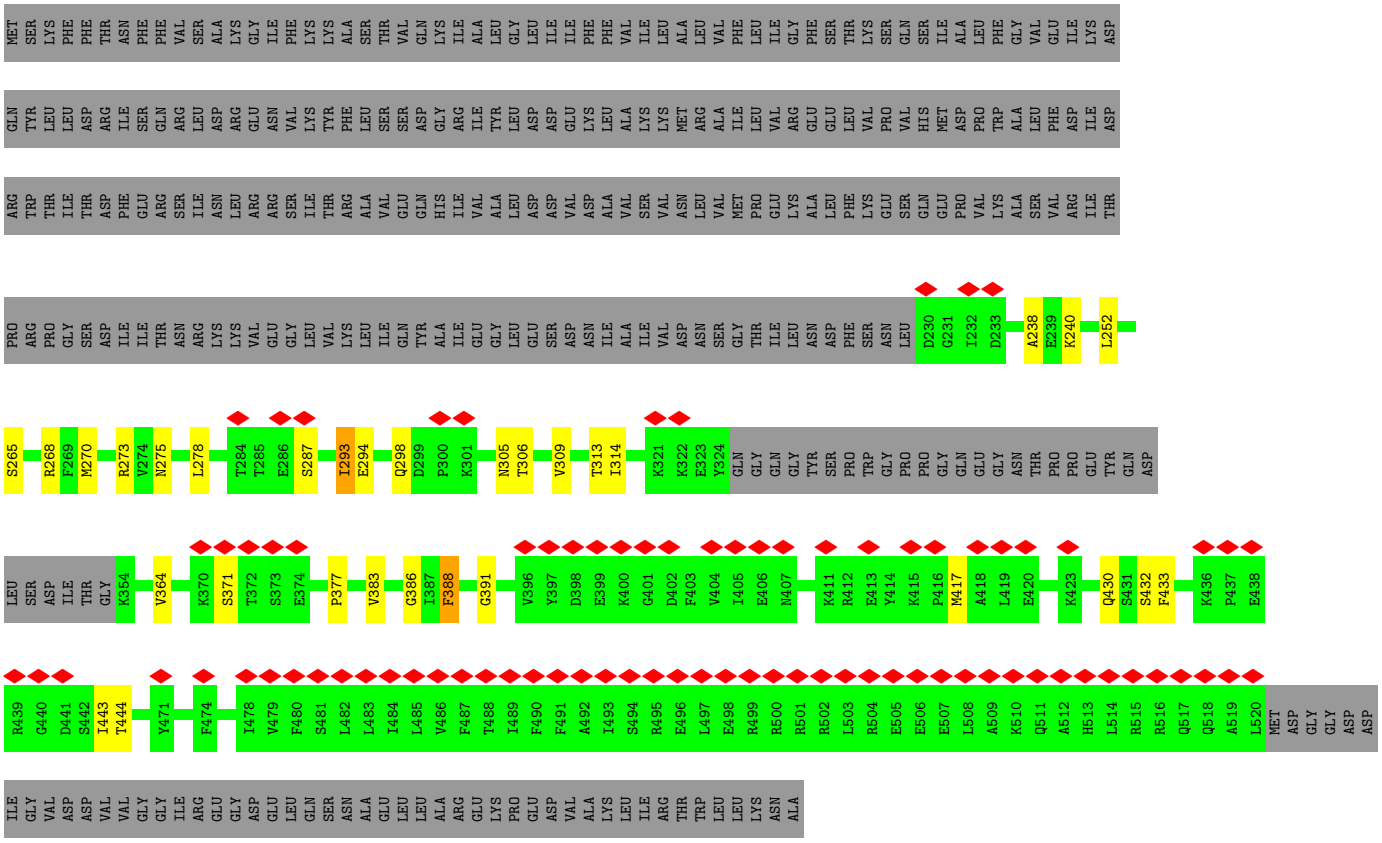




• Molecule 1: Flagellar M-ring protein

Chain j:

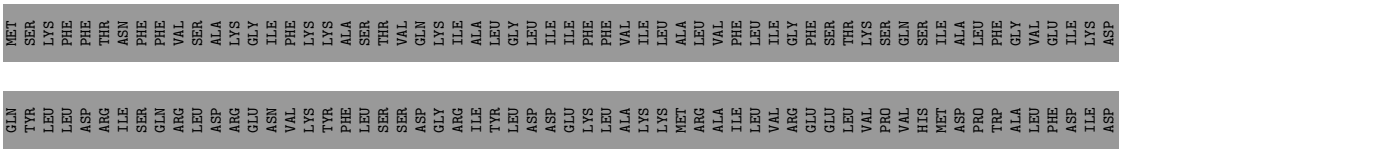


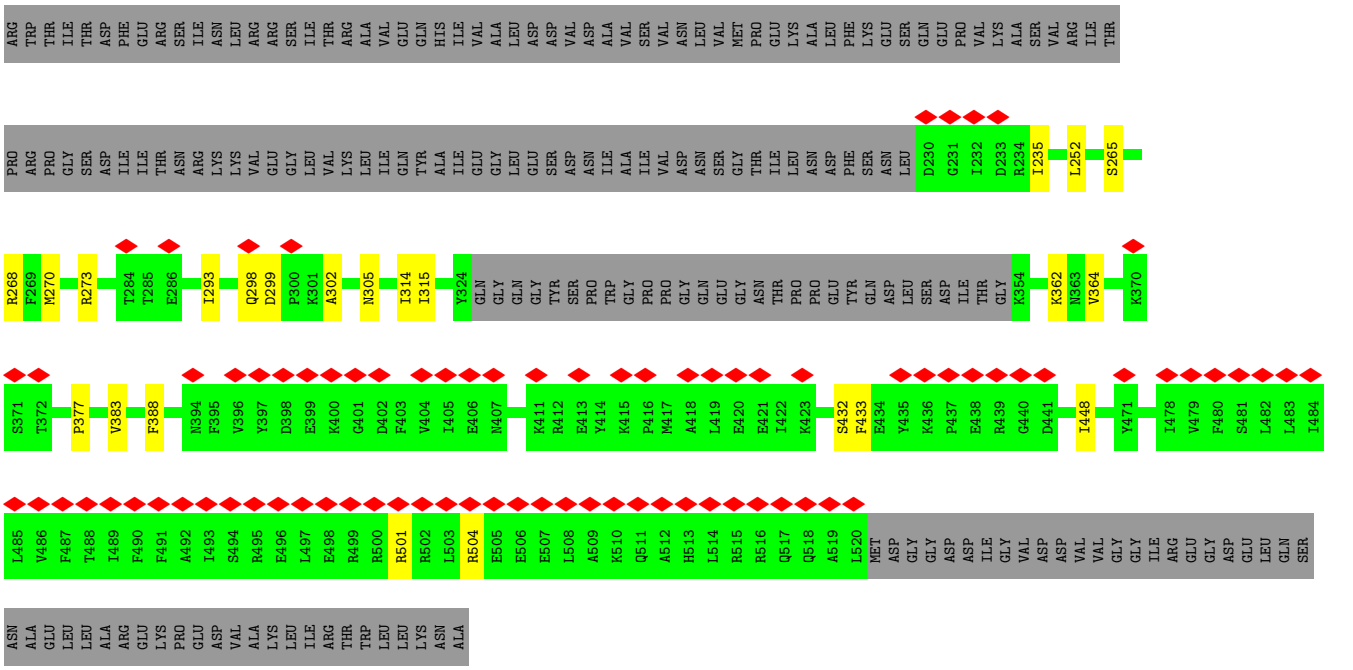


• Molecule 1: Flagellar M-ring protein

Chain k:



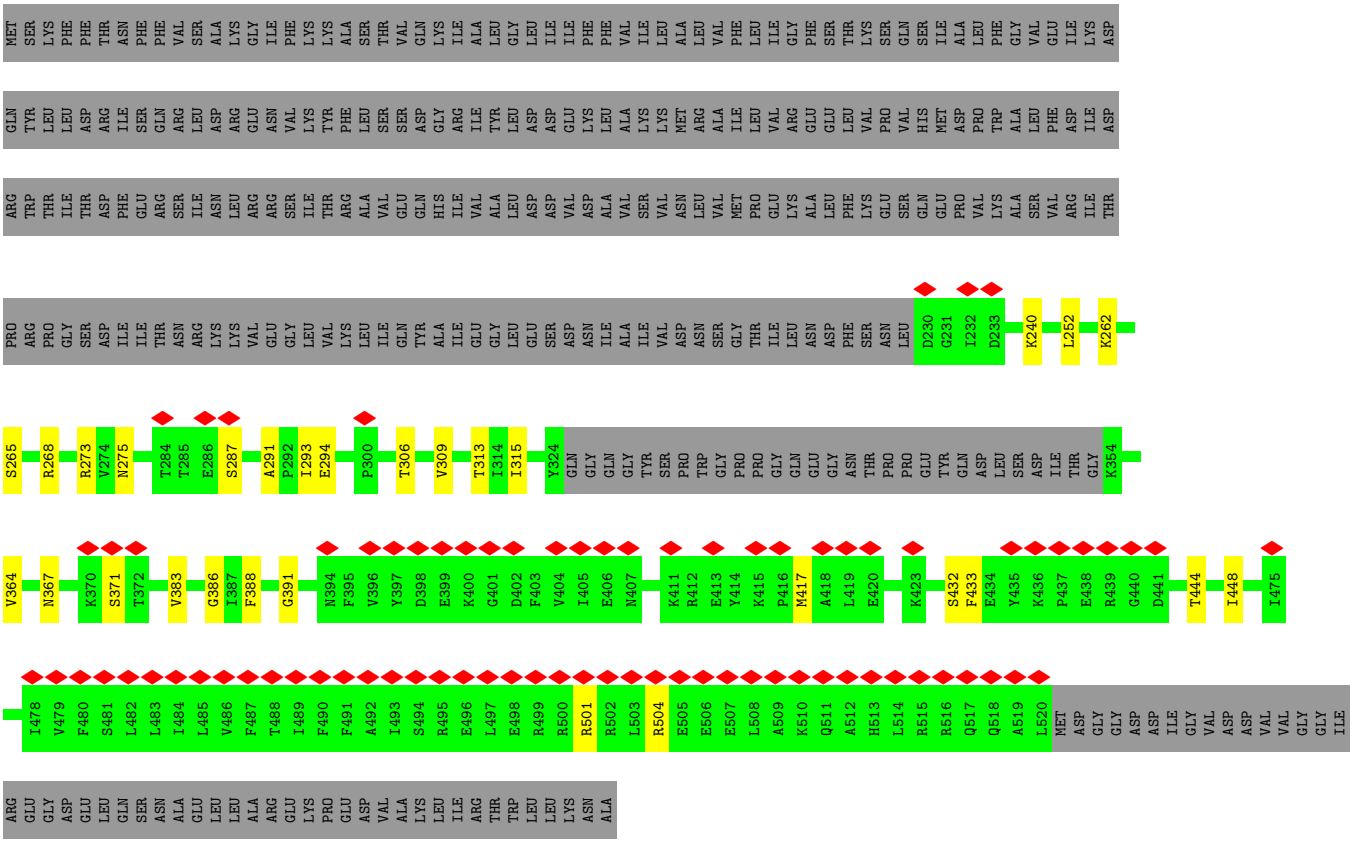




• Molecule 1: Flagellar M-ring protein

Chain l:

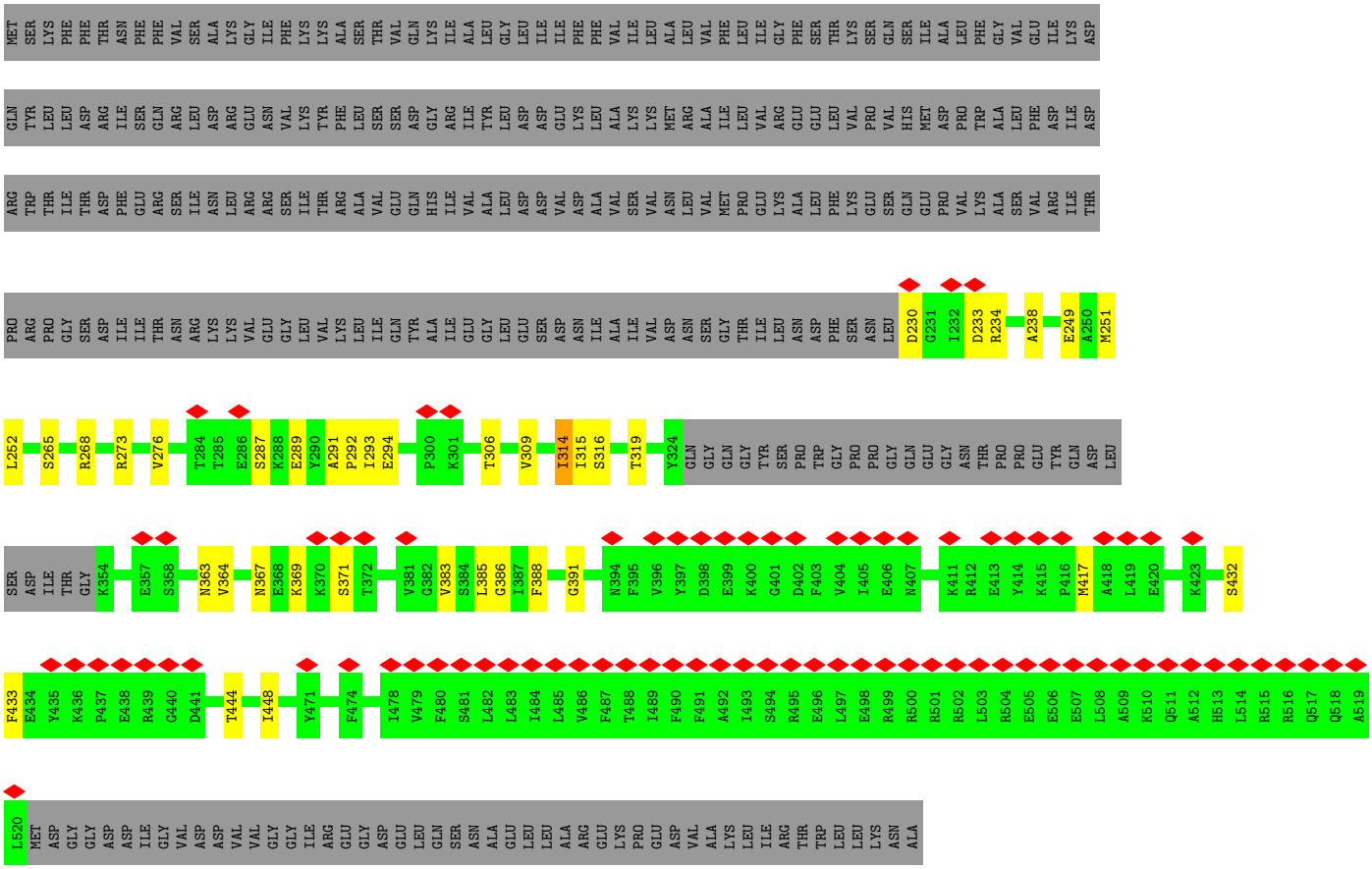




• Molecule 1: Flagellar M-ring protein

Chain m:

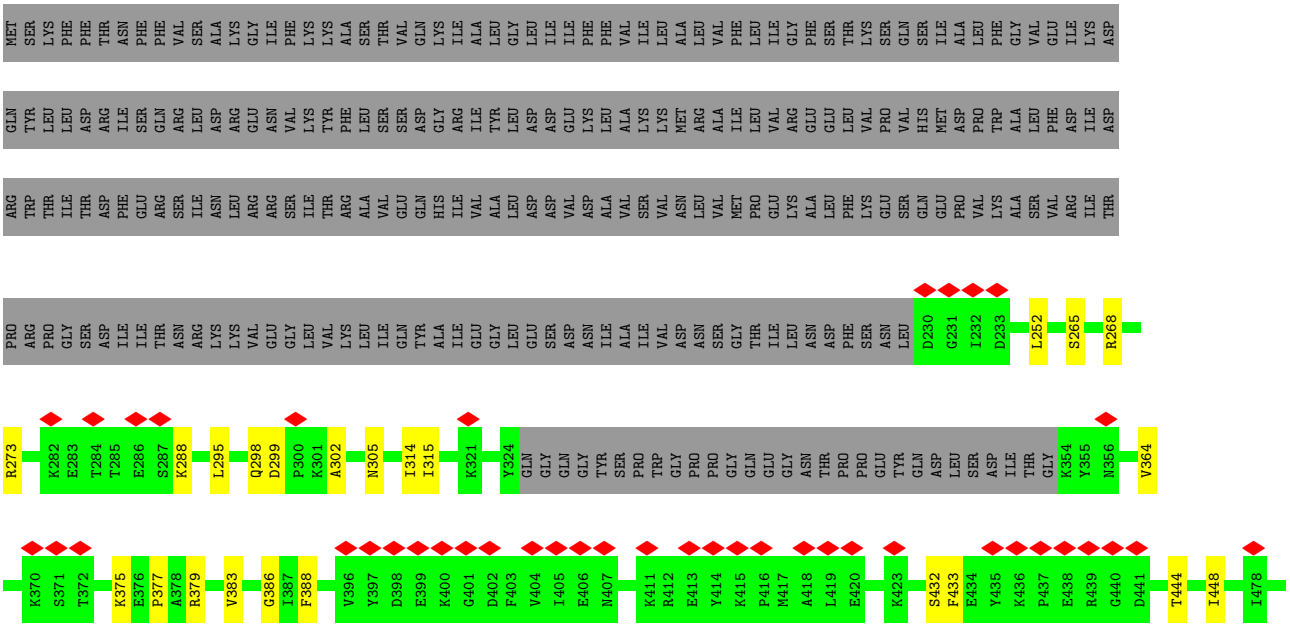


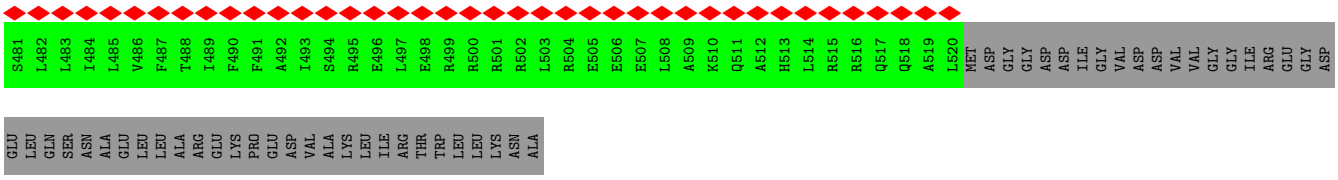


• Molecule 1: Flagellar M-ring protein

Chain n:



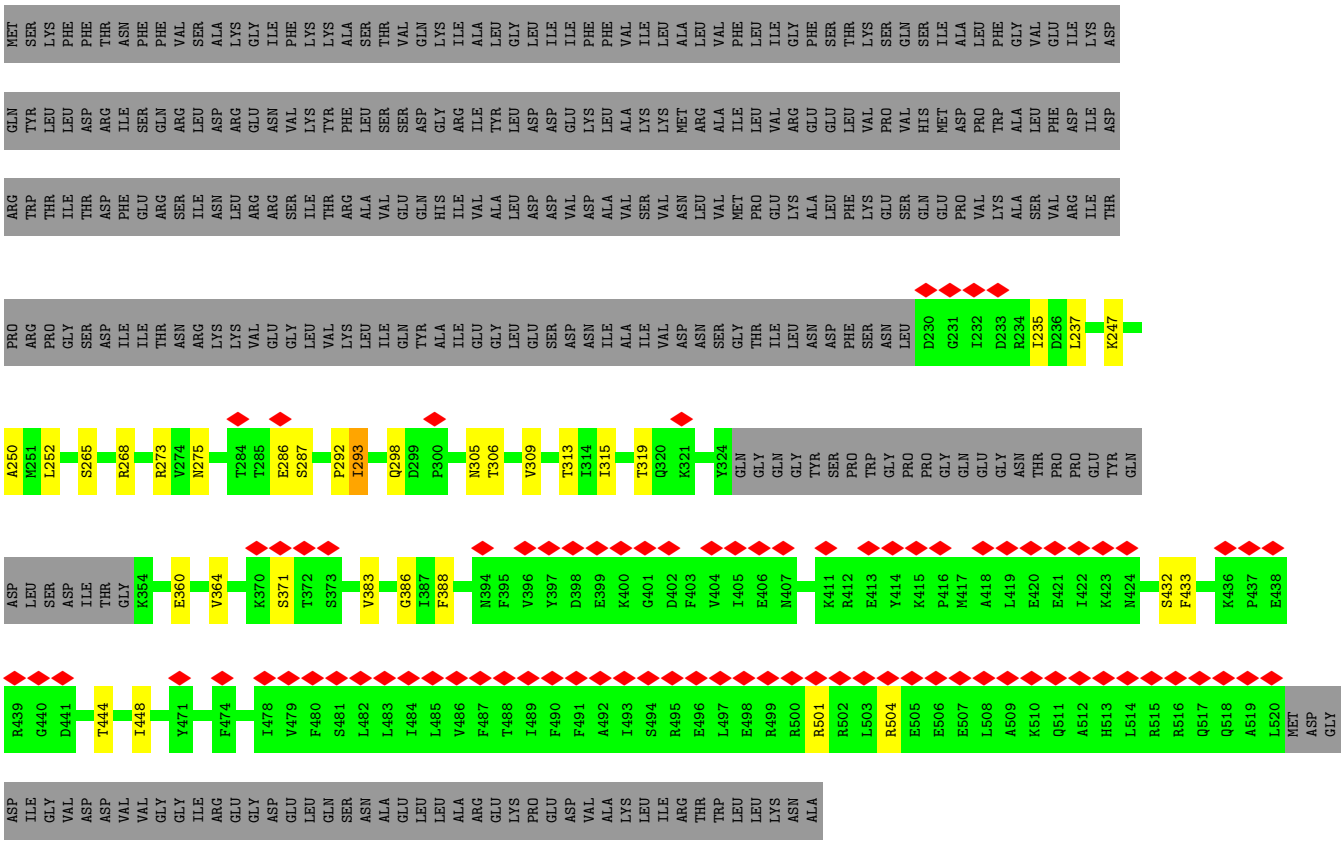




• Molecule 1: Flagellar M-ring protein

Chain o:

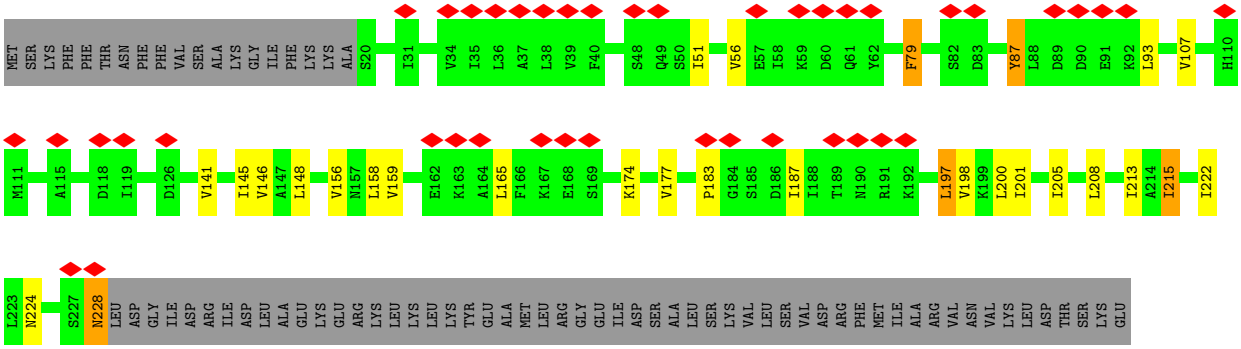


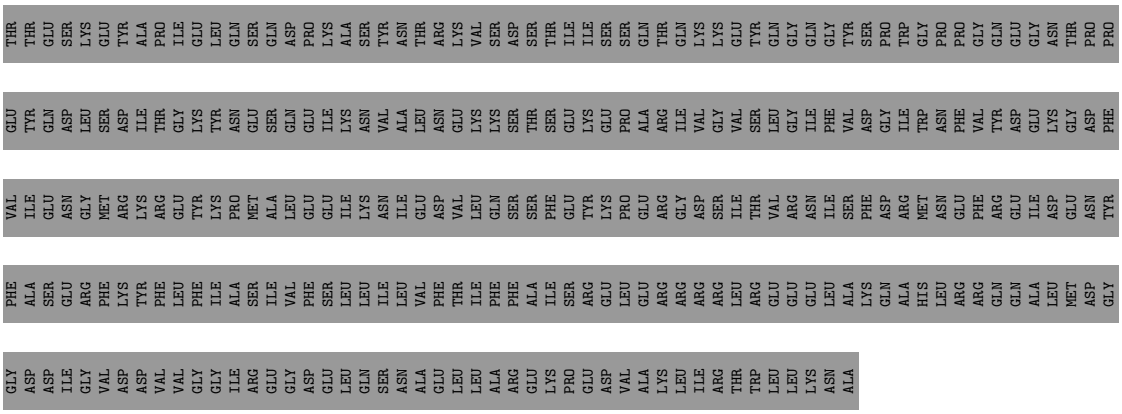


• Molecule 1: Flagellar M-ring protein

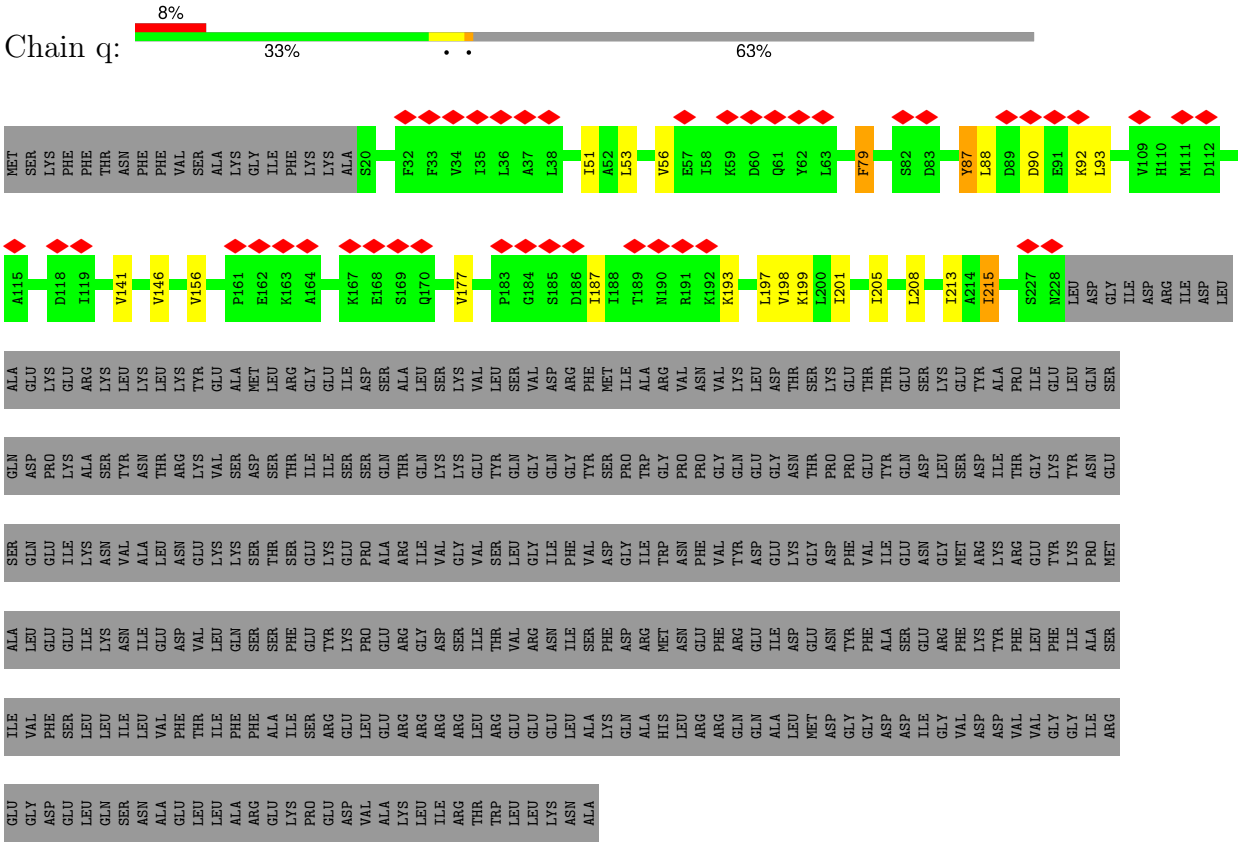
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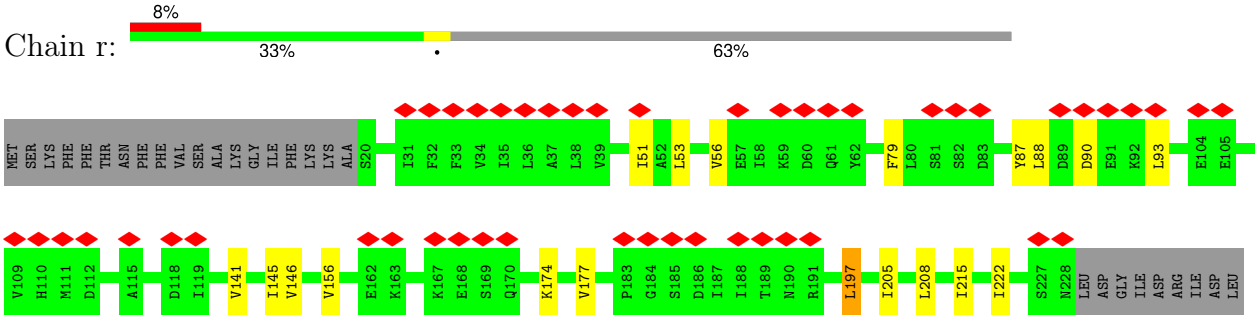


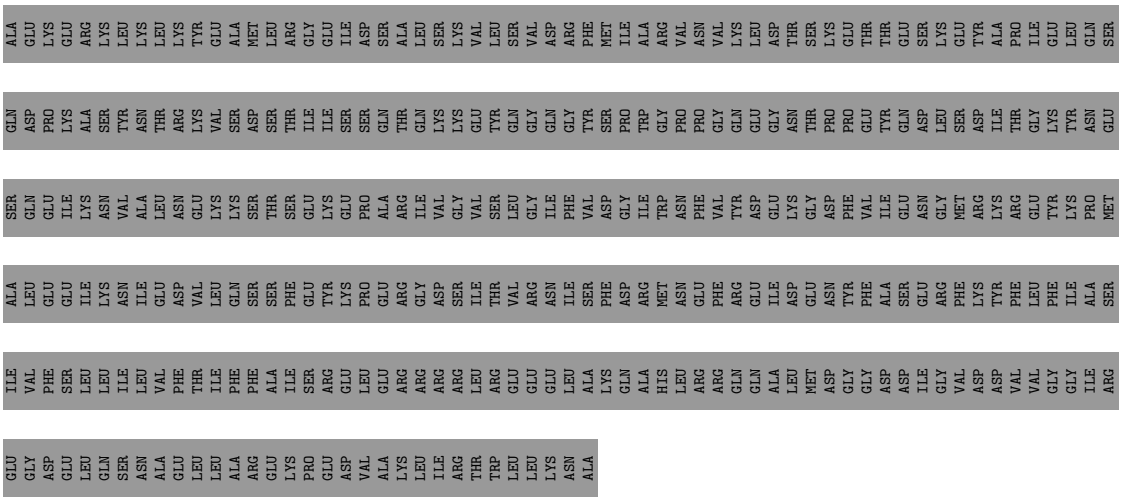


• Molecule 1: Flagellar M-ring protein

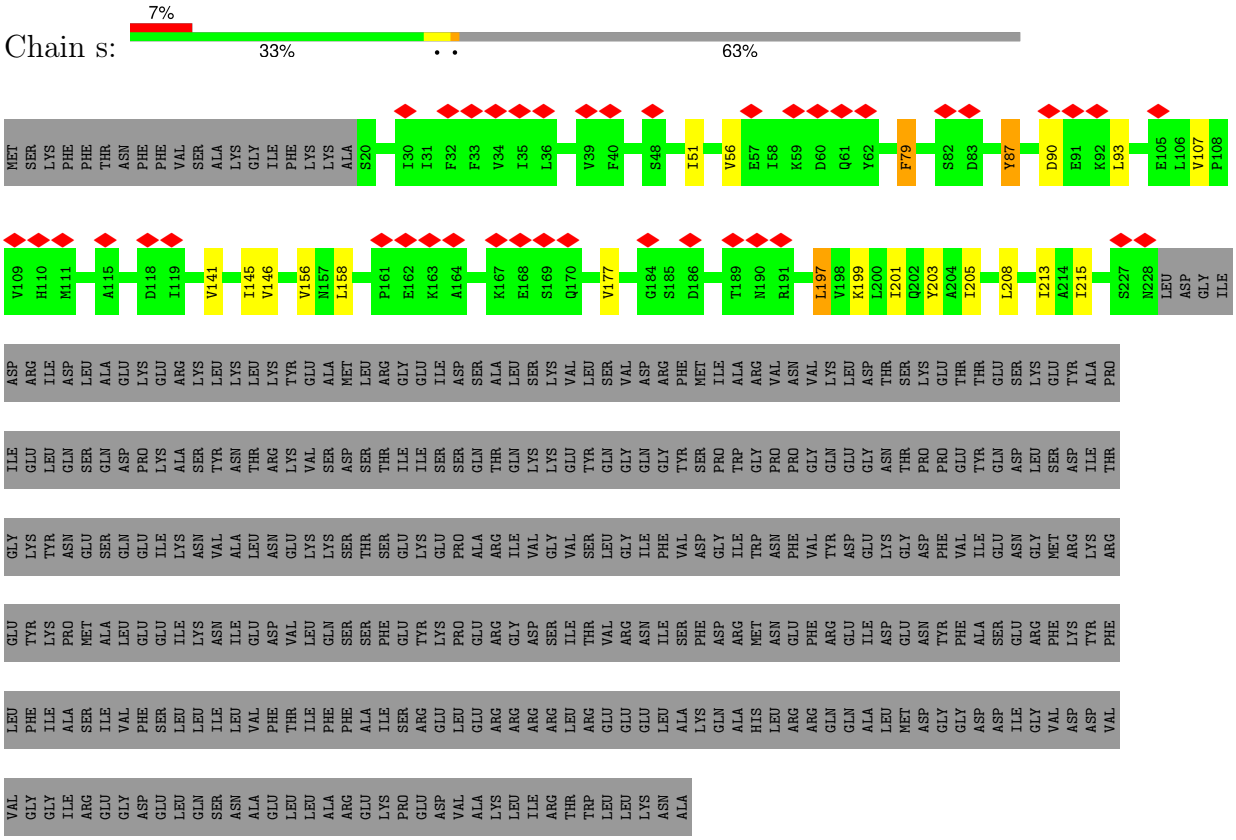


• Molecule 1: Flagellar M-ring protein

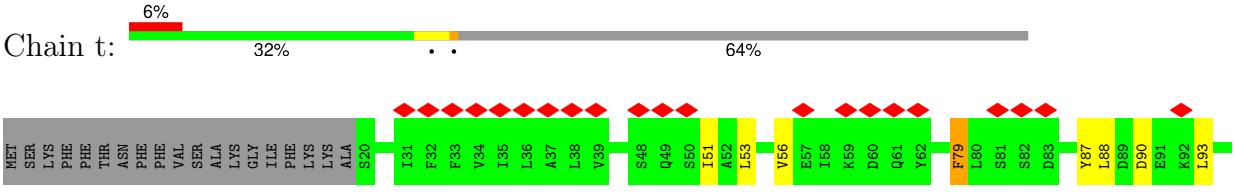


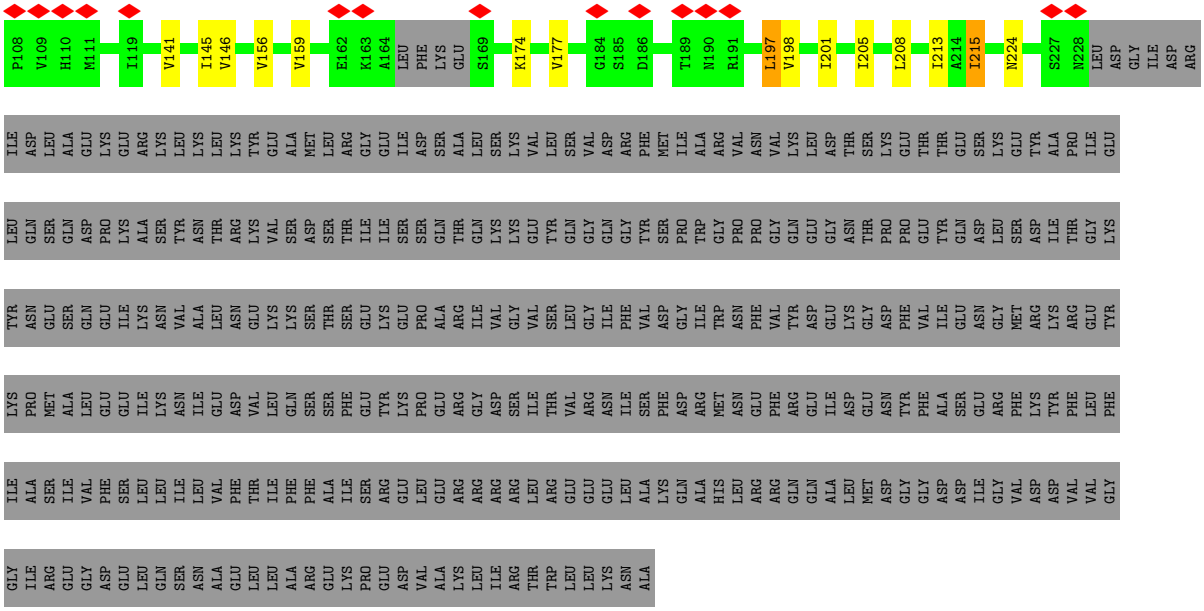


• Molecule 1: Flagellar M-ring protein



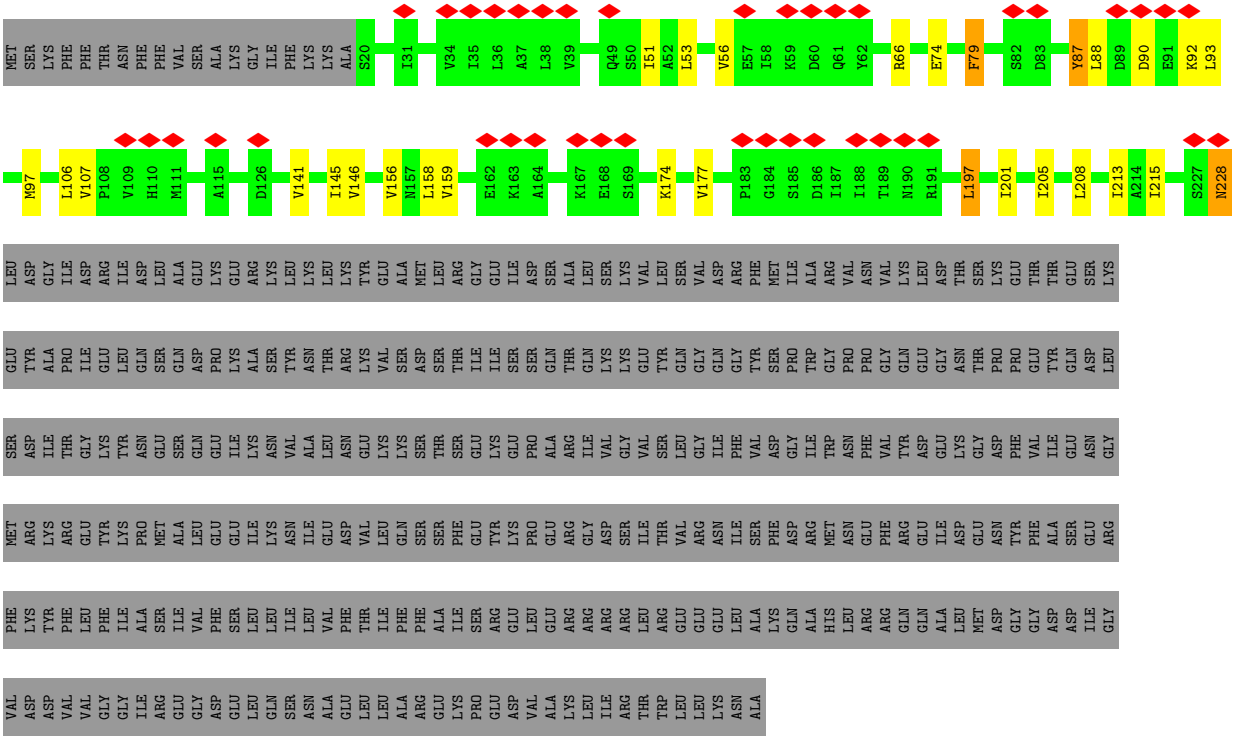
• Molecule 1: Flagellar M-ring protein





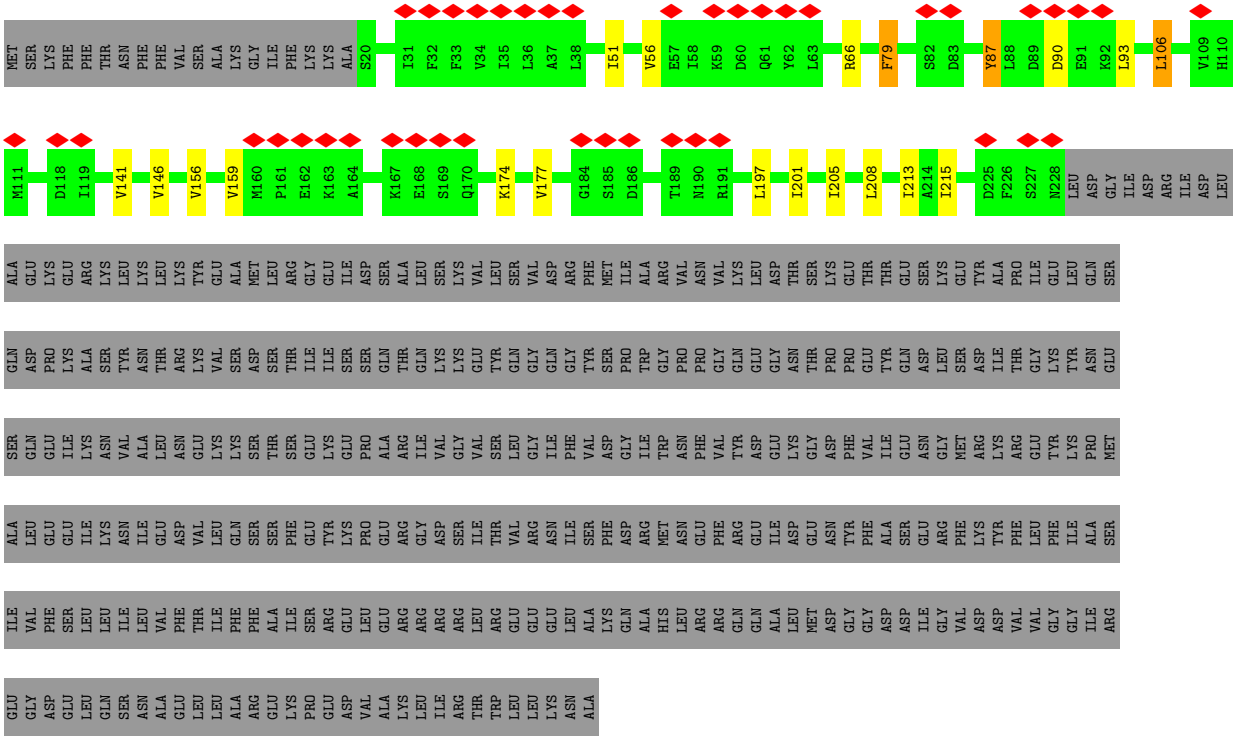
• Molecule 1: Flagellar M-ring protein



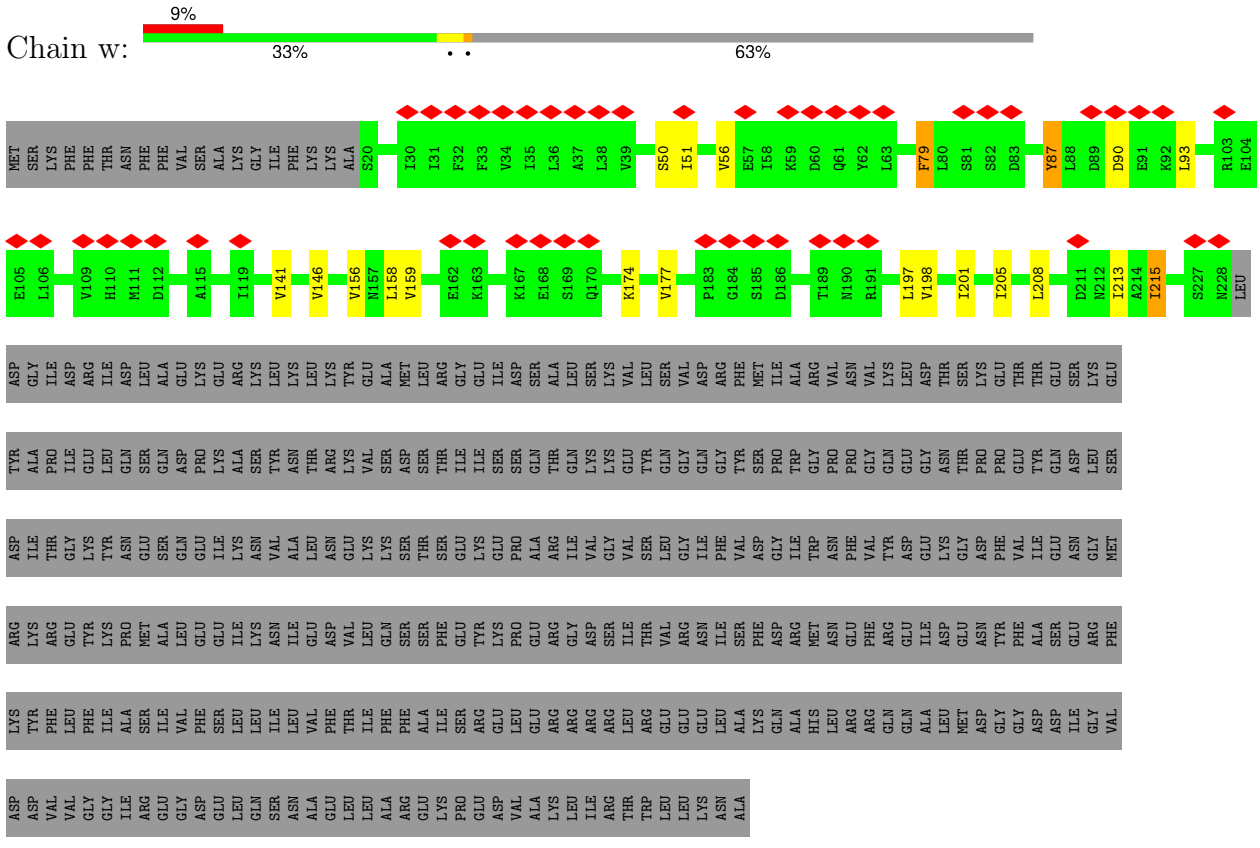


• Molecule 1: Flagellar M-ring protein



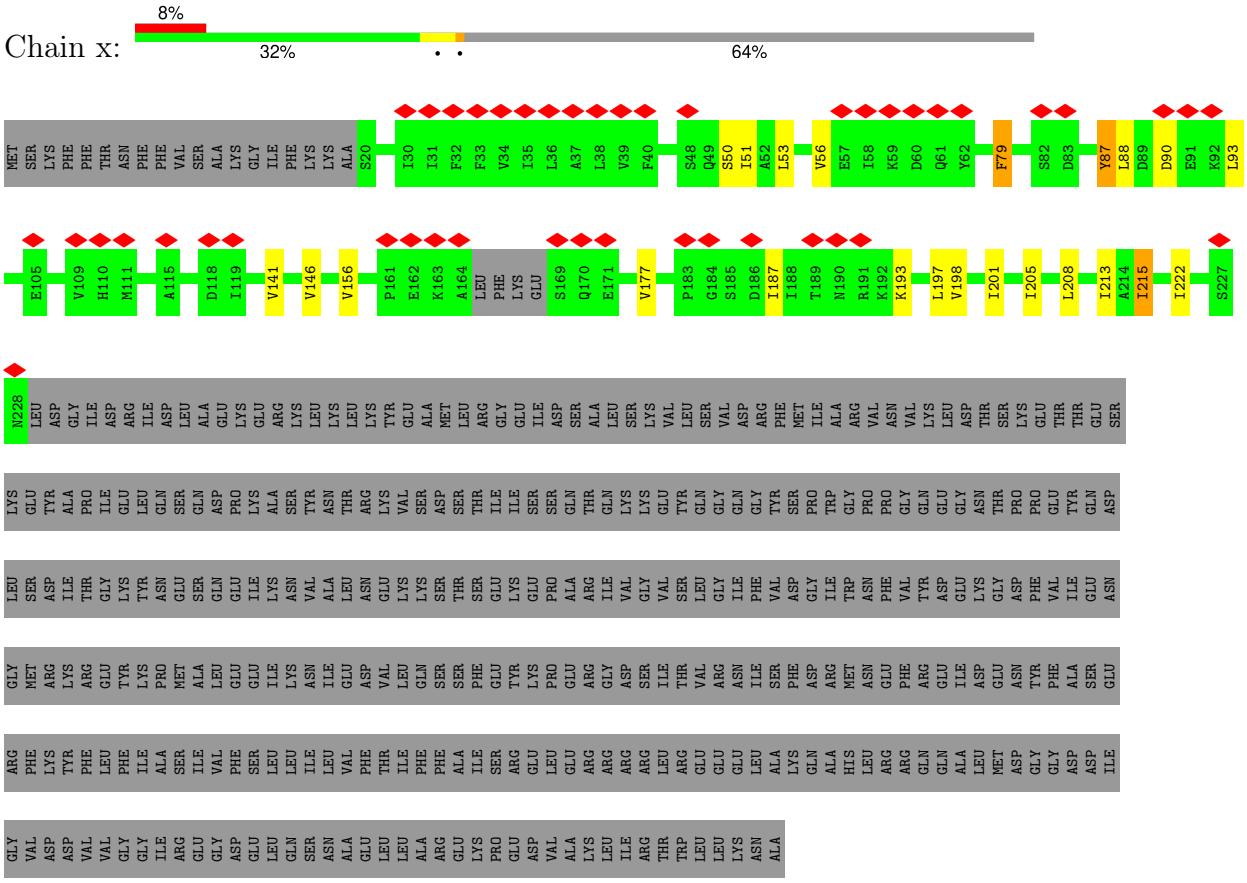


• Molecule 1: Flagellar M-ring protein



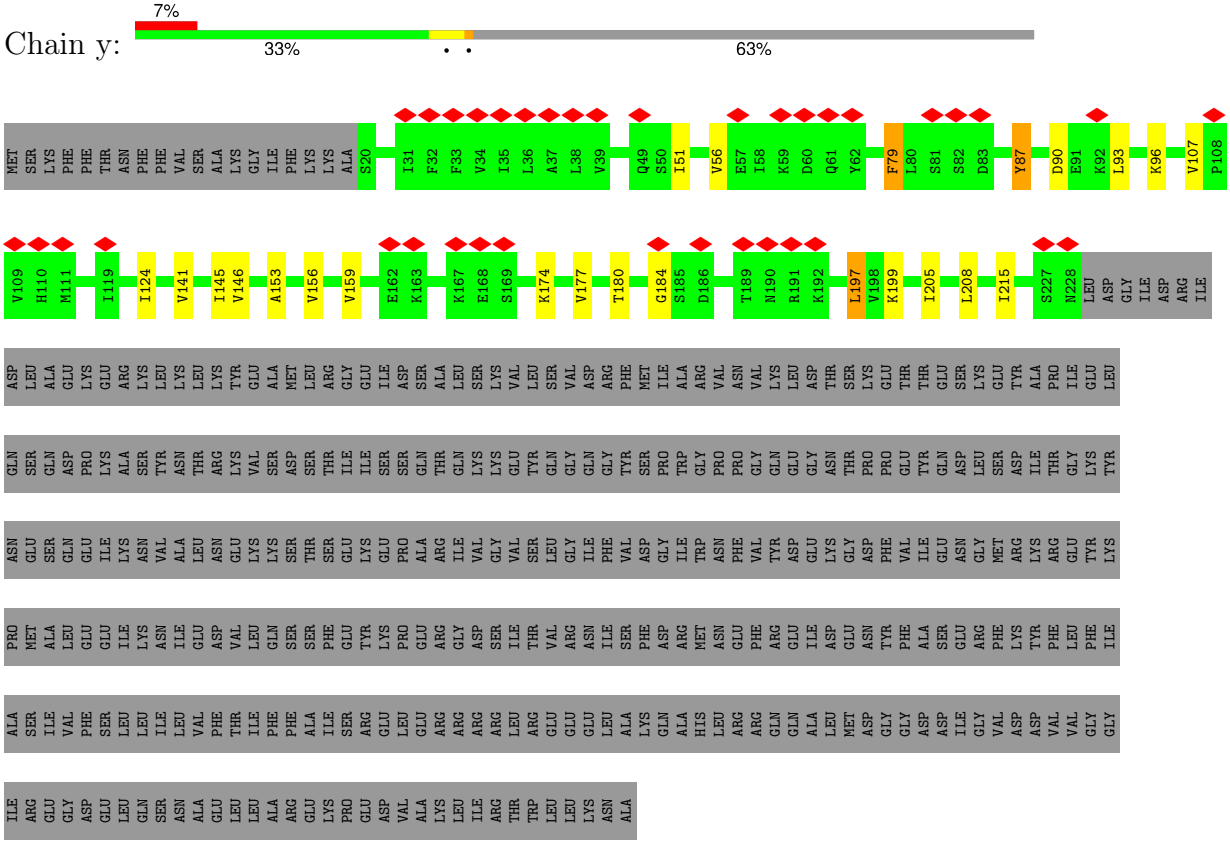
• Molecule 1: Flagellar M-ring protein

Chain x:



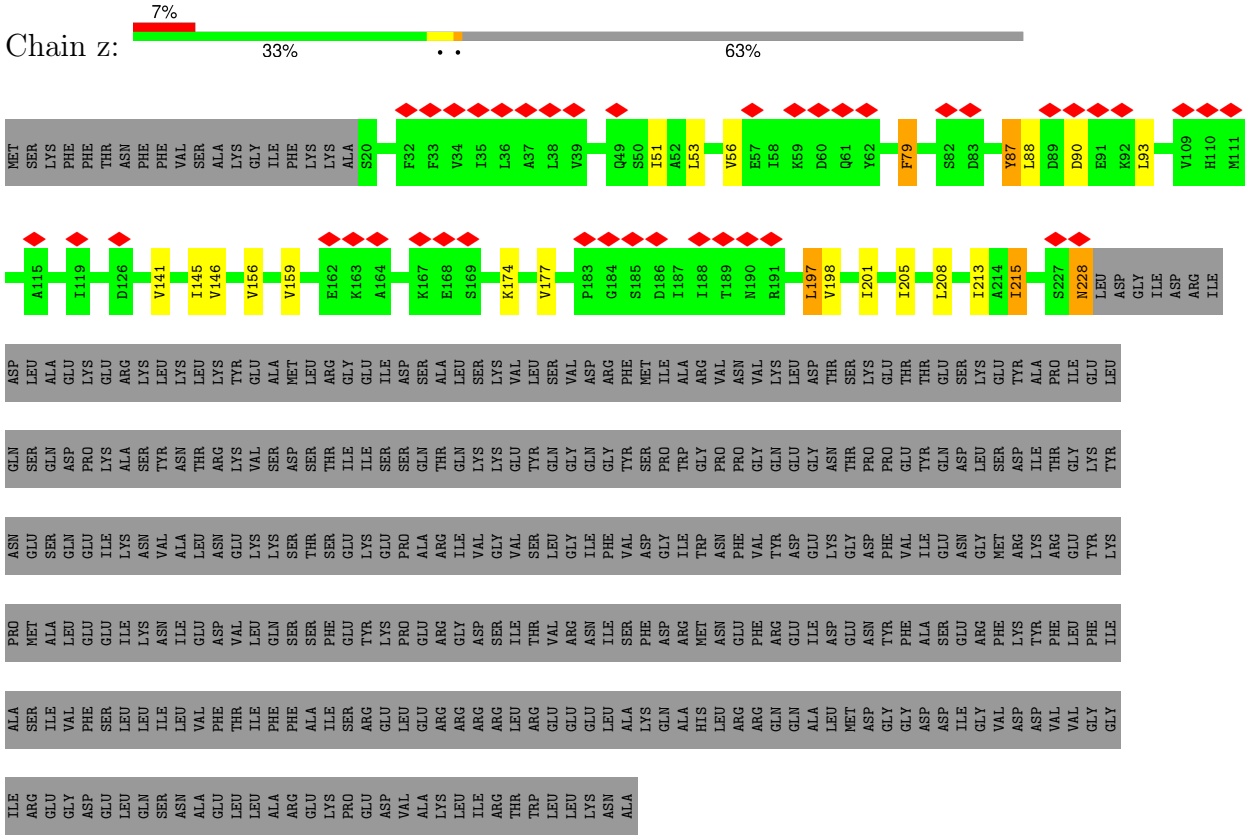
• Molecule 1: Flagellar M-ring protein

Chain y:



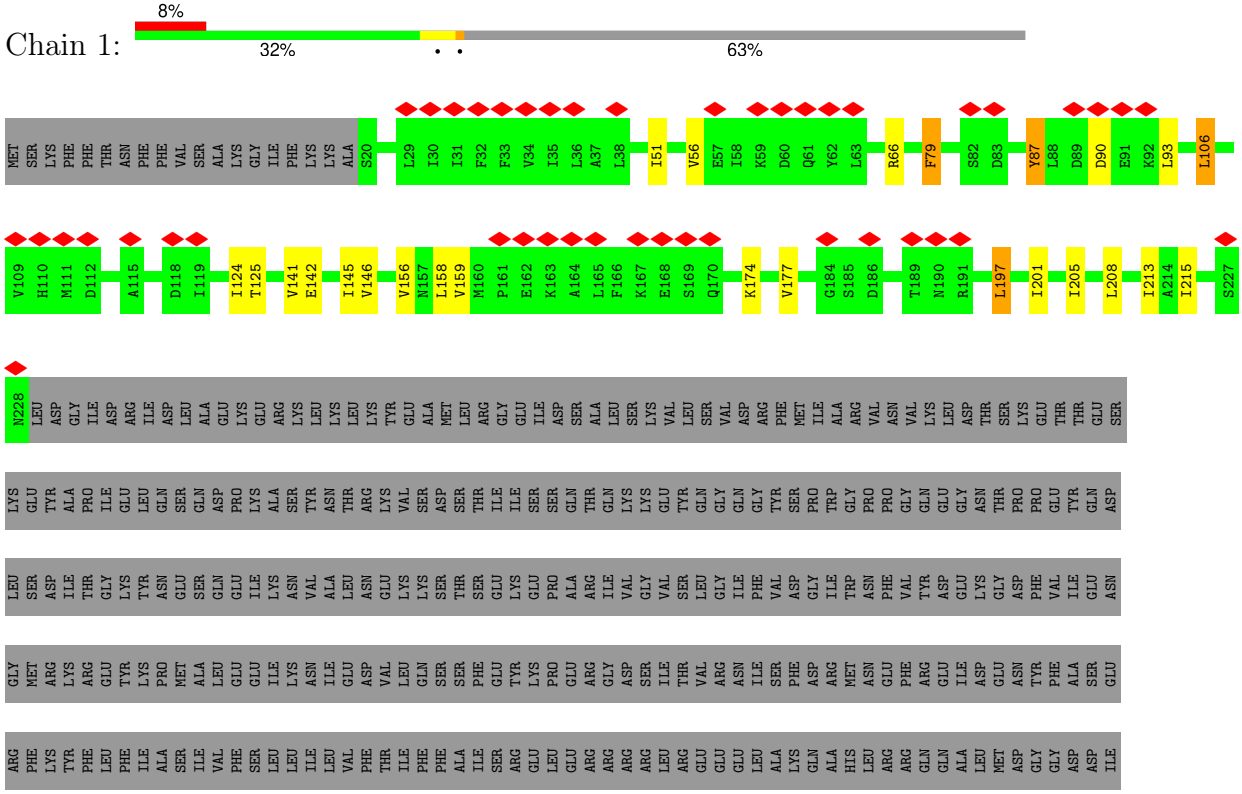
• Molecule 1: Flagellar M-ring protein

Chain z:



• Molecule 1: Flagellar M-ring protein

Chain 1:

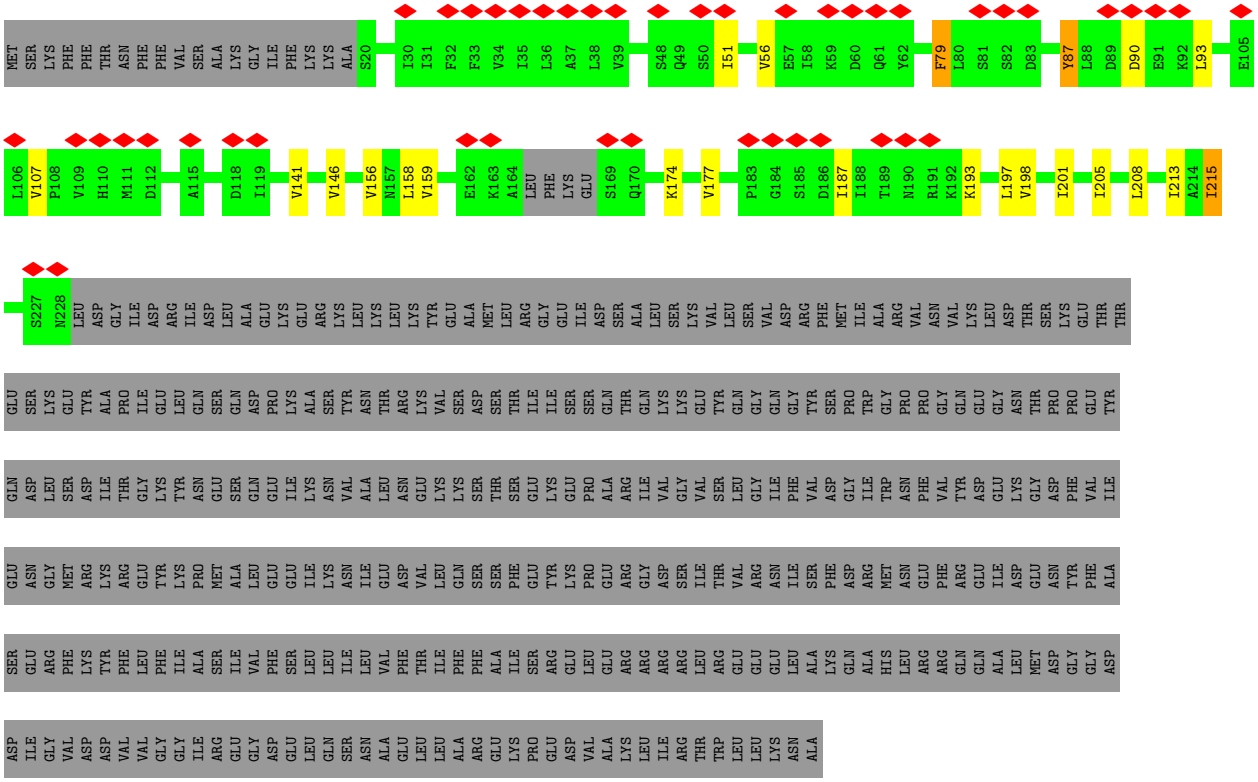




• Molecule 1: Flagellar M-ring protein

Chain 2:

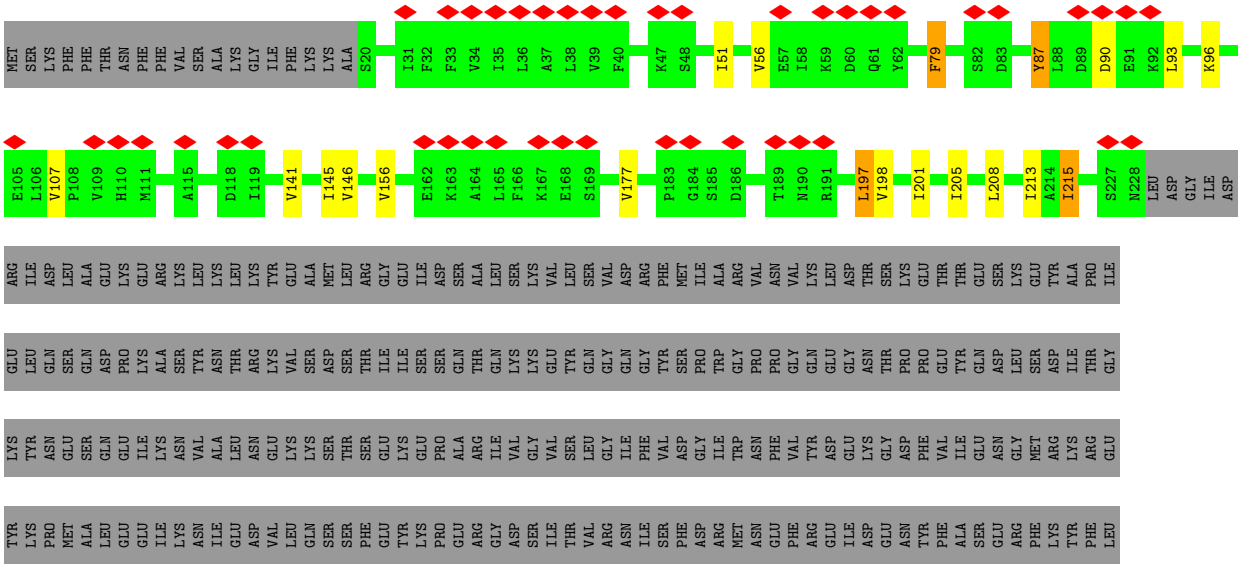


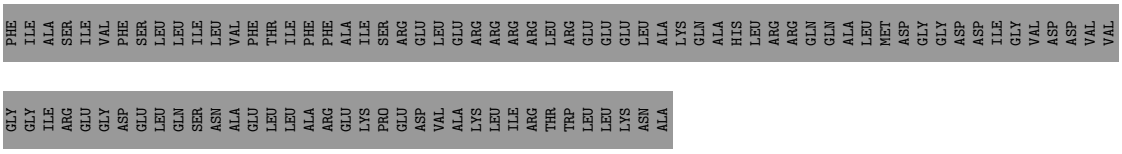


• Molecule 1: Flagellar M-ring protein

Chain 3:



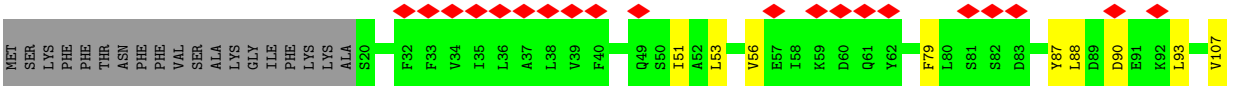


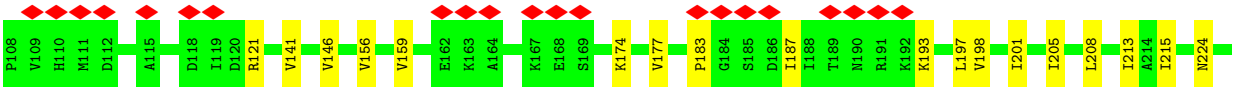


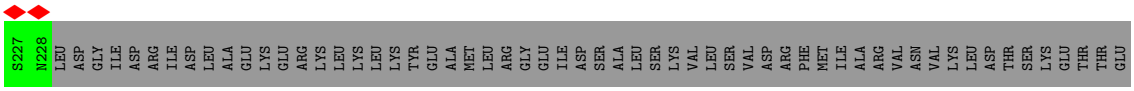
• Molecule 1: Flagellar M-ring protein

Chain 4:

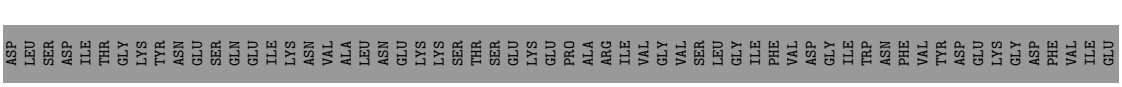


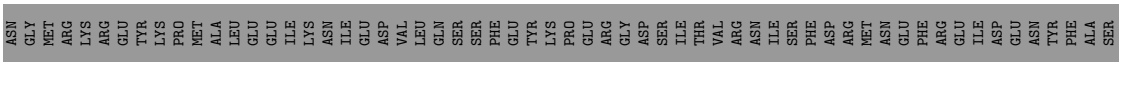


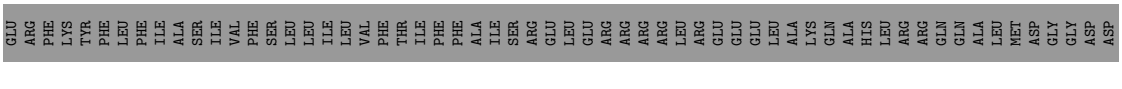










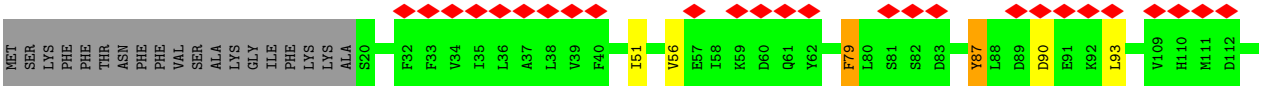


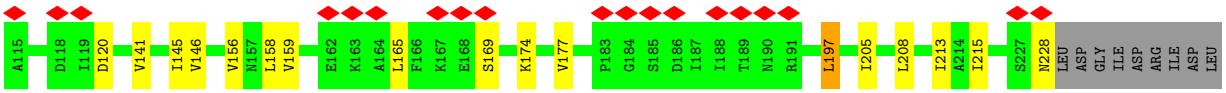


• Molecule 1: Flagellar M-ring protein

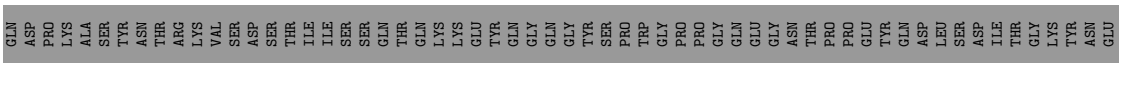
Chain 5:

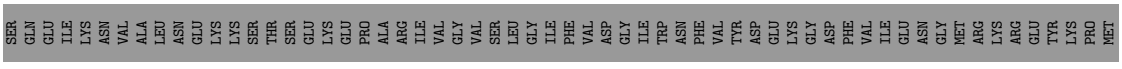


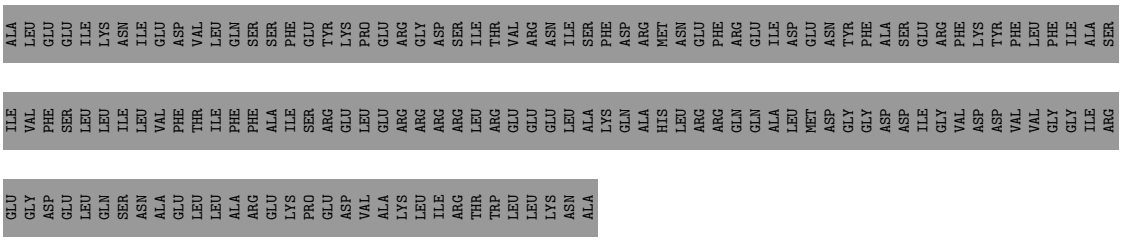








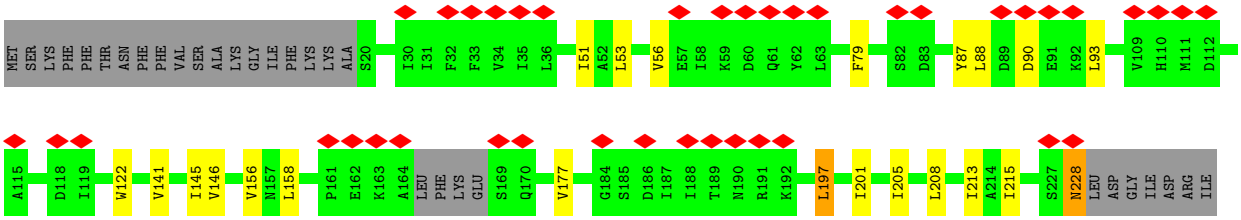




• Molecule 1: Flagellar M-ring protein

Chain 6:

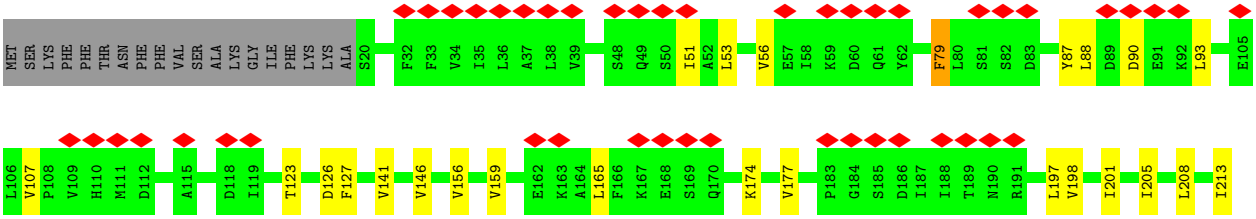


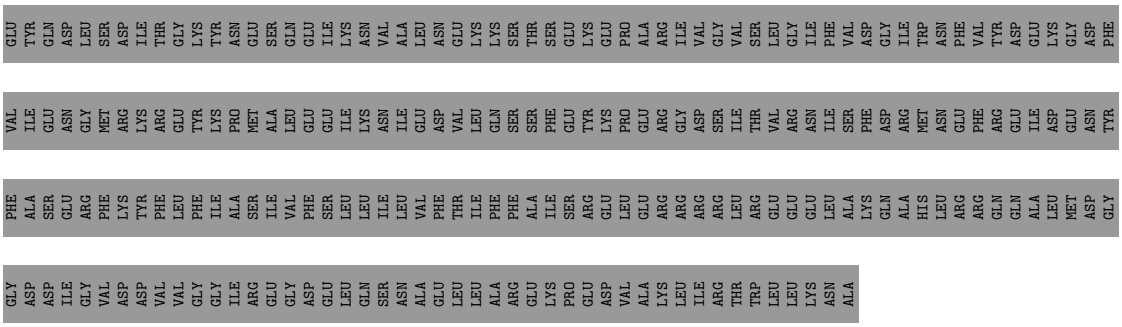


• Molecule 1: Flagellar M-ring protein

Chain 7:



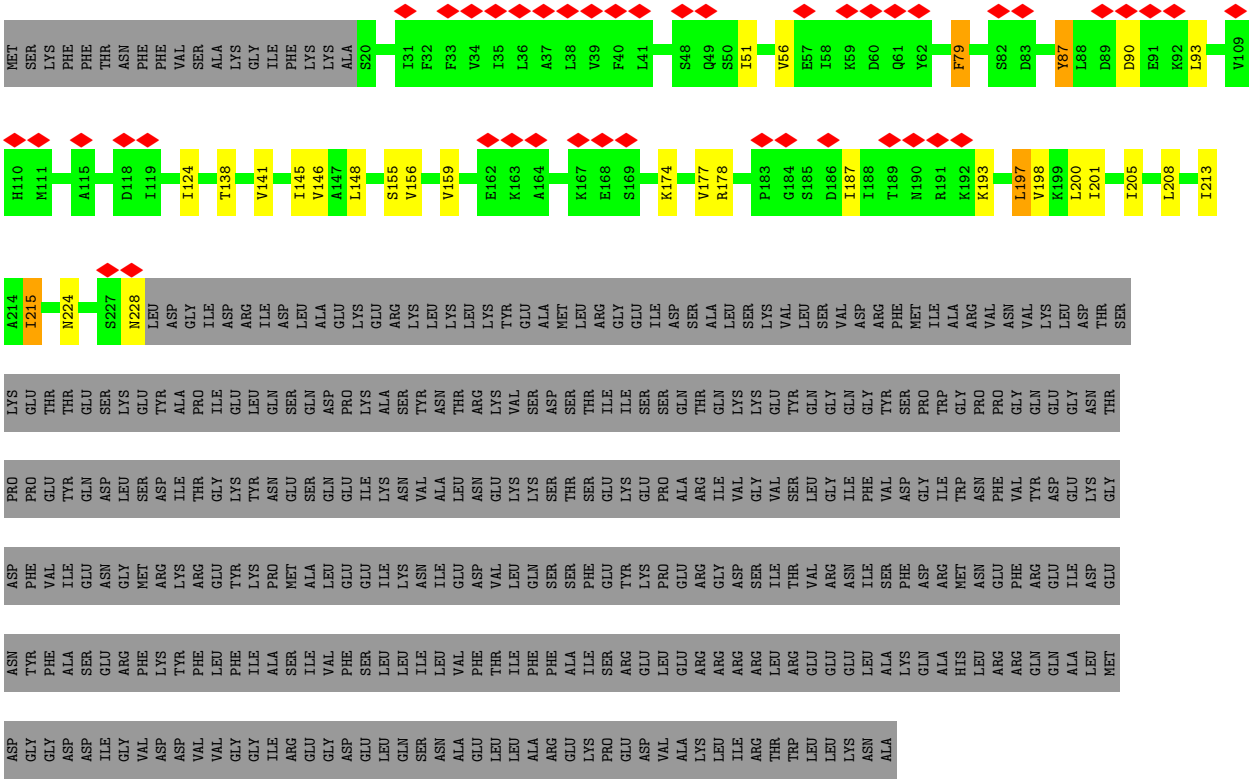




• Molecule 1: Flagellar M-ring protein

Chain 8:

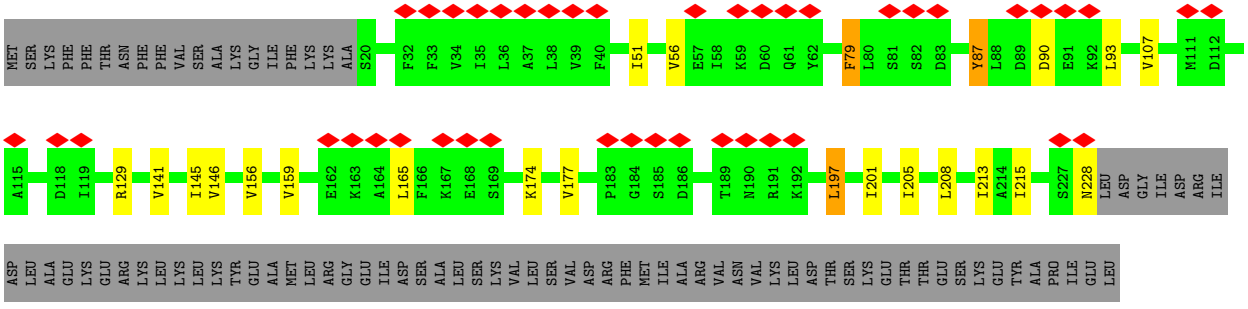


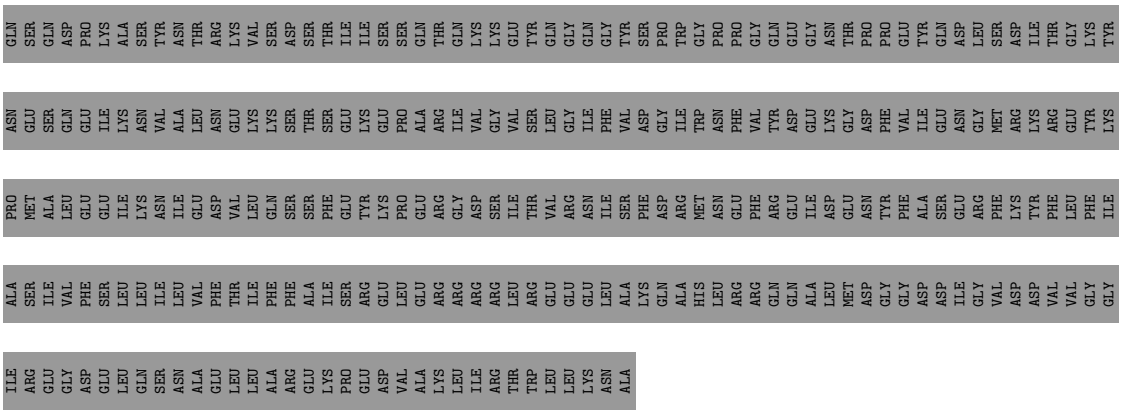


• Molecule 1: Flagellar M-ring protein

Chain 9:



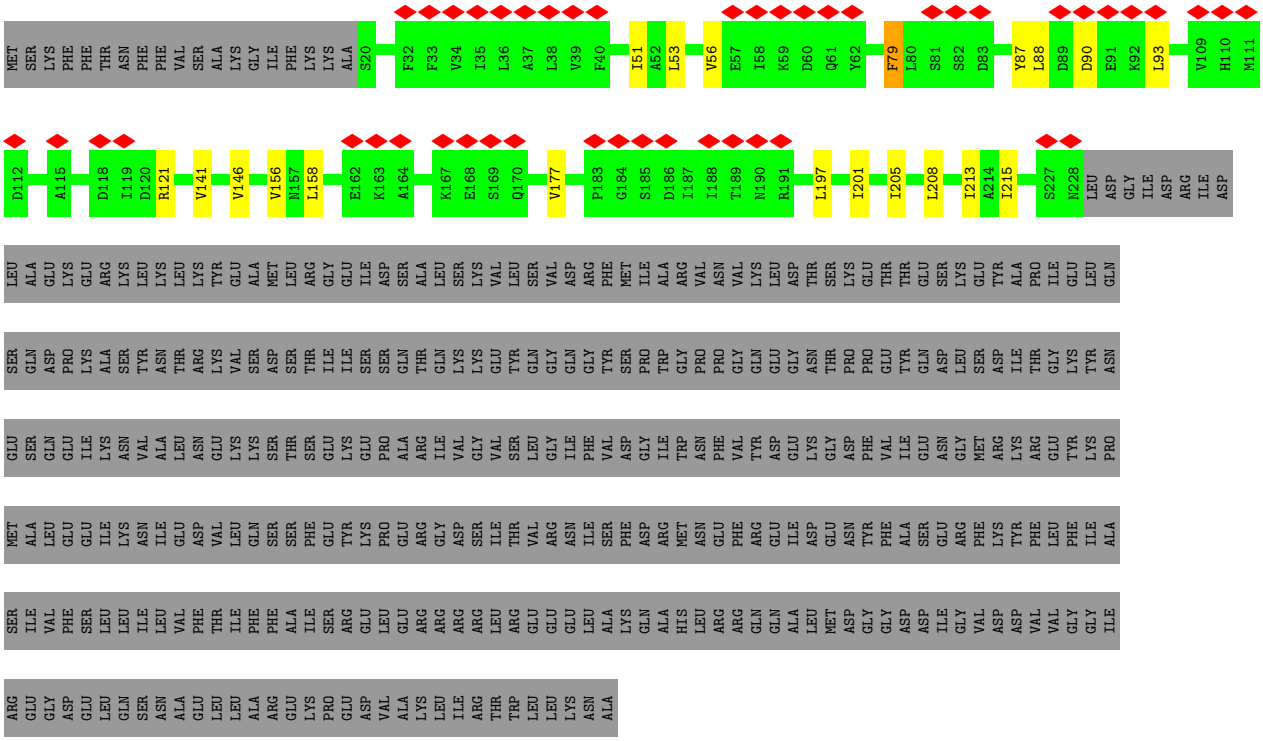




• Molecule 1: Flagellar M-ring protein

Chain 0:

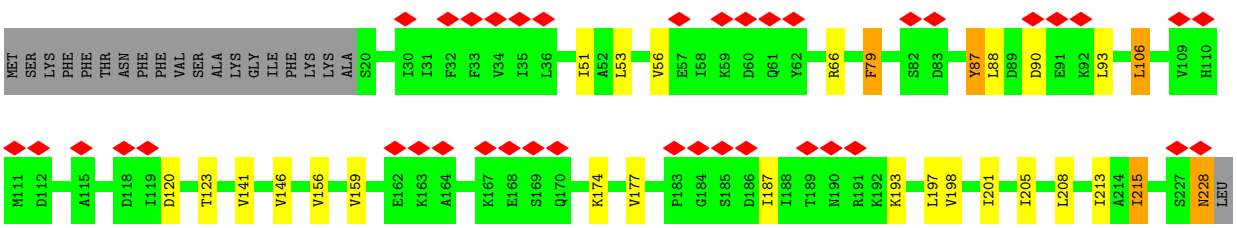


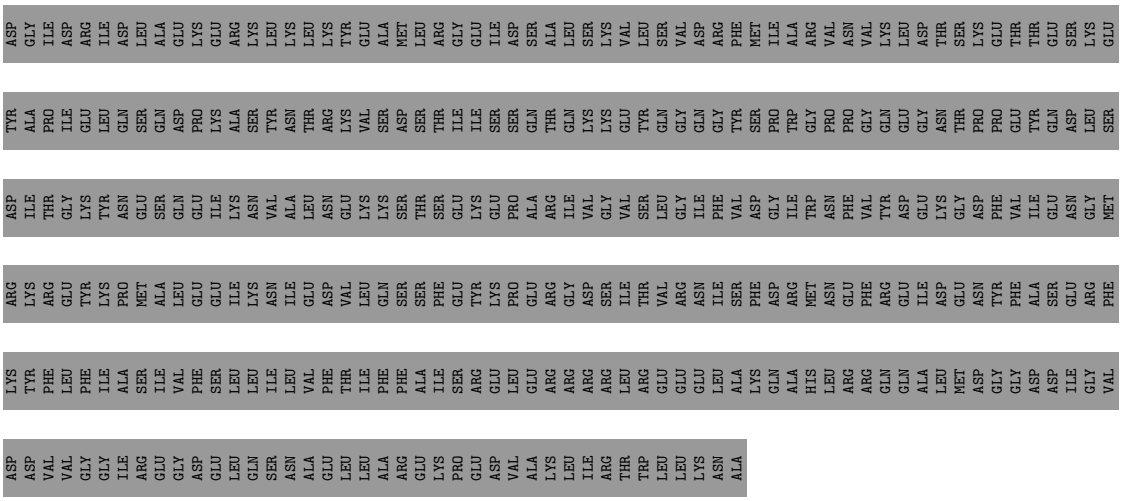


• Molecule 1: Flagellar M-ring protein

Chain AA:



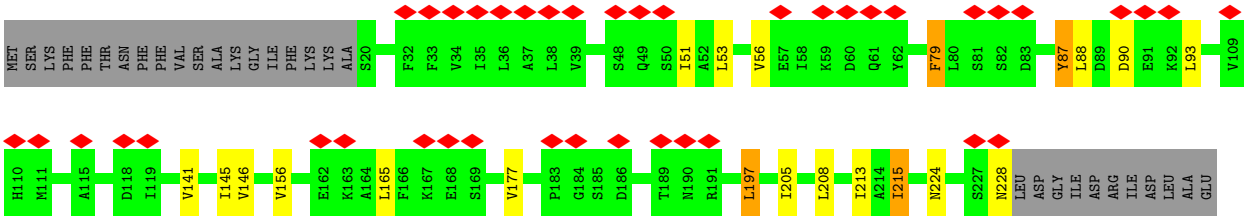




• Molecule 1: Flagellar M-ring protein

Chain AB:

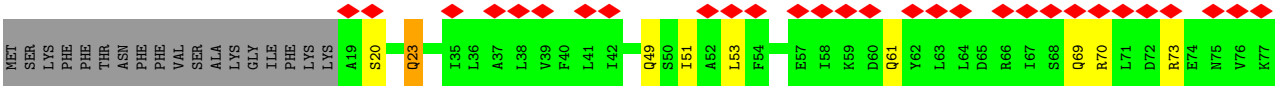


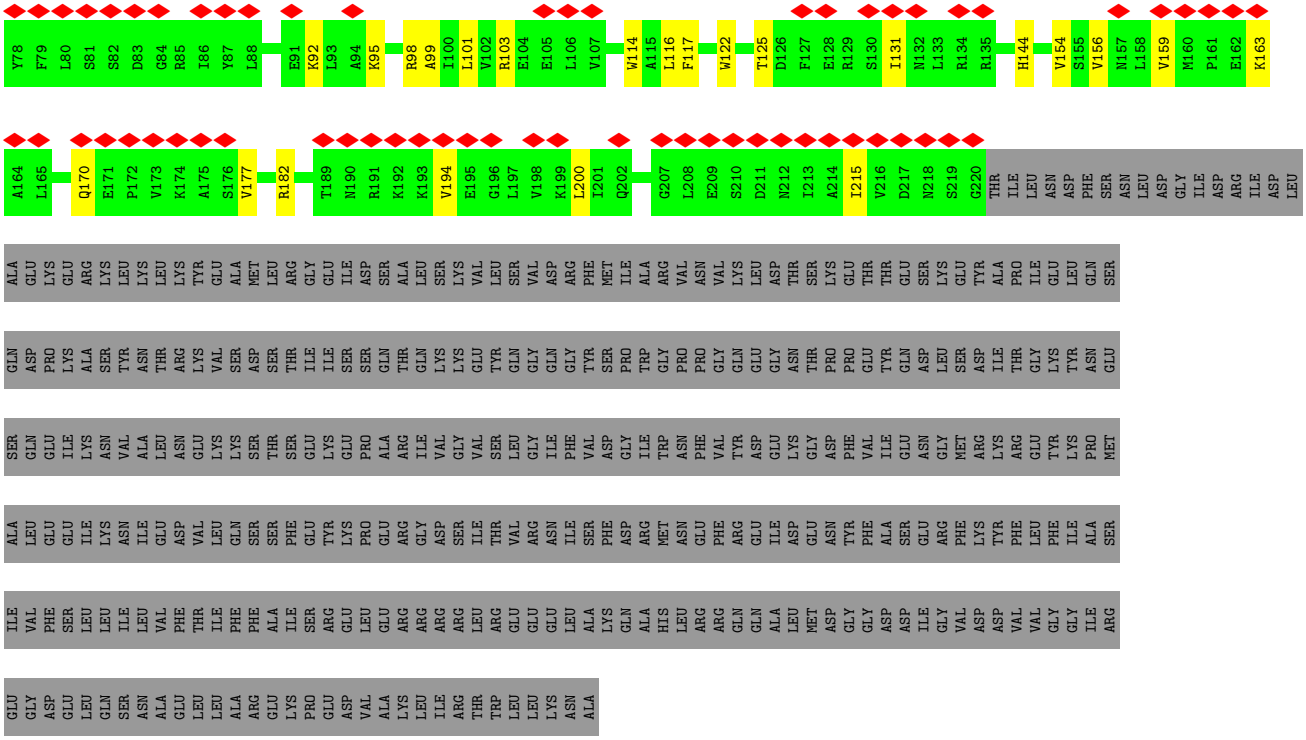


• Molecule 1: Flagellar M-ring protein

Chain AC:



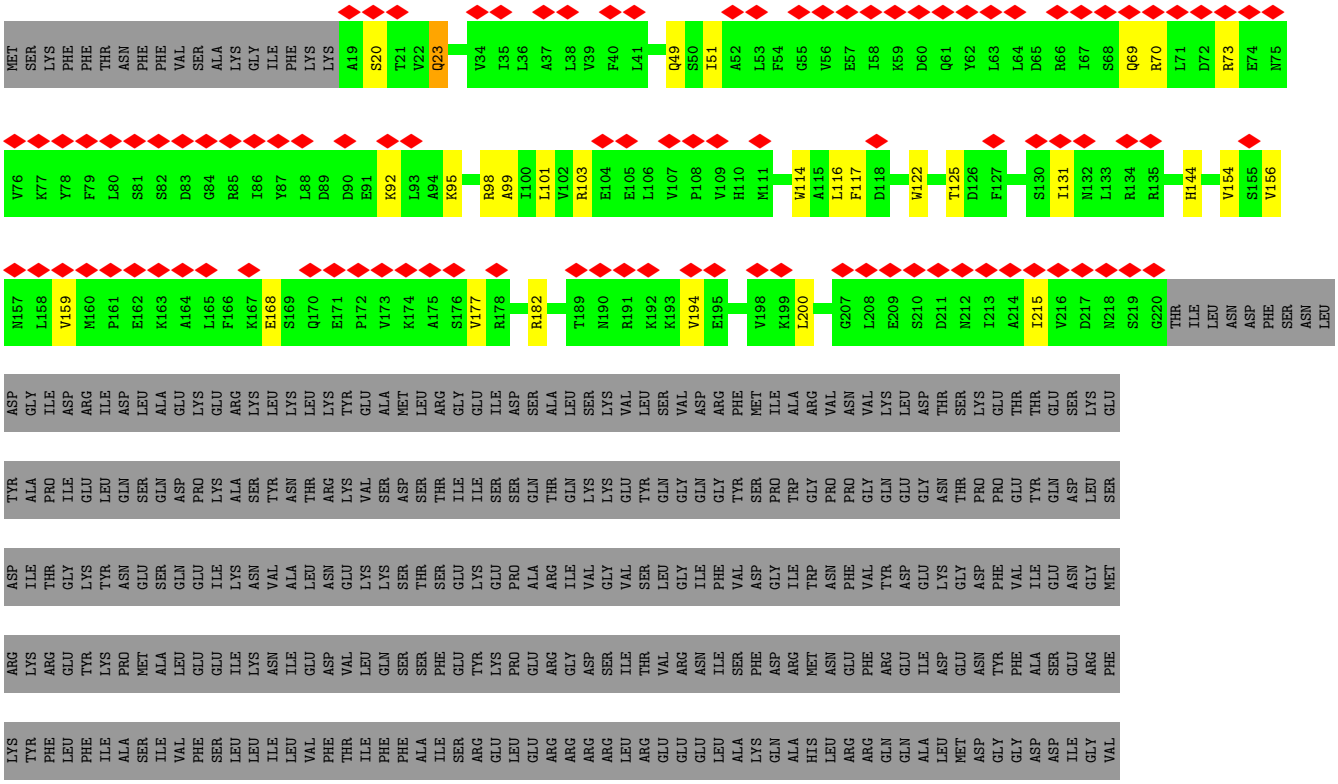




• Molecule 1: Flagellar M-ring protein

Chain AD:



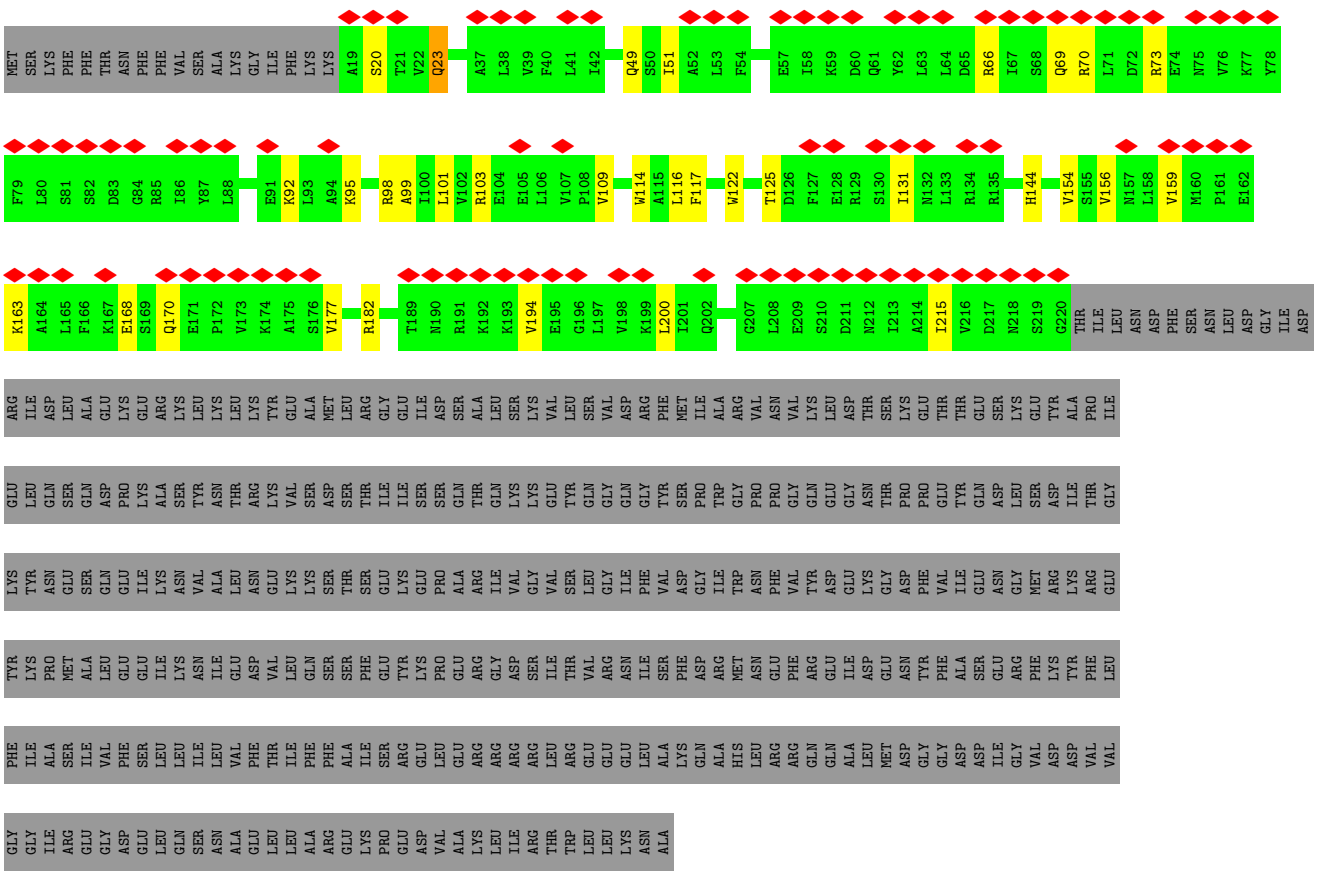




• Molecule 1: Flagellar M-ring protein

Chain AE:

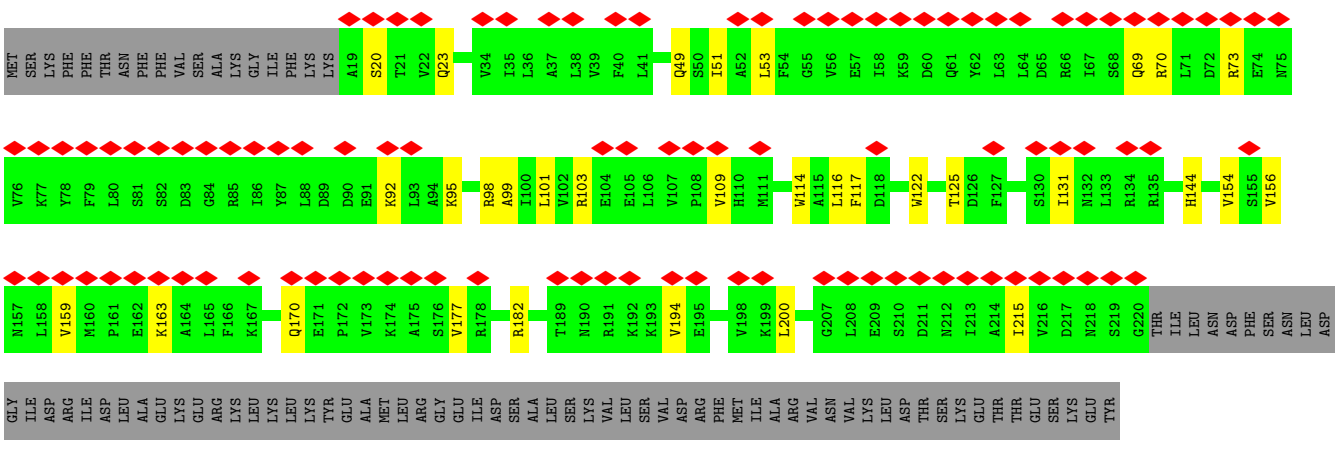


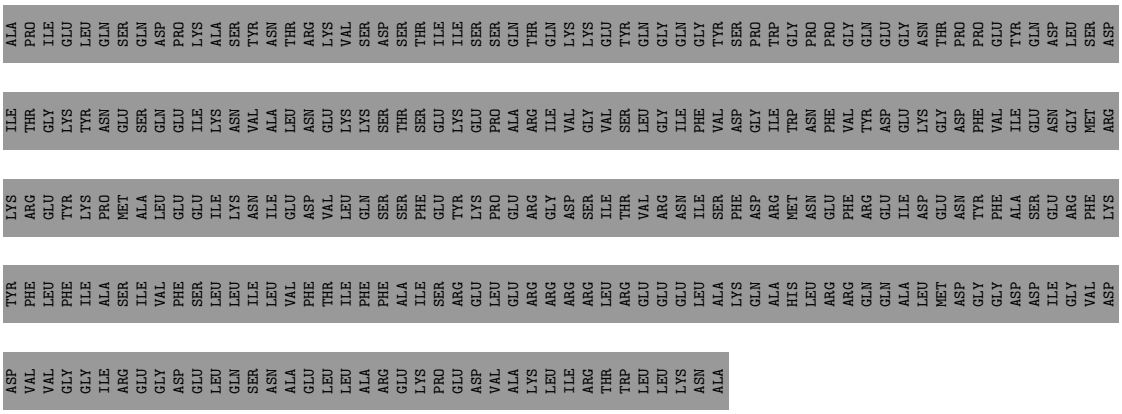


• Molecule 1: Flagellar M-ring protein

Chain AF:



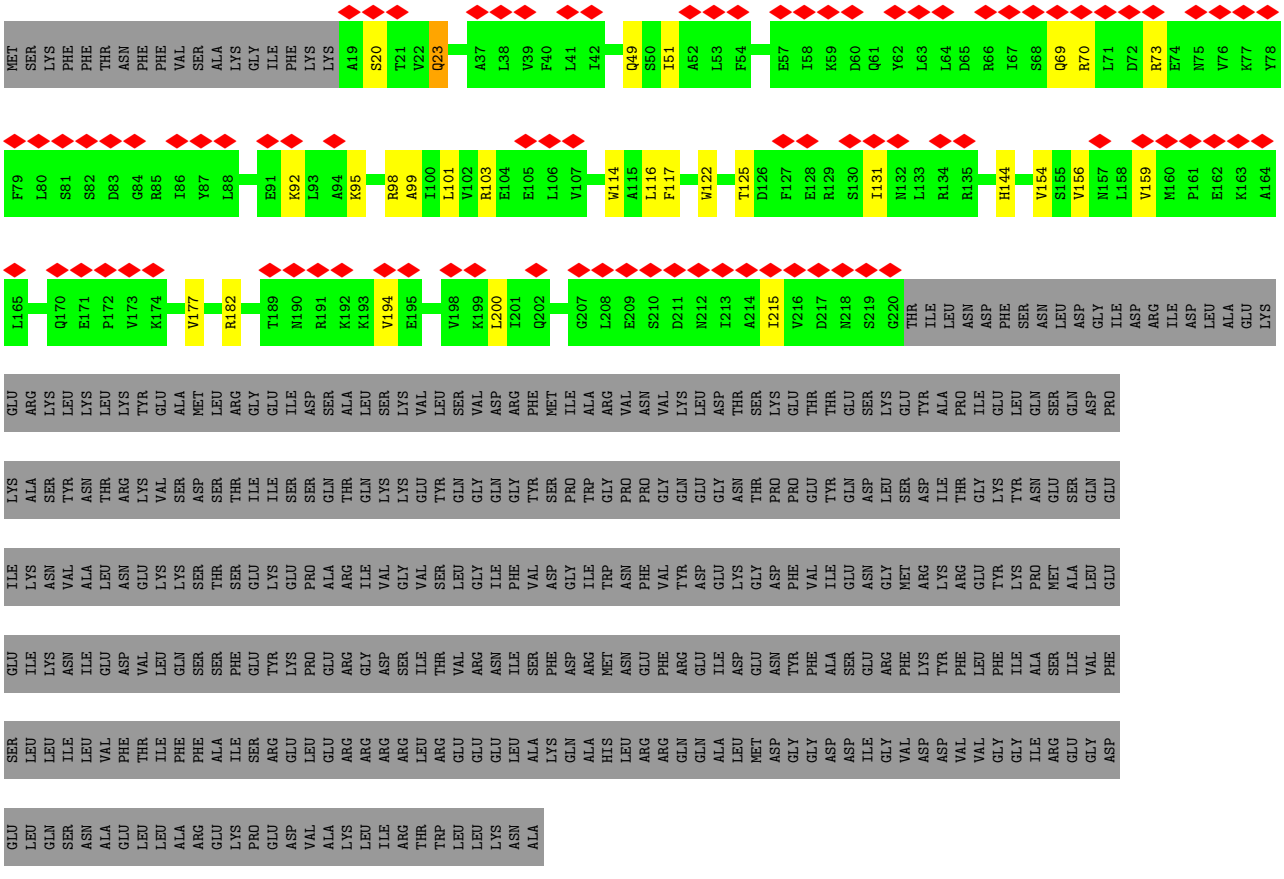




• Molecule 1: Flagellar M-ring protein

Chain AG:

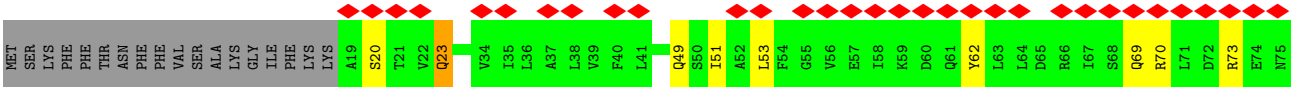


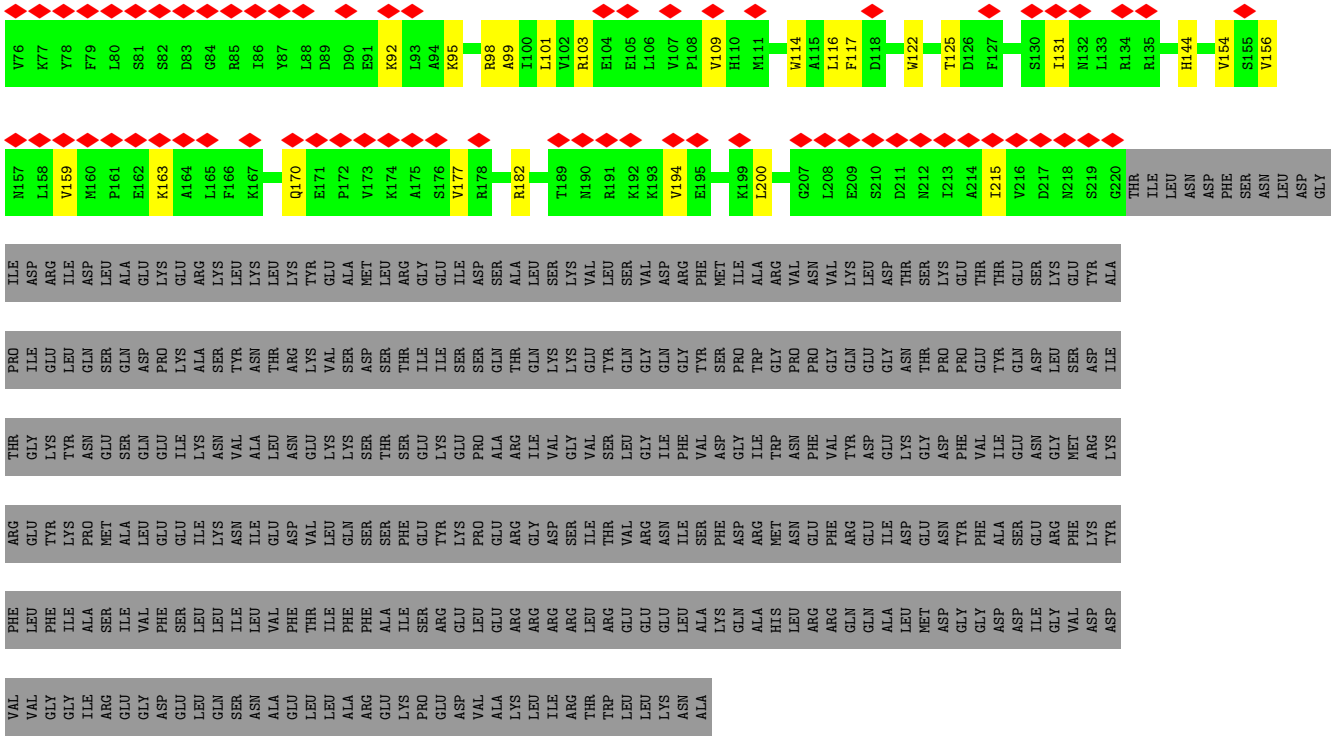


• Molecule 1: Flagellar M-ring protein

Chain AH:



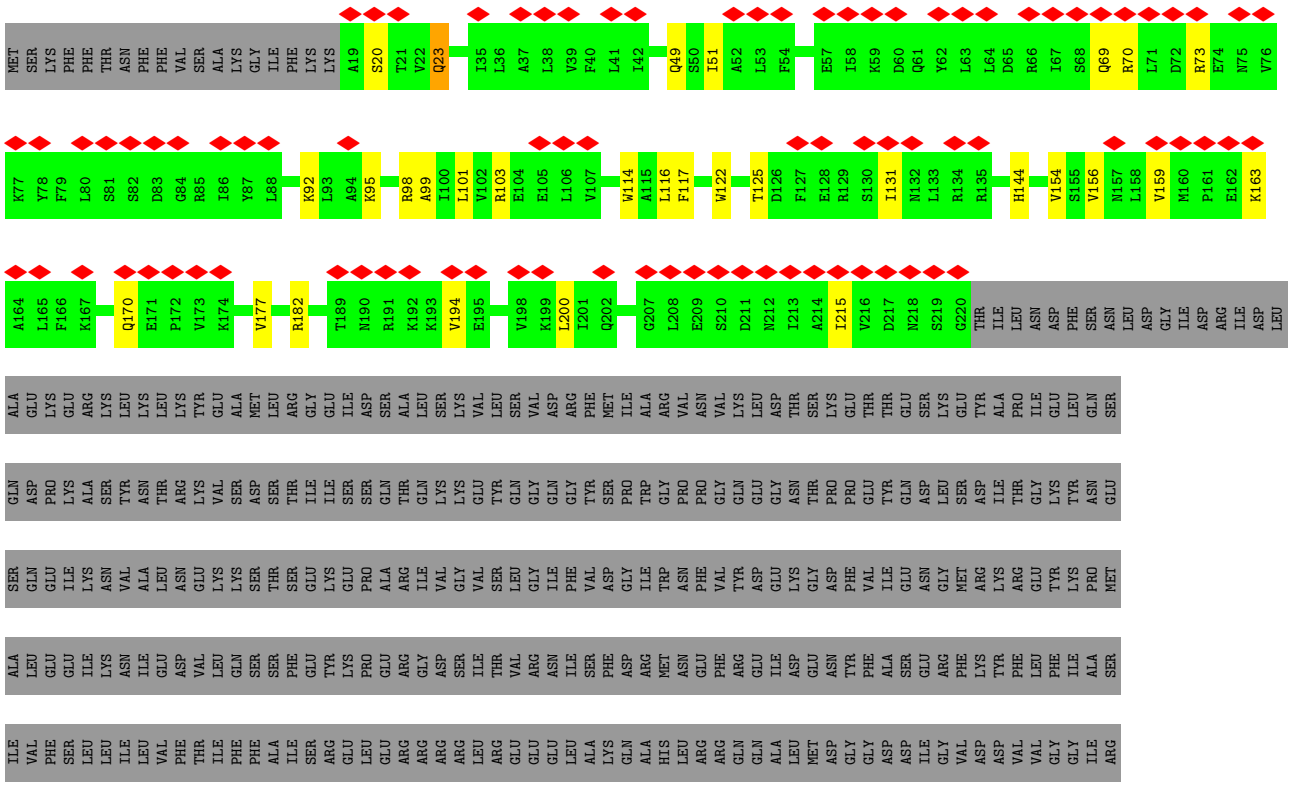




• Molecule 1: Flagellar M-ring protein

Chain AI:



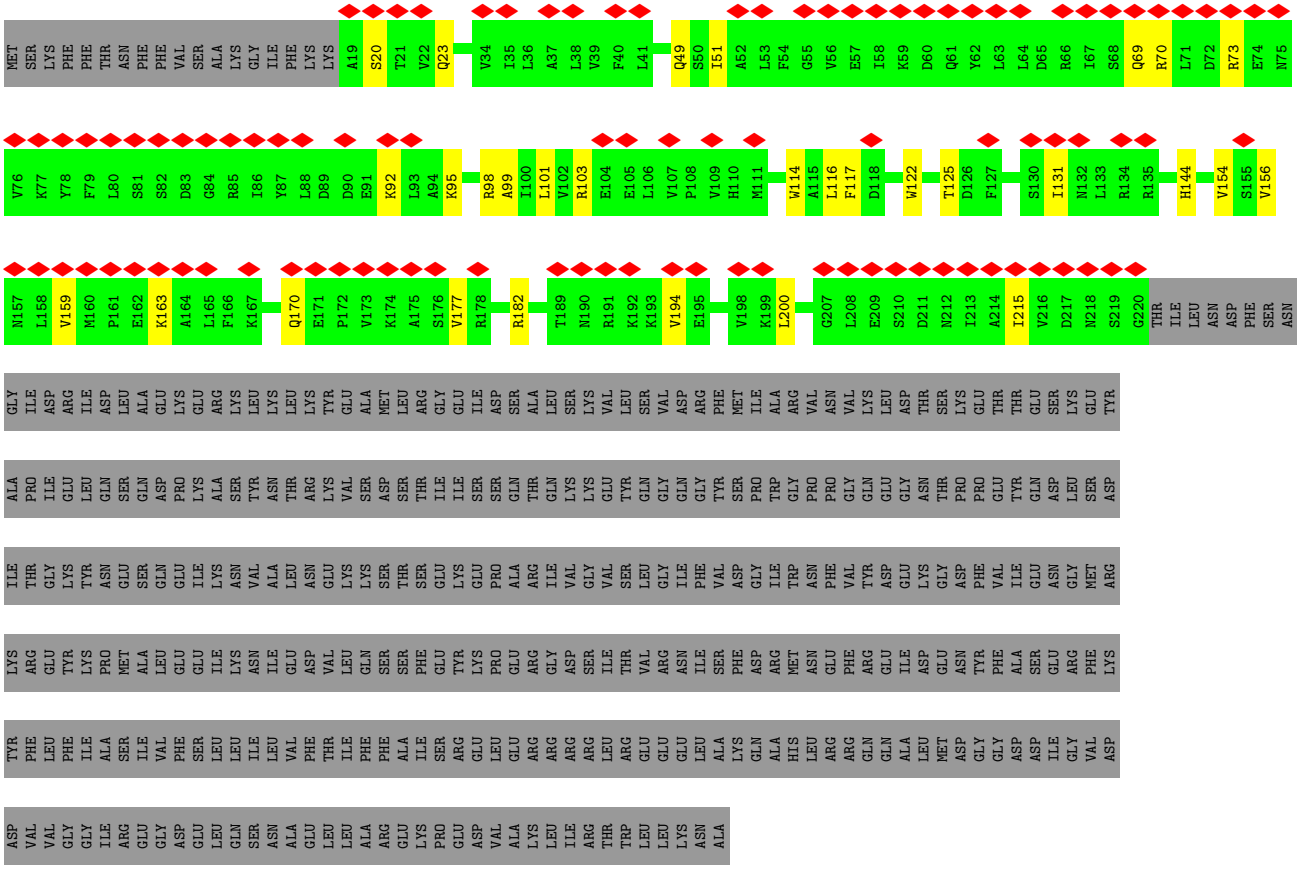




• Molecule 1: Flagellar M-ring protein

Chain AJ:

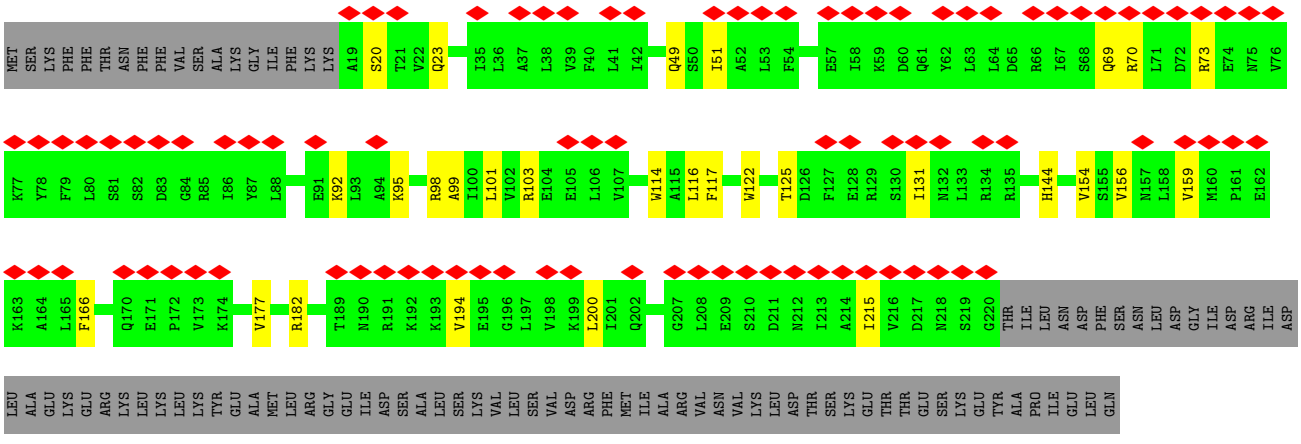


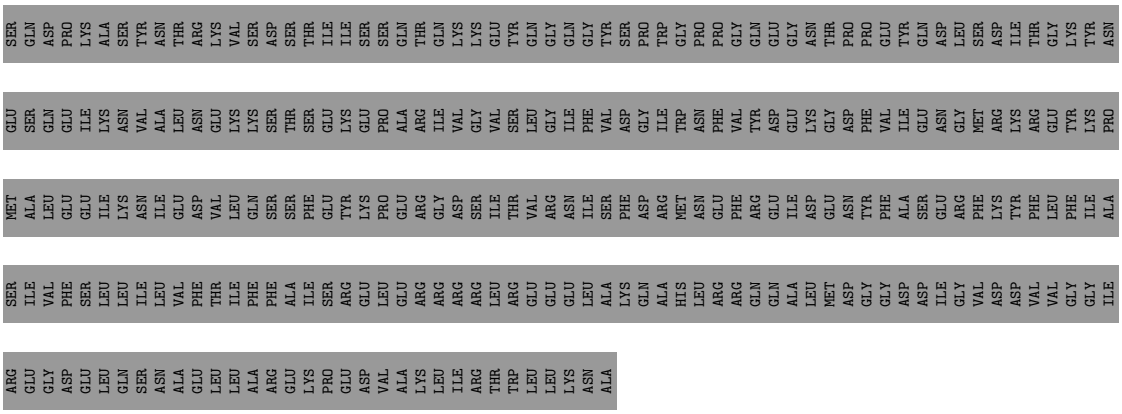


• Molecule 1: Flagellar M-ring protein

Chain AK:



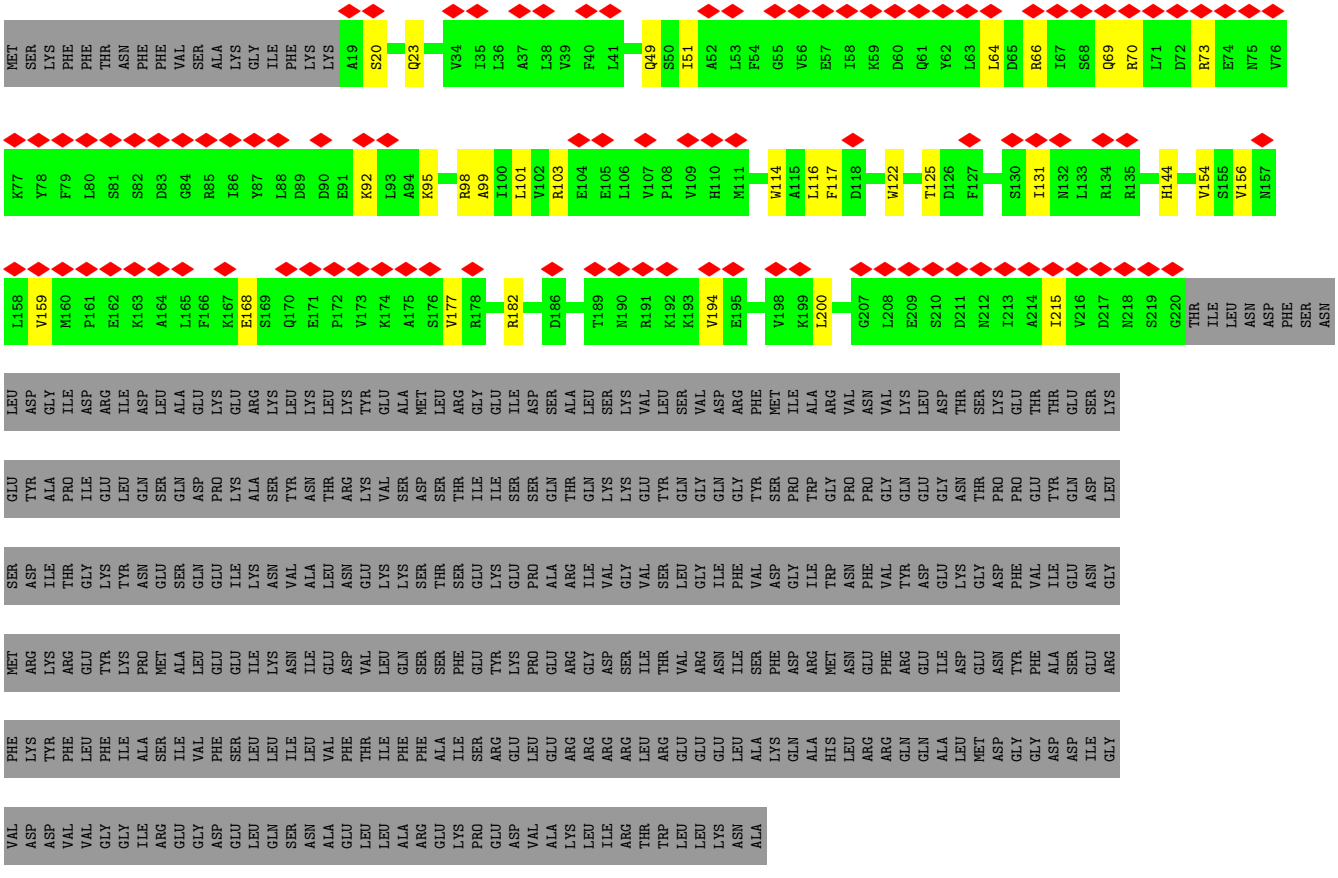




• Molecule 1: Flagellar M-ring protein

Chain AL:

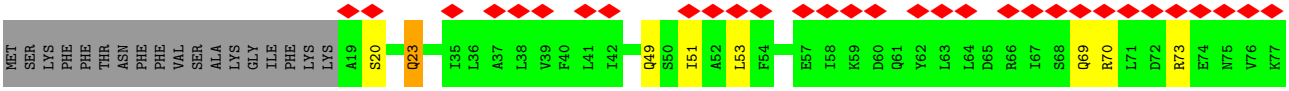


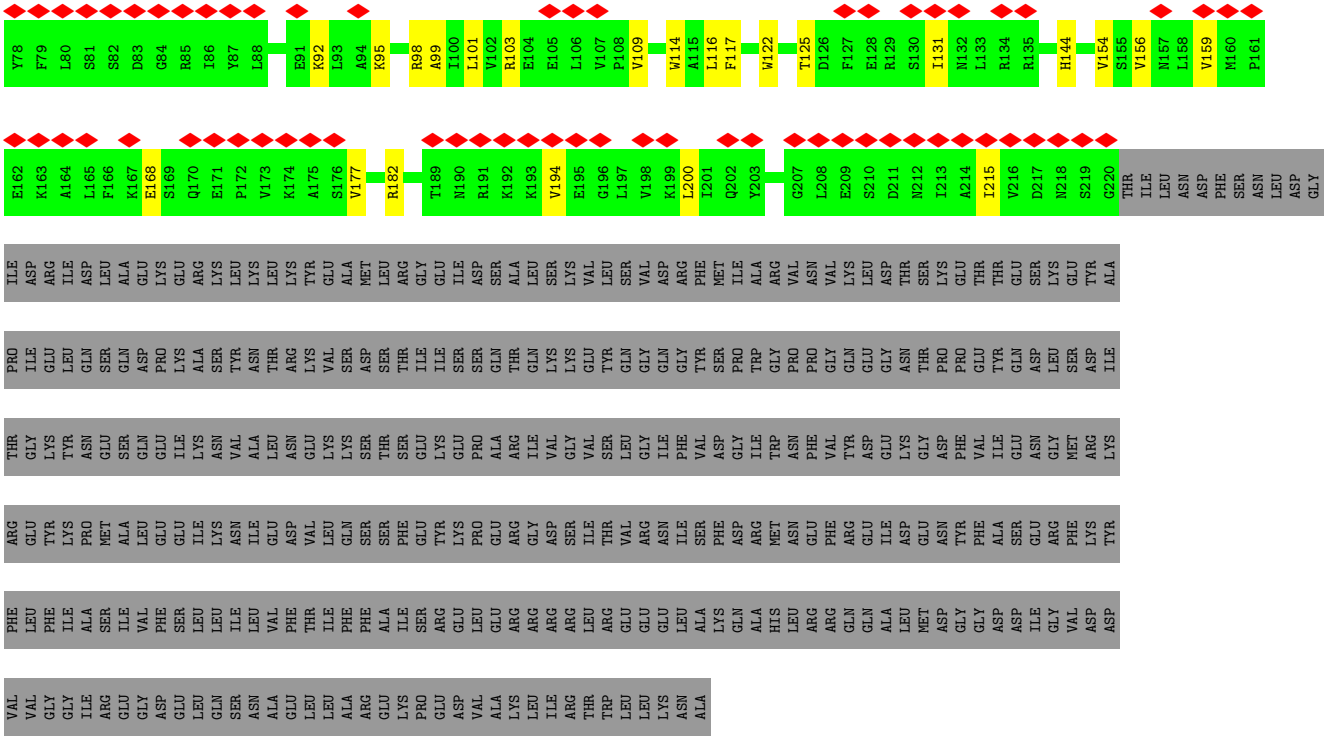


• Molecule 1: Flagellar M-ring protein

Chain AM:



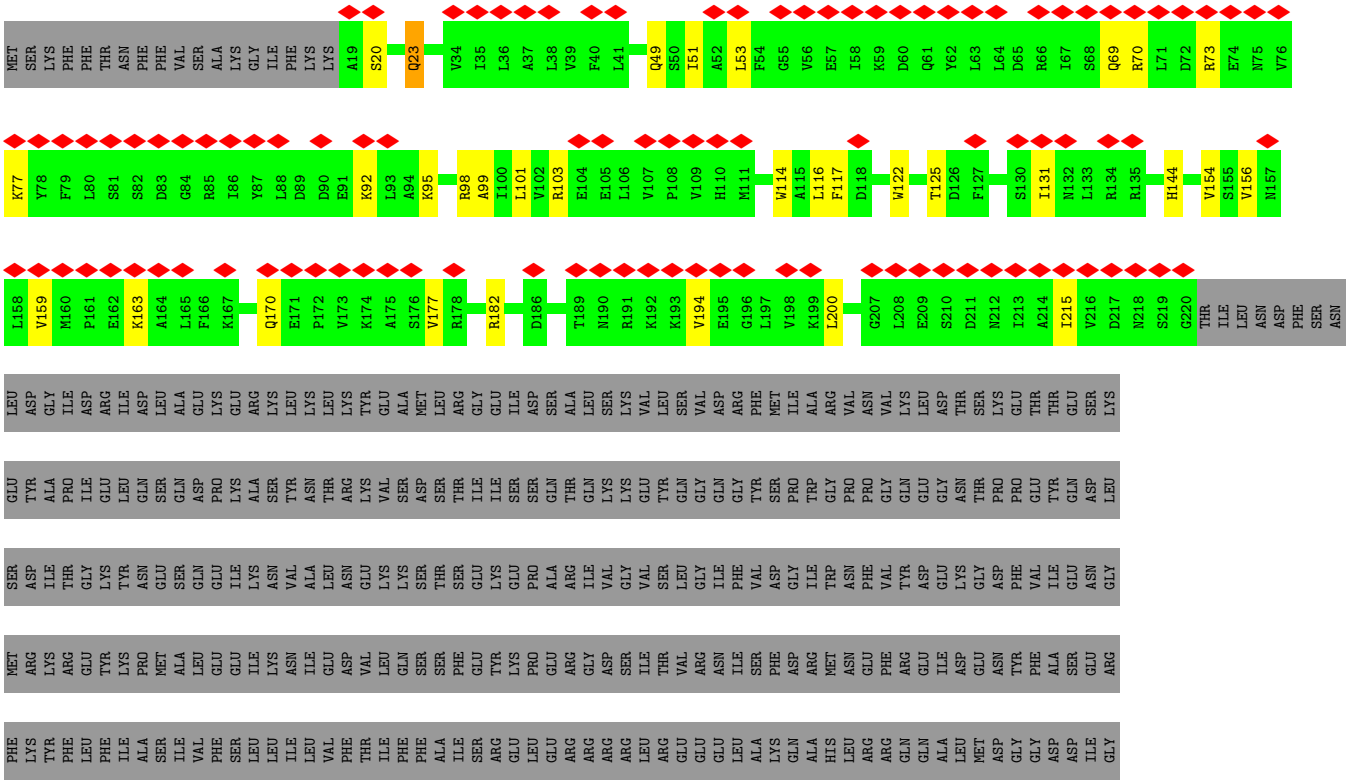


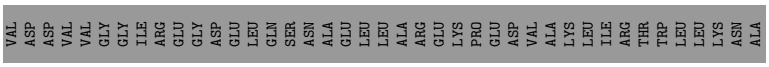


• Molecule 1: Flagellar M-ring protein

Chain AN:



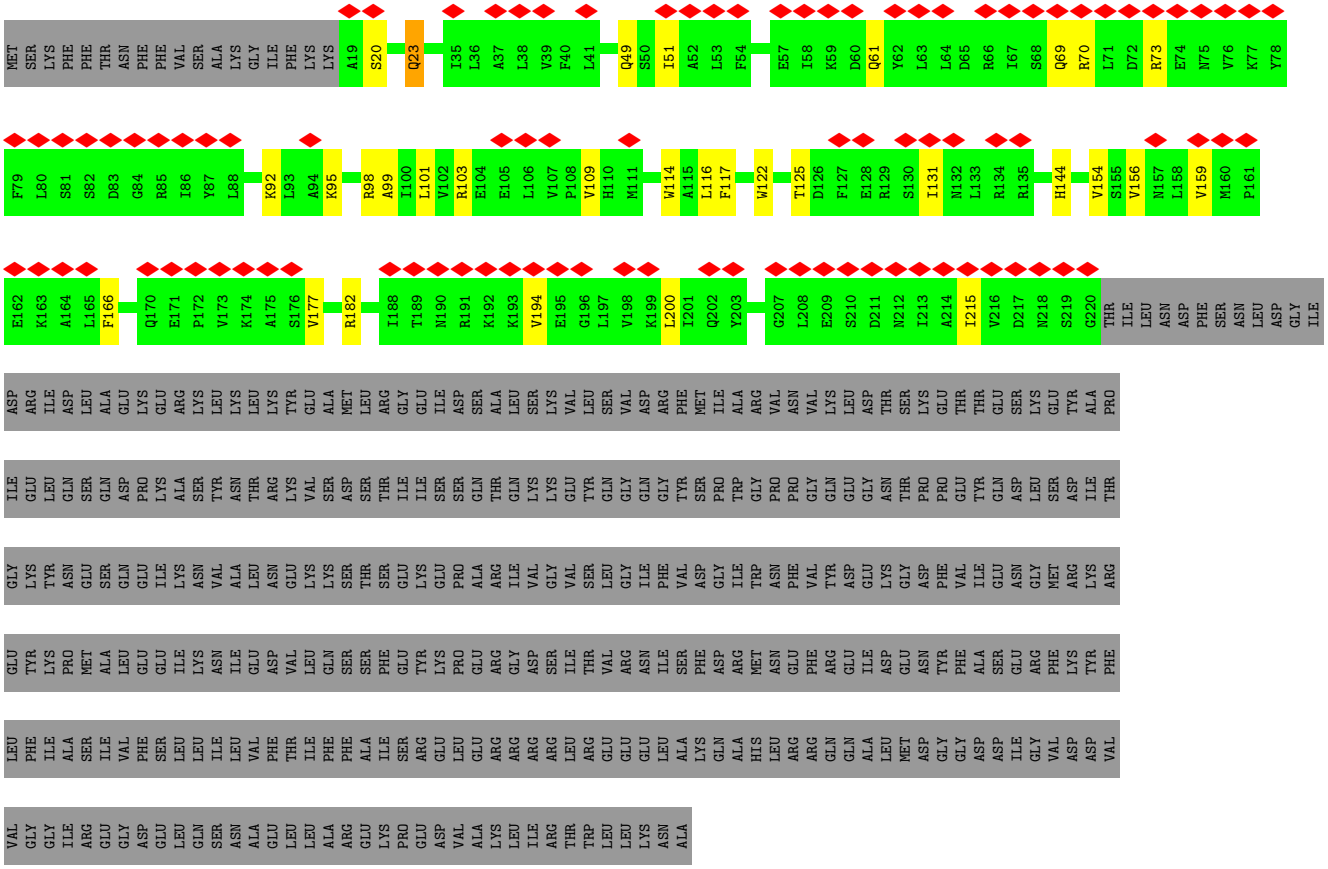




• Molecule 1: Flagellar M-ring protein

Chain AO:

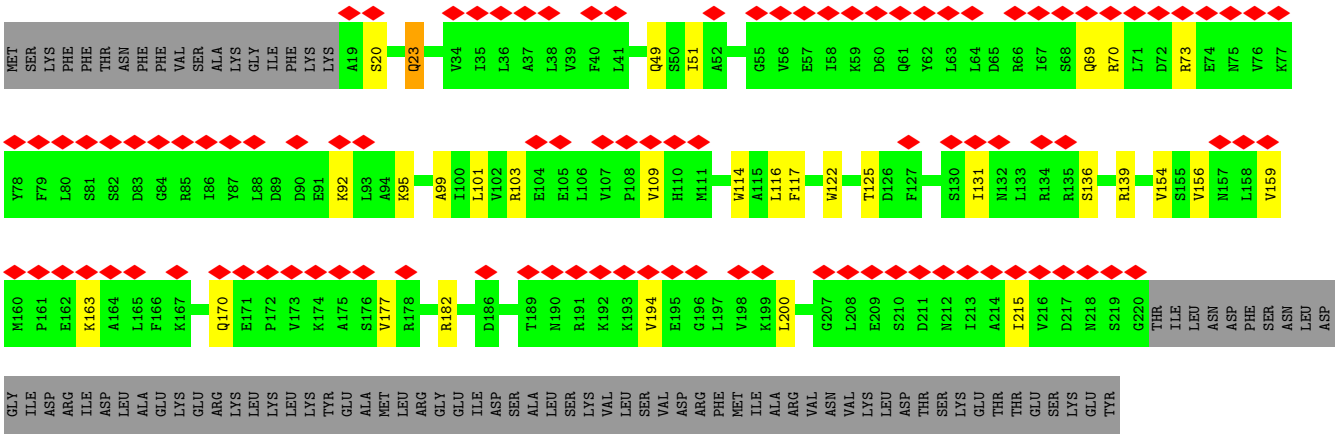


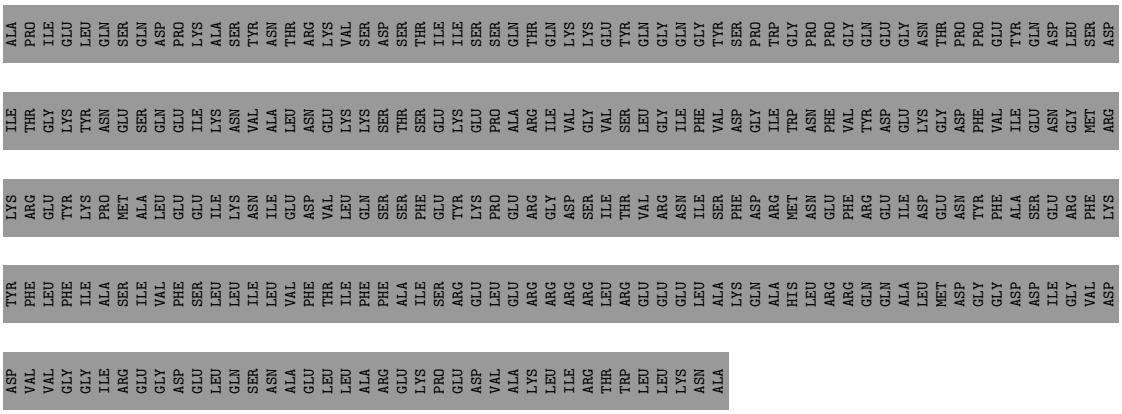


• Molecule 1: Flagellar M-ring protein

Chain AP:



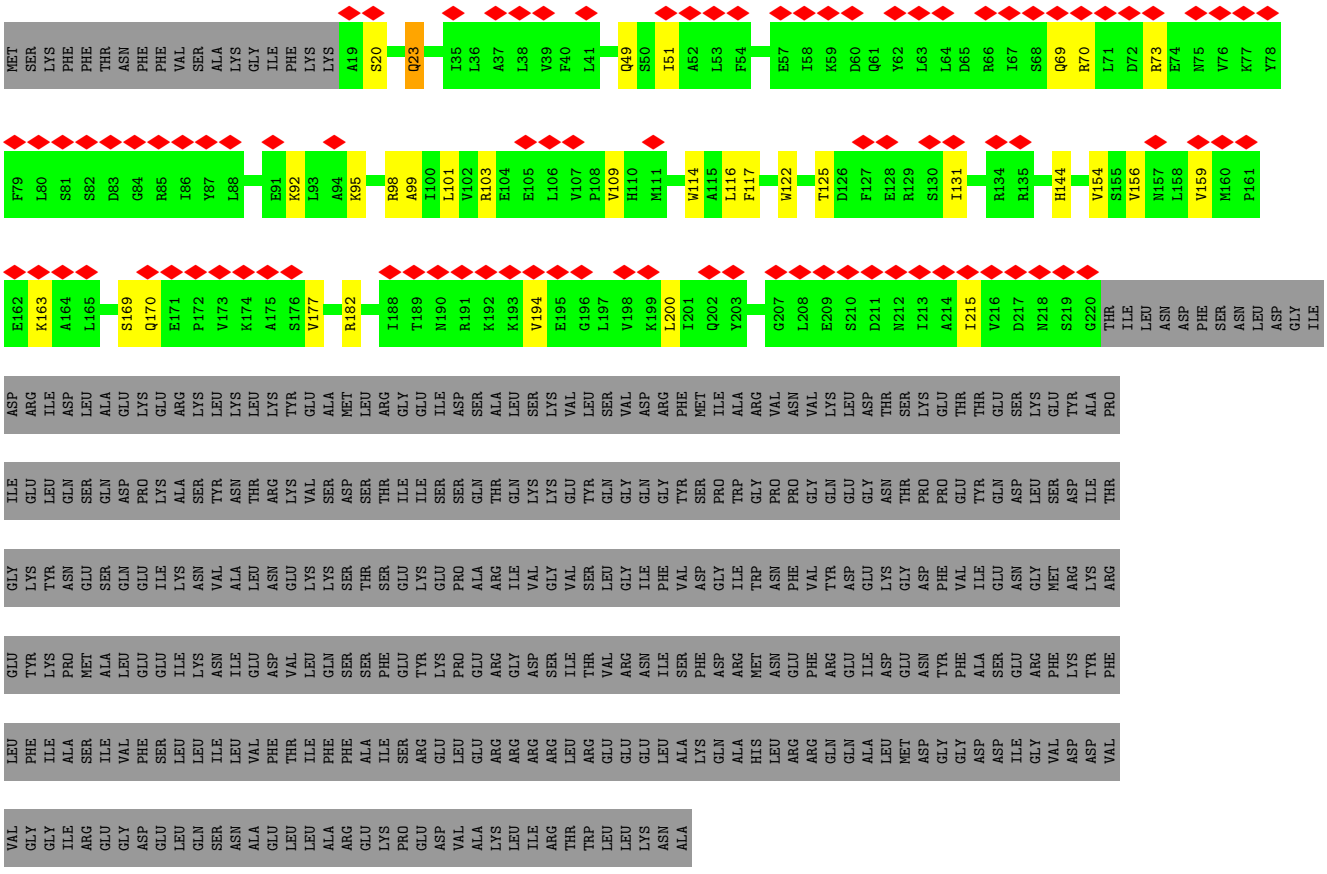




• Molecule 1: Flagellar M-ring protein

Chain AQ:

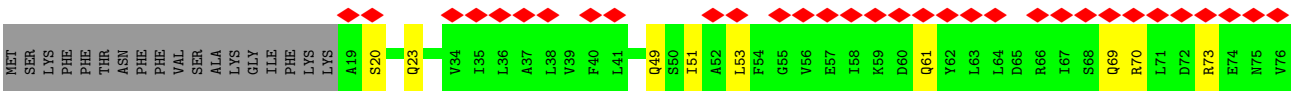


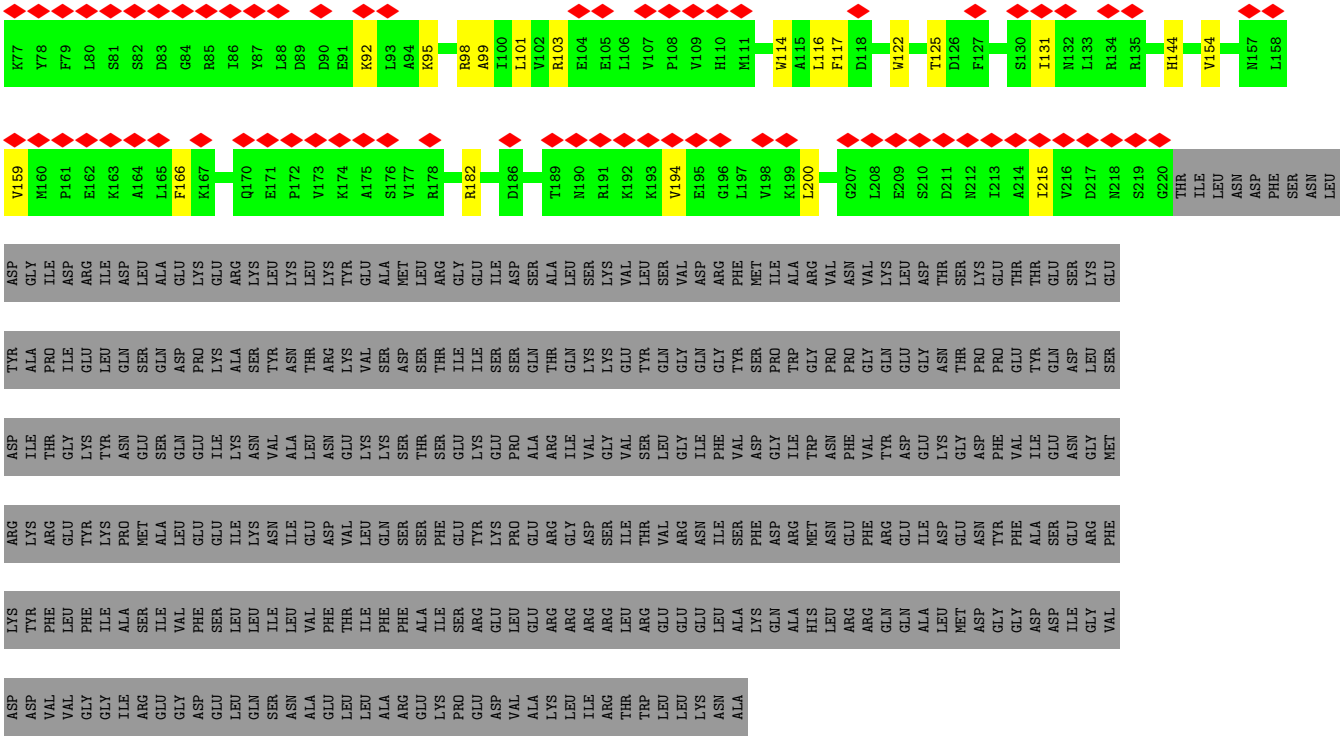


• Molecule 1: Flagellar M-ring protein

Chain AR:



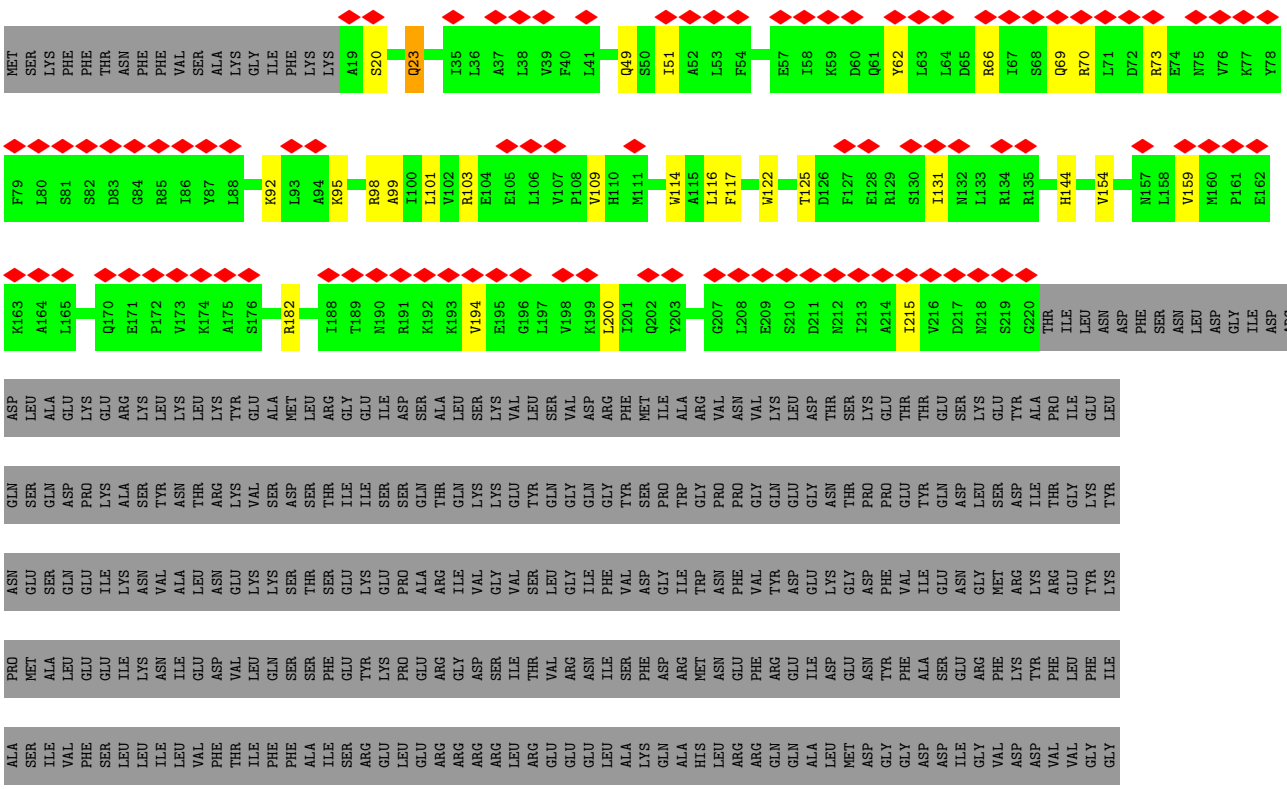




• Molecule 1: Flagellar M-ring protein

Chain AS:



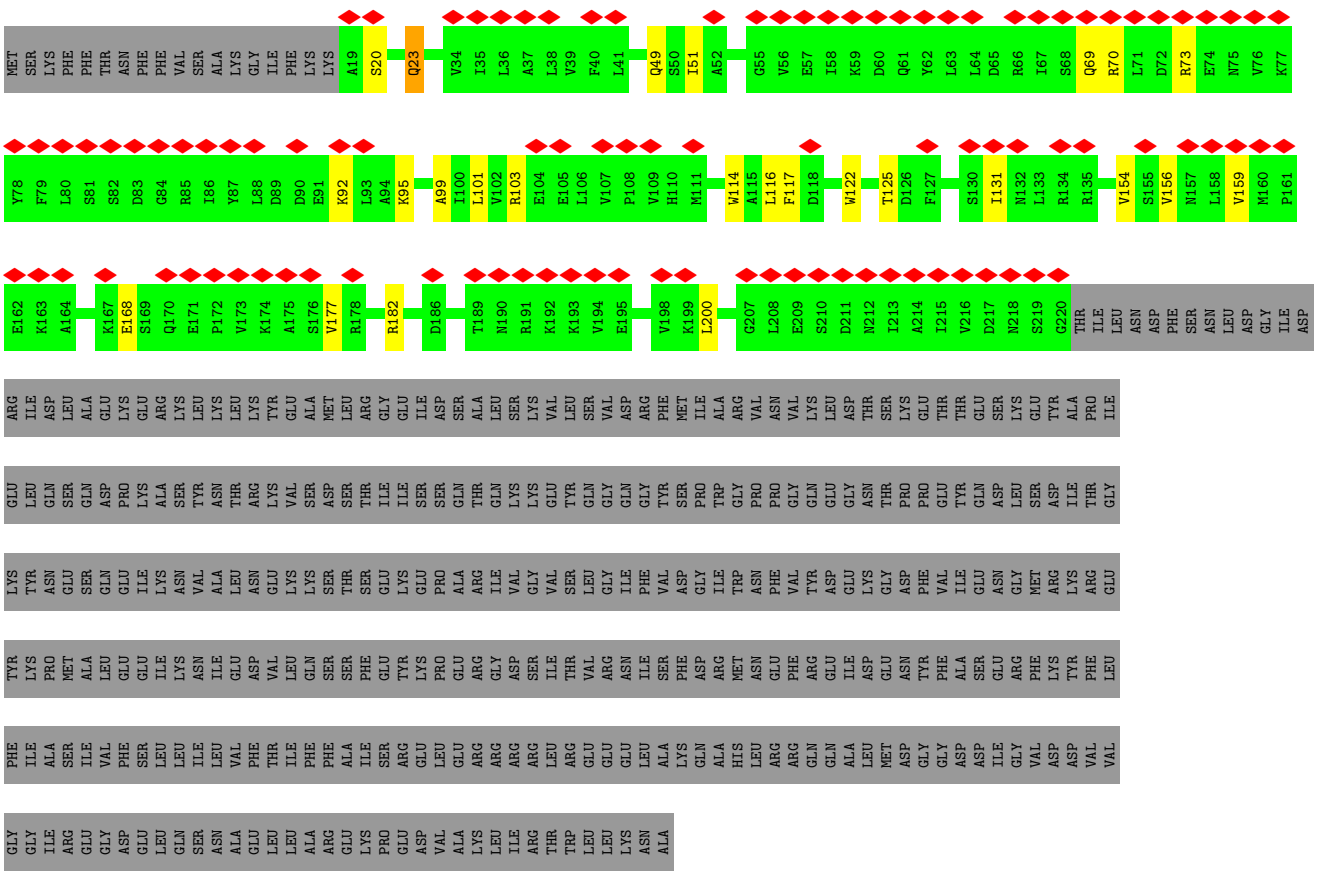




• Molecule 1: Flagellar M-ring protein

Chain AT:

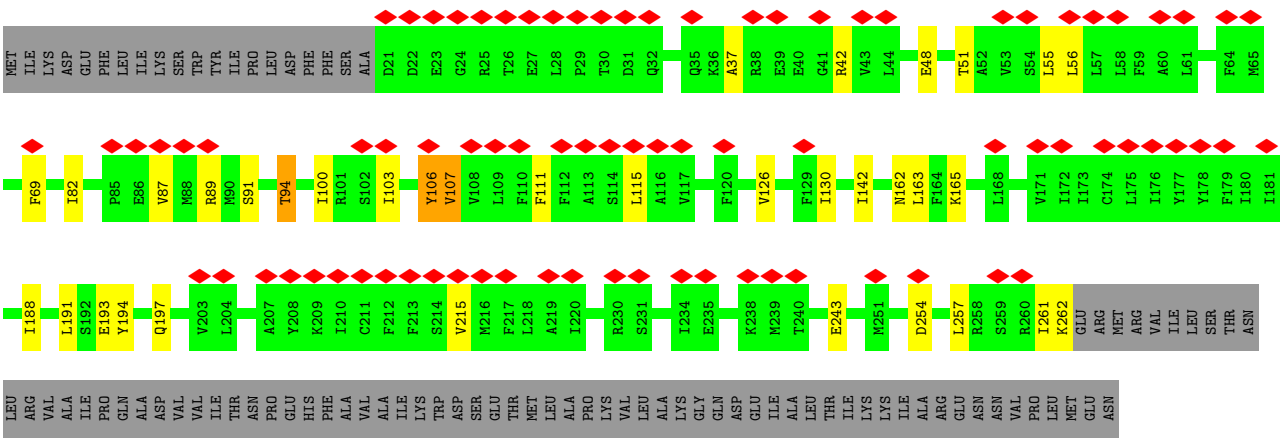




• Molecule 2: Flagellar biosynthetic protein FlhB

Chain AX:



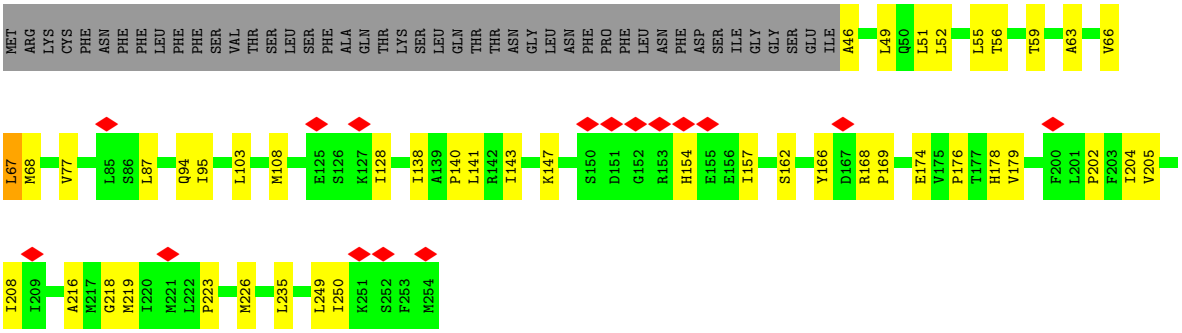




• Molecule 3: Flagellar biosynthetic protein FliP

Chain AY:

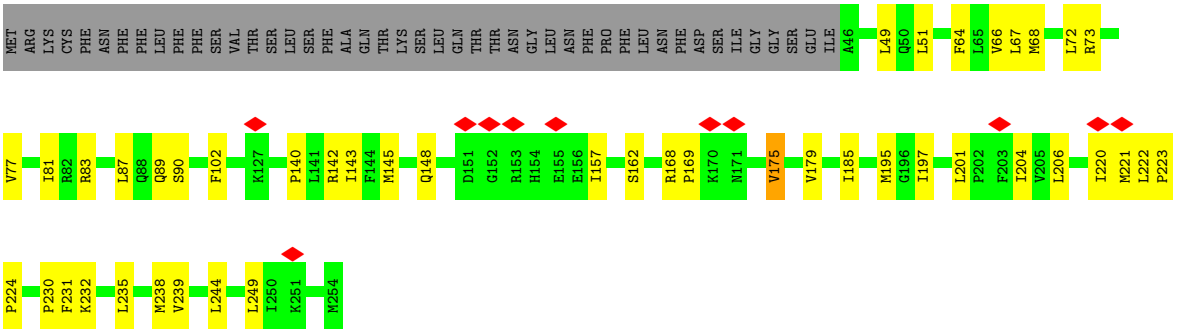




• Molecule 3: Flagellar biosynthetic protein FliP

Chain AZ:

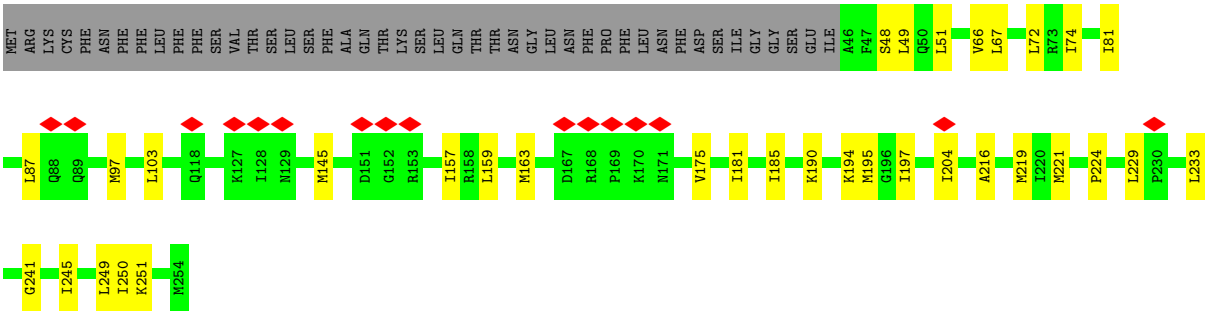




• Molecule 3: Flagellar biosynthetic protein FliP

Chain Aa:

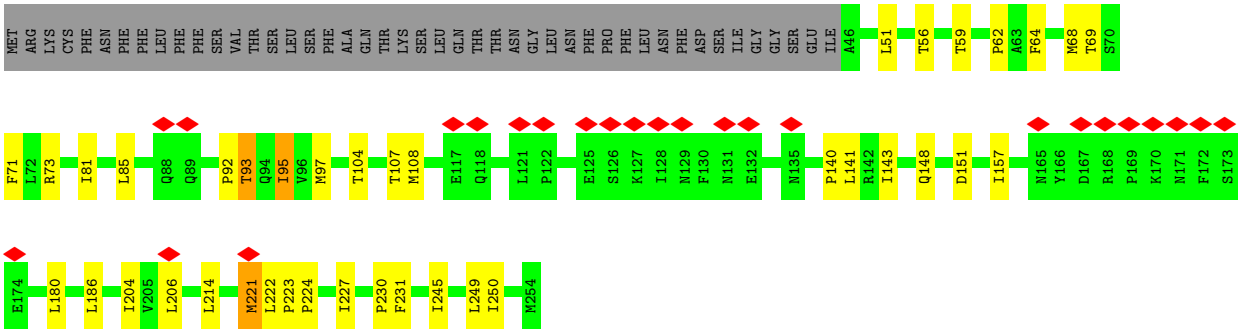




• Molecule 3: Flagellar biosynthetic protein FliP

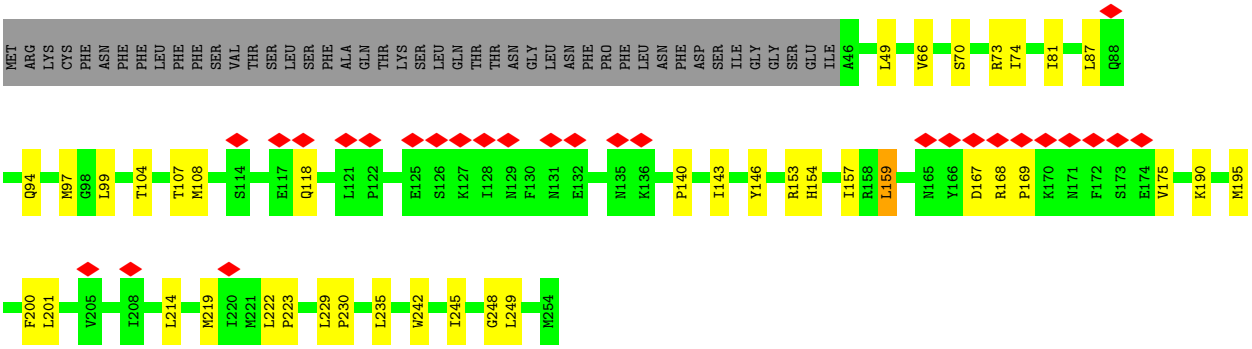
Chain Ab:



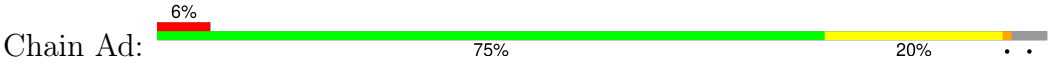


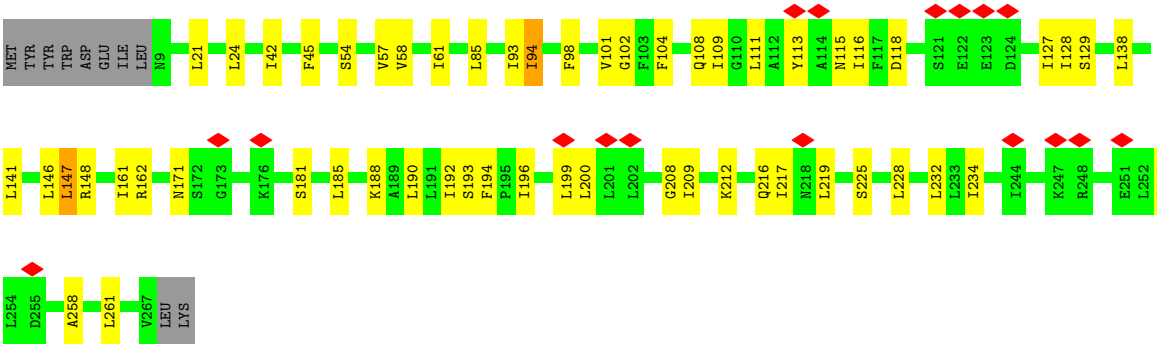
• Molecule 3: Flagellar biosynthetic protein FliP





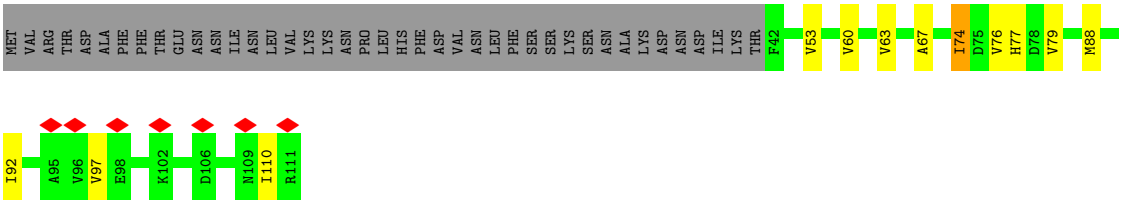
• Molecule 4: Flagellar biosynthetic protein FliR





• Molecule 5: Flagellar hook-basal body complex protein FliE

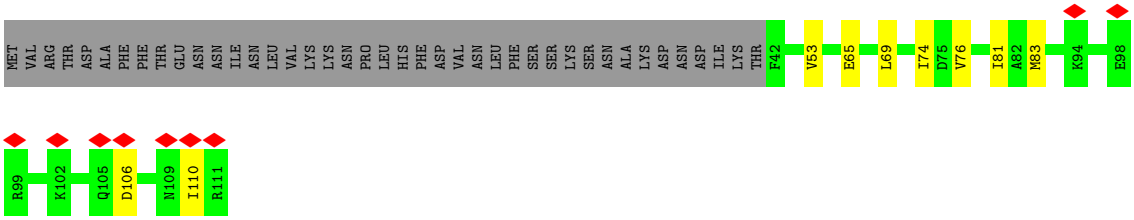




• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain Af:

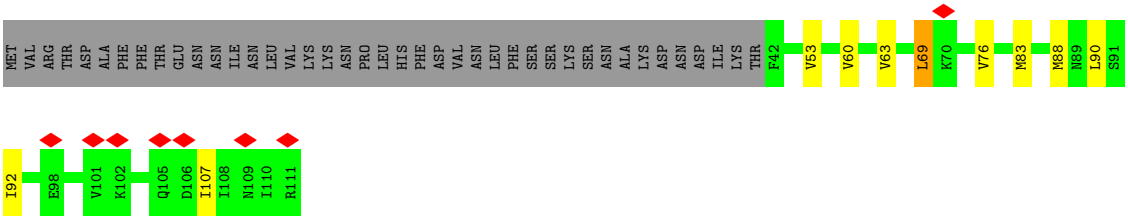




• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain Ag:

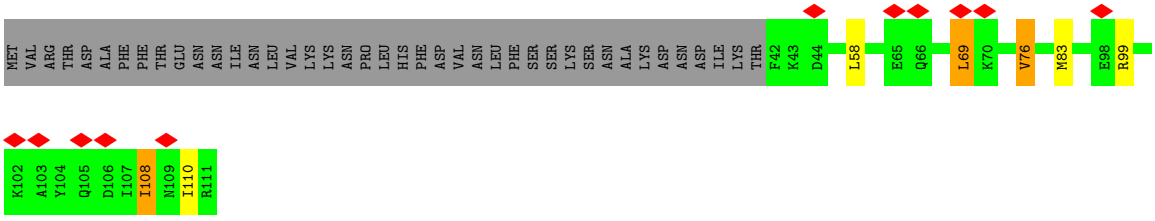




• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain Ah:

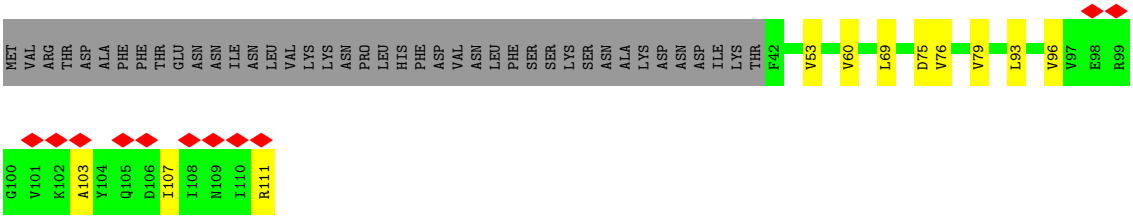




• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain Ai:

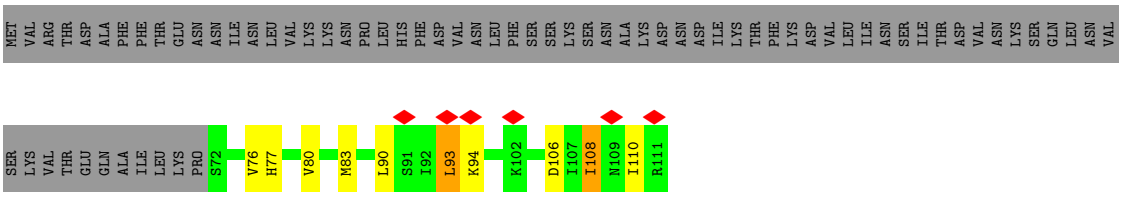




• Molecule 5: Flagellar hook-basal body complex protein FliE

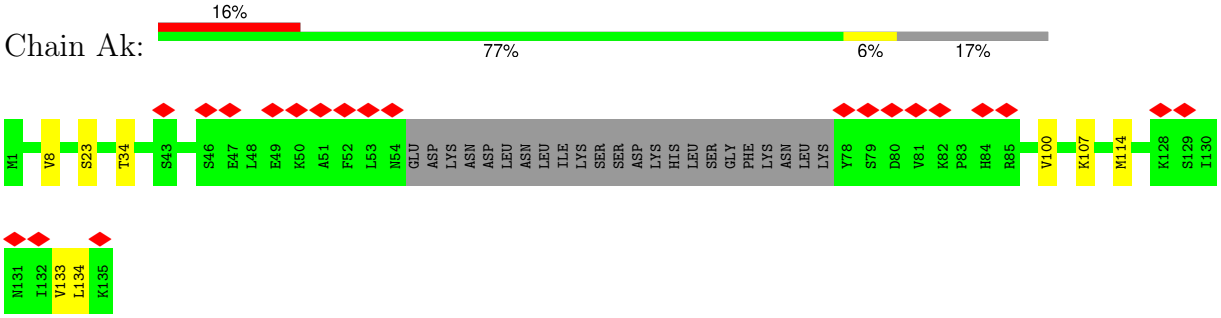
Chain Aj:





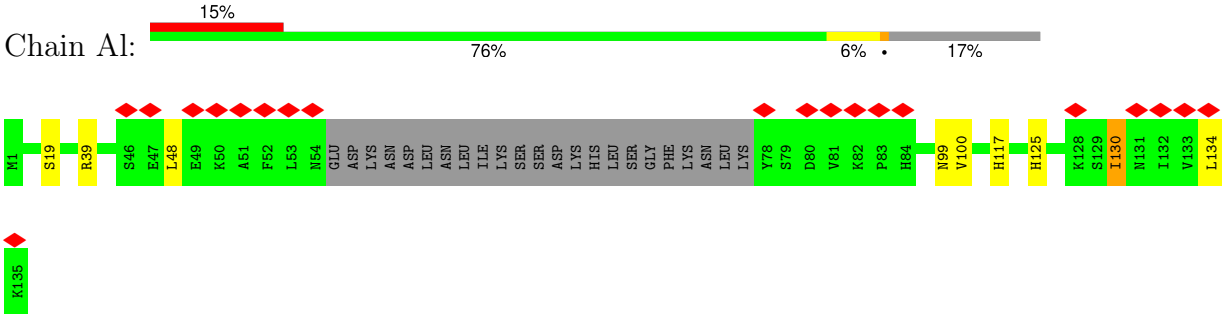
• Molecule 6: Flagellar basal body rod protein FlgB

Chain Ak:



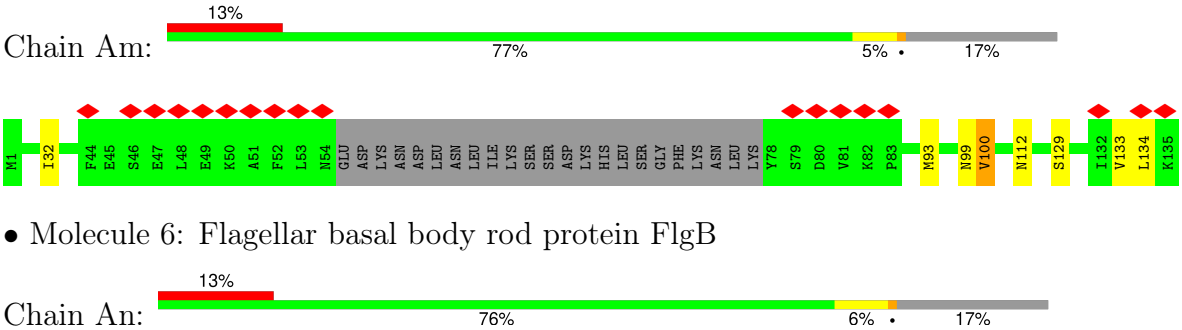
• Molecule 6: Flagellar basal body rod protein FlgB

Chain Al:



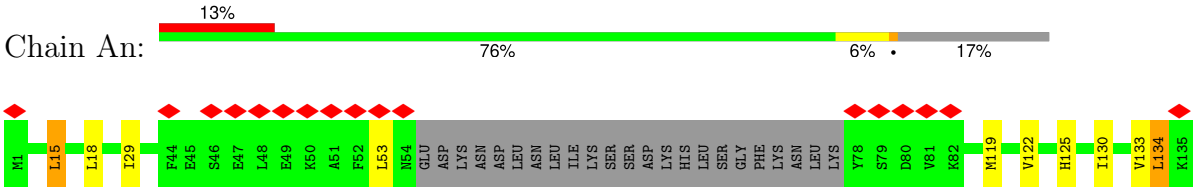
• Molecule 6: Flagellar basal body rod protein FlgB

Chain Am:



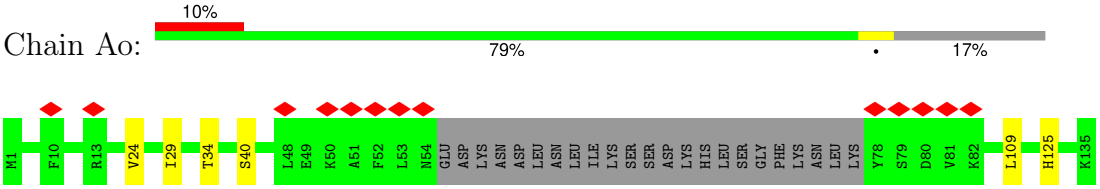
• Molecule 6: Flagellar basal body rod protein FlgB

Chain An:



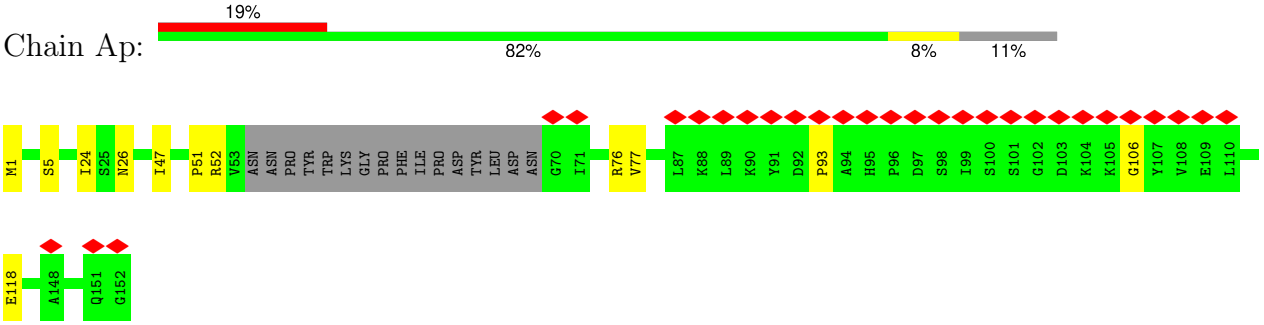
• Molecule 6: Flagellar basal body rod protein FlgB

Chain Ao:



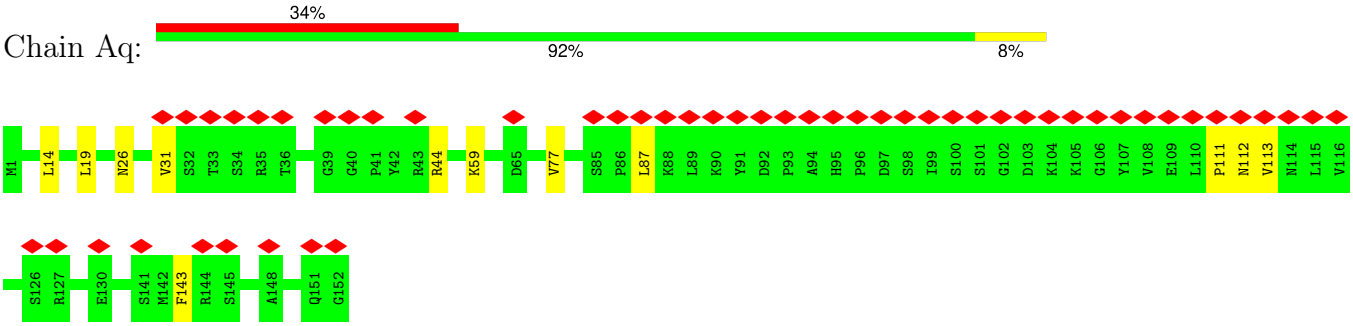
• Molecule 7: Flagellar basal-body rod protein FlgC

Chain Ap:



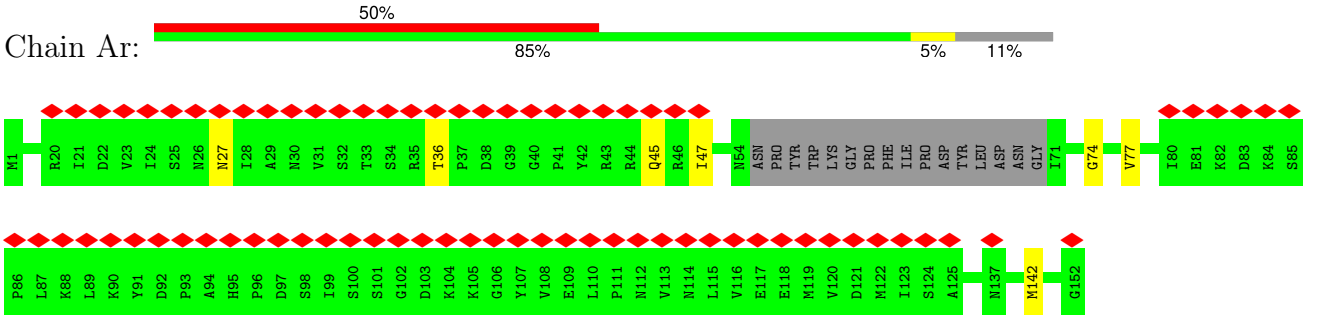
• Molecule 7: Flagellar basal-body rod protein FlgC

Chain Aq:



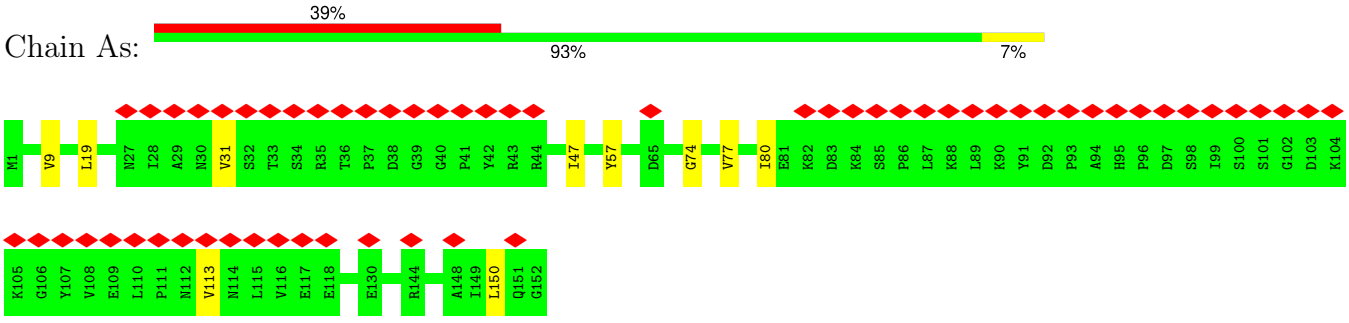
• Molecule 7: Flagellar basal-body rod protein FlgC

Chain Ar:



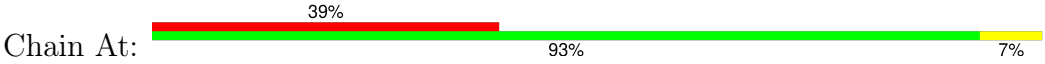
• Molecule 7: Flagellar basal-body rod protein FlgC

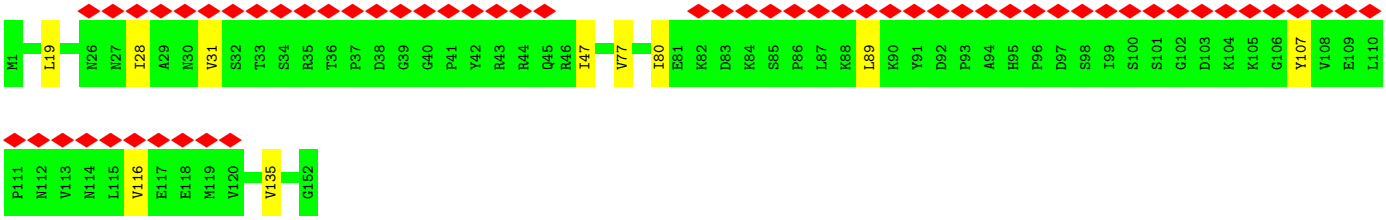
Chain As:



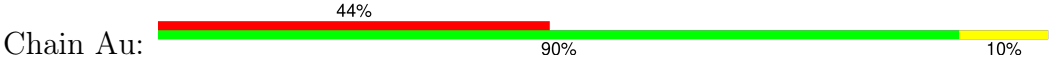
• Molecule 7: Flagellar basal-body rod protein FlgC

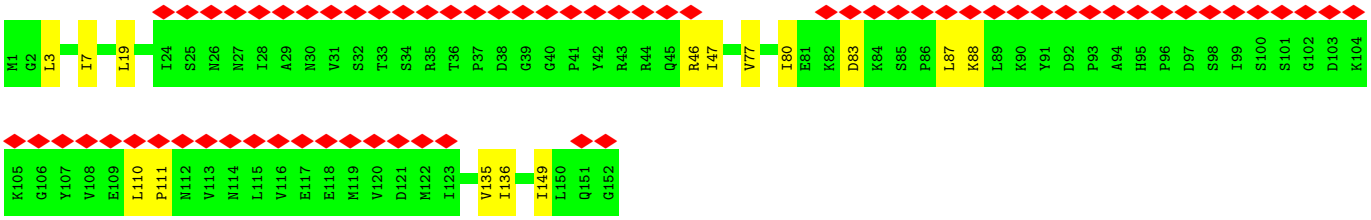
Chain At:



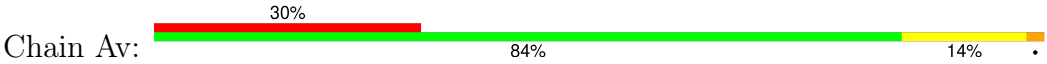


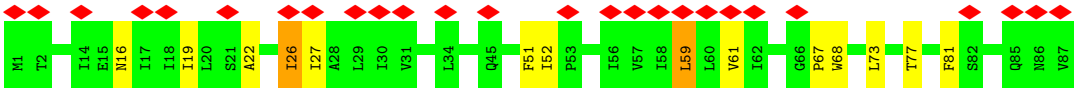
• Molecule 7: Flagellar basal-body rod protein FlgC





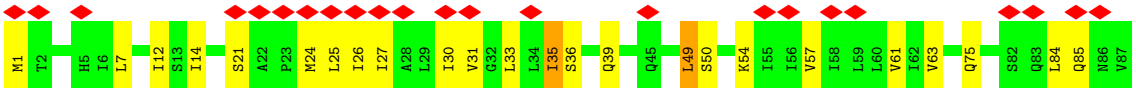
• Molecule 8: Flagellar biosynthetic protein FliQ



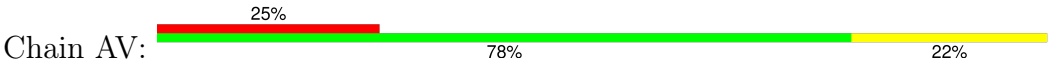


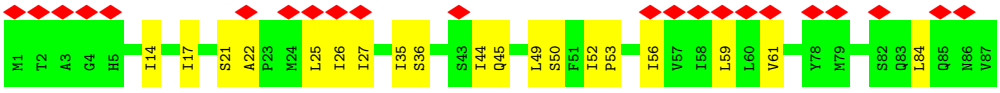
• Molecule 8: Flagellar biosynthetic protein FliQ



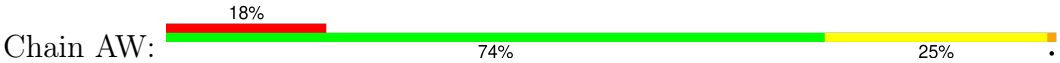


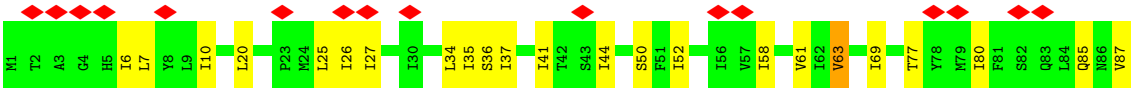
• Molecule 8: Flagellar biosynthetic protein FliQ





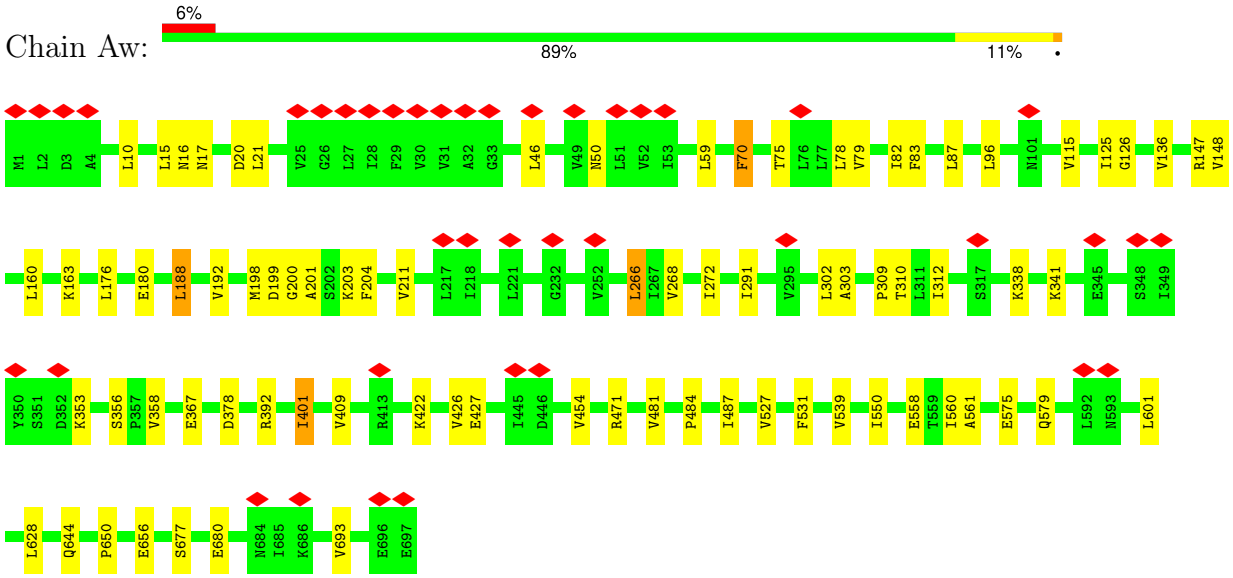
• Molecule 8: Flagellar biosynthetic protein FliQ





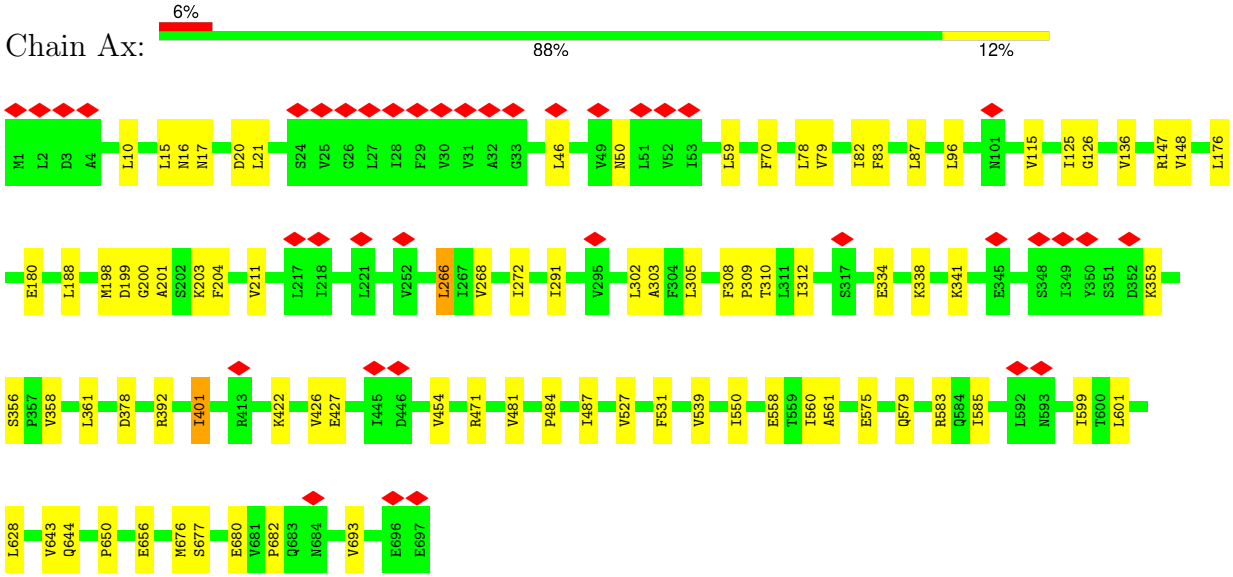
• Molecule 9: Flagellar biosynthesis protein FlhA

Chain Aw:



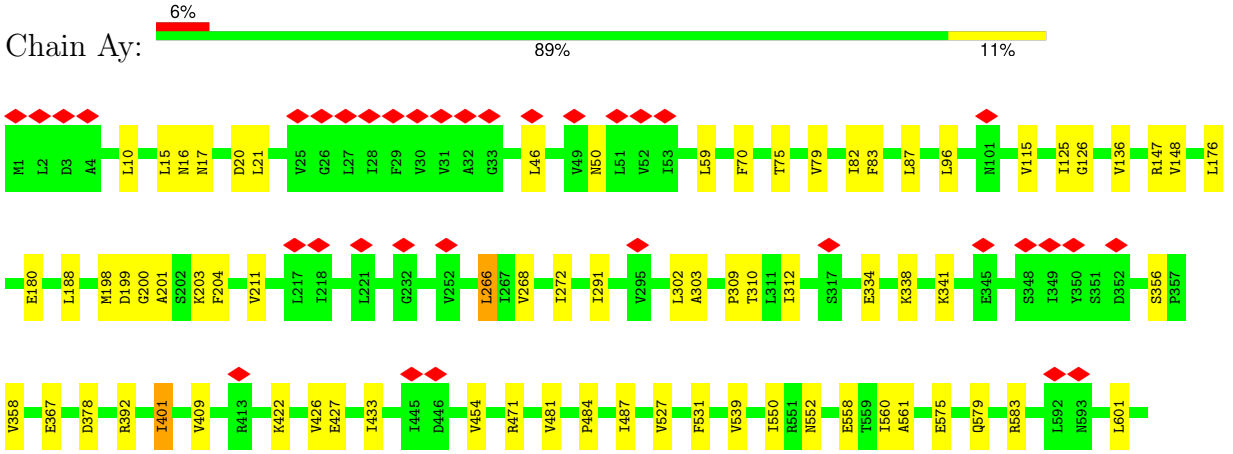
• Molecule 9: Flagellar biosynthesis protein FlhA

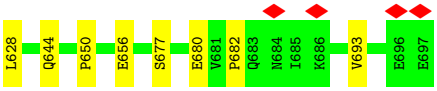
Chain Ax:



• Molecule 9: Flagellar biosynthesis protein FlhA

Chain Ay:

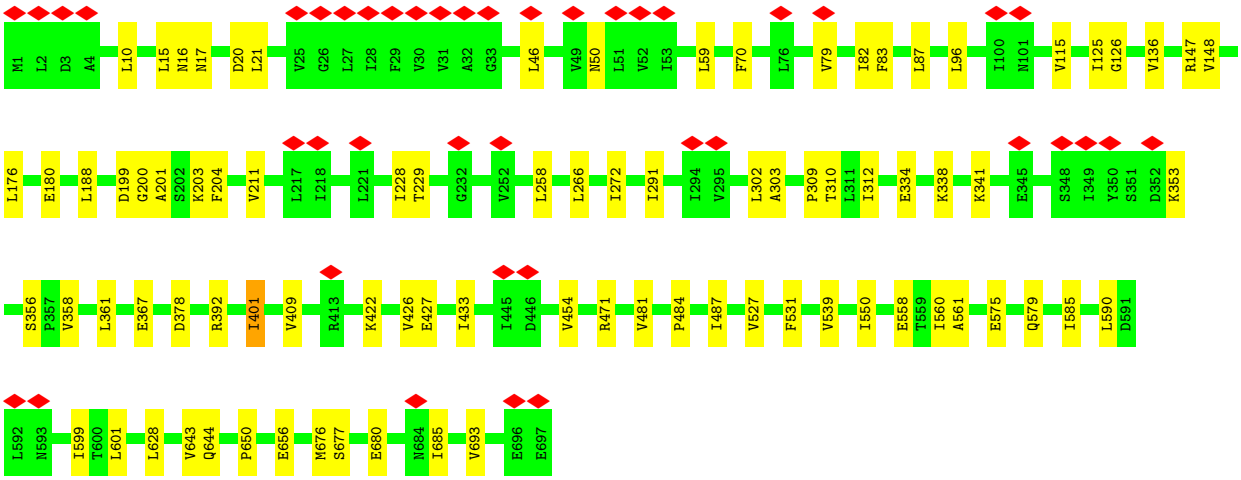




• Molecule 9: Flagellar biosynthesis protein FlhA

Chain Az:

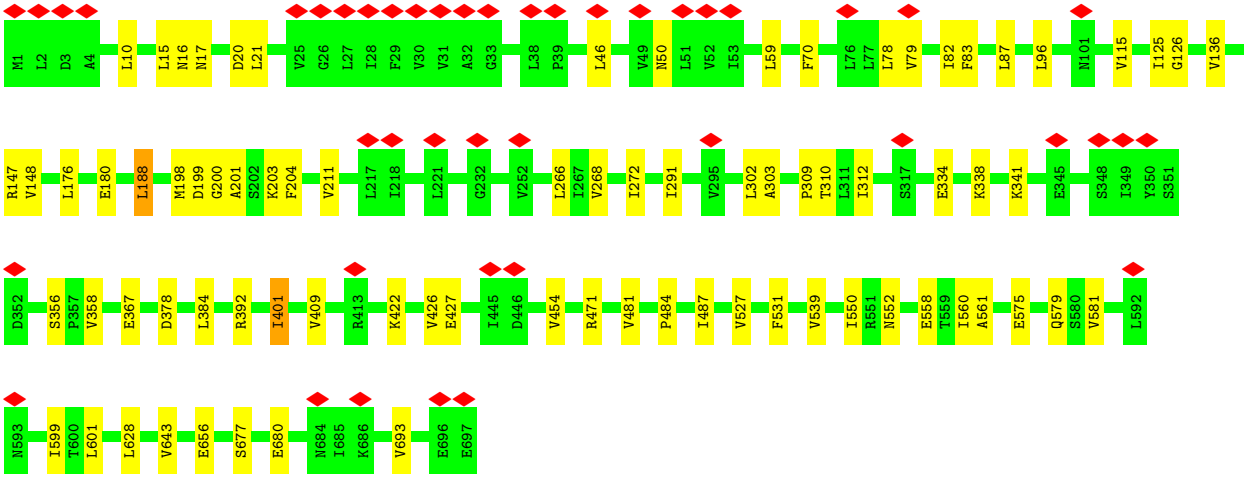




• Molecule 9: Flagellar biosynthesis protein FlhA

Chain A1:

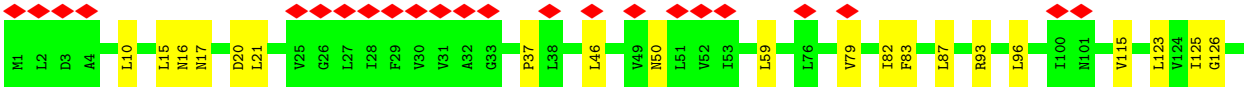


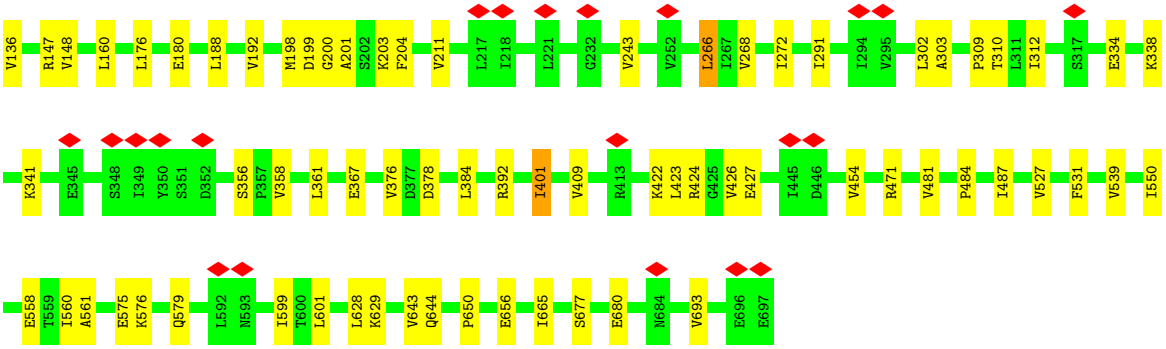


• Molecule 9: Flagellar biosynthesis protein FlhA

Chain A2:



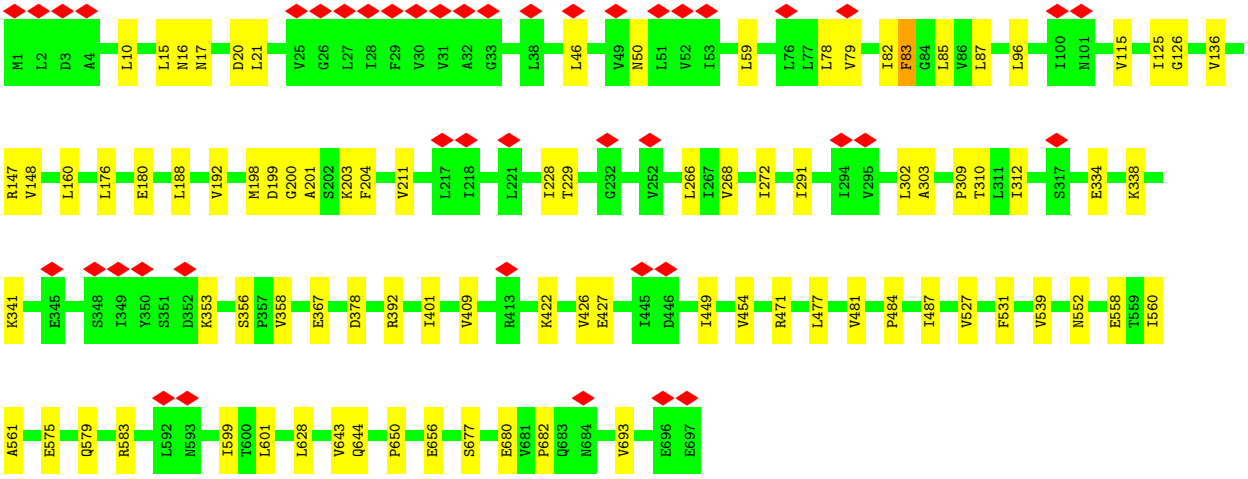




• Molecule 9: Flagellar biosynthesis protein FlhA

Chain A3:

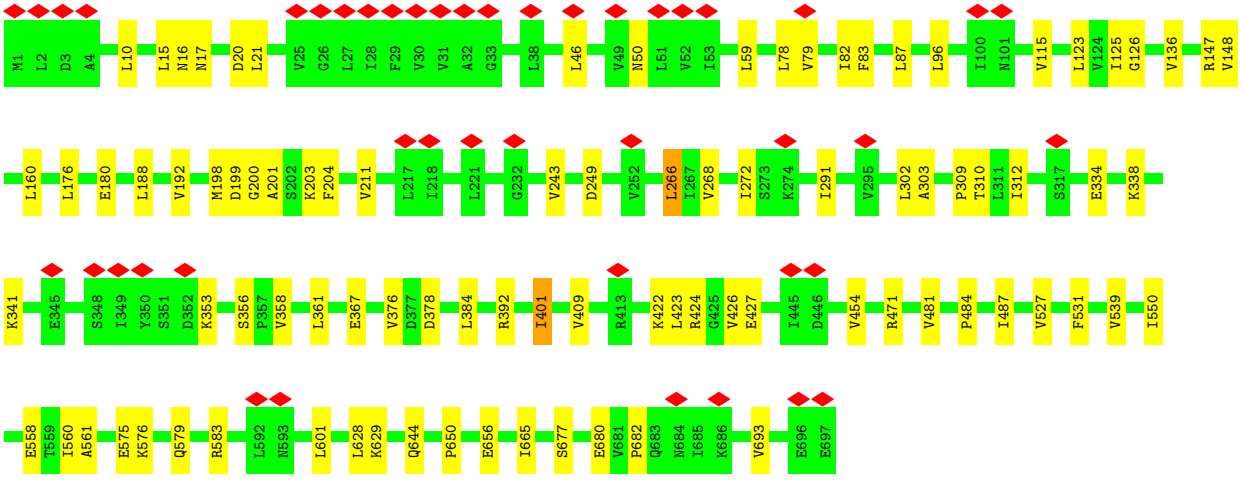




• Molecule 9: Flagellar biosynthesis protein FlhA

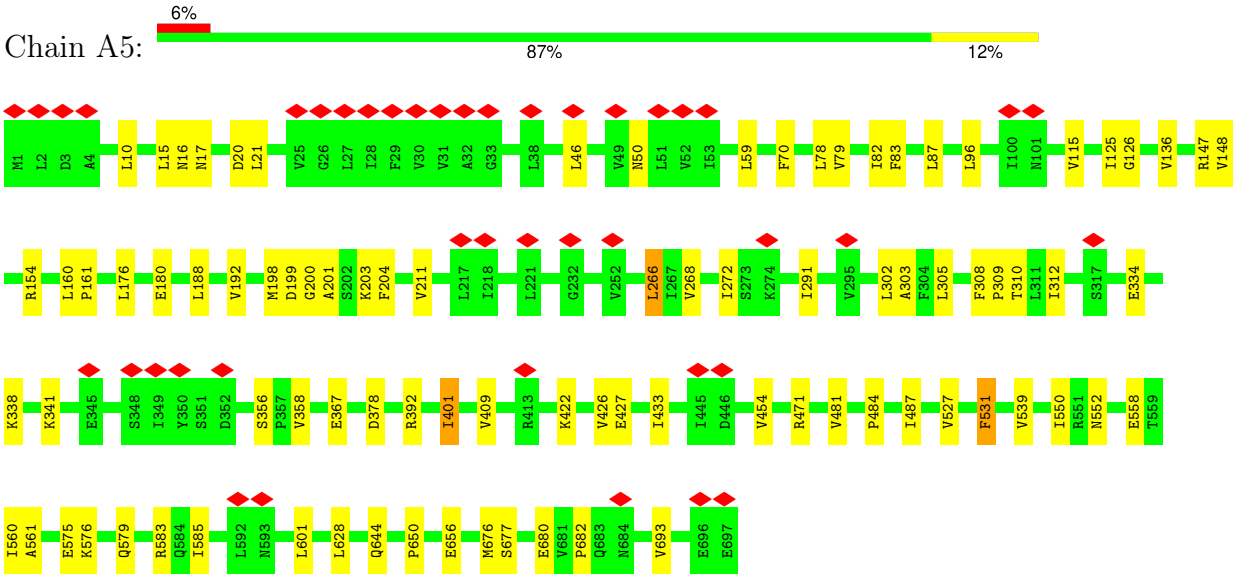
Chain A4:





• Molecule 9: Flagellar biosynthesis protein FlhA

Chain A5:


6%
87%
12%
M1 L2 D3 A4 L10 L15 N16 N17 D20 L21 V25 G26 L27 I28 F29 V30 V31 A32 G33 L38 L46 V49 N50 L51 V52 I53 L59 F70 L78 V79 I82 F83 L87 L96 I100 N101 V115 I125 G126 V136 R147 V148
R154 L160 P161 L176 E180 L188 V192 M198 D199 G200 A201 S202 K203 F204 V211 L217 I218 L221 G232 V252 L266 I267 V268 I272 S273 K274 I291 V295 L302 A303 F304 L305 F308 P309 T310 L311 I312 S317 E334
K338 K341 E345 S348 I349 Y350 S351 D352 S356 P357 V358 E367 D378 R392 I401 V409 R413 K422 V426 E427 I433 I445 D446 V454 R471 V481 P484 I487 V527 F531 V539 I550 R551 N552 E558 T559
I560 A561 E575 K576 Q579 R583 Q584 I585 L592 N593 L601 L628 Q644 P650 E656 M676 S677 E680 V681 P682 Q683 N684 V693 E696 E697

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C9	Depositor
Number of subtomograms used	4322	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.75	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.842	Depositor
Minimum map value	-5.454	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.342	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	691.2, 691.2, 691.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.7, 2.7, 2.7	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	0	0.13	0/1657	0.34	0/2246
1	1	0.13	0/1657	0.34	0/2246
1	2	0.19	1/1618 (0.1%)	0.35	0/2193
1	3	0.18	1/1657 (0.1%)	0.35	0/2246
1	4	0.19	1/1657 (0.1%)	0.37	0/2246
1	5	0.13	0/1657	0.35	0/2246
1	6	0.13	0/1618	0.34	0/2193
1	7	0.19	1/1657 (0.1%)	0.36	0/2246
1	8	0.13	0/1657	0.35	0/2246
1	9	0.18	1/1657 (0.1%)	0.35	0/2246
1	A	0.11	0/2132	0.24	0/2861
1	AA	0.13	0/1657	0.34	0/2246
1	AB	0.13	0/1657	0.34	0/2246
1	AC	0.12	0/1638	0.36	0/2214
1	AD	0.13	0/1638	0.37	0/2214
1	AE	0.13	0/1638	0.36	0/2214
1	AF	0.13	0/1638	0.36	0/2214
1	AG	0.13	0/1638	0.37	0/2214
1	AH	0.13	0/1638	0.35	0/2214
1	AI	0.12	0/1638	0.35	0/2214
1	AJ	0.13	0/1638	0.35	0/2214
1	AK	0.13	0/1638	0.36	0/2214
1	AL	0.13	0/1638	0.37	0/2214
1	AM	0.12	0/1638	0.36	0/2214
1	AN	0.13	0/1638	0.36	0/2214
1	AO	0.12	0/1638	0.35	0/2214
1	AP	0.12	0/1638	0.36	0/2214
1	AQ	0.12	0/1638	0.37	0/2214
1	AR	0.13	0/1638	0.37	0/2214
1	AS	0.13	0/1638	0.37	0/2214
1	AT	0.12	0/1638	0.37	0/2214
1	B	0.11	0/2132	0.26	0/2861
1	C	0.11	0/2132	0.27	0/2861
1	D	0.12	0/2132	0.25	0/2861

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	E	0.12	0/2132	0.27	0/2861
1	F	0.11	0/2132	0.27	0/2861
1	G	0.11	0/2132	0.26	0/2861
1	H	0.11	0/2132	0.26	0/2861
1	I	0.11	0/2132	0.24	0/2861
1	J	0.11	0/2132	0.27	0/2861
1	K	0.11	0/2132	0.24	0/2861
1	L	0.11	0/2132	0.25	0/2861
1	M	0.11	0/2132	0.26	0/2861
1	N	0.11	0/2132	0.28	0/2861
1	O	0.11	0/2132	0.25	0/2861
1	P	0.11	0/2132	0.26	0/2861
1	Q	0.11	0/2132	0.26	0/2861
1	R	0.11	0/2132	0.27	0/2861
1	S	0.11	0/2132	0.26	0/2861
1	T	0.11	0/2132	0.27	0/2861
1	U	0.11	0/2132	0.25	0/2861
1	V	0.11	0/2132	0.26	0/2861
1	W	0.12	0/2132	0.28	0/2861
1	X	0.12	0/2132	0.28	0/2861
1	Y	0.11	0/2132	0.26	0/2861
1	Z	0.11	0/2132	0.27	0/2861
1	a	0.11	0/2132	0.26	0/2861
1	b	0.11	0/2132	0.28	0/2861
1	c	0.11	0/2132	0.28	0/2861
1	d	0.11	0/2132	0.27	0/2861
1	e	0.11	0/2132	0.25	0/2861
1	f	0.11	0/2132	0.27	0/2861
1	g	0.11	0/2132	0.27	0/2861
1	h	0.12	0/2132	0.28	0/2861
1	i	0.11	0/2132	0.26	0/2861
1	j	0.11	0/2132	0.26	0/2861
1	k	0.11	0/2132	0.26	0/2861
1	l	0.11	0/2132	0.27	0/2861
1	m	0.11	0/2132	0.27	0/2861
1	n	0.11	0/2132	0.25	0/2861
1	o	0.11	0/2132	0.26	0/2861
1	p	0.18	1/1657 (0.1%)	0.34	0/2246
1	q	0.13	0/1657	0.34	0/2246
1	r	0.12	0/1657	0.35	0/2246
1	s	0.18	1/1657 (0.1%)	0.35	0/2246
1	t	0.13	0/1618	0.36	0/2193
1	u	0.18	1/1657 (0.1%)	0.34	0/2246

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	v	0.13	0/1657	0.33	0/2246
1	w	0.13	0/1657	0.33	0/2246
1	x	0.12	0/1618	0.35	0/2193
1	y	0.19	1/1657 (0.1%)	0.35	0/2246
1	z	0.13	0/1657	0.34	0/2246
2	AX	0.13	0/2033	0.31	0/2734
3	AY	0.16	0/1706	0.35	0/2313
3	AZ	0.15	0/1696	0.33	0/2300
3	Aa	0.15	0/1697	0.34	0/2300
3	Ab	0.16	0/1706	0.36	0/2312
3	Ac	0.15	0/1717	0.32	0/2325
4	Ad	0.13	0/2135	0.32	0/2892
5	Ae	0.13	0/545	0.30	0/734
5	Af	0.13	0/545	0.26	0/734
5	Ag	0.13	0/545	0.28	0/734
5	Ah	0.13	0/532	0.30	0/718
5	Ai	0.13	0/545	0.29	0/734
5	Aj	0.12	0/309	0.29	0/414
6	Ak	0.11	0/936	0.25	0/1259
6	Al	0.11	0/936	0.27	0/1259
6	Am	0.11	0/936	0.24	0/1259
6	An	0.11	0/936	0.28	0/1259
6	Ao	0.11	0/936	0.23	0/1259
7	Ap	0.11	0/1043	0.24	0/1405
7	Aq	0.12	0/1175	0.26	0/1593
7	Ar	0.12	0/1047	0.27	0/1411
7	As	0.11	0/1191	0.25	0/1612
7	At	0.11	0/1191	0.27	0/1612
7	Au	0.10	0/1191	0.26	0/1612
8	AU	0.16	0/694	0.35	0/946
8	AV	0.15	0/704	0.34	0/957
8	AW	0.15	0/704	0.32	0/957
8	Av	0.17	0/690	0.34	0/941
9	A1	0.14	0/5515	0.33	0/7477
9	A2	0.14	0/5515	0.33	0/7477
9	A3	0.14	0/5515	0.33	0/7477
9	A4	0.14	0/5515	0.33	0/7477
9	A5	0.14	0/5515	0.33	0/7477
9	Aw	0.14	0/5515	0.33	0/7477
9	Ax	0.14	0/5515	0.33	0/7477
9	Ay	0.14	0/5515	0.33	0/7477
9	Az	0.14	0/5515	0.33	0/7477
All	All	0.13	9/234507 (0.0%)	0.31	0/316477

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7	107	VAL	C-N	5.75	1.38	1.33
1	4	107	VAL	C-N	5.74	1.38	1.33
1	2	107	VAL	C-N	5.71	1.38	1.33
1	9	107	VAL	C-N	5.61	1.38	1.33
1	y	107	VAL	C-N	5.59	1.38	1.33
1	s	107	VAL	C-N	5.47	1.38	1.33
1	p	107	VAL	C-N	5.45	1.38	1.33
1	3	107	VAL	C-N	5.34	1.38	1.33
1	u	107	VAL	C-N	5.30	1.38	1.33

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	0	1632	0	1673	6	0
1	1	1632	0	1673	9	0
1	2	1595	0	1633	7	0
1	3	1632	0	1673	8	0
1	4	1632	0	1673	10	0
1	5	1632	0	1673	8	0
1	6	1595	0	1633	7	0
1	7	1632	0	1673	11	0
1	8	1632	0	1673	14	0
1	9	1632	0	1673	12	0
1	A	2104	0	2085	18	0
1	AA	1632	0	1673	12	0
1	AB	1632	0	1673	9	0
1	AC	1614	0	1677	18	0
1	AD	1614	0	1677	18	0
1	AE	1614	0	1677	18	0
1	AF	1614	0	1677	18	0
1	AG	1614	0	1677	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AH	1614	0	1677	17	0
1	AI	1614	0	1677	17	0
1	AJ	1614	0	1677	18	0
1	AK	1614	0	1677	17	0
1	AL	1614	0	1677	19	0
1	AM	1614	0	1677	17	0
1	AN	1614	0	1677	19	0
1	AO	1614	0	1677	18	0
1	AP	1614	0	1677	17	0
1	AQ	1614	0	1677	18	0
1	AR	1614	0	1677	17	0
1	AS	1614	0	1677	16	0
1	AT	1614	0	1677	16	0
1	B	2104	0	2085	19	0
1	C	2104	0	2085	20	0
1	D	2104	0	2085	21	0
1	E	2104	0	2085	21	0
1	F	2104	0	2085	17	0
1	G	2104	0	2085	20	0
1	H	2104	0	2085	18	0
1	I	2104	0	2085	18	0
1	J	2104	0	2085	15	0
1	K	2104	0	2085	15	0
1	L	2104	0	2085	17	0
1	M	2104	0	2085	16	0
1	N	2104	0	2085	27	0
1	O	2104	0	2085	20	0
1	P	2104	0	2085	19	0
1	Q	2104	0	2085	22	0
1	R	2104	0	2085	19	0
1	S	2104	0	2085	28	0
1	T	2104	0	2085	19	0
1	U	2104	0	2085	19	0
1	V	2104	0	2085	21	0
1	W	2104	0	2085	19	0
1	X	2104	0	2085	22	0
1	Y	2104	0	2085	14	0
1	Z	2104	0	2085	14	0
1	a	2104	0	2085	17	0
1	b	2104	0	2085	20	0
1	c	2104	0	2085	21	0
1	d	2104	0	2085	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	e	2104	0	2085	19	0
1	f	2104	0	2085	16	0
1	g	2104	0	2085	17	0
1	h	2104	0	2085	16	0
1	i	2104	0	2085	18	0
1	j	2104	0	2085	19	0
1	k	2104	0	2085	14	0
1	l	2104	0	2085	17	0
1	m	2104	0	2085	20	0
1	n	2104	0	2085	13	0
1	o	2104	0	2085	19	0
1	p	1632	0	1673	15	0
1	q	1632	0	1673	9	0
1	r	1632	0	1673	6	0
1	s	1632	0	1673	7	0
1	t	1595	0	1633	9	0
1	u	1632	0	1673	14	0
1	v	1632	0	1673	6	0
1	w	1632	0	1673	7	0
1	x	1595	0	1633	10	0
1	y	1632	0	1673	10	0
1	z	1632	0	1673	9	0
2	AX	1988	0	2043	22	0
3	AY	1665	0	1752	31	0
3	AZ	1656	0	1740	29	0
3	Aa	1657	0	1747	24	0
3	Ab	1666	0	1755	23	0
3	Ac	1676	0	1773	23	0
4	Ad	2083	0	2194	32	0
5	Ae	542	0	579	8	0
5	Af	542	0	579	4	0
5	Ag	542	0	579	7	0
5	Ah	530	0	561	7	0
5	Ai	542	0	579	8	0
5	Aj	308	0	327	7	0
6	Ak	920	0	896	6	0
6	Al	920	0	896	6	0
6	Am	920	0	896	5	0
6	An	920	0	896	11	0
6	Ao	920	0	896	4	0
7	Ap	1030	0	1055	8	0
7	Aq	1153	0	1150	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Ar	1034	0	1058	4	0
7	As	1169	0	1178	5	0
7	At	1169	0	1178	5	0
7	Au	1169	0	1178	9	0
8	AU	682	0	749	14	0
8	AV	692	0	771	10	0
8	AW	692	0	771	16	0
8	Av	678	0	743	12	0
9	A1	5429	0	5666	44	0
9	A2	5429	0	5666	47	0
9	A3	5429	0	5666	46	0
9	A4	5429	0	5666	50	0
9	A5	5429	0	5666	51	0
9	Aw	5429	0	5666	43	0
9	Ax	5429	0	5666	46	0
9	Ay	5429	0	5666	43	0
9	Az	5429	0	5666	44	0
All	All	231030	0	235503	1684	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 4.

All (1684) 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)
4:Ad:54:SER:O	4:Ad:58:VAL:HB	1.78	0.83
1:m:230:ASP:O	1:m:234:ARG:HB2	1.80	0.81
8:Av:22:ALA:O	8:Av:26:ILE:HB	1.83	0.78
8:AU:27:ILE:HG21	8:AU:61:VAL:HG21	1.65	0.77
3:AZ:64:PHE:O	3:AZ:68:MET:HB3	1.90	0.71
1:AE:69:GLN:HE22	1:AE:73:ARG:HH21	1.37	0.70
8:AV:22:ALA:O	8:AV:26:ILE:HB	1.92	0.70
1:X:287:SER:HB2	1:X:371:SER:HB3	1.75	0.69
1:AM:69:GLN:HE22	1:AM:73:ARG:HH21	1.41	0.69
1:H:231:GLY:H	1:6:228:ASN:HB2	1.58	0.68
1:R:287:SER:HB2	1:R:371:SER:HB3	1.75	0.68
1:p:183:PRO:HB2	1:AL:66:ARG:HD3	1.74	0.68
1:c:287:SER:HB2	1:c:371:SER:HB3	1.76	0.67
7:Ap:52:ARG:HE	7:Ap:76:ARG:HB2	1.59	0.67
8:Av:27:ILE:HG21	8:Av:61:VAL:HG21	1.77	0.67
1:N:287:SER:HB2	1:N:371:SER:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:69:GLN:HE22	1:AJ:73:ARG:HH21	1.43	0.66
1:A:287:SER:HB2	1:A:371:SER:HB3	1.77	0.66
1:N:230:ASP:O	1:N:234:ARG:HB2	1.94	0.66
1:m:287:SER:HB3	1:m:371:SER:HB3	1.78	0.66
9:Ax:471:ARG:HG3	9:Ax:481:VAL:HG11	1.78	0.66
1:AD:69:GLN:HE22	1:AD:73:ARG:HH21	1.43	0.65
3:Aa:157:ILE:HD11	3:Aa:175:VAL:HG11	1.78	0.65
1:B:287:SER:HB2	1:B:371:SER:HB3	1.78	0.65
1:E:287:SER:HB2	1:E:371:SER:HB3	1.77	0.65
9:Aw:291:ILE:HB	9:A5:59:LEU:HD23	1.78	0.65
9:Aw:471:ARG:HG3	9:Aw:481:VAL:HG11	1.79	0.65
9:Az:471:ARG:HG3	9:Az:481:VAL:HG11	1.79	0.65
1:AS:69:GLN:HE22	1:AS:73:ARG:HH21	1.42	0.65
9:A3:59:LEU:HD23	9:A4:291:ILE:HB	1.79	0.64
1:d:364:VAL:HG22	1:e:315:ILE:HA	1.80	0.64
9:A1:471:ARG:HG3	9:A1:481:VAL:HG11	1.79	0.64
1:j:287:SER:HB3	1:j:371:SER:HB3	1.79	0.64
1:I:287:SER:HB2	1:I:371:SER:HB3	1.80	0.64
9:Ay:471:ARG:HG3	9:Ay:481:VAL:HG11	1.80	0.64
1:AH:69:GLN:HE22	1:AH:73:ARG:HH21	1.43	0.64
1:AC:69:GLN:HE22	1:AC:73:ARG:HH21	1.45	0.63
9:A4:471:ARG:HG3	9:A4:481:VAL:HG11	1.79	0.63
1:l:287:SER:HB2	1:l:371:SER:HB3	1.81	0.63
8:AV:27:ILE:HG21	8:AV:61:VAL:HG21	1.80	0.63
9:A1:59:LEU:HD23	9:A2:291:ILE:HB	1.79	0.63
9:A2:471:ARG:HG3	9:A2:481:VAL:HG11	1.80	0.63
9:A3:471:ARG:HG3	9:A3:481:VAL:HG11	1.79	0.63
9:A4:59:LEU:HD23	9:A5:291:ILE:HB	1.79	0.63
1:AK:69:GLN:HE22	1:AK:73:ARG:HH21	1.46	0.63
9:Aw:59:LEU:HD23	9:Ax:291:ILE:HB	1.80	0.63
9:Ay:59:LEU:HD23	9:Az:291:ILE:HB	1.79	0.63
9:Az:59:LEU:HD23	9:A1:291:ILE:HB	1.80	0.63
1:AT:69:GLN:HE22	1:AT:73:ARG:HH21	1.43	0.63
4:Ad:190:LEU:O	4:Ad:194:PHE:HB2	1.99	0.63
1:J:287:SER:HB2	1:J:371:SER:HB3	1.81	0.63
9:Ax:59:LEU:HD23	9:Ay:291:ILE:HB	1.79	0.62
9:A5:471:ARG:HG3	9:A5:481:VAL:HG11	1.80	0.62
1:AN:69:GLN:HE22	1:AN:73:ARG:HH21	1.45	0.62
1:1:159:VAL:HB	1:1:174:LYS:HG3	1.82	0.62
1:AL:69:GLN:HE22	1:AL:73:ARG:HH21	1.45	0.62
1:AR:69:GLN:HE22	1:AR:73:ARG:HH21	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A2:59:LEU:HD23	9:A3:291:ILE:HB	1.80	0.61
1:AG:69:GLN:HE22	1:AG:73:ARG:HH21	1.47	0.61
2:AX:103:ILE:O	2:AX:107:VAL:HB	2.00	0.61
1:AO:69:GLN:HE22	1:AO:73:ARG:HH21	1.49	0.61
1:5:165:LEU:HB3	3:AY:162:SER:HB3	1.83	0.61
1:J:364:VAL:HG22	1:K:315:ILE:HA	1.82	0.61
1:AP:69:GLN:HE22	1:AP:73:ARG:HH21	1.48	0.61
9:A5:575:GLU:HG2	9:A5:656:GLU:HG3	1.83	0.61
1:AP:70:ARG:HG2	1:AP:101:LEU:HD11	1.83	0.61
2:AX:188:ILE:HD13	4:Ad:199:LEU:HD12	1.82	0.60
9:A4:361:LEU:HD11	9:A5:552:ASN:HA	1.83	0.60
1:U:364:VAL:HG22	1:V:315:ILE:HA	1.82	0.60
4:Ad:94:ILE:HD13	4:Ad:253:SER:HA	1.83	0.60
1:R:242:ARG:HH12	1:S:251:MET:HG3	1.65	0.60
1:4:183:PRO:HB2	1:AE:66:ARG:HD3	1.83	0.60
1:AI:69:GLN:HE22	1:AI:73:ARG:HH21	1.47	0.60
7:Au:47:ILE:HG22	7:Au:80:ILE:HG12	1.84	0.60
9:Aw:136:VAL:HG22	9:A5:211:VAL:HG21	1.82	0.60
1:M:287:SER:HB2	1:M:371:SER:HB3	1.84	0.60
9:Ay:211:VAL:HG21	9:Az:136:VAL:HG22	1.83	0.60
1:AF:116:LEU:HA	1:AF:122:TRP:HB2	1.84	0.60
1:y:184:GLY:HA3	1:AS:66:ARG:HH12	1.65	0.60
6:An:29:ILE:HG21	7:At:135:VAL:HG21	1.84	0.60
1:E:355:TYR:HA	1:F:323:GLU:HB3	1.84	0.60
2:AX:115:LEU:HB2	8:Av:52:ILE:HG21	1.82	0.60
2:AX:254:ASP:HB3	2:AX:257:LEU:HB2	1.84	0.60
1:Z:355:TYR:HA	1:a:323:GLU:HB3	1.84	0.60
1:f:235:ILE:HG21	1:g:240:LYS:HB3	1.84	0.60
9:Ay:96:LEU:HD13	9:Az:125:ILE:HD12	1.84	0.60
1:AQ:69:GLN:HE22	1:AQ:73:ARG:HH21	1.47	0.59
9:A3:575:GLU:HG2	9:A3:656:GLU:HG3	1.84	0.59
9:A2:575:GLU:HG2	9:A2:656:GLU:HG3	1.85	0.59
1:o:287:SER:HB2	1:o:371:SER:HB3	1.84	0.59
1:H:356:ASN:HB3	1:I:323:GLU:HB3	1.84	0.59
1:d:288:LYS:HE2	1:d:370:LYS:HE3	1.84	0.59
9:Az:361:LEU:HD11	9:A1:552:ASN:HA	1.84	0.59
1:W:287:SER:HB2	1:W:371:SER:HB3	1.83	0.59
1:AD:116:LEU:HA	1:AD:122:TRP:HB2	1.84	0.59
9:A2:96:LEU:HD13	9:A3:125:ILE:HD12	1.84	0.59
1:O:417:MET:H	1:O:447:ASN:HD21	1.51	0.59
1:l:364:VAL:HG22	1:m:315:ILE:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:As:47:ILE:HG12	7:As:80:ILE:HG12	1.84	0.59
9:A1:575:GLU:HG2	9:A1:656:GLU:HG3	1.85	0.59
1:AO:20:SER:HB3	1:AO:23:GLN:HE22	1.68	0.59
9:A2:115:VAL:HG13	9:A2:126:GLY:HA3	1.85	0.59
1:AI:70:ARG:HG2	1:AI:101:LEU:HD11	1.84	0.59
3:Aa:48:SER:HB2	6:Am:133:VAL:HG21	1.84	0.59
9:Aw:575:GLU:HG2	9:Aw:656:GLU:HG3	1.85	0.59
9:Ax:211:VAL:HG21	9:Ay:136:VAL:HG22	1.84	0.59
9:Az:575:GLU:HG2	9:Az:656:GLU:HG3	1.85	0.59
1:AE:70:ARG:HG2	1:AE:101:LEU:HD11	1.85	0.59
1:AT:116:LEU:HA	1:AT:122:TRP:HB2	1.85	0.59
9:Az:211:VAL:HG21	9:A1:136:VAL:HG22	1.84	0.59
1:V:316:SER:HB2	1:V:363:ASN:HB3	1.84	0.59
9:Az:115:VAL:HG13	9:Az:126:GLY:HA3	1.85	0.59
1:Q:231:GLY:H	1:AA:228:ASN:HB2	1.68	0.58
1:AC:20:SER:HB3	1:AC:23:GLN:HE22	1.68	0.58
3:Ac:73:ARG:HD3	3:Ac:195:MET:HE1	1.84	0.58
9:A3:211:VAL:HG21	9:A4:136:VAL:HG22	1.83	0.58
9:A4:115:VAL:HG13	9:A4:126:GLY:HA3	1.85	0.58
1:K:287:SER:HB2	1:K:371:SER:HB3	1.85	0.58
1:M:293:ILE:HD13	1:M:313:THR:HG21	1.85	0.58
1:AE:20:SER:HB3	1:AE:23:GLN:HE22	1.67	0.58
3:AY:169:PRO:HB3	3:AY:174:GLU:HG2	1.86	0.58
6:Ao:29:ILE:HG21	7:Au:135:VAL:HG21	1.84	0.58
9:A1:211:VAL:HG21	9:A2:136:VAL:HG22	1.85	0.58
9:A4:575:GLU:HG2	9:A4:656:GLU:HG3	1.85	0.58
1:V:364:VAL:HG22	1:W:315:ILE:HA	1.86	0.58
1:AO:70:ARG:HG2	1:AO:101:LEU:HD11	1.86	0.58
1:F:287:SER:HB3	1:F:371:SER:HB3	1.86	0.58
1:AP:20:SER:HB3	1:AP:23:GLN:HE22	1.69	0.58
7:Aq:19:LEU:HD23	7:Aq:77:VAL:HG21	1.86	0.58
7:As:19:LEU:HD23	7:As:77:VAL:HG21	1.84	0.58
1:AG:20:SER:HB3	1:AG:23:GLN:HE22	1.69	0.58
1:AN:20:SER:HB3	1:AN:23:GLN:HE22	1.69	0.58
9:Ax:575:GLU:HG2	9:Ax:656:GLU:HG3	1.85	0.58
1:H:364:VAL:HG22	1:I:315:ILE:HA	1.85	0.58
1:b:298:GLN:HE22	1:b:305:ASN:HA	1.69	0.58
1:AN:70:ARG:HG2	1:AN:101:LEU:HD11	1.86	0.58
1:AT:20:SER:HB3	1:AT:23:GLN:HE22	1.69	0.58
9:A1:96:LEU:HD13	9:A2:125:ILE:HD12	1.85	0.58
1:7:53:LEU:HG	1:7:88:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:116:LEU:HA	1:AH:122:TRP:HB2	1.86	0.58
9:Aw:211:VAL:HG21	9:Ax:136:VAL:HG22	1.85	0.57
9:A5:46:LEU:HB3	9:A5:87:LEU:HD21	1.85	0.57
3:AZ:64:PHE:O	3:AZ:68:MET:CB	2.52	0.57
9:Aw:46:LEU:HB3	9:Aw:87:LEU:HD21	1.86	0.57
1:4:53:LEU:HG	1:4:88:LEU:HD11	1.86	0.57
1:AC:116:LEU:HA	1:AC:122:TRP:HB2	1.85	0.57
1:AG:116:LEU:HA	1:AG:122:TRP:HB2	1.87	0.57
3:Ab:81:ILE:HD11	3:Ab:245:ILE:HG21	1.85	0.57
9:Az:96:LEU:HD13	9:A1:125:ILE:HD12	1.85	0.57
1:A:364:VAL:HG22	1:B:315:ILE:HA	1.85	0.57
1:G:287:SER:HB2	1:G:371:SER:HB3	1.86	0.57
1:AC:70:ARG:HG2	1:AC:101:LEU:HD11	1.85	0.57
1:AK:116:LEU:HA	1:AK:122:TRP:HB2	1.86	0.57
1:AH:20:SER:HB3	1:AH:23:GLN:HE22	1.70	0.57
1:AL:116:LEU:HA	1:AL:122:TRP:HB2	1.84	0.57
1:AQ:70:ARG:HG2	1:AQ:101:LEU:HD11	1.85	0.57
9:A3:46:LEU:HB3	9:A3:87:LEU:HD21	1.85	0.57
9:A4:46:LEU:HB3	9:A4:87:LEU:HD21	1.86	0.57
9:A4:211:VAL:HG21	9:A5:136:VAL:HG22	1.85	0.57
1:H:287:SER:HB2	1:H:371:SER:HB3	1.86	0.57
1:r:53:LEU:HG	1:r:88:LEU:HD11	1.85	0.57
1:AS:70:ARG:HG2	1:AS:101:LEU:HD11	1.87	0.57
9:A1:46:LEU:HB3	9:A1:87:LEU:HD21	1.85	0.57
9:A3:96:LEU:HD13	9:A4:125:ILE:HD12	1.86	0.57
9:A4:96:LEU:HD13	9:A5:125:ILE:HD12	1.84	0.57
1:i:273:ARG:HB2	1:j:432:SER:HB2	1.86	0.57
1:AE:116:LEU:HA	1:AE:122:TRP:HB2	1.86	0.57
1:AE:163:LYS:HG3	1:AE:170:GLN:HE22	1.70	0.57
1:AJ:20:SER:HB3	1:AJ:23:GLN:HE22	1.70	0.57
1:AR:116:LEU:HA	1:AR:122:TRP:HB2	1.85	0.57
9:A2:211:VAL:HG21	9:A3:136:VAL:HG22	1.85	0.57
1:b:501:ARG:HG2	1:b:504:ARG:HH21	1.70	0.57
1:AN:116:LEU:HA	1:AN:122:TRP:HB2	1.86	0.57
1:t:53:LEU:HG	1:t:88:LEU:HD11	1.87	0.57
1:6:53:LEU:HG	1:6:88:LEU:HD11	1.85	0.57
1:AI:116:LEU:HA	1:AI:122:TRP:HB2	1.87	0.57
1:AQ:20:SER:HB3	1:AQ:23:GLN:HE22	1.69	0.57
3:AZ:51:LEU:HD11	5:Ae:92:ILE:HD11	1.86	0.57
9:Ax:46:LEU:HB3	9:Ax:87:LEU:HD21	1.87	0.57
1:d:233:ASP:HB2	1:u:228:ASN:HD21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:265:SER:HB2	1:o:268:ARG:HG3	1.87	0.56
1:AP:163:LYS:HG3	1:AP:170:GLN:HE22	1.70	0.56
3:AZ:235:LEU:HD21	8:Av:73:LEU:HB3	1.87	0.56
1:AJ:70:ARG:HG2	1:AJ:101:LEU:HD11	1.87	0.56
1:AM:116:LEU:HA	1:AM:122:TRP:HB2	1.86	0.56
9:A2:46:LEU:HB3	9:A2:87:LEU:HD21	1.85	0.56
1:B:501:ARG:HG2	1:B:504:ARG:HH21	1.70	0.56
1:M:316:SER:HB2	1:M:363:ASN:HB3	1.85	0.56
1:X:273:ARG:HB2	1:Y:432:SER:HB3	1.87	0.56
1:n:298:GLN:HE22	1:n:305:ASN:HA	1.71	0.56
1:AK:20:SER:HB3	1:AK:23:GLN:HE22	1.70	0.56
1:AK:70:ARG:HG2	1:AK:101:LEU:HD11	1.87	0.56
1:AP:116:LEU:HA	1:AP:122:TRP:HB2	1.86	0.56
1:AQ:116:LEU:HA	1:AQ:122:TRP:HB2	1.85	0.56
7:At:47:ILE:HG12	7:At:80:ILE:HG12	1.86	0.56
8:AU:35:ILE:HD11	8:AU:54:LYS:HZ2	1.70	0.56
9:Aw:125:ILE:HD12	9:A5:96:LEU:HD13	1.87	0.56
9:Ay:46:LEU:HB3	9:Ay:87:LEU:HD21	1.86	0.56
1:N:251:MET:HE2	1:N:255:GLU:HG3	1.87	0.56
1:AD:70:ARG:HG2	1:AD:101:LEU:HD11	1.87	0.56
1:AF:69:GLN:HE22	1:AF:73:ARG:HH21	1.51	0.56
1:AF:70:ARG:HG2	1:AF:101:LEU:HD11	1.88	0.56
1:AJ:116:LEU:HA	1:AJ:122:TRP:HB2	1.87	0.56
1:AO:116:LEU:HA	1:AO:122:TRP:HB2	1.86	0.56
3:Ac:235:LEU:HD11	8:AW:77:THR:HG21	1.85	0.56
9:Ax:115:VAL:HG13	9:Ax:126:GLY:HA3	1.87	0.56
9:A5:176:LEU:HD22	9:A5:180:GLU:HG2	1.87	0.56
1:S:273:ARG:HB2	1:T:432:SER:HB2	1.86	0.56
9:Ax:96:LEU:HD13	9:Ay:125:ILE:HD12	1.86	0.56
1:AS:116:LEU:HA	1:AS:122:TRP:HB2	1.86	0.56
9:A3:203:LYS:HG3	9:A4:147:ARG:HG2	1.87	0.56
1:L:232:ILE:H	1:8:228:ASN:HB2	1.71	0.56
1:T:316:SER:HB2	1:T:363:ASN:HB3	1.88	0.56
1:AT:70:ARG:HG2	1:AT:101:LEU:HD11	1.87	0.56
1:S:238:ALA:HB2	1:T:377:PRO:HB2	1.88	0.56
1:AH:70:ARG:HG2	1:AH:101:LEU:HD11	1.87	0.56
1:AM:70:ARG:HG2	1:AM:101:LEU:HD11	1.87	0.56
1:AR:70:ARG:HG2	1:AR:101:LEU:HD11	1.88	0.56
9:Aw:96:LEU:HD13	9:Ax:125:ILE:HD12	1.88	0.56
1:D:501:ARG:HG2	1:D:504:ARG:HH21	1.71	0.56
1:n:364:VAL:HG22	1:o:315:ILE:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:70:ARG:HG2	1:AG:101:LEU:HD11	1.85	0.56
1:AI:20:SER:HB3	1:AI:23:GLN:HE22	1.71	0.56
1:G:364:VAL:HG22	1:H:315:ILE:HA	1.87	0.55
1:O:287:SER:HB2	1:O:371:SER:HB3	1.88	0.55
1:O:501:ARG:HG2	1:O:504:ARG:HH21	1.71	0.55
2:AX:55:LEU:HD13	4:Ad:212:LYS:HG2	1.88	0.55
2:AX:69:PHE:HA	2:AX:106:TYR:HE2	1.71	0.55
9:Az:46:LEU:HB3	9:Az:87:LEU:HD21	1.87	0.55
1:o:501:ARG:HG2	1:o:504:ARG:HH21	1.70	0.55
1:AB:215:ILE:HB	1:AB:224:ASN:HB2	1.88	0.55
1:I:265:SER:HB2	1:I:268:ARG:HG3	1.89	0.55
1:AC:182:ARG:HH21	1:AT:125:THR:HB	1.71	0.55
9:A5:115:VAL:HG13	9:A5:126:GLY:HA3	1.88	0.55
1:E:293:ILE:HD13	1:E:313:THR:HG21	1.88	0.55
1:I:391:GLY:HA2	1:I:417:MET:HG3	1.88	0.55
1:Y:316:SER:HB2	1:Y:363:ASN:HB3	1.88	0.55
1:a:265:SER:HB3	1:a:268:ARG:HG3	1.88	0.55
2:AX:100:ILE:HG23	8:Av:59:LEU:HD12	1.88	0.55
9:A3:176:LEU:HD22	9:A3:180:GLU:HG2	1.88	0.55
1:E:501:ARG:HG2	1:E:504:ARG:HH21	1.72	0.55
1:9:79:PHE:HB2	1:9:87:TYR:HB3	1.88	0.55
1:AF:20:SER:HB3	1:AF:23:GLN:HE22	1.71	0.55
9:A1:115:VAL:HG13	9:A1:126:GLY:HA3	1.89	0.55
3:AZ:197:ILE:HD11	3:Aa:233:LEU:HB2	1.89	0.55
3:Ac:214:LEU:HD11	3:Ac:222:LEU:HD23	1.89	0.55
1:A:501:ARG:HG2	1:A:504:ARG:HH21	1.71	0.55
1:N:230:ASP:HA	1:9:228:ASN:HB3	1.88	0.55
1:AR:20:SER:HB3	1:AR:23:GLN:HE22	1.70	0.55
9:Aw:147:ARG:HG2	9:A5:203:LYS:HG3	1.89	0.55
1:N:265:SER:HB2	1:N:268:ARG:HG3	1.89	0.55
9:A1:203:LYS:HG3	9:A2:147:ARG:HG2	1.89	0.55
1:H:265:SER:HB2	1:H:268:ARG:HG3	1.89	0.55
1:L:294:GLU:HA	1:L:309:VAL:HG12	1.88	0.55
1:T:265:SER:HB3	1:T:268:ARG:HG3	1.88	0.55
1:AG:125:THR:HB	1:AH:182:ARG:HH21	1.71	0.55
3:AY:218:GLY:HA3	4:Ad:212:LYS:HD3	1.89	0.55
1:A:355:TYR:HA	1:B:323:GLU:HB3	1.88	0.54
1:K:364:VAL:HG22	1:L:315:ILE:HA	1.89	0.54
1:Z:293:ILE:HD13	1:Z:313:THR:HG21	1.90	0.54
8:AV:53:PRO:HA	8:AV:56:ILE:HG22	1.89	0.54
9:Ay:115:VAL:HG13	9:Ay:126:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Ay:203:LYS:HG3	9:Az:147:ARG:HG2	1.89	0.54
1:F:388:PHE:HD1	1:F:448:ILE:HD12	1.73	0.54
2:AX:257:LEU:HG	9:A5:161:PRO:HG3	1.90	0.54
3:AZ:49:LEU:HD21	5:Af:53:VAL:HG12	1.89	0.54
9:Aw:115:VAL:HG13	9:Aw:126:GLY:HA3	1.89	0.54
1:G:294:GLU:HA	1:G:309:VAL:HG12	1.89	0.54
1:h:501:ARG:HG2	1:h:504:ARG:HH21	1.71	0.54
1:x:79:PHE:HB2	1:x:87:TYR:HB3	1.89	0.54
9:Ay:575:GLU:HG2	9:Ay:656:GLU:HG3	1.88	0.54
1:U:235:ILE:HG21	1:V:240:LYS:HG3	1.89	0.54
1:W:364:VAL:HG22	1:X:315:ILE:HA	1.88	0.54
9:A2:361:LEU:HD11	9:A3:552:ASN:HA	1.89	0.54
9:A3:115:VAL:HG13	9:A3:126:GLY:HA3	1.90	0.54
1:l:501:ARG:HG2	1:l:504:ARG:HH21	1.73	0.54
1:1:79:PHE:HB2	1:1:87:TYR:HB3	1.89	0.54
1:4:121:ARG:HH11	1:5:120:ASP:HB2	1.72	0.54
4:Ad:196:ILE:HA	4:Ad:234:ILE:HD13	1.89	0.54
9:Ay:401:ILE:HG23	9:Ay:550:ILE:HD11	1.89	0.54
1:e:265:SER:HB3	1:e:268:ARG:HG3	1.89	0.54
1:5:79:PHE:HB2	1:5:87:TYR:HB3	1.90	0.54
3:AZ:206:LEU:HD22	3:AZ:232:LYS:HG3	1.90	0.54
1:A:294:GLU:HA	1:A:309:VAL:HG12	1.90	0.54
1:K:273:ARG:HB2	1:L:432:SER:HB2	1.89	0.54
1:j:364:VAL:HG22	1:k:315:ILE:HA	1.90	0.54
1:AA:79:PHE:HB2	1:AA:87:TYR:HB3	1.90	0.54
3:Aa:103:LEU:HD22	3:Aa:250:ILE:HD11	1.89	0.54
9:Ax:203:LYS:HG3	9:Ay:147:ARG:HG2	1.89	0.54
9:Az:401:ILE:HG23	9:Az:550:ILE:HD11	1.88	0.54
9:Az:677:SER:HB3	9:Az:680:GLU:HG3	1.90	0.54
1:M:273:ARG:HB2	1:N:432:SER:HB2	1.88	0.54
1:J:319:THR:HG22	1:J:360:GLU:HG3	1.89	0.54
1:AI:125:THR:HB	1:AJ:182:ARG:HH21	1.73	0.54
1:AL:20:SER:HB3	1:AL:23:GLN:HE22	1.73	0.54
9:Aw:203:LYS:HG3	9:Ax:147:ARG:HG2	1.89	0.54
9:A2:203:LYS:HG3	9:A3:147:ARG:HG2	1.88	0.54
9:A4:677:SER:HB3	9:A4:680:GLU:HG3	1.90	0.54
1:O:391:GLY:HA2	1:O:417:MET:HG3	1.90	0.54
1:o:293:ILE:HD13	1:o:313:THR:HG21	1.89	0.54
1:0:53:LEU:HG	1:0:88:LEU:HD11	1.88	0.54
1:A:265:SER:HB2	1:A:268:ARG:HG3	1.91	0.53
1:C:501:ARG:HG2	1:C:504:ARG:HH21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:289:GLU:HB2	1:m:369:LYS:HB3	1.90	0.53
3:Aa:224:PRO:HD3	3:Ab:221:MET:HE1	1.89	0.53
1:Q:273:ARG:HB2	1:R:432:SER:HB2	1.89	0.53
1:AL:125:THR:HB	1:AM:182:ARG:HH21	1.72	0.53
9:Az:176:LEU:HD22	9:Az:180:GLU:HG2	1.88	0.53
1:d:391:GLY:HA2	1:d:417:MET:HG3	1.90	0.53
1:AE:125:THR:HB	1:AF:182:ARG:HH21	1.72	0.53
1:AS:125:THR:HB	1:AT:182:ARG:HH21	1.72	0.53
2:AX:56:LEU:HD13	2:AX:215:VAL:HG11	1.90	0.53
9:A4:203:LYS:HG3	9:A5:147:ARG:HG2	1.89	0.53
1:V:501:ARG:HG2	1:V:504:ARG:HH21	1.74	0.53
1:j:314:ILE:HA	1:j:364:VAL:HG12	1.90	0.53
1:AB:53:LEU:HG	1:AB:88:LEU:HD11	1.90	0.53
3:AY:94:GLN:HA	5:Aj:108:ILE:HG13	1.90	0.53
9:Aw:601:LEU:HD23	9:Aw:693:VAL:HB	1.90	0.53
9:Ay:527:VAL:HG22	9:Ay:561:ALA:HB2	1.91	0.53
9:A4:583:ARG:HG2	9:A4:682:PRO:HG3	1.90	0.53
1:L:265:SER:HB2	1:L:268:ARG:HG3	1.91	0.53
4:Ad:199:LEU:HD22	4:Ad:234:ILE:HD11	1.90	0.53
8:AU:31:VAL:HG11	8:AU:57:VAL:HG11	1.89	0.53
1:E:265:SER:HB2	1:E:268:ARG:HG3	1.91	0.53
1:G:273:ARG:HB2	1:H:432:SER:HB2	1.90	0.53
1:d:265:SER:HB3	1:d:268:ARG:HG3	1.89	0.53
1:m:265:SER:HB3	1:m:268:ARG:HG3	1.91	0.53
1:AH:125:THR:HB	1:AI:182:ARG:HH21	1.73	0.53
1:AN:125:THR:HB	1:AO:182:ARG:HH21	1.74	0.53
8:AW:27:ILE:HG21	8:AW:61:VAL:HG21	1.91	0.53
9:A1:677:SER:HB3	9:A1:680:GLU:HG3	1.91	0.53
1:I:235:ILE:HG21	1:J:240:LYS:HB3	1.90	0.53
1:O:294:GLU:HA	1:O:309:VAL:HG12	1.90	0.53
1:a:316:SER:HB2	1:a:363:ASN:HB3	1.91	0.53
1:b:294:GLU:HA	1:b:309:VAL:HG12	1.90	0.53
1:l:265:SER:HB2	1:l:268:ARG:HG3	1.91	0.53
3:Ab:69:THR:HG22	3:Ab:108:MET:HE2	1.91	0.53
7:Ap:1:MET:HE3	7:Ap:5:SER:HB3	1.90	0.53
1:G:265:SER:HB2	1:G:268:ARG:HG3	1.91	0.53
1:J:501:ARG:HG2	1:J:504:ARG:HH21	1.74	0.53
1:P:265:SER:HB3	1:P:268:ARG:HG3	1.91	0.53
1:U:265:SER:HB2	1:U:268:ARG:HG3	1.90	0.53
1:X:265:SER:HB2	1:X:268:ARG:HG3	1.91	0.53
4:Ad:98:PHE:HA	4:Ad:101:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Az:203:LYS:HG3	9:A1:147:ARG:HG2	1.90	0.53
1:A:240:LYS:HB3	1:o:235:ILE:HG21	1.91	0.53
1:M:501:ARG:HG2	1:M:504:ARG:HH21	1.74	0.53
1:Z:238:ALA:HB2	1:a:377:PRO:HB2	1.89	0.53
1:c:294:GLU:HA	1:c:309:VAL:HG12	1.90	0.53
1:AJ:125:THR:HB	1:AK:182:ARG:HH21	1.73	0.53
9:A5:677:SER:HB3	9:A5:680:GLU:HG3	1.91	0.53
1:D:265:SER:HB2	1:D:268:ARG:HG3	1.92	0.52
1:E:388:PHE:HD1	1:E:448:ILE:HD12	1.74	0.52
1:N:319:THR:HG22	1:N:360:GLU:HG3	1.91	0.52
1:P:501:ARG:HG2	1:P:504:ARG:HH21	1.74	0.52
3:Ac:159:LEU:HB2	4:Ad:147:LEU:HD12	1.91	0.52
9:Aw:677:SER:HB3	9:Aw:680:GLU:HG3	1.91	0.52
9:A2:677:SER:HB3	9:A2:680:GLU:HG3	1.90	0.52
9:A4:338:LYS:HA	9:A4:341:LYS:HE2	1.90	0.52
9:A4:601:LEU:HD23	9:A4:693:VAL:HB	1.91	0.52
1:O:265:SER:HB2	1:O:268:ARG:HG3	1.91	0.52
1:5:169:SER:HB3	3:AY:168:ARG:HH11	1.75	0.52
1:W:252:LEU:HD13	1:W:433:PHE:HE2	1.75	0.52
1:c:501:ARG:HG2	1:c:504:ARG:HH21	1.75	0.52
1:f:388:PHE:HD1	1:f:448:ILE:HD12	1.74	0.52
1:g:265:SER:HB3	1:g:268:ARG:HG3	1.92	0.52
1:l:293:ILE:HD13	1:l:313:THR:HG21	1.91	0.52
1:n:265:SER:HB3	1:n:268:ARG:HG3	1.91	0.52
1:AD:20:SER:HB3	1:AD:23:GLN:HE22	1.74	0.52
3:AY:103:LEU:HD22	3:AY:250:ILE:HD11	1.90	0.52
9:Ax:176:LEU:HD22	9:Ax:180:GLU:HG2	1.91	0.52
1:S:388:PHE:HD1	1:S:448:ILE:HD12	1.74	0.52
1:3:79:PHE:HB2	1:3:87:TYR:HB3	1.91	0.52
1:AM:103:ARG:HD3	1:AM:200:LEU:HD22	1.92	0.52
5:Ag:92:ILE:HG12	6:An:134:LEU:HD11	1.91	0.52
9:Ax:677:SER:HB3	9:Ax:680:GLU:HG3	1.91	0.52
1:O:324:TYR:HA	1:O:354:LYS:HA	1.91	0.52
1:S:230:ASP:O	1:S:234:ARG:HB2	2.09	0.52
1:S:293:ILE:HD13	1:S:313:THR:HG21	1.91	0.52
1:T:430:GLN:HA	1:T:443:ILE:HD12	1.92	0.52
1:a:294:GLU:HA	1:a:309:VAL:HG12	1.91	0.52
1:AK:125:THR:HB	1:AL:182:ARG:HH21	1.75	0.52
3:Ac:201:LEU:HD21	8:AW:10:ILE:HD13	1.92	0.52
9:Ax:303:ALA:HB1	9:Ax:310:THR:HG23	1.92	0.52
9:Ax:422:LYS:HG2	9:Ax:427:GLU:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ARG:HB2	1:C:432:SER:HB2	1.90	0.52
1:a:364:VAL:HG22	1:b:315:ILE:HA	1.92	0.52
1:k:364:VAL:HG22	1:l:315:ILE:HA	1.92	0.52
1:l:294:GLU:HA	1:l:309:VAL:HG12	1.91	0.52
1:AR:125:THR:HB	1:AS:182:ARG:HH21	1.75	0.52
3:Ab:157:ILE:HD11	3:Ab:180:LEU:HA	1.90	0.52
7:Ap:47:ILE:HG23	7:Ap:77:VAL:HG13	1.91	0.52
9:Ay:422:LYS:HG2	9:Ay:427:GLU:HA	1.92	0.52
9:Az:422:LYS:HG2	9:Az:427:GLU:HA	1.92	0.52
9:A5:338:LYS:HA	9:A5:341:LYS:HE2	1.90	0.52
1:D:238:ALA:HB2	1:E:377:PRO:HB2	1.92	0.52
1:o:273:ARG:HH12	1:o:275:ASN:HB2	1.75	0.52
1:1:66:ARG:HE	1:1:106:LEU:HD21	1.74	0.52
1:AD:125:THR:HB	1:AE:182:ARG:HH21	1.75	0.52
1:AQ:125:THR:HB	1:AR:182:ARG:HH21	1.75	0.52
9:A4:422:LYS:HG2	9:A4:427:GLU:HA	1.91	0.52
1:F:265:SER:HB3	1:F:268:ARG:HG3	1.92	0.52
1:Q:294:GLU:HA	1:Q:309:VAL:HG12	1.92	0.52
1:Z:294:GLU:HA	1:Z:309:VAL:HG12	1.91	0.52
1:f:501:ARG:HG2	1:f:504:ARG:HH21	1.75	0.52
1:k:235:ILE:HG21	1:l:240:LYS:HB3	1.92	0.52
1:z:79:PHE:HB2	1:z:87:TYR:HB3	1.92	0.52
1:AP:125:THR:HB	1:AQ:182:ARG:HH21	1.75	0.52
3:AZ:195:MET:HE1	3:AZ:249:LEU:HD13	1.91	0.52
9:Ax:338:LYS:HA	9:Ax:341:LYS:HE2	1.91	0.52
1:AF:125:THR:HB	1:AG:182:ARG:HH21	1.73	0.52
9:A3:338:LYS:HA	9:A3:341:LYS:HE2	1.91	0.52
1:C:314:ILE:HA	1:C:364:VAL:HG12	1.92	0.52
1:G:430:GLN:HA	1:G:443:ILE:HD12	1.92	0.52
1:H:501:ARG:HG2	1:H:504:ARG:HH21	1.74	0.52
1:J:265:SER:HB3	1:J:268:ARG:HG3	1.92	0.52
1:K:294:GLU:HA	1:K:309:VAL:HG12	1.92	0.52
1:Y:265:SER:HB2	1:Y:268:ARG:HG3	1.92	0.52
1:a:293:ILE:HD13	1:a:313:THR:HG21	1.90	0.52
1:h:355:TYR:HA	1:i:323:GLU:HB3	1.92	0.52
3:AY:219:MET:HE3	4:Ad:208:GLY:HA3	1.91	0.52
8:AV:36:SER:HB2	8:AW:44:ILE:HG21	1.92	0.52
9:Ay:677:SER:HB3	9:Ay:680:GLU:HG3	1.92	0.52
9:Az:644:GLN:HE21	9:Az:650:PRO:HG3	1.75	0.52
9:A2:356:SER:HB3	9:A3:392:ARG:HH21	1.75	0.52
9:A2:422:LYS:HG2	9:A2:427:GLU:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:388:PHE:HD1	1:P:448:ILE:HD12	1.75	0.51
1:Q:265:SER:HB2	1:Q:268:ARG:HG3	1.93	0.51
1:Q:501:ARG:HG2	1:Q:504:ARG:HH21	1.75	0.51
1:c:273:ARG:HB2	1:d:432:SER:HB2	1.91	0.51
8:AU:35:ILE:HD12	8:AU:50:SER:HA	1.92	0.51
9:A3:677:SER:HB3	9:A3:680:GLU:HG3	1.91	0.51
9:A4:303:ALA:HB1	9:A4:310:THR:HG23	1.92	0.51
1:j:430:GLN:HA	1:j:443:ILE:HD12	1.92	0.51
9:A1:527:VAL:HG22	9:A1:561:ALA:HB2	1.93	0.51
9:A2:303:ALA:HB1	9:A2:310:THR:HG23	1.92	0.51
9:A2:539:VAL:HG11	9:A2:560:ILE:HD11	1.93	0.51
9:A3:601:LEU:HD23	9:A3:693:VAL:HB	1.91	0.51
1:D:324:TYR:HA	1:D:354:LYS:HA	1.91	0.51
1:N:273:ARG:HB2	1:O:432:SER:HB2	1.92	0.51
1:N:293:ILE:HD13	1:N:313:THR:HG21	1.92	0.51
9:Ay:303:ALA:HB1	9:Ay:310:THR:HG23	1.92	0.51
9:A1:338:LYS:HA	9:A1:341:LYS:HE2	1.91	0.51
9:A2:338:LYS:HA	9:A2:341:LYS:HE2	1.91	0.51
1:D:294:GLU:HA	1:D:309:VAL:HG12	1.92	0.51
1:E:273:ARG:HB2	1:F:432:SER:HB2	1.91	0.51
1:H:273:ARG:HB2	1:I:432:SER:HB2	1.92	0.51
1:Y:364:VAL:HG22	1:Z:315:ILE:HA	1.91	0.51
1:u:141:VAL:HG21	1:u:205:ILE:HD11	1.93	0.51
4:Ad:258:ALA:HA	4:Ad:261:LEU:HD12	1.91	0.51
9:Aw:422:LYS:HG2	9:Aw:427:GLU:HA	1.92	0.51
9:Az:303:ALA:HB1	9:Az:310:THR:HG23	1.93	0.51
1:G:391:GLY:HA2	1:G:417:MET:HG3	1.93	0.51
1:e:501:ARG:HG2	1:e:504:ARG:HH21	1.75	0.51
1:f:265:SER:HB3	1:f:268:ARG:HG3	1.91	0.51
1:g:388:PHE:HD1	1:g:448:ILE:HD12	1.75	0.51
1:y:79:PHE:HB2	1:y:87:TYR:HB3	1.92	0.51
1:AA:123:THR:HA	2:AX:197:GLN:HB3	1.93	0.51
9:A5:527:VAL:HG22	9:A5:561:ALA:HB2	1.93	0.51
1:B:388:PHE:HD1	1:B:448:ILE:HD12	1.75	0.51
1:H:294:GLU:HA	1:H:309:VAL:HG12	1.91	0.51
1:N:501:ARG:HG2	1:N:504:ARG:HH21	1.75	0.51
1:S:265:SER:HB2	1:S:268:ARG:HG3	1.93	0.51
1:a:391:GLY:HA2	1:a:417:MET:HG3	1.92	0.51
1:k:501:ARG:HG2	1:k:504:ARG:HH21	1.75	0.51
1:AN:103:ARG:HD3	1:AN:200:LEU:HD22	1.92	0.51
5:Ai:53:VAL:HG11	5:Ai:93:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A1:303:ALA:HB1	9:A1:310:THR:HG23	1.93	0.51
9:A5:422:LYS:HG2	9:A5:427:GLU:HA	1.91	0.51
1:X:294:GLU:HA	1:X:309:VAL:HG12	1.92	0.51
1:n:388:PHE:HD1	1:n:448:ILE:HD12	1.76	0.51
3:AY:140:PRO:HA	3:AY:143:ILE:HG12	1.93	0.51
3:Ab:73:ARG:HH22	3:Ab:148:GLN:HE21	1.59	0.51
3:Ac:222:LEU:HD12	3:Ac:223:PRO:HD2	1.91	0.51
9:Aw:303:ALA:HB1	9:Aw:310:THR:HG23	1.92	0.51
9:A3:527:VAL:HG22	9:A3:561:ALA:HB2	1.93	0.51
9:A5:303:ALA:HB1	9:A5:310:THR:HG23	1.93	0.51
1:B:294:GLU:HA	1:B:309:VAL:HG12	1.91	0.51
1:I:388:PHE:HD1	1:I:448:ILE:HD12	1.75	0.51
1:S:316:SER:HB2	1:S:363:ASN:HB3	1.92	0.51
1:U:258:SER:HB3	1:AK:166:PHE:HE2	1.76	0.51
1:W:388:PHE:HD1	1:W:448:ILE:HD12	1.76	0.51
1:e:299:ASP:HB2	1:e:302:ALA:HB2	1.92	0.51
1:h:252:LEU:HD13	1:h:433:PHE:HE1	1.76	0.51
3:Aa:194:LYS:HA	3:Aa:197:ILE:HD12	1.92	0.51
7:Au:19:LEU:HD23	7:Au:77:VAL:HG21	1.92	0.51
9:A2:201:ALA:HA	9:A2:204:PHE:HD2	1.76	0.51
9:A3:303:ALA:HB1	9:A3:310:THR:HG23	1.93	0.51
1:J:388:PHE:HD1	1:J:448:ILE:HD12	1.76	0.51
1:U:501:ARG:HG2	1:U:504:ARG:HH21	1.74	0.51
1:Z:273:ARG:HB2	1:a:432:SER:HB2	1.92	0.51
1:AP:103:ARG:HD3	1:AP:200:LEU:HD22	1.93	0.51
4:Ad:61:ILE:HG12	4:Ad:162:ARG:HH22	1.76	0.51
9:A1:422:LYS:HG2	9:A1:427:GLU:HA	1.93	0.51
1:G:235:ILE:HG21	1:H:240:LYS:HB3	1.93	0.51
1:J:315:ILE:HD13	1:J:365:ALA:HB2	1.93	0.51
1:L:388:PHE:HD1	1:L:448:ILE:HD12	1.76	0.51
1:P:235:ILE:HG21	1:Q:240:LYS:HB3	1.92	0.51
1:S:294:GLU:HA	1:S:309:VAL:HG12	1.93	0.51
1:U:293:ILE:HD13	1:U:313:THR:HG21	1.92	0.51
1:W:501:ARG:HG2	1:W:504:ARG:HH21	1.75	0.51
1:X:356:ASN:HB2	1:Y:323:GLU:HB2	1.93	0.51
9:Az:338:LYS:HA	9:Az:341:LYS:HE2	1.93	0.51
9:A2:176:LEU:HD22	9:A2:180:GLU:HG2	1.93	0.51
1:B:235:ILE:HG21	1:C:240:LYS:HB3	1.93	0.50
1:K:501:ARG:HG2	1:K:504:ARG:HH21	1.77	0.50
1:L:430:GLN:HA	1:L:443:ILE:HD12	1.92	0.50
1:h:288:LYS:HE2	1:h:370:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:391:GLY:HA2	1:j:417:MET:HG3	1.93	0.50
1:AR:103:ARG:HD3	1:AR:200:LEU:HD22	1.93	0.50
1:AS:20:SER:HB3	1:AS:23:GLN:HE22	1.75	0.50
9:A3:539:VAL:HG11	9:A3:560:ILE:HD11	1.93	0.50
1:U:294:GLU:HA	1:U:309:VAL:HG12	1.92	0.50
1:f:293:ILE:HD13	1:f:313:THR:HG21	1.93	0.50
1:h:388:PHE:HD1	1:h:448:ILE:HD12	1.77	0.50
1:l:388:PHE:HD1	1:l:448:ILE:HD12	1.77	0.50
1:u:79:PHE:HB2	1:u:87:TYR:HB3	1.93	0.50
1:2:79:PHE:HB2	1:2:87:TYR:HB3	1.93	0.50
3:Aa:190:LYS:HE2	8:AU:1:MET:HE2	1.93	0.50
7:As:47:ILE:HG23	7:As:77:VAL:HG13	1.92	0.50
9:Aw:392:ARG:HH21	9:A5:356:SER:HB3	1.75	0.50
9:A5:539:VAL:HG11	9:A5:560:ILE:HD11	1.92	0.50
1:C:293:ILE:HD13	1:C:313:THR:HG21	1.92	0.50
1:E:409:MET:HE2	1:E:457:ARG:HE	1.76	0.50
1:L:501:ARG:HG2	1:L:504:ARG:HH21	1.77	0.50
1:Q:316:SER:HB2	1:Q:363:ASN:HB3	1.94	0.50
1:q:79:PHE:HB2	1:q:87:TYR:HB3	1.93	0.50
1:AC:103:ARG:HD3	1:AC:200:LEU:HD22	1.92	0.50
1:AI:194:VAL:HG13	1:AI:215:ILE:HD12	1.93	0.50
1:AM:125:THR:HB	1:AN:182:ARG:HH21	1.76	0.50
1:AP:99:ALA:HA	1:AP:103:ARG:HH21	1.76	0.50
3:AY:49:LEU:HD21	5:Ae:53:VAL:HG12	1.92	0.50
9:Ay:338:LYS:HA	9:Ay:341:LYS:HE2	1.93	0.50
9:A1:176:LEU:HD22	9:A1:180:GLU:HG2	1.92	0.50
1:N:238:ALA:HB2	1:O:377:PRO:HB2	1.94	0.50
1:O:388:PHE:HD1	1:O:448:ILE:HD12	1.75	0.50
1:Z:265:SER:HB3	1:Z:268:ARG:HG3	1.92	0.50
1:c:391:GLY:HA2	1:c:417:MET:HG3	1.93	0.50
1:d:298:GLN:HE22	1:d:305:ASN:HA	1.76	0.50
1:r:141:VAL:HG21	1:r:205:ILE:HD11	1.94	0.50
3:Ac:168:ARG:HE	3:Ac:169:PRO:HD2	1.76	0.50
5:Ag:92:ILE:HA	6:An:134:LEU:HD21	1.93	0.50
9:Aw:527:VAL:HG22	9:Aw:561:ALA:HB2	1.92	0.50
9:Az:601:LEU:HD23	9:Az:693:VAL:HB	1.92	0.50
9:A4:176:LEU:HD22	9:A4:180:GLU:HG2	1.94	0.50
9:A5:160:LEU:HD11	9:A5:192:VAL:HG21	1.94	0.50
1:L:273:ARG:HB2	1:M:432:SER:HB2	1.92	0.50
1:b:230:ASP:O	1:b:234:ARG:HB2	2.12	0.50
4:Ad:108:GLN:HG3	4:Ad:200:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:An:122:VAL:HA	6:An:125:HIS:CD2	2.46	0.50
9:Ay:601:LEU:HD23	9:Ay:693:VAL:HB	1.93	0.50
9:A2:200:GLY:HA3	9:A3:148:VAL:HG22	1.94	0.50
1:C:265:SER:HB2	1:C:268:ARG:HG3	1.94	0.50
1:I:294:GLU:HA	1:I:309:VAL:HG12	1.92	0.50
1:K:265:SER:HB3	1:K:268:ARG:HG3	1.94	0.50
1:K:391:GLY:HA2	1:K:417:MET:HG3	1.94	0.50
1:R:265:SER:HB2	1:R:268:ARG:HG3	1.94	0.50
1:U:388:PHE:HD1	1:U:448:ILE:HD12	1.77	0.50
1:Y:293:ILE:HD13	1:Y:313:THR:HG21	1.93	0.50
1:AJ:194:VAL:HG13	1:AJ:215:ILE:HD12	1.94	0.50
3:Aa:204:ILE:HG13	3:Ab:230:PRO:HG2	1.92	0.50
4:Ad:161:ILE:HD11	4:Ad:261:LEU:HA	1.93	0.50
9:A1:356:SER:HB3	9:A2:392:ARG:HH21	1.77	0.50
1:M:298:GLN:HE22	1:M:305:ASN:HA	1.75	0.50
1:T:364:VAL:HG22	1:U:315:ILE:HA	1.93	0.50
1:j:252:LEU:HD13	1:j:433:PHE:HE2	1.76	0.50
1:j:265:SER:HB3	1:j:268:ARG:HG3	1.94	0.50
1:m:391:GLY:HA2	1:m:417:MET:HG3	1.94	0.50
1:9:141:VAL:HG21	1:9:205:ILE:HD11	1.93	0.50
1:AE:103:ARG:HD3	1:AE:200:LEU:HD22	1.93	0.50
9:Ax:539:VAL:HG11	9:Ax:560:ILE:HD11	1.93	0.50
1:E:294:GLU:HA	1:E:309:VAL:HG12	1.92	0.50
1:R:298:GLN:HE22	1:R:305:ASN:HA	1.77	0.50
1:T:273:ARG:HB2	1:U:432:SER:HB2	1.92	0.50
1:W:286:GLU:HB3	1:X:370:LYS:HB2	1.93	0.50
1:Z:316:SER:HB2	1:Z:363:ASN:HB3	1.93	0.50
1:i:316:SER:HB2	1:i:363:ASN:HB3	1.93	0.50
1:p:156:VAL:HG12	1:p:177:VAL:HG13	1.94	0.50
1:y:141:VAL:HG21	1:y:205:ILE:HD11	1.94	0.50
1:0:141:VAL:HG21	1:0:205:ILE:HD11	1.93	0.50
9:Aw:338:LYS:HA	9:Aw:341:LYS:HE2	1.93	0.50
1:N:233:ASP:HB2	1:9:228:ASN:HB2	1.94	0.50
1:k:252:LEU:HD13	1:k:433:PHE:HE2	1.77	0.50
3:AY:216:ALA:HA	8:Av:51:PHE:HZ	1.77	0.50
3:Aa:195:MET:HG2	8:AU:84:LEU:HD11	1.94	0.50
3:Ab:107:THR:HG22	3:Ab:250:ILE:HG23	1.94	0.50
5:Ae:67:ALA:HB2	5:Ae:74:ILE:HD11	1.93	0.50
9:Ax:361:LEU:HD11	9:Ay:552:ASN:HA	1.94	0.50
9:Ay:356:SER:HB3	9:Az:392:ARG:HH21	1.76	0.50
1:M:265:SER:HB3	1:M:268:ARG:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:388:PHE:HD1	1:V:448:ILE:HD12	1.77	0.49
1:h:314:ILE:HA	1:h:364:VAL:HG12	1.93	0.49
1:p:141:VAL:HG21	1:p:205:ILE:HD11	1.94	0.49
1:AI:103:ARG:HD3	1:AI:200:LEU:HD22	1.93	0.49
3:AY:68:MET:HE1	3:AY:108:MET:HE1	1.94	0.49
9:Az:539:VAL:HG11	9:Az:560:ILE:HD11	1.94	0.49
9:A2:601:LEU:HD23	9:A2:693:VAL:HB	1.93	0.49
1:E:391:GLY:HA2	1:E:417:MET:HG3	1.95	0.49
1:N:388:PHE:HD1	1:N:448:ILE:HD12	1.77	0.49
1:S:430:GLN:HA	1:S:443:ILE:HD12	1.94	0.49
1:Z:501:ARG:HG2	1:Z:504:ARG:HH21	1.77	0.49
1:c:364:VAL:HG22	1:d:315:ILE:HA	1.94	0.49
1:2:156:VAL:HG12	1:2:177:VAL:HG13	1.94	0.49
1:AC:125:THR:HB	1:AD:182:ARG:HH21	1.76	0.49
3:AZ:201:LEU:HA	3:AZ:204:ILE:HD12	1.94	0.49
9:Ax:200:GLY:HA3	9:Ay:148:VAL:HG22	1.94	0.49
9:A4:50:ASN:HB2	9:A4:83:PHE:HE2	1.77	0.49
1:A:252:LEU:HD13	1:A:433:PHE:HE1	1.77	0.49
1:V:430:GLN:HA	1:V:443:ILE:HD12	1.93	0.49
1:j:238:ALA:HB2	1:k:377:PRO:HB2	1.93	0.49
1:o:298:GLN:HE22	1:o:305:ASN:HA	1.77	0.49
1:p:215:ILE:HB	1:p:224:ASN:HB2	1.93	0.49
1:AS:99:ALA:HA	1:AS:103:ARG:HH21	1.77	0.49
3:Ac:74:ILE:HG12	3:Ac:249:LEU:HD21	1.95	0.49
6:Ak:23:SER:HB3	7:Ap:1:MET:HE2	1.93	0.49
9:Ax:401:ILE:HG23	9:Ax:550:ILE:HD11	1.94	0.49
1:f:252:LEU:HD13	1:f:433:PHE:HE1	1.78	0.49
1:AF:194:VAL:HG13	1:AF:215:ILE:HD12	1.95	0.49
1:AT:114:TRP:HD1	1:AT:117:PHE:HD2	1.60	0.49
3:AY:202:PRO:HA	3:AY:205:VAL:HG12	1.93	0.49
4:Ad:115:ASN:HA	4:Ad:118:ASP:HB2	1.94	0.49
9:Aw:148:VAL:HG22	9:A5:200:GLY:HA3	1.95	0.49
9:A3:422:LYS:HG2	9:A3:427:GLU:HA	1.93	0.49
9:A4:334:GLU:HG2	9:A4:338:LYS:HE3	1.94	0.49
1:R:294:GLU:HA	1:R:309:VAL:HG12	1.94	0.49
1:a:252:LEU:HD13	1:a:433:PHE:HE2	1.78	0.49
1:a:319:THR:HG22	1:a:360:GLU:HG3	1.93	0.49
1:d:388:PHE:HD1	1:d:448:ILE:HD12	1.77	0.49
1:5:156:VAL:HG12	1:5:177:VAL:HG13	1.95	0.49
1:8:79:PHE:HB2	1:8:87:TYR:HB3	1.94	0.49
1:AQ:99:ALA:HA	1:AQ:103:ARG:HH21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AY:223:PRO:HB2	3:AY:226:MET:HG2	1.95	0.49
7:Ap:26:ASN:HD22	7:Ar:74:GLY:H	1.59	0.49
9:A2:527:VAL:HG22	9:A2:561:ALA:HB2	1.94	0.49
9:A3:356:SER:HB3	9:A4:392:ARG:HH21	1.77	0.49
9:A5:601:LEU:HD23	9:A5:693:VAL:HB	1.94	0.49
1:c:273:ARG:HH12	1:c:275:ASN:HB2	1.78	0.49
1:e:314:ILE:HA	1:e:364:VAL:HG12	1.95	0.49
1:AS:103:ARG:HH11	1:AS:200:LEU:HD22	1.78	0.49
4:Ad:21:LEU:HD22	5:Aj:93:LEU:HD22	1.94	0.49
9:Aw:176:LEU:HD22	9:Aw:180:GLU:HG2	1.94	0.49
9:Ay:50:ASN:HB2	9:Ay:83:PHE:HE2	1.78	0.49
9:A4:356:SER:HB3	9:A5:392:ARG:HH21	1.77	0.49
1:P:364:VAL:HG22	1:Q:315:ILE:HA	1.94	0.49
1:Q:364:VAL:HG22	1:R:315:ILE:HA	1.95	0.49
1:W:294:GLU:HA	1:W:309:VAL:HG12	1.94	0.49
1:b:291:ALA:HB3	1:b:367:ASN:HB2	1.93	0.49
1:b:314:ILE:HA	1:b:364:VAL:HG12	1.95	0.49
1:g:273:ARG:HB2	1:h:432:SER:HB2	1.94	0.49
1:i:388:PHE:HD1	1:i:448:ILE:HD12	1.76	0.49
1:m:314:ILE:HA	1:m:364:VAL:HG12	1.94	0.49
1:3:141:VAL:HG21	1:3:205:ILE:HD11	1.94	0.49
1:7:156:VAL:HG12	1:7:177:VAL:HG13	1.95	0.49
1:AJ:99:ALA:HA	1:AJ:103:ARG:HH21	1.77	0.49
1:AL:70:ARG:HG2	1:AL:101:LEU:HD11	1.93	0.49
1:AL:114:TRP:HD1	1:AL:117:PHE:HD2	1.61	0.49
1:P:238:ALA:HB2	1:Q:377:PRO:HB2	1.95	0.49
1:T:294:GLU:HA	1:T:309:VAL:HG12	1.94	0.49
1:W:265:SER:HB2	1:W:268:ARG:HG3	1.95	0.49
1:o:388:PHE:HD1	1:o:448:ILE:HD12	1.77	0.49
1:AG:103:ARG:HD3	1:AG:200:LEU:HD22	1.94	0.49
1:AQ:114:TRP:HD1	1:AQ:117:PHE:HD2	1.59	0.49
2:AX:111:PHE:HD1	8:Av:52:ILE:HG23	1.77	0.49
5:Ae:77:HIS:HE1	6:Al:19:SER:HB2	1.77	0.49
7:At:47:ILE:HG23	7:At:77:VAL:HG13	1.95	0.49
9:A1:401:ILE:HG23	9:A1:550:ILE:HD11	1.93	0.49
1:M:388:PHE:HD1	1:M:448:ILE:HD12	1.76	0.49
1:N:391:GLY:HA2	1:N:417:MET:HG3	1.95	0.49
1:V:294:GLU:HA	1:V:309:VAL:HG12	1.94	0.49
1:Y:314:ILE:HA	1:Y:364:VAL:HG12	1.94	0.49
1:e:273:ARG:HH22	1:e:275:ASN:HD22	1.60	0.49
1:k:388:PHE:HD1	1:k:448:ILE:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:156:VAL:HG12	1:w:177:VAL:HG13	1.94	0.49
1:z:177:VAL:HG21	1:z:201:ILE:HD13	1.95	0.49
1:AB:141:VAL:HG21	1:AB:205:ILE:HD11	1.95	0.49
3:AY:51:LEU:HD21	6:Ak:134:LEU:HD13	1.95	0.49
9:Aw:200:GLY:HA3	9:Ax:148:VAL:HG22	1.95	0.49
9:Ax:601:LEU:HD23	9:Ax:693:VAL:HB	1.94	0.49
9:Az:201:ALA:HA	9:Az:204:PHE:HD2	1.77	0.49
9:A3:200:GLY:HA3	9:A4:148:VAL:HG22	1.95	0.49
1:J:294:GLU:HA	1:J:309:VAL:HG12	1.95	0.49
1:T:252:LEU:HD13	1:T:433:PHE:HE2	1.78	0.49
1:c:388:PHE:HD1	1:c:448:ILE:HD12	1.78	0.49
1:e:316:SER:HB2	1:e:363:ASN:HB3	1.95	0.49
1:f:314:ILE:HA	1:f:364:VAL:HG12	1.95	0.49
1:l:273:ARG:HB2	1:m:432:SER:HB2	1.95	0.49
1:y:156:VAL:HG12	1:y:177:VAL:HG13	1.95	0.49
1:0:156:VAL:HG12	1:0:177:VAL:HG13	1.95	0.49
1:AL:103:ARG:HD3	1:AL:200:LEU:HD22	1.95	0.49
1:AM:114:TRP:HD1	1:AM:117:PHE:HD2	1.59	0.49
9:A1:601:LEU:HD23	9:A1:693:VAL:HB	1.95	0.49
9:A4:579:GLN:HA	9:A4:680:GLU:HG2	1.94	0.49
1:E:314:ILE:HA	1:E:364:VAL:HG12	1.95	0.48
1:N:364:VAL:HG22	1:O:315:ILE:HA	1.95	0.48
1:Y:252:LEU:HD13	1:Y:433:PHE:HE1	1.78	0.48
1:AD:103:ARG:HD3	1:AD:200:LEU:HD22	1.94	0.48
1:AQ:103:ARG:HD3	1:AQ:200:LEU:HD22	1.95	0.48
3:AY:56:THR:HA	3:AY:59:THR:HG22	1.94	0.48
9:Aw:579:GLN:HA	9:Aw:680:GLU:HG2	1.94	0.48
9:A2:579:GLN:HA	9:A2:680:GLU:HG2	1.94	0.48
1:A:388:PHE:HD1	1:A:448:ILE:HD12	1.78	0.48
1:P:314:ILE:HA	1:P:364:VAL:HG12	1.95	0.48
1:Q:298:GLN:HE22	1:Q:305:ASN:HA	1.77	0.48
1:Q:388:PHE:HD1	1:Q:448:ILE:HD12	1.78	0.48
1:q:156:VAL:HG12	1:q:177:VAL:HG13	1.95	0.48
1:5:141:VAL:HG21	1:5:205:ILE:HD11	1.95	0.48
1:AO:114:TRP:HD1	1:AO:117:PHE:HD2	1.62	0.48
9:Az:50:ASN:HB2	9:Az:83:PHE:HE2	1.78	0.48
9:Az:579:GLN:HA	9:Az:680:GLU:HG2	1.94	0.48
9:A1:539:VAL:HG11	9:A1:560:ILE:HD11	1.95	0.48
9:A2:334:GLU:HG2	9:A2:338:LYS:HE3	1.96	0.48
1:F:294:GLU:HA	1:F:309:VAL:HG12	1.94	0.48
1:G:291:ALA:HB3	1:G:367:ASN:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:252:LEU:HD13	1:U:433:PHE:HE2	1.79	0.48
1:f:238:ALA:HB2	1:g:377:PRO:HB2	1.94	0.48
1:AE:99:ALA:HA	1:AE:103:ARG:HH21	1.79	0.48
9:Ay:539:VAL:HG11	9:Ay:560:ILE:HD11	1.95	0.48
9:A5:579:GLN:HA	9:A5:680:GLU:HG2	1.95	0.48
1:D:364:VAL:HG22	1:E:315:ILE:HA	1.94	0.48
1:b:268:ARG:HH12	1:b:417:MET:HE2	1.78	0.48
1:f:294:GLU:HA	1:f:309:VAL:HG12	1.95	0.48
1:q:141:VAL:HG21	1:q:205:ILE:HD11	1.95	0.48
1:s:141:VAL:HG21	1:s:205:ILE:HD11	1.96	0.48
1:u:156:VAL:HG12	1:u:177:VAL:HG13	1.94	0.48
1:4:141:VAL:HG21	1:4:205:ILE:HD11	1.95	0.48
1:7:165:LEU:HD21	3:AY:147:LYS:HB2	1.95	0.48
1:AC:194:VAL:HG13	1:AC:215:ILE:HD12	1.95	0.48
1:AK:103:ARG:HD3	1:AK:200:LEU:HD22	1.95	0.48
1:AP:103:ARG:HH11	1:AP:200:LEU:HD22	1.79	0.48
7:Aq:111:PRO:HB2	7:Aq:113:VAL:HG23	1.95	0.48
9:Ay:176:LEU:HD22	9:Ay:180:GLU:HG2	1.94	0.48
1:H:388:PHE:HD1	1:H:448:ILE:HD12	1.79	0.48
1:b:364:VAL:HG22	1:c:315:ILE:HA	1.95	0.48
1:AA:141:VAL:HG21	1:AA:205:ILE:HD11	1.95	0.48
3:AZ:206:LEU:HD12	3:AZ:235:LEU:HD22	1.95	0.48
9:Az:200:GLY:HA3	9:A1:148:VAL:HG22	1.95	0.48
9:A1:15:LEU:HB3	9:A1:21:LEU:HD12	1.94	0.48
9:A1:200:GLY:HA3	9:A2:148:VAL:HG22	1.95	0.48
9:A1:579:GLN:HA	9:A1:680:GLU:HG2	1.94	0.48
1:I:319:THR:HG22	1:I:360:GLU:HG3	1.96	0.48
1:R:388:PHE:HD1	1:R:448:ILE:HD12	1.78	0.48
1:v:156:VAL:HG12	1:v:177:VAL:HG13	1.94	0.48
1:1:141:VAL:HG21	1:1:205:ILE:HD11	1.95	0.48
3:AY:138:ILE:HD12	3:AY:141:LEU:HD12	1.95	0.48
9:Aw:356:SER:HB3	9:Ax:392:ARG:HH21	1.77	0.48
9:Ax:50:ASN:HB2	9:Ax:83:PHE:HE2	1.78	0.48
9:Ax:579:GLN:HA	9:Ax:680:GLU:HG2	1.95	0.48
9:Ay:17:ASN:HB3	9:Ay:20:ASP:HB2	1.96	0.48
9:A3:17:ASN:HB3	9:A3:20:ASP:HB2	1.96	0.48
1:Q:252:LEU:HD13	1:Q:433:PHE:HE1	1.78	0.48
1:T:388:PHE:HD1	1:T:448:ILE:HD12	1.77	0.48
1:W:375:LYS:HG3	1:W:379:ARG:HH21	1.79	0.48
1:j:298:GLN:HE22	1:j:305:ASN:HA	1.79	0.48
1:w:79:PHE:HB2	1:w:87:TYR:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:156:VAL:HG12	1:6:177:VAL:HG13	1.96	0.48
1:AJ:103:ARG:HD3	1:AJ:200:LEU:HD22	1.94	0.48
3:Aa:81:ILE:HD11	3:Aa:245:ILE:HG21	1.96	0.48
9:Aw:17:ASN:HB3	9:Aw:20:ASP:HB2	1.95	0.48
1:A:273:ARG:HB2	1:B:432:SER:HB2	1.95	0.48
1:A:432:SER:HB2	1:o:273:ARG:HB2	1.95	0.48
1:G:238:ALA:HB2	1:H:377:PRO:HB2	1.96	0.48
1:G:293:ILE:HD13	1:G:313:THR:HG21	1.94	0.48
1:X:316:SER:HB2	1:X:363:ASN:HB3	1.96	0.48
1:Y:298:GLN:HE22	1:Y:305:ASN:HA	1.79	0.48
1:c:293:ILE:HD13	1:c:313:THR:HG21	1.95	0.48
1:g:298:GLN:HE22	1:g:305:ASN:HA	1.79	0.48
1:g:314:ILE:HA	1:g:364:VAL:HG12	1.96	0.48
1:i:265:SER:HB3	1:i:268:ARG:HG3	1.96	0.48
1:k:270:MET:HE3	1:l:262:LYS:HG3	1.95	0.48
1:l:273:ARG:HH12	1:l:275:ASN:HB2	1.77	0.48
1:u:159:VAL:HB	1:u:174:LYS:HG3	1.95	0.48
1:AE:194:VAL:HG13	1:AE:215:ILE:HD12	1.96	0.48
1:AF:99:ALA:HA	1:AF:103:ARG:HH21	1.79	0.48
1:AI:114:TRP:HD1	1:AI:117:PHE:HD2	1.60	0.48
1:AR:114:TRP:HD1	1:AR:117:PHE:HD2	1.62	0.48
9:Aw:50:ASN:HB2	9:Aw:83:PHE:HE2	1.77	0.48
9:A3:10:LEU:HG	9:A3:16:ASN:HA	1.95	0.48
1:B:265:SER:HB2	1:B:268:ARG:HG3	1.95	0.48
1:B:319:THR:HG22	1:B:360:GLU:HG3	1.96	0.48
1:N:294:GLU:HA	1:N:309:VAL:HG12	1.96	0.48
1:Q:314:ILE:HA	1:Q:364:VAL:HG12	1.95	0.48
1:R:252:LEU:HD13	1:R:433:PHE:HE1	1.78	0.48
1:S:232:ILE:HD13	1:T:240:LYS:HG3	1.96	0.48
1:d:501:ARG:HG2	1:d:504:ARG:HH21	1.79	0.48
1:m:388:PHE:HD1	1:m:448:ILE:HD12	1.78	0.48
1:s:79:PHE:HB2	1:s:87:TYR:HB3	1.95	0.48
1:AG:99:ALA:HA	1:AG:103:ARG:HH21	1.79	0.48
1:AO:103:ARG:HH11	1:AO:200:LEU:HD22	1.78	0.48
3:Ac:248:GLY:HA2	8:AW:85:GLN:HG2	1.94	0.48
9:Ax:527:VAL:HG22	9:Ax:561:ALA:HB2	1.95	0.48
9:Ay:579:GLN:HA	9:Ay:680:GLU:HG2	1.95	0.48
9:Az:527:VAL:HG22	9:Az:561:ALA:HB2	1.95	0.48
9:A4:17:ASN:HB3	9:A4:20:ASP:HB2	1.96	0.48
1:I:252:LEU:HD13	1:I:433:PHE:HE1	1.79	0.48
1:S:232:ILE:H	1:AB:228:ASN:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:265:SER:HB2	1:V:268:ARG:HG3	1.96	0.48
1:X:314:ILE:HA	1:X:364:VAL:HG12	1.96	0.48
1:d:273:ARG:HB2	1:e:432:SER:HB2	1.96	0.48
1:g:501:ARG:HG2	1:g:504:ARG:HH21	1.79	0.48
1:3:156:VAL:HG12	1:3:177:VAL:HG13	1.96	0.48
1:AH:103:ARG:HD3	1:AH:200:LEU:HD22	1.94	0.48
2:AX:163:LEU:HB2	8:AW:41:ILE:HD11	1.96	0.48
9:Aw:539:VAL:HG11	9:Aw:560:ILE:HD11	1.94	0.48
9:Ay:200:GLY:HA3	9:Az:148:VAL:HG22	1.95	0.48
9:Az:334:GLU:HG2	9:Az:338:LYS:HE3	1.96	0.48
1:b:265:SER:HB2	1:b:268:ARG:HG3	1.96	0.47
1:p:145:ILE:HG23	1:p:197:LEU:HD21	1.95	0.47
1:v:79:PHE:HB2	1:v:87:TYR:HB3	1.96	0.47
1:5:145:ILE:HG23	1:5:197:LEU:HD21	1.96	0.47
1:AH:114:TRP:HD1	1:AH:117:PHE:HD2	1.62	0.47
9:A2:50:ASN:HB2	9:A2:83:PHE:HE2	1.79	0.47
9:A4:200:GLY:HA3	9:A5:148:VAL:HG22	1.96	0.47
1:8:141:VAL:HG21	1:8:205:ILE:HD11	1.95	0.47
1:AM:98:ARG:HH21	1:AM:144:HIS:HE1	1.62	0.47
4:Ad:141:LEU:HD13	4:Ad:146:LEU:HD22	1.95	0.47
6:Am:93:MET:H	6:Am:99:ASN:HA	1.78	0.47
9:A3:15:LEU:HB3	9:A3:21:LEU:HD12	1.96	0.47
9:A5:50:ASN:HB2	9:A5:83:PHE:HE2	1.78	0.47
9:A5:201:ALA:HA	9:A5:204:PHE:HD2	1.79	0.47
1:B:375:LYS:HG3	1:B:379:ARG:HH21	1.79	0.47
1:D:388:PHE:HD1	1:D:448:ILE:HD12	1.78	0.47
1:F:286:GLU:HB3	1:G:370:LYS:HB2	1.96	0.47
1:b:386:GLY:HA2	1:b:444:THR:O	2.15	0.47
1:e:364:VAL:HG22	1:f:315:ILE:HA	1.96	0.47
1:h:250:ALA:HB1	1:AQ:169:SER:HB3	1.96	0.47
1:h:364:VAL:HG22	1:i:315:ILE:HA	1.96	0.47
1:AE:114:TRP:HD1	1:AE:117:PHE:HD2	1.61	0.47
1:AG:114:TRP:HD1	1:AG:117:PHE:HD2	1.61	0.47
1:AH:194:VAL:HG13	1:AH:215:ILE:HD12	1.97	0.47
1:AS:114:TRP:HD1	1:AS:117:PHE:HD2	1.60	0.47
5:Ai:103:ALA:HB1	5:Aj:90:LEU:HD23	1.95	0.47
8:AU:27:ILE:HA	8:AU:30:ILE:HG22	1.96	0.47
9:Ax:356:SER:HB3	9:Ay:392:ARG:HH21	1.79	0.47
9:A4:15:LEU:HB3	9:A4:21:LEU:HD12	1.97	0.47
1:S:232:ILE:HG22	1:AB:228:ASN:HB2	1.95	0.47
1:W:238:ALA:HB2	1:X:377:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:293:ILE:HD13	1:X:313:THR:HG21	1.95	0.47
1:f:316:SER:HB2	1:f:363:ASN:HB3	1.97	0.47
1:g:252:LEU:HD13	1:g:433:PHE:HE2	1.78	0.47
1:AF:114:TRP:HD1	1:AF:117:PHE:HD2	1.62	0.47
1:AN:114:TRP:HD1	1:AN:117:PHE:HD2	1.62	0.47
1:AT:103:ARG:HD3	1:AT:200:LEU:HD22	1.95	0.47
9:A1:50:ASN:HB2	9:A1:83:PHE:HE2	1.78	0.47
9:A4:539:VAL:HG11	9:A4:560:ILE:HD11	1.96	0.47
1:O:314:ILE:HA	1:O:364:VAL:HG12	1.96	0.47
1:S:501:ARG:HG2	1:S:504:ARG:HH21	1.79	0.47
1:e:388:PHE:HD1	1:e:448:ILE:HD12	1.79	0.47
1:h:265:SER:HB3	1:h:268:ARG:HG3	1.96	0.47
1:i:252:LEU:HD13	1:i:433:PHE:HE1	1.80	0.47
1:p:79:PHE:HB2	1:p:87:TYR:HB3	1.95	0.47
1:w:141:VAL:HG21	1:w:205:ILE:HD11	1.97	0.47
6:Ak:114:MET:HE3	7:Aq:143:PHE:CG	2.50	0.47
7:As:9:VAL:HG13	7:As:74:GLY:HA2	1.97	0.47
8:AW:35:ILE:HD13	8:AW:50:SER:HA	1.97	0.47
9:Ay:201:ALA:HA	9:Ay:204:PHE:HD2	1.80	0.47
1:B:364:VAL:HG22	1:C:315:ILE:HA	1.96	0.47
1:F:364:VAL:HG22	1:G:315:ILE:HA	1.97	0.47
1:N:273:ARG:HH12	1:N:275:ASN:HB2	1.79	0.47
1:m:238:ALA:HB2	1:n:377:PRO:HB2	1.97	0.47
1:AB:156:VAL:HG12	1:AB:177:VAL:HG13	1.97	0.47
1:AK:114:TRP:HD1	1:AK:117:PHE:HD2	1.62	0.47
9:Az:15:LEU:HB3	9:Az:21:LEU:HD12	1.97	0.47
9:A2:10:LEU:HG	9:A2:16:ASN:HA	1.96	0.47
1:B:386:GLY:HA2	1:B:444:THR:O	2.15	0.47
1:E:386:GLY:HA2	1:E:444:THR:O	2.15	0.47
1:N:298:GLN:HE22	1:N:305:ASN:HA	1.80	0.47
1:S:391:GLY:HA2	1:S:417:MET:HG3	1.97	0.47
1:W:319:THR:HG22	1:W:360:GLU:HG3	1.95	0.47
1:Y:287:SER:HB2	1:Y:371:SER:HB3	1.96	0.47
1:Y:388:PHE:HD1	1:Y:448:ILE:HD12	1.80	0.47
1:b:388:PHE:HD1	1:b:448:ILE:HD12	1.79	0.47
1:f:273:ARG:HB2	1:g:432:SER:HB2	1.96	0.47
1:i:314:ILE:HA	1:i:364:VAL:HG12	1.97	0.47
1:k:314:ILE:HA	1:k:364:VAL:HG12	1.96	0.47
1:s:156:VAL:HG12	1:s:177:VAL:HG13	1.96	0.47
1:AA:66:ARG:HE	1:AA:106:LEU:HD21	1.80	0.47
1:AA:198:VAL:HG12	1:AA:215:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AL:99:ALA:HA	1:AL:103:ARG:HH21	1.80	0.47
1:AN:99:ALA:HA	1:AN:103:ARG:HH21	1.79	0.47
1:AP:114:TRP:HD1	1:AP:117:PHE:HD2	1.63	0.47
3:AZ:220:ILE:HG13	3:AZ:221:MET:HG2	1.96	0.47
9:Ay:644:GLN:HE21	9:Ay:650:PRO:HG3	1.80	0.47
9:A1:201:ALA:HA	9:A1:204:PHE:HD2	1.79	0.47
9:A2:15:LEU:HB3	9:A2:21:LEU:HD12	1.96	0.47
9:A3:334:GLU:HG2	9:A3:338:LYS:HE3	1.97	0.47
1:F:391:GLY:HA2	1:F:417:MET:HG3	1.97	0.47
1:m:386:GLY:HA2	1:m:444:THR:O	2.14	0.47
1:p:159:VAL:HB	1:p:174:LYS:HG3	1.96	0.47
1:r:156:VAL:HG12	1:r:177:VAL:HG13	1.97	0.47
1:t:141:VAL:HG21	1:t:205:ILE:HD11	1.97	0.47
1:x:141:VAL:HG21	1:x:205:ILE:HD11	1.97	0.47
1:AH:163:LYS:HG3	1:AH:170:GLN:HE22	1.80	0.47
1:AK:99:ALA:HA	1:AK:103:ARG:HH21	1.80	0.47
3:AY:205:VAL:HA	3:AY:208:ILE:HG22	1.96	0.47
9:Aw:309:PRO:HB2	9:Aw:312:ILE:HG22	1.97	0.47
9:Ax:17:ASN:HB3	9:Ax:20:ASP:HB2	1.97	0.47
9:Ax:309:PRO:HB2	9:Ax:312:ILE:HG22	1.97	0.47
9:A3:50:ASN:HB2	9:A3:83:PHE:HE2	1.79	0.47
9:A5:17:ASN:HB3	9:A5:20:ASP:HB2	1.97	0.47
1:K:319:THR:HG22	1:K:360:GLU:HG3	1.97	0.47
1:N:314:ILE:HA	1:N:364:VAL:HG12	1.96	0.47
1:U:231:GLY:HA3	1:V:237:LEU:HG	1.96	0.47
1:p:222:ILE:HG21	1:q:199:LYS:HZ3	1.80	0.47
1:2:198:VAL:HG12	1:2:215:ILE:HD13	1.96	0.47
1:AC:99:ALA:HA	1:AC:103:ARG:HH21	1.79	0.47
1:AG:103:ARG:HH11	1:AG:200:LEU:HD22	1.80	0.47
1:AO:103:ARG:HD3	1:AO:200:LEU:HD22	1.97	0.47
3:Ab:186:LEU:HD22	3:Ac:242:TRP:HB3	1.97	0.47
7:Aq:31:VAL:HG23	7:Aq:113:VAL:HB	1.96	0.47
9:Ay:15:LEU:HB3	9:Ay:21:LEU:HD12	1.96	0.47
9:A4:309:PRO:HB2	9:A4:312:ILE:HG22	1.97	0.47
1:O:273:ARG:HB2	1:P:432:SER:HB2	1.95	0.47
1:a:273:ARG:HB2	1:b:432:SER:HB2	1.97	0.47
1:i:235:ILE:HG21	1:j:240:LYS:HB3	1.97	0.47
1:k:265:SER:HB3	1:k:268:ARG:HG3	1.96	0.47
1:7:123:THR:HA	2:AX:94:THR:HB	1.97	0.47
1:AF:103:ARG:HD3	1:AF:200:LEU:HD22	1.96	0.47
1:AF:103:ARG:HH11	1:AF:200:LEU:HD22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:103:ARG:HH11	1:AH:200:LEU:HD22	1.80	0.47
5:Ah:83:MET:HG2	6:An:125:HIS:CD2	2.50	0.47
9:A4:10:LEU:HG	9:A4:16:ASN:HA	1.97	0.47
9:A4:527:VAL:HG22	9:A4:561:ALA:HB2	1.96	0.47
9:A5:10:LEU:HG	9:A5:16:ASN:HA	1.97	0.47
1:T:293:ILE:HD13	1:T:313:THR:HG21	1.96	0.46
1:X:388:PHE:HD1	1:X:448:ILE:HD12	1.78	0.46
1:l:291:ALA:HB3	1:l:367:ASN:HB2	1.96	0.46
1:m:294:GLU:HA	1:m:309:VAL:HG12	1.96	0.46
1:7:141:VAL:HG21	1:7:205:ILE:HD11	1.96	0.46
1:8:177:VAL:HG21	1:8:201:ILE:HD13	1.95	0.46
1:9:156:VAL:HG12	1:9:177:VAL:HG13	1.98	0.46
1:AB:165:LEU:HD21	4:Ad:148:ARG:HE	1.80	0.46
1:AH:99:ALA:HA	1:AH:103:ARG:HH21	1.79	0.46
1:AJ:103:ARG:HH11	1:AJ:200:LEU:HD22	1.80	0.46
1:AM:20:SER:HB3	1:AM:23:GLN:HE22	1.80	0.46
1:AO:125:THR:HB	1:AP:182:ARG:HH21	1.79	0.46
1:AS:103:ARG:HD3	1:AS:200:LEU:HD22	1.95	0.46
3:Ab:224:PRO:HG2	3:Ac:222:LEU:HD13	1.97	0.46
4:Ad:225:SER:HB2	8:AW:25:LEU:HD22	1.96	0.46
5:Af:83:MET:HG3	6:Al:125:HIS:CG	2.50	0.46
6:Ao:109:LEU:HD22	7:Au:135:VAL:HG22	1.97	0.46
9:A3:579:GLN:HA	9:A3:680:GLU:HG2	1.97	0.46
9:A4:644:GLN:HE21	9:A4:650:PRO:HG3	1.79	0.46
1:X:386:GLY:HA2	1:X:444:THR:O	2.15	0.46
1:c:298:GLN:HE22	1:c:305:ASN:HA	1.81	0.46
1:c:314:ILE:HA	1:c:364:VAL:HG12	1.96	0.46
1:AT:99:ALA:HA	1:AT:103:ARG:HH21	1.80	0.46
3:AZ:157:ILE:HD12	3:AZ:175:VAL:HG21	1.96	0.46
4:Ad:217:ILE:HG12	8:AW:36:SER:HB2	1.96	0.46
7:Au:7:ILE:HG23	7:Au:136:ILE:HD11	1.96	0.46
9:Aw:401:ILE:HG23	9:Aw:550:ILE:HD11	1.96	0.46
9:Ax:15:LEU:HB3	9:Ax:21:LEU:HD12	1.97	0.46
9:Az:309:PRO:HB2	9:Az:312:ILE:HG22	1.97	0.46
9:A2:17:ASN:HB3	9:A2:20:ASP:HB2	1.97	0.46
9:A4:629:LYS:HE3	9:A4:665:ILE:HG23	1.97	0.46
1:G:252:LEU:HD13	1:G:433:PHE:HE1	1.80	0.46
1:L:252:LEU:HD13	1:L:433:PHE:HE1	1.81	0.46
1:e:386:GLY:HA2	1:e:444:THR:O	2.15	0.46
1:i:280:THR:HG22	1:i:378:ALA:HA	1.97	0.46
1:t:156:VAL:HG12	1:t:177:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:79:PHE:HB2	1:AB:87:TYR:HB3	1.98	0.46
1:AN:163:LYS:HG3	1:AN:170:GLN:HE22	1.80	0.46
1:AP:156:VAL:HG22	1:AP:177:VAL:HG22	1.97	0.46
3:AY:204:ILE:HG13	3:AZ:230:PRO:HG2	1.97	0.46
3:AZ:83:ARG:HH12	3:Aa:87:LEU:HA	1.80	0.46
9:Aw:201:ALA:HA	9:Aw:204:PHE:HD2	1.80	0.46
1:C:430:GLN:HA	1:C:443:ILE:HD12	1.98	0.46
1:G:386:GLY:HA2	1:G:444:THR:O	2.16	0.46
1:O:364:VAL:HG22	1:P:315:ILE:HA	1.96	0.46
1:P:430:GLN:HA	1:P:443:ILE:HD12	1.96	0.46
1:S:252:LEU:HD13	1:S:433:PHE:HE1	1.81	0.46
1:V:252:LEU:HD13	1:V:433:PHE:HE1	1.81	0.46
1:l:391:GLY:HA2	1:l:417:MET:HG3	1.98	0.46
1:2:141:VAL:HG21	1:2:205:ILE:HD11	1.98	0.46
1:AL:103:ARG:HH11	1:AL:200:LEU:HD22	1.79	0.46
9:Az:10:LEU:HG	9:Az:16:ASN:HA	1.96	0.46
9:Az:17:ASN:HB3	9:Az:20:ASP:HB2	1.97	0.46
9:A2:644:GLN:HE21	9:A2:650:PRO:HG3	1.80	0.46
9:A3:583:ARG:HG2	9:A3:682:PRO:HG3	1.98	0.46
9:A5:309:PRO:HB2	9:A5:312:ILE:HG22	1.97	0.46
1:a:314:ILE:HA	1:a:364:VAL:HG12	1.98	0.46
1:b:252:LEU:HD13	1:b:433:PHE:HE2	1.81	0.46
1:v:141:VAL:HG21	1:v:205:ILE:HD11	1.98	0.46
1:x:156:VAL:HG12	1:x:177:VAL:HG13	1.97	0.46
1:1:156:VAL:HG12	1:1:177:VAL:HG13	1.98	0.46
1:AC:103:ARG:HH11	1:AC:200:LEU:HD22	1.80	0.46
1:AD:103:ARG:HH11	1:AD:200:LEU:HD22	1.80	0.46
1:AE:103:ARG:HH11	1:AE:200:LEU:HD22	1.80	0.46
1:AI:99:ALA:HA	1:AI:103:ARG:HH21	1.80	0.46
1:AI:103:ARG:HH11	1:AI:200:LEU:HD22	1.80	0.46
1:AK:103:ARG:HH11	1:AK:200:LEU:HD22	1.79	0.46
1:AM:194:VAL:HG13	1:AM:215:ILE:HD12	1.97	0.46
3:AY:52:LEU:HD11	5:Ae:97:VAL:HG11	1.96	0.46
3:AZ:238:MET:HE3	3:AZ:238:MET:HB3	1.78	0.46
5:Ae:88:MET:HE2	6:Al:130:ILE:HG21	1.97	0.46
9:Az:356:SER:HB3	9:A1:392:ARG:HH21	1.80	0.46
1:I:501:ARG:HG2	1:I:504:ARG:HH21	1.81	0.46
1:M:252:LEU:HD13	1:M:433:PHE:HE1	1.81	0.46
1:W:235:ILE:HG21	1:X:240:LYS:HB3	1.98	0.46
1:m:364:VAL:HG22	1:n:315:ILE:HA	1.97	0.46
1:z:159:VAL:HB	1:z:174:LYS:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:103:ARG:HH11	1:AR:200:LEU:HD22	1.80	0.46
1:AR:194:VAL:HG13	1:AR:215:ILE:HD12	1.98	0.46
3:Aa:51:LEU:HD21	6:Am:134:LEU:HD13	1.97	0.46
3:Ab:51:LEU:HD23	6:An:133:VAL:HG13	1.97	0.46
4:Ad:93:ILE:HG21	4:Ad:181:SER:HB3	1.98	0.46
9:Ax:644:GLN:HE21	9:Ax:650:PRO:HG3	1.81	0.46
9:A2:629:LYS:HE3	9:A2:665:ILE:HG23	1.96	0.46
1:T:238:ALA:HB2	1:U:377:PRO:HB2	1.97	0.46
1:X:430:GLN:HA	1:X:443:ILE:HD12	1.97	0.46
1:b:235:ILE:HG21	1:c:240:LYS:HB3	1.97	0.46
1:c:289:GLU:HB2	1:c:369:LYS:HB3	1.98	0.46
1:e:315:ILE:HD13	1:e:365:ALA:HB2	1.98	0.46
1:7:177:VAL:HG21	1:7:201:ILE:HD13	1.98	0.46
1:AA:156:VAL:HG12	1:AA:177:VAL:HG13	1.98	0.46
1:AI:163:LYS:HG3	1:AI:170:GLN:HE22	1.80	0.46
1:AO:99:ALA:HA	1:AO:103:ARG:HH21	1.81	0.46
3:Aa:97:MET:HE1	5:Af:110:ILE:HD12	1.98	0.46
3:Ab:92:PRO:HB2	3:Ab:95:ILE:HG23	1.98	0.46
9:A3:78:LEU:HD23	9:A4:266:LEU:HD12	1.97	0.46
1:F:252:LEU:HD13	1:F:433:PHE:HE2	1.81	0.46
1:M:294:GLU:HA	1:M:309:VAL:HG12	1.97	0.46
1:R:364:VAL:HG22	1:S:315:ILE:HA	1.98	0.46
1:c:291:ALA:HB3	1:c:367:ASN:HB2	1.98	0.46
1:d:238:ALA:HB2	1:e:377:PRO:HB2	1.97	0.46
1:i:238:ALA:HB2	1:j:377:PRO:HB2	1.97	0.46
1:q:198:VAL:HG12	1:q:215:ILE:HD13	1.98	0.46
1:AC:114:TRP:HD1	1:AC:117:PHE:HD2	1.63	0.46
1:AJ:114:TRP:HD1	1:AJ:117:PHE:HD2	1.62	0.46
3:AY:154:HIS:HD2	3:AY:157:ILE:HD12	1.81	0.46
3:Aa:163:MET:HE3	3:Aa:163:MET:HB3	1.85	0.46
9:A5:583:ARG:HG2	9:A5:682:PRO:HG3	1.98	0.46
1:B:252:LEU:HD13	1:B:433:PHE:HE2	1.81	0.46
1:C:270:MET:HB3	1:C:388:PHE:HD1	1.81	0.46
1:D:239:GLU:HG3	1:D:242:ARG:HH21	1.81	0.46
1:P:273:ARG:HB2	1:Q:432:SER:HB2	1.97	0.46
1:T:391:GLY:HA2	1:T:417:MET:HG3	1.98	0.46
1:T:501:ARG:HG2	1:T:504:ARG:HH21	1.81	0.46
1:V:315:ILE:HD13	1:V:365:ALA:HB2	1.98	0.46
1:X:391:GLY:HA2	1:X:417:MET:HG3	1.98	0.46
1:Z:314:ILE:HA	1:Z:364:VAL:HG12	1.98	0.46
1:g:316:SER:HB2	1:g:363:ASN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:145:ILE:HG23	1:1:197:LEU:HD21	1.98	0.46
1:AC:163:LYS:HG3	1:AC:170:GLN:HE22	1.80	0.46
1:AN:103:ARG:HH11	1:AN:200:LEU:HD22	1.81	0.46
1:AQ:103:ARG:HH11	1:AQ:200:LEU:HD22	1.80	0.46
1:AT:103:ARG:HH11	1:AT:200:LEU:HD22	1.80	0.46
3:AY:55:LEU:HD11	6:Ak:134:LEU:HD12	1.98	0.46
3:Ab:56:THR:HA	3:Ab:59:THR:HG22	1.97	0.46
9:Ax:201:ALA:HA	9:Ax:204:PHE:HD2	1.81	0.46
9:A1:334:GLU:HG2	9:A1:338:LYS:HE3	1.98	0.46
1:C:252:LEU:HD13	1:C:433:PHE:HE1	1.81	0.46
1:K:252:LEU:HD13	1:K:433:PHE:HE1	1.81	0.46
1:K:388:PHE:HD1	1:K:448:ILE:HD12	1.81	0.46
1:M:314:ILE:HA	1:M:364:VAL:HG12	1.98	0.46
1:k:273:ARG:HB2	1:l:432:SER:HB2	1.98	0.46
1:3:145:ILE:HG23	1:3:197:LEU:HD21	1.97	0.46
1:AP:122:TRP:CE2	1:AQ:182:ARG:HD2	2.51	0.46
9:A2:309:PRO:HB2	9:A2:312:ILE:HG22	1.97	0.46
1:D:386:GLY:HA2	1:D:444:THR:O	2.16	0.45
1:R:273:ARG:HB2	1:S:432:SER:HB2	1.97	0.45
1:W:273:ARG:HB2	1:X:432:SER:HB2	1.97	0.45
1:Y:238:ALA:HB2	1:Z:377:PRO:HB2	1.97	0.45
1:o:250:ALA:HB3	1:AT:168:GLU:HB2	1.98	0.45
1:t:177:VAL:HG21	1:t:201:ILE:HD13	1.98	0.45
1:1:125:THR:HG22	8:AU:75:GLN:HB2	1.97	0.45
1:AN:98:ARG:HH21	1:AN:144:HIS:HE1	1.64	0.45
4:Ad:109:ILE:HD12	4:Ad:228:LEU:HA	1.98	0.45
5:Ae:92:ILE:HD13	6:Al:134:LEU:HD21	1.98	0.45
9:Ay:198:MET:HE3	9:Ay:198:MET:HB3	1.84	0.45
9:A1:17:ASN:HB3	9:A1:20:ASP:HB2	1.97	0.45
9:A2:401:ILE:HG23	9:A2:550:ILE:HD11	1.97	0.45
1:L:316:SER:HB2	1:L:363:ASN:HB3	1.98	0.45
1:U:386:GLY:HA2	1:U:444:THR:O	2.16	0.45
1:Z:364:VAL:HG22	1:a:315:ILE:HA	1.98	0.45
1:c:316:SER:HB2	1:c:363:ASN:HB3	1.96	0.45
1:f:386:GLY:HA2	1:f:444:THR:O	2.15	0.45
1:g:386:GLY:HA2	1:g:444:THR:O	2.16	0.45
1:o:386:GLY:HA2	1:o:444:THR:O	2.16	0.45
1:t:159:VAL:HB	1:t:174:LYS:HG3	1.97	0.45
1:AG:122:TRP:CE2	1:AH:182:ARG:HD2	2.51	0.45
7:Ap:93:PRO:HA	7:Ap:106:GLY:HA2	1.98	0.45
9:Aw:15:LEU:HB3	9:Aw:21:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A1:10:LEU:HG	9:A1:16:ASN:HA	1.98	0.45
1:D:273:ARG:HB2	1:E:432:SER:HB2	1.98	0.45
1:Z:270:MET:HB3	1:Z:388:PHE:HD1	1.82	0.45
1:a:388:PHE:HD1	1:a:448:ILE:HD12	1.81	0.45
1:c:252:LEU:HD13	1:c:433:PHE:HE1	1.82	0.45
1:4:187:ILE:HG13	1:4:193:LYS:HB3	1.97	0.45
1:AI:122:TRP:CE2	1:AJ:182:ARG:HD2	2.51	0.45
3:AY:176:PRO:HG2	3:AY:179:VAL:HG12	1.98	0.45
1:C:238:ALA:HB2	1:D:377:PRO:HB2	1.97	0.45
1:I:364:VAL:HG22	1:J:315:ILE:HA	1.97	0.45
1:J:252:LEU:HD13	1:J:433:PHE:HE1	1.82	0.45
1:K:235:ILE:HG21	1:L:240:LYS:HB3	1.98	0.45
1:N:252:LEU:HD13	1:N:433:PHE:HE1	1.81	0.45
1:V:235:ILE:HG21	1:W:240:LYS:HB3	1.98	0.45
1:W:386:GLY:HA2	1:W:444:THR:O	2.16	0.45
1:5:159:VAL:HB	1:5:174:LYS:HG3	1.97	0.45
3:Ac:107:THR:HG23	3:Ac:108:MET:HG3	1.98	0.45
6:An:119:MET:HA	6:An:122:VAL:HG22	1.98	0.45
1:C:386:GLY:HA2	1:C:444:THR:O	2.17	0.45
1:F:430:GLN:HA	1:F:443:ILE:HD12	1.99	0.45
1:G:298:GLN:HE22	1:G:305:ASN:HA	1.82	0.45
1:W:362:LYS:HG2	1:X:317:SER:HB3	1.97	0.45
1:d:242:ARG:HH12	1:e:251:MET:HG3	1.80	0.45
1:e:430:GLN:HA	1:e:443:ILE:HD12	1.98	0.45
1:AE:122:TRP:CE2	1:AF:182:ARG:HD2	2.51	0.45
1:AK:122:TRP:CE2	1:AL:182:ARG:HD2	2.52	0.45
1:AR:122:TRP:CE2	1:AS:182:ARG:HD2	2.51	0.45
9:A3:201:ALA:HA	9:A3:204:PHE:HD2	1.82	0.45
9:A5:644:GLN:HE21	9:A5:650:PRO:HG3	1.81	0.45
1:C:391:GLY:HA2	1:C:417:MET:HG3	1.99	0.45
1:o:252:LEU:HD13	1:o:433:PHE:HE1	1.81	0.45
1:1:177:VAL:HG21	1:1:201:ILE:HD13	1.99	0.45
1:8:138:THR:HG23	1:8:156:VAL:HG23	1.99	0.45
1:9:165:LEU:HD22	4:Ad:171:ASN:HA	1.97	0.45
1:AD:99:ALA:HA	1:AD:103:ARG:HH21	1.82	0.45
1:AM:122:TRP:CE2	1:AN:182:ARG:HD2	2.52	0.45
1:AQ:98:ARG:HH21	1:AQ:144:HIS:HE1	1.64	0.45
1:G:388:PHE:HD1	1:G:448:ILE:HD12	1.82	0.45
1:M:386:GLY:HA2	1:M:444:THR:O	2.17	0.45
1:U:273:ARG:HB2	1:V:432:SER:HB2	1.98	0.45
1:i:386:GLY:HA2	1:i:444:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:177:VAL:HG21	1:v:201:ILE:HD13	1.99	0.45
1:w:159:VAL:HB	1:w:174:LYS:HG3	1.97	0.45
5:Ah:83:MET:HE2	6:An:125:HIS:HB2	1.98	0.45
1:A:315:ILE:HA	1:o:364:VAL:HG22	1.98	0.45
1:a:238:ALA:HB2	1:b:377:PRO:HB2	1.99	0.45
1:4:215:ILE:HB	1:4:224:ASN:HB2	1.98	0.45
1:AD:194:VAL:HG13	1:AD:215:ILE:HD12	1.99	0.45
3:Aa:251:LYS:HE2	8:AU:85:GLN:HE22	1.82	0.45
3:Ac:70:SER:HB2	3:Ac:104:THR:HG22	1.98	0.45
7:Ap:24:ILE:HG23	7:Ap:118:GLU:HG3	1.98	0.45
9:Ay:309:PRO:HB2	9:Ay:312:ILE:HG22	1.97	0.45
1:R:238:ALA:HB2	1:S:377:PRO:HB2	1.99	0.45
1:V:273:ARG:HB2	1:W:432:SER:HB2	1.98	0.45
1:k:299:ASP:HB2	1:k:302:ALA:HB2	1.98	0.45
1:m:273:ARG:HB2	1:n:432:SER:HB2	1.98	0.45
1:z:141:VAL:HG21	1:z:205:ILE:HD11	1.99	0.45
1:7:159:VAL:HB	1:7:174:LYS:HG3	1.98	0.45
1:AA:177:VAL:HG21	1:AA:201:ILE:HD13	1.99	0.45
1:AK:194:VAL:HG13	1:AK:215:ILE:HD12	1.99	0.45
1:AS:122:TRP:CE2	1:AT:182:ARG:HD2	2.52	0.45
1:T:314:ILE:HA	1:T:364:VAL:HG12	2.00	0.45
1:X:273:ARG:HH12	1:X:275:ASN:HB2	1.82	0.45
1:d:386:GLY:HA2	1:d:444:THR:O	2.17	0.45
1:j:294:GLU:HA	1:j:309:VAL:HG12	1.98	0.45
1:6:177:VAL:HG21	1:6:201:ILE:HD13	1.99	0.45
1:AG:92:LYS:HA	1:AG:95:LYS:HE3	1.99	0.45
1:AM:156:VAL:HG22	1:AM:177:VAL:HG22	1.99	0.45
7:Aq:59:LYS:HD2	7:Aq:59:LYS:HA	1.82	0.45
9:Aw:644:GLN:HE21	9:Aw:650:PRO:HG3	1.81	0.45
9:Ax:334:GLU:HG2	9:Ax:338:LYS:HE3	1.98	0.45
9:A4:401:ILE:HG23	9:A4:550:ILE:HD11	1.98	0.45
1:R:314:ILE:HA	1:R:364:VAL:HG12	1.99	0.44
1:8:198:VAL:HG12	1:8:215:ILE:HD13	1.98	0.44
1:AC:182:ARG:HD2	1:AT:122:TRP:CE2	2.52	0.44
1:AE:156:VAL:HG22	1:AE:177:VAL:HG22	2.00	0.44
9:A1:309:PRO:HB2	9:A1:312:ILE:HG22	1.98	0.44
1:A:386:GLY:HA2	1:A:444:THR:O	2.18	0.44
1:B:314:ILE:HA	1:B:364:VAL:HG12	2.00	0.44
1:L:314:ILE:HA	1:L:364:VAL:HG12	1.99	0.44
1:L:386:GLY:HA2	1:L:444:THR:O	2.16	0.44
1:b:280:THR:HG22	1:b:378:ALA:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:386:GLY:HA2	1:c:444:THR:O	2.17	0.44
1:l:252:LEU:HD13	1:l:433:PHE:HE2	1.82	0.44
1:u:74:GLU:HB2	1:u:97:MET:HE1	1.99	0.44
1:x:198:VAL:HG12	1:x:215:ILE:HD13	1.99	0.44
1:AF:122:TRP:CE2	1:AG:182:ARG:HD2	2.53	0.44
1:AJ:156:VAL:HG22	1:AJ:177:VAL:HG22	1.99	0.44
1:AM:103:ARG:HH11	1:AM:200:LEU:HD22	1.81	0.44
3:Ab:140:PRO:HA	3:Ab:143:ILE:HG22	1.98	0.44
4:Ad:102:GLY:HA3	4:Ad:129:SER:HA	1.98	0.44
9:Ax:78:LEU:HD23	9:Ay:266:LEU:HD12	1.99	0.44
9:A3:309:PRO:HB2	9:A3:312:ILE:HG22	1.97	0.44
1:H:386:GLY:HA2	1:H:444:THR:O	2.18	0.44
1:I:386:GLY:HA2	1:I:444:THR:O	2.16	0.44
1:N:291:ALA:HB3	1:N:367:ASN:HB2	1.99	0.44
1:S:314:ILE:HA	1:S:364:VAL:HG12	1.99	0.44
1:u:53:LEU:HD21	1:u:88:LEU:HD22	1.99	0.44
1:x:177:VAL:HG21	1:x:201:ILE:HD13	2.00	0.44
1:z:145:ILE:HG23	1:z:197:LEU:HD21	1.97	0.44
1:9:159:VAL:HB	1:9:174:LYS:HG3	1.99	0.44
1:AQ:163:LYS:HG3	1:AQ:170:GLN:HE22	1.82	0.44
4:Ad:111:LEU:O	4:Ad:115:ASN:HB2	2.17	0.44
9:Aw:10:LEU:HG	9:Aw:16:ASN:HA	1.98	0.44
9:Ay:484:PRO:HA	9:Ay:487:ILE:HD12	1.99	0.44
1:P:286:GLU:HB3	1:Q:370:LYS:HB2	1.99	0.44
1:x:53:LEU:HD21	1:x:88:LEU:HD22	1.99	0.44
1:AC:122:TRP:CE2	1:AD:182:ARG:HD2	2.52	0.44
1:AE:98:ARG:HH21	1:AE:144:HIS:HE1	1.64	0.44
1:AG:98:ARG:HH21	1:AG:144:HIS:HE1	1.64	0.44
1:AM:99:ALA:HA	1:AM:103:ARG:HH21	1.81	0.44
1:AN:122:TRP:CE2	1:AO:182:ARG:HD2	2.52	0.44
1:AQ:122:TRP:CE2	1:AR:182:ARG:HD2	2.52	0.44
3:Ab:214:LEU:HD13	3:Ab:222:LEU:HD23	1.99	0.44
8:AU:36:SER:HB2	8:AV:44:ILE:HG23	1.98	0.44
9:Az:484:PRO:HA	9:Az:487:ILE:HD12	2.00	0.44
1:D:314:ILE:HA	1:D:364:VAL:HG12	1.99	0.44
1:i:291:ALA:HB3	1:i:367:ASN:HB2	1.98	0.44
1:AC:92:LYS:HA	1:AC:95:LYS:HE3	2.00	0.44
1:AF:98:ARG:HH21	1:AF:144:HIS:HE1	1.65	0.44
1:AK:92:LYS:HA	1:AK:95:LYS:HE3	2.00	0.44
9:A5:334:GLU:HG2	9:A5:338:LYS:HE3	1.99	0.44
1:A:286:GLU:HB3	1:B:370:LYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:LEU:HD13	1:D:433:PHE:HE1	1.83	0.44
1:H:252:LEU:HD13	1:H:433:PHE:HE1	1.83	0.44
1:I:359:GLN:HA	1:J:320:GLN:HA	1.99	0.44
1:q:187:ILE:HG13	1:q:193:LYS:HB3	1.99	0.44
1:4:156:VAL:HG12	1:4:177:VAL:HG13	2.00	0.44
1:0:121:ARG:HH11	1:AA:120:ASP:HB2	1.81	0.44
1:AD:114:TRP:HD1	1:AD:117:PHE:HD2	1.64	0.44
1:AL:156:VAL:HG22	1:AL:177:VAL:HG22	2.00	0.44
5:Ai:60:VAL:HG21	6:Ao:125:HIS:CE1	2.53	0.44
9:Ax:10:LEU:HG	9:Ax:16:ASN:HA	1.99	0.44
9:A3:198:MET:HE3	9:A3:198:MET:HB3	1.83	0.44
1:E:251:MET:HE2	1:AD:168:GLU:HB2	1.98	0.44
1:Q:238:ALA:HB2	1:R:377:PRO:HB2	2.00	0.44
1:X:291:ALA:HB3	1:X:367:ASN:HB2	2.00	0.44
1:h:294:GLU:HA	1:h:309:VAL:HG12	1.99	0.44
1:h:324:TYR:HA	1:h:354:LYS:HA	2.00	0.44
1:p:148:LEU:HD11	1:p:200:LEU:HD21	1.99	0.44
1:t:79:PHE:HD1	1:t:79:PHE:HA	1.74	0.44
1:AH:122:TRP:CE2	1:AI:182:ARG:HD2	2.52	0.44
1:AJ:92:LYS:HA	1:AJ:95:LYS:HE3	2.00	0.44
1:AR:99:ALA:HA	1:AR:103:ARG:HH21	1.82	0.44
3:AZ:140:PRO:HA	3:AZ:143:ILE:HG22	1.99	0.44
3:Ab:204:ILE:HD11	3:Ac:230:PRO:HG2	1.99	0.44
9:A1:78:LEU:HD23	9:A2:266:LEU:HD12	1.99	0.44
1:C:273:ARG:HH12	1:C:275:ASN:HB2	1.82	0.44
1:E:252:LEU:HD13	1:E:433:PHE:HE1	1.83	0.44
1:n:375:LYS:HG3	1:n:379:ARG:HH21	1.83	0.44
1:x:222:ILE:HG21	1:y:199:LYS:HZ3	1.83	0.44
1:z:53:LEU:HD21	1:z:88:LEU:HD22	2.00	0.44
1:AP:194:VAL:HG13	1:AP:215:ILE:HD12	1.99	0.44
1:AR:98:ARG:HH21	1:AR:144:HIS:HE1	1.64	0.44
3:AY:77:VAL:HG11	3:AY:249:LEU:HD22	2.00	0.44
3:Ac:190:LYS:HG3	4:Ad:141:LEU:HD12	1.99	0.44
5:Ah:69:LEU:HD13	5:Ah:69:LEU:HA	1.85	0.44
9:A3:644:GLN:HE21	9:A3:650:PRO:HG3	1.81	0.44
1:A:370:LYS:HB2	1:o:286:GLU:HB3	2.00	0.44
1:U:291:ALA:HB3	1:U:367:ASN:HB2	1.99	0.44
1:V:293:ILE:HD13	1:V:313:THR:HG21	1.98	0.44
1:f:364:VAL:HG22	1:g:315:ILE:HA	1.98	0.44
1:y:153:ALA:HB3	1:y:180:THR:HB	1.98	0.44
1:AI:156:VAL:HG22	1:AI:177:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:98:ARG:HH21	1:AS:144:HIS:HE1	1.64	0.44
9:Ax:484:PRO:HA	9:Ax:487:ILE:HD12	2.00	0.44
9:A2:376:VAL:HG22	9:A2:384:LEU:HD12	2.00	0.44
1:M:364:VAL:HG22	1:N:315:ILE:HA	1.99	0.43
1:R:291:ALA:HB3	1:R:367:ASN:HB2	1.99	0.43
1:V:298:GLN:HE22	1:V:305:ASN:HA	1.83	0.43
1:AD:98:ARG:HH21	1:AD:144:HIS:HE1	1.65	0.43
1:AK:156:VAL:HG22	1:AK:177:VAL:HG22	2.00	0.43
2:AX:37:ALA:HB1	2:AX:42:ARG:HG3	1.99	0.43
3:AZ:87:LEU:HD13	3:AZ:90:SER:HB2	2.00	0.43
7:Ar:142:MET:HE2	7:Ar:142:MET:HB2	1.91	0.43
9:A5:198:MET:HE3	9:A5:198:MET:HB3	1.85	0.43
1:U:316:SER:HB2	1:U:363:ASN:HB3	2.00	0.43
1:e:252:LEU:HD13	1:e:433:PHE:HE2	1.83	0.43
1:z:156:VAL:HG12	1:z:177:VAL:HG13	2.00	0.43
1:AM:92:LYS:HA	1:AM:95:LYS:HE3	2.01	0.43
1:AO:98:ARG:HH21	1:AO:144:HIS:HE1	1.66	0.43
1:AO:122:TRP:CE2	1:AP:182:ARG:HD2	2.53	0.43
1:AP:92:LYS:HA	1:AP:95:LYS:HE3	2.00	0.43
1:AQ:194:VAL:HG13	1:AQ:215:ILE:HD12	1.99	0.43
1:AS:92:LYS:HA	1:AS:95:LYS:HE3	2.00	0.43
7:Au:87:LEU:HD12	7:Au:111:PRO:HA	2.00	0.43
7:Au:88:LYS:HB2	7:Au:110:LEU:HB2	1.99	0.43
9:A4:376:VAL:HG22	9:A4:384:LEU:HD12	1.98	0.43
9:A5:15:LEU:HB3	9:A5:21:LEU:HD12	2.00	0.43
1:Q:314:ILE:HG12	1:Q:362:LYS:HE3	2.01	0.43
1:l:386:GLY:HA2	1:l:444:THR:O	2.17	0.43
1:x:187:ILE:HG13	1:x:193:LYS:HB3	1.99	0.43
1:AA:53:LEU:HD21	1:AA:88:LEU:HD22	2.00	0.43
1:AH:98:ARG:HH21	1:AH:144:HIS:HE1	1.65	0.43
3:Ab:93:THR:HG22	3:Ab:97:MET:HE2	2.00	0.43
7:At:28:ILE:HA	7:At:31:VAL:HG23	2.00	0.43
1:D:316:SER:HB2	1:D:363:ASN:HB3	2.00	0.43
1:S:232:ILE:HD12	1:S:235:ILE:HB	1.99	0.43
1:h:273:ARG:HB2	1:i:432:SER:HB2	2.00	0.43
1:AH:92:LYS:HA	1:AH:95:LYS:HE3	2.01	0.43
3:AZ:239:VAL:HG21	8:Av:77:THR:HG21	2.00	0.43
1:C:364:VAL:HG22	1:D:315:ILE:HA	2.00	0.43
1:N:230:ASP:N	1:9:228:ASN:HD22	2.17	0.43
1:e:238:ALA:HB2	1:f:377:PRO:HB2	2.00	0.43
1:j:270:MET:HB3	1:j:388:PHE:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:79:PHE:HD1	1:9:79:PHE:HA	1.74	0.43
1:AF:156:VAL:HG22	1:AF:177:VAL:HG22	2.01	0.43
1:AG:194:VAL:HG13	1:AG:215:ILE:HD12	2.00	0.43
3:Aa:241:GLY:O	3:Aa:245:ILE:HB	2.17	0.43
9:Aw:266:LEU:HD12	9:A5:78:LEU:HD23	2.01	0.43
9:A2:423:LEU:HG	9:A2:424:ARG:HD2	1.99	0.43
9:A2:484:PRO:HA	9:A2:487:ILE:HD12	1.99	0.43
9:A3:484:PRO:HA	9:A3:487:ILE:HD12	1.99	0.43
9:A4:423:LEU:HG	9:A4:424:ARG:HD2	2.00	0.43
1:P:292:PRO:HB2	1:P:309:VAL:HB	1.99	0.43
1:w:50:SER:HA	1:w:87:TYR:HD2	1.84	0.43
1:9:145:ILE:HG23	1:9:197:LEU:HD21	2.00	0.43
1:AI:92:LYS:HA	1:AI:95:LYS:HE3	2.01	0.43
1:AL:122:TRP:CE2	1:AM:182:ARG:HD2	2.53	0.43
7:Ar:27:ASN:HD21	7:Ar:45:GLN:H	1.66	0.43
1:L:288:LYS:HD3	1:L:370:LYS:HD3	2.01	0.43
1:T:291:ALA:HB3	1:T:367:ASN:HB2	2.00	0.43
1:p:165:LEU:HB2	3:Ac:153:ARG:HH21	1.84	0.43
1:q:92:LYS:HD2	1:AL:64:LEU:HD21	2.00	0.43
1:r:145:ILE:HG23	1:r:197:LEU:HD21	2.01	0.43
1:z:198:VAL:HG12	1:z:215:ILE:HD13	2.01	0.43
1:6:141:VAL:HG21	1:6:205:ILE:HD11	2.01	0.43
1:AD:122:TRP:CE2	1:AE:182:ARG:HD2	2.53	0.43
1:AL:101:LEU:HD13	1:AL:101:LEU:HA	1.94	0.43
3:AY:87:LEU:HD11	4:Ad:104:PHE:HE1	1.83	0.43
3:Ab:71:PHE:HB2	3:Ab:104:THR:HG21	2.00	0.43
9:Aw:484:PRO:HA	9:Aw:487:ILE:HD12	2.00	0.43
1:F:238:ALA:HB2	1:G:377:PRO:HB2	2.00	0.43
1:P:294:GLU:HA	1:P:309:VAL:HG12	2.00	0.43
1:Q:391:GLY:HA2	1:Q:417:MET:HG3	2.01	0.43
1:j:273:ARG:HB2	1:k:432:SER:HB2	2.00	0.43
1:u:66:ARG:HE	1:u:106:LEU:HD21	1.84	0.43
1:3:177:VAL:HG21	1:3:201:ILE:HD13	2.01	0.43
1:AE:92:LYS:HA	1:AE:95:LYS:HE3	2.01	0.43
1:G:418:ALA:HB3	1:G:421:GLU:HG2	1.99	0.43
1:H:293:ILE:HD13	1:H:313:THR:HG21	1.99	0.43
1:O:386:GLY:HA2	1:O:444:THR:O	2.18	0.43
1:Y:294:GLU:HA	1:Y:309:VAL:HG12	1.99	0.43
1:i:293:ILE:HD13	1:i:313:THR:HG21	2.01	0.43
1:2:177:VAL:HG21	1:2:201:ILE:HD13	2.00	0.43
1:AI:98:ARG:HH21	1:AI:144:HIS:HE1	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AO:194:VAL:HG13	1:AO:215:ILE:HD12	2.00	0.43
1:AQ:92:LYS:HA	1:AQ:95:LYS:HE3	2.01	0.43
5:Ai:75:ASP:O	5:Ai:79:VAL:HG13	2.18	0.43
9:Ax:585:ILE:HG22	9:Ax:676:MET:HE2	2.00	0.43
1:B:293:ILE:HD13	1:B:313:THR:HG21	2.01	0.43
1:I:316:SER:HB2	1:I:363:ASN:HB3	2.00	0.43
1:K:316:SER:HB2	1:K:363:ASN:HB3	2.01	0.43
1:M:286:GLU:HB3	1:N:370:LYS:HB2	1.99	0.43
1:O:293:ILE:HD13	1:O:313:THR:HG21	2.01	0.43
1:Q:293:ILE:HD13	1:Q:313:THR:HG21	1.99	0.43
1:S:273:ARG:HH12	1:S:275:ASN:HB2	1.84	0.43
1:c:238:ALA:HB2	1:d:377:PRO:HB2	2.00	0.43
1:g:364:VAL:HG22	1:h:315:ILE:HA	2.00	0.43
1:n:386:GLY:HA2	1:n:444:THR:O	2.18	0.43
1:p:228:ASN:HD22	1:p:228:ASN:N	2.17	0.43
1:2:187:ILE:HG13	1:2:193:LYS:HB3	2.00	0.43
1:3:96:LYS:HE3	1:AC:61:GLN:HG3	2.01	0.43
1:AQ:156:VAL:HG22	1:AQ:177:VAL:HG22	2.00	0.43
3:AZ:206:LEU:HD21	3:AZ:231:PHE:HB2	2.01	0.43
9:A4:198:MET:HE3	9:A4:198:MET:HB3	1.84	0.43
9:A5:484:PRO:HA	9:A5:487:ILE:HD12	2.00	0.43
1:n:273:ARG:HB2	1:o:432:SER:HB2	2.01	0.42
1:u:145:ILE:HG23	1:u:197:LEU:HD21	2.01	0.42
1:AJ:122:TRP:CE2	1:AK:182:ARG:HD2	2.54	0.42
3:Aa:204:ILE:HD12	3:Ab:227:ILE:HD13	2.01	0.42
8:AV:35:ILE:HG21	8:AV:50:SER:HA	2.00	0.42
9:Ax:79:VAL:HA	9:Ax:82:ILE:HG12	2.01	0.42
1:A:299:ASP:HB2	1:A:302:ALA:HB2	2.01	0.42
1:N:245:LYS:O	1:N:249:GLU:HG3	2.19	0.42
1:S:386:GLY:HA2	1:S:444:THR:O	2.19	0.42
1:s:145:ILE:HG23	1:s:197:LEU:HD21	2.01	0.42
1:4:198:VAL:HG12	1:4:215:ILE:HD13	2.01	0.42
1:7:126:ASP:HB3	2:AX:89:ARG:HG2	2.00	0.42
1:8:187:ILE:HG13	1:8:193:LYS:HB3	2.00	0.42
1:AH:156:VAL:HG22	1:AH:177:VAL:HG22	2.01	0.42
6:An:15:LEU:HD13	6:An:15:LEU:HA	1.93	0.42
6:Ao:24:VAL:HG13	6:Ao:40:SER:HB2	2.00	0.42
9:A3:79:VAL:HA	9:A3:82:ILE:HG12	2.01	0.42
9:A3:198:MET:HE2	9:A3:268:VAL:HB	2.01	0.42
1:L:364:VAL:HG22	1:M:315:ILE:HA	2.00	0.42
1:P:291:ALA:HB3	1:P:367:ASN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:386:GLY:HA2	1:R:444:THR:O	2.19	0.42
1:V:386:GLY:HA2	1:V:444:THR:O	2.19	0.42
1:e:298:GLN:HE22	1:e:305:ASN:HA	1.84	0.42
1:q:177:VAL:HG21	1:q:201:ILE:HD13	2.01	0.42
1:0:79:PHE:HD1	1:0:79:PHE:HA	1.75	0.42
1:AD:92:LYS:HA	1:AD:95:LYS:HE3	2.02	0.42
1:AF:92:LYS:HA	1:AF:95:LYS:HE3	2.01	0.42
3:AY:68:MET:HE3	3:AY:68:MET:HB3	1.91	0.42
3:AZ:77:VAL:O	3:AZ:81:ILE:HG12	2.19	0.42
3:AZ:244:LEU:HD23	8:Av:81:PHE:HD2	1.83	0.42
9:Ay:79:VAL:HA	9:Ay:82:ILE:HG12	2.02	0.42
9:Az:79:VAL:HA	9:Az:82:ILE:HG12	2.02	0.42
1:P:314:ILE:HG12	1:P:362:LYS:HE3	2.02	0.42
1:n:299:ASP:HB2	1:n:302:ALA:HB2	2.00	0.42
1:AN:156:VAL:HG22	1:AN:177:VAL:HG22	2.02	0.42
5:Aj:106:ASP:O	5:Aj:110:ILE:HG13	2.19	0.42
7:At:89:LEU:HB3	7:At:107:TYR:HD2	1.84	0.42
9:A3:367:GLU:HA	9:A3:409:VAL:O	2.20	0.42
9:A4:198:MET:HE2	9:A4:268:VAL:HB	2.01	0.42
9:A4:201:ALA:HA	9:A4:204:PHE:HD2	1.83	0.42
9:A5:585:ILE:HG22	9:A5:676:MET:HE2	2.01	0.42
1:C:294:GLU:HA	1:C:309:VAL:HG12	2.01	0.42
1:E:289:GLU:HB2	1:E:369:LYS:HB3	2.01	0.42
1:b:273:ARG:HB2	1:c:432:SER:HB2	2.01	0.42
1:p:177:VAL:HG21	1:p:201:ILE:HD13	2.00	0.42
1:y:79:PHE:HD1	1:y:79:PHE:HA	1.74	0.42
1:8:79:PHE:HD1	1:8:79:PHE:HA	1.72	0.42
1:9:177:VAL:HG21	1:9:201:ILE:HD13	2.01	0.42
3:Aa:145:MET:HE1	3:Aa:181:ILE:HG12	2.01	0.42
5:Ai:96:VAL:HG23	5:Aj:83:MET:HE3	2.00	0.42
6:Al:39:ARG:HG2	6:Al:99:ASN:HD21	1.84	0.42
8:AU:14:ILE:HD12	8:AV:59:LEU:HD22	2.01	0.42
9:A5:79:VAL:HA	9:A5:82:ILE:HG12	2.01	0.42
9:A5:154:ARG:HA	9:A5:154:ARG:HD2	1.89	0.42
1:C:273:ARG:HB2	1:D:432:SER:HB2	2.01	0.42
1:d:233:ASP:HB2	1:u:228:ASN:ND2	2.34	0.42
1:m:252:LEU:HD13	1:m:433:PHE:HE1	1.85	0.42
1:r:222:ILE:HG21	1:s:199:LYS:HZ3	1.84	0.42
1:0:177:VAL:HG21	1:0:201:ILE:HD13	2.02	0.42
1:AS:194:VAL:HG13	1:AS:215:ILE:HD12	2.01	0.42
3:AY:63:ALA:O	3:AY:67:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Ac:81:ILE:HD11	3:Ac:245:ILE:HD13	2.01	0.42
8:AU:21:SER:HB2	8:AU:25:LEU:HD13	2.00	0.42
9:Aw:367:GLU:HA	9:Aw:409:VAL:O	2.20	0.42
9:Az:367:GLU:HA	9:Az:409:VAL:O	2.19	0.42
9:A2:367:GLU:HA	9:A2:409:VAL:O	2.19	0.42
9:A5:198:MET:HE2	9:A5:268:VAL:HB	2.01	0.42
1:F:501:ARG:HG2	1:F:504:ARG:HH21	1.85	0.42
1:H:291:ALA:HB3	1:H:367:ASN:HB2	2.02	0.42
1:I:247:LYS:HE3	1:I:247:LYS:HB3	1.95	0.42
1:I:314:ILE:HA	1:I:364:VAL:HG12	2.02	0.42
1:d:294:GLU:HA	1:d:309:VAL:HG12	2.01	0.42
1:m:291:ALA:HB3	1:m:367:ASN:HB2	2.01	0.42
1:s:177:VAL:HG21	1:s:201:ILE:HD13	2.02	0.42
1:t:198:VAL:HG12	1:t:215:ILE:HD13	2.01	0.42
1:x:50:SER:HA	1:x:87:TYR:HD2	1.85	0.42
1:4:159:VAL:HB	1:4:174:LYS:HG3	2.02	0.42
1:9:129:ARG:HH12	2:AX:82:ILE:HD12	1.84	0.42
1:AA:187:ILE:HG13	1:AA:193:LYS:HB3	2.01	0.42
1:AC:98:ARG:HH21	1:AC:144:HIS:HE1	1.67	0.42
1:AG:156:VAL:HG22	1:AG:177:VAL:HG22	2.02	0.42
1:AL:92:LYS:HA	1:AL:95:LYS:HE3	2.02	0.42
1:AL:98:ARG:HH21	1:AL:144:HIS:HE1	1.66	0.42
1:AR:92:LYS:HA	1:AR:95:LYS:HE3	2.02	0.42
3:Aa:72:LEU:HD13	3:Ab:95:ILE:HG21	2.02	0.42
3:Ac:154:HIS:HD2	3:Ac:157:ILE:HD12	1.83	0.42
9:Aw:78:LEU:HD23	9:Ax:266:LEU:HD12	2.02	0.42
9:Aw:79:VAL:HA	9:Aw:82:ILE:HG12	2.01	0.42
9:Ay:10:LEU:HG	9:Ay:16:ASN:HA	2.01	0.42
1:P:386:GLY:HA2	1:P:444:THR:O	2.20	0.42
1:Z:230:ASP:O	1:Z:234:ARG:HB2	2.20	0.42
1:g:362:LYS:HB2	1:h:317:SER:HB3	2.01	0.42
1:7:79:PHE:HD1	1:7:79:PHE:HA	1.76	0.42
1:AO:156:VAL:HG22	1:AO:177:VAL:HG22	2.01	0.42
3:AZ:73:ARG:HH22	3:AZ:148:GLN:HE21	1.66	0.42
6:Al:39:ARG:HB3	6:Al:100:VAL:HG22	2.01	0.42
8:AW:20:LEU:HD22	8:AW:69:ILE:HG23	2.02	0.42
9:A1:79:VAL:HA	9:A1:82:ILE:HG12	2.01	0.42
9:A4:78:LEU:HD23	9:A5:266:LEU:HD12	2.02	0.42
1:R:286:GLU:HB3	1:S:370:LYS:HB2	2.02	0.42
1:S:287:SER:HB3	1:S:371:SER:HB3	2.01	0.42
1:AF:163:LYS:HG3	1:AF:170:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AN:92:LYS:HA	1:AN:95:LYS:HE3	2.02	0.42
1:AN:194:VAL:HG13	1:AN:215:ILE:HD12	2.01	0.42
1:AO:92:LYS:HA	1:AO:95:LYS:HE3	2.02	0.42
5:Ag:69:LEU:HD13	5:Ag:69:LEU:HA	1.90	0.42
8:AV:14:ILE:HG21	8:AW:63:VAL:HB	2.01	0.42
9:Aw:160:LEU:HD11	9:Aw:192:VAL:HG21	2.02	0.42
1:A:240:LYS:HD3	1:A:240:LYS:HA	1.93	0.42
1:K:238:ALA:HB2	1:L:377:PRO:HB2	2.02	0.42
1:O:356:ASN:H	1:P:323:GLU:HB3	1.84	0.42
1:P:391:GLY:HA2	1:P:417:MET:HG3	2.02	0.42
1:X:238:ALA:HB2	1:Y:377:PRO:HB2	2.00	0.42
1:j:273:ARG:HH12	1:j:275:ASN:HB2	1.84	0.42
1:p:79:PHE:HD1	1:p:79:PHE:HA	1.75	0.42
1:2:159:VAL:HB	1:2:174:LYS:HG3	2.00	0.42
1:4:177:VAL:HG21	1:4:201:ILE:HD13	2.02	0.42
3:AY:178:HIS:HA	3:AZ:102:PHE:HE2	1.84	0.42
3:Ac:49:LEU:HD11	5:Ai:53:VAL:HG12	2.02	0.42
3:Ac:219:MET:HE3	3:Ac:219:MET:HB3	1.95	0.42
5:Ai:107:ILE:HD12	5:Aj:94:LYS:HG3	2.02	0.42
6:Am:32:ILE:HA	6:Am:100:VAL:HG11	2.01	0.42
9:Aw:70:PHE:HD1	9:Aw:70:PHE:HA	1.74	0.42
9:Ay:367:GLU:HA	9:Ay:409:VAL:O	2.19	0.42
9:A1:484:PRO:HA	9:A1:487:ILE:HD12	2.00	0.42
9:A3:228:ILE:HG13	9:A3:229:THR:HG23	2.02	0.42
1:C:292:PRO:HB2	1:C:309:VAL:HB	2.01	0.41
1:D:293:ILE:HD13	1:D:313:THR:HG21	2.02	0.41
1:E:238:ALA:HB2	1:F:377:PRO:HB2	2.02	0.41
1:J:292:PRO:HB2	1:J:309:VAL:HB	2.01	0.41
1:d:356:ASN:H	1:e:323:GLU:HB3	1.85	0.41
1:g:289:GLU:HB2	1:g:369:LYS:HB3	2.02	0.41
1:k:298:GLN:HE22	1:k:305:ASN:HA	1.84	0.41
1:m:316:SER:HB2	1:m:363:ASN:HB3	2.01	0.41
1:t:145:ILE:HG23	1:t:197:LEU:HD21	2.01	0.41
1:u:79:PHE:HD1	1:u:79:PHE:HA	1.73	0.41
1:3:198:VAL:HG12	1:3:215:ILE:HD13	2.01	0.41
1:7:127:PHE:HB2	2:AX:89:ARG:HD2	2.02	0.41
1:8:215:ILE:HB	1:8:224:ASN:HB2	2.01	0.41
1:AD:156:VAL:HG22	1:AD:177:VAL:HG22	2.02	0.41
1:AJ:98:ARG:HH21	1:AJ:144:HIS:HE1	1.67	0.41
1:AR:101:LEU:HD13	1:AR:101:LEU:HA	1.96	0.41
5:Ah:110:ILE:HA	5:Ai:111:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Ak:34:THR:HG21	7:Ap:51:PRO:HD3	2.02	0.41
6:An:122:VAL:HA	6:An:125:HIS:NE2	2.34	0.41
9:Ax:599:ILE:HD11	9:Ax:643:VAL:HG21	2.02	0.41
9:Ay:583:ARG:HG2	9:Ay:682:PRO:HG3	2.01	0.41
9:A5:401:ILE:HG23	9:A5:550:ILE:HD11	2.02	0.41
1:q:53:LEU:HD21	1:q:88:LEU:HD22	2.02	0.41
1:y:96:LYS:HB2	1:AR:61:GLN:HG3	2.02	0.41
1:AC:156:VAL:HG22	1:AC:177:VAL:HG22	2.01	0.41
1:AJ:163:LYS:HG3	1:AJ:170:GLN:HE22	1.84	0.41
3:AY:46:ALA:HB3	3:AY:49:LEU:HB2	2.02	0.41
3:Ab:206:LEU:HD21	3:Ab:231:PHE:HB2	2.01	0.41
9:A3:449:ILE:HD11	9:A3:477:LEU:HD12	2.01	0.41
1:O:291:ALA:HB3	1:O:367:ASN:HB2	2.02	0.41
1:d:230:ASP:HA	1:u:228:ASN:ND2	2.35	0.41
1:d:293:ILE:HD13	1:d:313:THR:HG21	2.02	0.41
1:i:294:GLU:HA	1:i:309:VAL:HG12	2.02	0.41
1:o:247:LYS:HD3	1:AT:168:GLU:HB3	2.03	0.41
1:AA:159:VAL:HB	1:AA:174:LYS:HG3	2.02	0.41
1:AM:101:LEU:HD13	1:AM:101:LEU:HA	1.96	0.41
3:AZ:222:LEU:H	3:Aa:221:MET:HG3	1.86	0.41
5:Ah:99:ARG:HD3	5:Ah:99:ARG:HA	1.95	0.41
6:Ak:107:LYS:HE3	6:Ak:107:LYS:HB3	1.89	0.41
8:AV:25:LEU:HD13	8:AW:52:ILE:HG23	2.03	0.41
9:Az:353:LYS:HD3	9:Az:353:LYS:HA	1.86	0.41
9:Az:599:ILE:HD11	9:Az:643:VAL:HG21	2.03	0.41
9:A4:484:PRO:HA	9:A4:487:ILE:HD12	2.01	0.41
9:A5:305:LEU:HD23	9:A5:308:PHE:HE1	1.85	0.41
1:i:391:GLY:HA2	1:i:417:MET:HG3	2.01	0.41
1:i:501:ARG:HG2	1:i:504:ARG:HH21	1.86	0.41
9:Ax:198:MET:HE2	9:Ax:268:VAL:HB	2.02	0.41
9:Ax:353:LYS:HD3	9:Ax:353:LYS:HA	1.85	0.41
9:A2:79:VAL:HA	9:A2:82:ILE:HG12	2.02	0.41
1:F:275:ASN:O	1:F:383:VAL:HA	2.19	0.41
1:d:291:ALA:HB3	1:d:367:ASN:HB2	2.03	0.41
1:j:293:ILE:HD13	1:j:313:THR:HG21	2.02	0.41
1:8:156:VAL:HG12	1:8:177:VAL:HG22	2.01	0.41
1:AK:98:ARG:HH21	1:AK:144:HIS:HE1	1.68	0.41
1:AO:23:GLN:HE21	1:AO:23:GLN:HB2	1.71	0.41
2:AX:162:ASN:HA	2:AX:165:LYS:HG2	2.01	0.41
3:AZ:67:LEU:HB2	3:AZ:185:ILE:HD11	2.02	0.41
7:As:31:VAL:HG23	7:As:113:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AU:39:GLN:HE21	8:AU:49:LEU:HD12	1.85	0.41
8:AW:58:ILE:HD13	8:AW:58:ILE:HA	1.92	0.41
9:Ay:198:MET:HE2	9:Ay:268:VAL:HB	2.02	0.41
9:A1:367:GLU:HA	9:A1:409:VAL:O	2.20	0.41
1:V:314:ILE:HA	1:V:364:VAL:HG12	2.02	0.41
1:n:252:LEU:HD13	1:n:433:PHE:HE2	1.86	0.41
1:u:177:VAL:HG21	1:u:201:ILE:HD13	2.03	0.41
1:y:145:ILE:HG23	1:y:197:LEU:HD21	2.02	0.41
1:y:159:VAL:HB	1:y:174:LYS:HG3	2.01	0.41
1:3:79:PHE:HD1	1:3:79:PHE:HA	1.75	0.41
1:6:122:TRP:HB3	8:Av:67:PRO:HB2	2.02	0.41
1:7:198:VAL:HG12	1:7:215:ILE:HD13	2.03	0.41
1:8:148:LEU:HD11	1:8:200:LEU:HD21	2.02	0.41
3:AZ:168:ARG:HD2	3:AZ:169:PRO:HD2	2.01	0.41
3:Ab:223:PRO:HA	3:Ab:224:PRO:HD3	1.86	0.41
5:Ag:90:LEU:HD23	6:Am:129:SER:HB2	2.02	0.41
7:Ar:47:ILE:HG23	7:Ar:77:VAL:HG13	2.02	0.41
9:A1:384:LEU:HD23	9:A1:384:LEU:HA	1.89	0.41
9:A2:123:LEU:HD21	9:A2:243:VAL:HB	2.03	0.41
9:A2:198:MET:HE2	9:A2:268:VAL:HB	2.02	0.41
9:A4:353:LYS:HA	9:A4:353:LYS:HD3	1.84	0.41
1:E:286:GLU:HB3	1:F:370:LYS:HB2	2.02	0.41
1:O:314:ILE:HG12	1:O:362:LYS:HD2	2.03	0.41
1:R:235:ILE:HG21	1:S:240:LYS:HB3	2.02	0.41
1:c:235:ILE:HG21	1:d:240:LYS:HB3	2.03	0.41
1:m:233:ASP:HB2	1:z:228:ASN:OD1	2.21	0.41
1:w:177:VAL:HG21	1:w:201:ILE:HD13	2.02	0.41
1:x:79:PHE:HD1	1:x:79:PHE:HA	1.76	0.41
2:AX:191:LEU:HD12	2:AX:194:TYR:HD2	1.86	0.41
3:AY:166:TYR:HE2	3:AY:176:PRO:HG3	1.85	0.41
4:Ad:101:VAL:HG21	4:Ad:192:ILE:HB	2.03	0.41
7:Aq:44:ARG:HD2	7:Aq:113:VAL:HA	2.01	0.41
8:AW:37:ILE:HD13	8:AW:37:ILE:HA	1.92	0.41
9:Aw:353:LYS:HA	9:Aw:353:LYS:HD3	1.85	0.41
9:A2:576:LYS:HD3	9:A2:576:LYS:HA	1.89	0.41
9:A3:160:LEU:HD11	9:A3:192:VAL:HG21	2.03	0.41
9:A4:576:LYS:HD3	9:A4:576:LYS:HA	1.88	0.41
9:A5:433:ILE:HD12	9:A5:484:PRO:HB3	2.03	0.41
1:G:231:GLY:HA3	1:H:237:LEU:HG	2.01	0.41
1:o:319:THR:HG22	1:o:360:GLU:HG3	2.01	0.41
1:AB:145:ILE:HG23	1:AB:197:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AF:101:LEU:HD13	1:AF:101:LEU:HA	1.95	0.41
3:AZ:142:ARG:HA	3:AZ:145:MET:HE3	2.02	0.41
3:Ab:62:PRO:HA	5:Ag:107:ILE:HD11	2.02	0.41
3:Ac:94:GLN:HE22	5:Ah:108:ILE:HB	1.85	0.41
8:Av:59:LEU:HD13	8:Av:59:LEU:HA	1.86	0.41
9:Aw:198:MET:HE2	9:Aw:268:VAL:HB	2.01	0.41
9:A5:367:GLU:HA	9:A5:409:VAL:O	2.21	0.41
1:B:238:ALA:HB2	1:C:377:PRO:HB2	2.02	0.41
1:J:273:ARG:HB2	1:K:432:SER:HB2	2.03	0.41
1:U:319:THR:HG22	1:U:360:GLU:HG3	2.03	0.41
1:f:315:ILE:HD13	1:f:365:ALA:HB2	2.03	0.41
1:j:386:GLY:HA2	1:j:444:THR:O	2.21	0.41
1:m:292:PRO:HG3	1:n:295:LEU:HA	2.03	0.41
1:r:174:LYS:HB2	1:s:203:TYR:HD1	1.86	0.41
1:u:92:LYS:HG3	1:AO:61:GLN:HE22	1.86	0.41
1:6:145:ILE:HG23	1:6:197:LEU:HD21	2.02	0.41
1:8:145:ILE:HG23	1:8:197:LEU:HD21	2.03	0.41
1:AL:194:VAL:HG13	1:AL:215:ILE:HD12	2.02	0.41
1:AT:92:LYS:HA	1:AT:95:LYS:HE3	2.03	0.41
2:AX:48:GLU:HA	2:AX:51:THR:HG22	2.02	0.41
3:Aa:216:ALA:HB2	8:AV:52:ILE:HD11	2.02	0.41
3:Ac:140:PRO:HA	3:Ac:143:ILE:HG12	2.03	0.41
4:Ad:138:LEU:HD11	8:AW:6:ILE:HG21	2.03	0.41
5:Ae:63:VAL:HG13	5:Ae:79:VAL:HG23	2.03	0.41
5:Aj:77:HIS:HA	5:Aj:80:VAL:HG12	2.03	0.41
8:AW:26:ILE:HD12	8:AW:26:ILE:HA	1.95	0.41
9:A1:599:ILE:HD11	9:A1:643:VAL:HG21	2.03	0.41
9:A5:531:PHE:HD1	9:A5:531:PHE:HA	1.71	0.41
1:J:316:SER:HB2	1:J:363:ASN:HB3	2.03	0.41
1:N:316:SER:HB2	1:N:363:ASN:HB3	2.03	0.41
1:O:323:GLU:HG3	1:O:324:TYR:H	1.86	0.41
1:V:292:PRO:HB2	1:V:309:VAL:HB	2.03	0.41
1:b:287:SER:O	1:b:370:LYS:HA	2.21	0.41
1:o:292:PRO:HB2	1:o:309:VAL:HB	2.03	0.41
3:AZ:223:PRO:HA	3:AZ:224:PRO:HD3	1.92	0.41
3:Ab:64:PHE:O	3:Ab:68:MET:CB	2.69	0.41
5:Af:74:ILE:HD12	5:Af:74:ILE:HA	1.90	0.41
5:Ah:76:VAL:HG13	7:Au:3:LEU:HD11	2.02	0.41
9:A1:188:LEU:HD13	9:A1:188:LEU:HA	1.96	0.41
9:A1:198:MET:HB3	9:A1:198:MET:HE3	1.83	0.41
9:A4:123:LEU:HD21	9:A4:243:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:LYS:O	1:C:249:GLU:HG3	2.21	0.40
1:D:323:GLU:HG3	1:D:324:TYR:H	1.87	0.40
1:N:386:GLY:HA2	1:N:444:THR:O	2.21	0.40
1:R:262:LYS:HE3	1:R:262:LYS:HB3	1.92	0.40
1:S:234:ARG:HG2	1:T:377:PRO:HG3	2.03	0.40
1:S:364:VAL:HG22	1:T:315:ILE:HA	2.02	0.40
1:W:262:LYS:HE3	1:W:262:LYS:HB3	1.92	0.40
1:j:278:LEU:HD23	1:j:278:LEU:HA	1.94	0.40
1:t:215:ILE:HB	1:t:224:ASN:HB2	2.02	0.40
1:v:159:VAL:HB	1:v:174:LYS:HG3	2.02	0.40
1:AN:77:LYS:HE2	1:AN:77:LYS:HB2	1.97	0.40
2:AX:111:PHE:CZ	3:AY:216:ALA:HB2	2.56	0.40
2:AX:261:ILE:HG22	2:AX:262:LYS:HG2	2.03	0.40
3:AZ:201:LEU:HD23	3:AZ:204:ILE:HD12	2.03	0.40
9:Az:590:LEU:HD21	9:Az:685:ILE:HD13	2.03	0.40
9:A4:160:LEU:HD11	9:A4:192:VAL:HG21	2.03	0.40
9:A5:576:LYS:HA	9:A5:576:LYS:HD3	1.89	0.40
1:Q:245:LYS:O	1:Q:249:GLU:HG3	2.21	0.40
1:AN:101:LEU:HD13	1:AN:101:LEU:HA	1.96	0.40
3:Aa:49:LEU:HD11	5:Ag:53:VAL:HG12	2.02	0.40
3:Aa:74:ILE:HG12	3:Aa:249:LEU:HD21	2.03	0.40
3:Ac:87:LEU:HD21	3:Ac:229:LEU:HD21	2.02	0.40
8:Av:16:ASN:HA	8:Av:19:ILE:HG22	2.02	0.40
9:Ax:305:LEU:HD23	9:Ax:308:PHE:HE1	1.86	0.40
9:A1:198:MET:HE2	9:A1:268:VAL:HB	2.02	0.40
9:A1:552:ASN:HD22	9:A1:581:VAL:HG12	1.85	0.40
9:A3:599:ILE:HD11	9:A3:643:VAL:HG21	2.03	0.40
9:A4:367:GLU:HA	9:A4:409:VAL:O	2.20	0.40
1:D:390:ASP:CG	1:D:452:ARG:HH21	2.30	0.40
1:Q:262:LYS:HE3	1:Q:262:LYS:HB3	1.94	0.40
1:m:249:GLU:HG2	1:m:276:VAL:HG23	2.03	0.40
1:AJ:101:LEU:HD13	1:AJ:101:LEU:HA	1.95	0.40
3:Aa:67:LEU:HD22	3:Aa:185:ILE:HD11	2.04	0.40
8:AU:26:ILE:HD12	8:AU:26:ILE:HA	1.94	0.40
9:Ay:334:GLU:HG2	9:Ay:338:LYS:HE3	2.03	0.40
1:A:262:LYS:HE3	1:A:262:LYS:HB3	1.94	0.40
1:F:386:GLY:HA2	1:F:444:THR:O	2.21	0.40
1:U:357:GLU:HA	1:V:322:LYS:HA	2.02	0.40
1:X:501:ARG:HG2	1:X:504:ARG:HH21	1.86	0.40
1:a:356:ASN:H	1:b:323:GLU:HB3	1.87	0.40
1:p:198:VAL:HG12	1:p:215:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:198:VAL:HG12	1:w:215:ILE:HD13	2.02	0.40
1:8:155:SER:HB3	1:8:178:ARG:HE	1.86	0.40
1:AP:136:SER:O	1:AP:139:ARG:HG3	2.22	0.40
1:AT:156:VAL:HG22	1:AT:177:VAL:HG22	2.03	0.40
7:Aq:87:LEU:HD23	7:Aq:112:ASN:HD22	1.85	0.40
9:Aw:163:LYS:HD3	9:Aw:188:LEU:HD11	2.02	0.40
9:Ax:583:ARG:HG2	9:Ax:682:PRO:HG3	2.03	0.40
9:Ay:433:ILE:HD12	9:Ay:484:PRO:HB3	2.03	0.40
9:Az:433:ILE:HD13	9:Az:433:ILE:HA	1.96	0.40
9:Az:585:ILE:HG22	9:Az:676:MET:HE2	2.03	0.40
9:A2:160:LEU:HD11	9:A2:192:VAL:HG21	2.04	0.40
1:D:286:GLU:HB3	1:E:370:LYS:HB2	2.03	0.40
1:D:299:ASP:HB2	1:D:302:ALA:HB2	2.03	0.40
1:g:235:ILE:HG21	1:h:240:LYS:HB3	2.03	0.40
1:p:187:ILE:HD11	1:p:197:LEU:HD12	2.04	0.40
1:v:66:ARG:HE	1:v:106:LEU:HD21	1.87	0.40
1:1:142:GLU:HG3	1:1:156:VAL:HG22	2.04	0.40
1:8:159:VAL:HB	1:8:174:LYS:HG3	2.04	0.40
1:AD:101:LEU:HD13	1:AD:101:LEU:HA	1.97	0.40
4:Ad:101:VAL:HG23	4:Ad:193:SER:HB3	2.04	0.40
4:Ad:188:LYS:HD3	4:Ad:188:LYS:HA	1.90	0.40
5:Ag:88:MET:HE2	6:An:130:ILE:HG21	2.02	0.40
7:Au:46:ARG:HH12	7:Au:83:ASP:HA	1.86	0.40
9:Ax:198:MET:HE3	9:Ax:198:MET:HB3	1.83	0.40
9:Az:228:ILE:HG13	9:Az:229:THR:HG23	2.04	0.40
9:A2:599:ILE:HD11	9:A2:643:VAL:HG21	2.04	0.40
9:A3:353:LYS:HD3	9:A3:353:LYS:HA	1.87	0.40
9:A4:79:VAL:HA	9:A4:82:ILE:HG12	2.01	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	0	207/569 (36%)	201 (97%)	5 (2%)	1 (0%)	24	63
1	1	207/569 (36%)	200 (97%)	6 (3%)	1 (0%)	24	63
1	2	201/569 (35%)	195 (97%)	5 (2%)	1 (0%)	24	63
1	3	207/569 (36%)	200 (97%)	6 (3%)	1 (0%)	24	63
1	4	207/569 (36%)	198 (96%)	8 (4%)	1 (0%)	24	63
1	5	207/569 (36%)	198 (96%)	8 (4%)	1 (0%)	24	63
1	6	201/569 (35%)	194 (96%)	6 (3%)	1 (0%)	24	63
1	7	207/569 (36%)	199 (96%)	7 (3%)	1 (0%)	24	63
1	8	207/569 (36%)	196 (95%)	10 (5%)	1 (0%)	24	63
1	9	207/569 (36%)	199 (96%)	7 (3%)	1 (0%)	24	63
1	A	258/569 (45%)	253 (98%)	5 (2%)	0	100	100
1	AA	207/569 (36%)	200 (97%)	6 (3%)	1 (0%)	24	63
1	AB	207/569 (36%)	200 (97%)	6 (3%)	1 (0%)	24	63
1	AC	200/569 (35%)	185 (92%)	14 (7%)	1 (0%)	24	63
1	AD	200/569 (35%)	184 (92%)	15 (8%)	1 (0%)	24	63
1	AE	200/569 (35%)	185 (92%)	14 (7%)	1 (0%)	24	63
1	AF	200/569 (35%)	186 (93%)	13 (6%)	1 (0%)	24	63
1	AG	200/569 (35%)	186 (93%)	13 (6%)	1 (0%)	24	63
1	AH	200/569 (35%)	184 (92%)	15 (8%)	1 (0%)	24	63
1	AI	200/569 (35%)	185 (92%)	14 (7%)	1 (0%)	24	63
1	AJ	200/569 (35%)	185 (92%)	14 (7%)	1 (0%)	24	63
1	AK	200/569 (35%)	184 (92%)	15 (8%)	1 (0%)	24	63
1	AL	200/569 (35%)	186 (93%)	13 (6%)	1 (0%)	24	63
1	AM	200/569 (35%)	185 (92%)	14 (7%)	1 (0%)	24	63
1	AN	200/569 (35%)	185 (92%)	14 (7%)	1 (0%)	24	63
1	AO	200/569 (35%)	184 (92%)	15 (8%)	1 (0%)	24	63
1	AP	200/569 (35%)	184 (92%)	15 (8%)	1 (0%)	24	63
1	AQ	200/569 (35%)	186 (93%)	13 (6%)	1 (0%)	24	63
1	AR	200/569 (35%)	186 (93%)	13 (6%)	1 (0%)	24	63
1	AS	200/569 (35%)	185 (92%)	14 (7%)	1 (0%)	24	63
1	AT	200/569 (35%)	186 (93%)	13 (6%)	1 (0%)	24	63
1	B	258/569 (45%)	250 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	258/569 (45%)	251 (97%)	7 (3%)	0	100	100
1	D	258/569 (45%)	253 (98%)	5 (2%)	0	100	100
1	E	258/569 (45%)	248 (96%)	10 (4%)	0	100	100
1	F	258/569 (45%)	251 (97%)	7 (3%)	0	100	100
1	G	258/569 (45%)	246 (95%)	12 (5%)	0	100	100
1	H	258/569 (45%)	251 (97%)	7 (3%)	0	100	100
1	I	258/569 (45%)	252 (98%)	6 (2%)	0	100	100
1	J	258/569 (45%)	250 (97%)	8 (3%)	0	100	100
1	K	258/569 (45%)	255 (99%)	3 (1%)	0	100	100
1	L	258/569 (45%)	253 (98%)	5 (2%)	0	100	100
1	M	258/569 (45%)	250 (97%)	8 (3%)	0	100	100
1	N	258/569 (45%)	250 (97%)	8 (3%)	0	100	100
1	O	258/569 (45%)	251 (97%)	7 (3%)	0	100	100
1	P	258/569 (45%)	249 (96%)	9 (4%)	0	100	100
1	Q	258/569 (45%)	249 (96%)	9 (4%)	0	100	100
1	R	258/569 (45%)	250 (97%)	8 (3%)	0	100	100
1	S	258/569 (45%)	250 (97%)	8 (3%)	0	100	100
1	T	258/569 (45%)	249 (96%)	9 (4%)	0	100	100
1	U	258/569 (45%)	254 (98%)	4 (2%)	0	100	100
1	V	258/569 (45%)	249 (96%)	9 (4%)	0	100	100
1	W	258/569 (45%)	251 (97%)	7 (3%)	0	100	100
1	X	258/569 (45%)	250 (97%)	8 (3%)	0	100	100
1	Y	258/569 (45%)	250 (97%)	8 (3%)	0	100	100
1	Z	258/569 (45%)	250 (97%)	8 (3%)	0	100	100
1	a	258/569 (45%)	252 (98%)	6 (2%)	0	100	100
1	b	258/569 (45%)	249 (96%)	9 (4%)	0	100	100
1	c	258/569 (45%)	250 (97%)	8 (3%)	0	100	100
1	d	258/569 (45%)	252 (98%)	6 (2%)	0	100	100
1	e	258/569 (45%)	255 (99%)	3 (1%)	0	100	100
1	f	258/569 (45%)	250 (97%)	8 (3%)	0	100	100
1	g	258/569 (45%)	251 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h	258/569 (45%)	251 (97%)	7 (3%)	0	100	100
1	i	258/569 (45%)	249 (96%)	9 (4%)	0	100	100
1	j	258/569 (45%)	251 (97%)	7 (3%)	0	100	100
1	k	258/569 (45%)	251 (97%)	7 (3%)	0	100	100
1	l	258/569 (45%)	252 (98%)	6 (2%)	0	100	100
1	m	258/569 (45%)	248 (96%)	10 (4%)	0	100	100
1	n	258/569 (45%)	253 (98%)	5 (2%)	0	100	100
1	o	258/569 (45%)	248 (96%)	10 (4%)	0	100	100
1	p	207/569 (36%)	200 (97%)	7 (3%)	0	100	100
1	q	207/569 (36%)	200 (97%)	6 (3%)	1 (0%)	24	63
1	r	207/569 (36%)	199 (96%)	7 (3%)	1 (0%)	24	63
1	s	207/569 (36%)	201 (97%)	5 (2%)	1 (0%)	24	63
1	t	201/569 (35%)	194 (96%)	6 (3%)	1 (0%)	24	63
1	u	207/569 (36%)	200 (97%)	6 (3%)	1 (0%)	24	63
1	v	207/569 (36%)	200 (97%)	6 (3%)	1 (0%)	24	63
1	w	207/569 (36%)	200 (97%)	6 (3%)	1 (0%)	24	63
1	x	201/569 (35%)	194 (96%)	6 (3%)	1 (0%)	24	63
1	y	207/569 (36%)	201 (97%)	5 (2%)	1 (0%)	24	63
1	z	207/569 (36%)	200 (97%)	6 (3%)	1 (0%)	24	63
2	AX	240/372 (64%)	236 (98%)	3 (1%)	1 (0%)	30	67
3	AY	207/254 (82%)	205 (99%)	2 (1%)	0	100	100
3	AZ	207/254 (82%)	201 (97%)	6 (3%)	0	100	100
3	Aa	207/254 (82%)	201 (97%)	6 (3%)	0	100	100
3	Ab	207/254 (82%)	202 (98%)	5 (2%)	0	100	100
3	Ac	207/254 (82%)	204 (99%)	3 (1%)	0	100	100
4	Ad	257/269 (96%)	248 (96%)	9 (4%)	0	100	100
5	Ae	68/111 (61%)	65 (96%)	3 (4%)	0	100	100
5	Af	68/111 (61%)	67 (98%)	1 (2%)	0	100	100
5	Ag	68/111 (61%)	68 (100%)	0	0	100	100
5	Ah	68/111 (61%)	67 (98%)	1 (2%)	0	100	100
5	Ai	68/111 (61%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Aj	38/111 (34%)	37 (97%)	1 (3%)	0	100	100
6	Ak	108/135 (80%)	107 (99%)	1 (1%)	0	100	100
6	Al	108/135 (80%)	106 (98%)	2 (2%)	0	100	100
6	Am	108/135 (80%)	107 (99%)	1 (1%)	0	100	100
6	An	108/135 (80%)	105 (97%)	3 (3%)	0	100	100
6	Ao	108/135 (80%)	104 (96%)	4 (4%)	0	100	100
7	Ap	132/152 (87%)	132 (100%)	0	0	100	100
7	Aq	150/152 (99%)	145 (97%)	5 (3%)	0	100	100
7	Ar	132/152 (87%)	128 (97%)	4 (3%)	0	100	100
7	As	150/152 (99%)	148 (99%)	2 (1%)	0	100	100
7	At	150/152 (99%)	148 (99%)	2 (1%)	0	100	100
7	Au	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
8	AU	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
8	AV	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
8	AW	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
8	Av	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
9	A1	695/697 (100%)	680 (98%)	15 (2%)	0	100	100
9	A2	695/697 (100%)	680 (98%)	15 (2%)	0	100	100
9	A3	695/697 (100%)	680 (98%)	15 (2%)	0	100	100
9	A4	695/697 (100%)	680 (98%)	15 (2%)	0	100	100
9	A5	695/697 (100%)	681 (98%)	14 (2%)	0	100	100
9	Aw	695/697 (100%)	679 (98%)	16 (2%)	0	100	100
9	Ax	695/697 (100%)	681 (98%)	14 (2%)	0	100	100
9	Ay	695/697 (100%)	680 (98%)	15 (2%)	0	100	100
9	Az	695/697 (100%)	680 (98%)	15 (2%)	0	100	100
All	All	28824/57443 (50%)	27875 (97%)	908 (3%)	41 (0%)	49	83

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AC	131	ILE
1	AD	131	ILE
1	AE	131	ILE

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Mol	Chain	Res	Type
1	AF	131	ILE
1	AG	131	ILE
1	AH	131	ILE
1	AI	131	ILE
1	AJ	131	ILE
1	AK	131	ILE
1	AL	131	ILE
1	AM	131	ILE
1	AN	131	ILE
1	AO	131	ILE
1	AP	131	ILE
1	AQ	131	ILE
1	AR	131	ILE
1	AS	131	ILE
1	AT	131	ILE
2	AX	91	SER
1	w	90	ASP
1	2	90	ASP
1	9	90	ASP
1	q	90	ASP
1	r	90	ASP
1	s	90	ASP
1	t	90	ASP
1	u	90	ASP
1	v	90	ASP
1	x	90	ASP
1	y	90	ASP
1	z	90	ASP
1	1	90	ASP
1	3	90	ASP
1	4	90	ASP
1	5	90	ASP
1	6	90	ASP
1	7	90	ASP
1	8	90	ASP
1	0	90	ASP
1	AA	90	ASP
1	AB	90	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	178/506 (35%)	167 (94%)	11 (6%)	16	38
1	1	178/506 (35%)	165 (93%)	13 (7%)	13	34
1	2	174/506 (34%)	163 (94%)	11 (6%)	16	37
1	3	178/506 (35%)	168 (94%)	10 (6%)	19	40
1	4	178/506 (35%)	169 (95%)	9 (5%)	21	42
1	5	178/506 (35%)	166 (93%)	12 (7%)	15	36
1	6	174/506 (34%)	162 (93%)	12 (7%)	14	36
1	7	178/506 (35%)	169 (95%)	9 (5%)	21	42
1	8	178/506 (35%)	167 (94%)	11 (6%)	16	38
1	9	178/506 (35%)	168 (94%)	10 (6%)	19	40
1	A	226/506 (45%)	221 (98%)	5 (2%)	45	64
1	AA	178/506 (35%)	166 (93%)	12 (7%)	15	36
1	AB	178/506 (35%)	168 (94%)	10 (6%)	19	40
1	AC	180/506 (36%)	174 (97%)	6 (3%)	33	55
1	AD	180/506 (36%)	175 (97%)	5 (3%)	38	60
1	AE	180/506 (36%)	173 (96%)	7 (4%)	28	49
1	AF	180/506 (36%)	174 (97%)	6 (3%)	33	55
1	AG	180/506 (36%)	175 (97%)	5 (3%)	38	60
1	AH	180/506 (36%)	172 (96%)	8 (4%)	25	47
1	AI	180/506 (36%)	175 (97%)	5 (3%)	38	60
1	AJ	180/506 (36%)	176 (98%)	4 (2%)	45	64
1	AK	180/506 (36%)	176 (98%)	4 (2%)	45	64
1	AL	180/506 (36%)	175 (97%)	5 (3%)	38	60
1	AM	180/506 (36%)	172 (96%)	8 (4%)	25	47
1	AN	180/506 (36%)	174 (97%)	6 (3%)	33	55
1	AO	180/506 (36%)	173 (96%)	7 (4%)	28	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AP	180/506 (36%)	174 (97%)	6 (3%)	33	55
1	AQ	180/506 (36%)	174 (97%)	6 (3%)	33	55
1	AR	180/506 (36%)	174 (97%)	6 (3%)	33	55
1	AS	180/506 (36%)	173 (96%)	7 (4%)	28	49
1	AT	180/506 (36%)	175 (97%)	5 (3%)	38	60
1	B	226/506 (45%)	221 (98%)	5 (2%)	45	64
1	C	226/506 (45%)	221 (98%)	5 (2%)	45	64
1	D	226/506 (45%)	221 (98%)	5 (2%)	45	64
1	E	226/506 (45%)	221 (98%)	5 (2%)	45	64
1	F	226/506 (45%)	223 (99%)	3 (1%)	61	74
1	G	226/506 (45%)	223 (99%)	3 (1%)	61	74
1	H	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	I	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	J	226/506 (45%)	221 (98%)	5 (2%)	45	64
1	K	226/506 (45%)	219 (97%)	7 (3%)	35	56
1	L	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	M	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	N	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	O	226/506 (45%)	223 (99%)	3 (1%)	61	74
1	P	226/506 (45%)	223 (99%)	3 (1%)	61	74
1	Q	226/506 (45%)	221 (98%)	5 (2%)	45	64
1	R	226/506 (45%)	223 (99%)	3 (1%)	61	74
1	S	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	T	226/506 (45%)	223 (99%)	3 (1%)	61	74
1	U	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	V	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	W	226/506 (45%)	221 (98%)	5 (2%)	45	64
1	X	226/506 (45%)	223 (99%)	3 (1%)	61	74
1	Y	226/506 (45%)	221 (98%)	5 (2%)	45	64
1	Z	226/506 (45%)	221 (98%)	5 (2%)	45	64
1	a	226/506 (45%)	222 (98%)	4 (2%)	51	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	226/506 (45%)	221 (98%)	5 (2%)	45	64
1	c	226/506 (45%)	223 (99%)	3 (1%)	61	74
1	d	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	e	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	f	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	g	226/506 (45%)	220 (97%)	6 (3%)	39	61
1	h	226/506 (45%)	223 (99%)	3 (1%)	61	74
1	i	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	j	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	k	226/506 (45%)	223 (99%)	3 (1%)	61	74
1	l	226/506 (45%)	224 (99%)	2 (1%)	70	79
1	m	226/506 (45%)	219 (97%)	7 (3%)	35	56
1	n	226/506 (45%)	223 (99%)	3 (1%)	61	74
1	o	226/506 (45%)	222 (98%)	4 (2%)	51	68
1	p	178/506 (35%)	166 (93%)	12 (7%)	15	36
1	q	178/506 (35%)	168 (94%)	10 (6%)	19	40
1	r	178/506 (35%)	169 (95%)	9 (5%)	21	42
1	s	178/506 (35%)	167 (94%)	11 (6%)	16	38
1	t	174/506 (34%)	164 (94%)	10 (6%)	18	40
1	u	178/506 (35%)	166 (93%)	12 (7%)	15	36
1	v	178/506 (35%)	167 (94%)	11 (6%)	16	38
1	w	178/506 (35%)	167 (94%)	11 (6%)	16	38
1	x	174/506 (34%)	164 (94%)	10 (6%)	18	40
1	y	178/506 (35%)	168 (94%)	10 (6%)	19	40
1	z	178/506 (35%)	167 (94%)	11 (6%)	16	38
2	AX	217/335 (65%)	208 (96%)	9 (4%)	27	49
3	AY	187/232 (81%)	182 (97%)	5 (3%)	39	61
3	AZ	185/232 (80%)	179 (97%)	6 (3%)	34	56
3	Aa	185/232 (80%)	181 (98%)	4 (2%)	45	64
3	Ab	187/232 (81%)	180 (96%)	7 (4%)	30	51
3	Ac	189/232 (82%)	180 (95%)	9 (5%)	23	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Ad	236/249 (95%)	220 (93%)	16 (7%)	14	36
5	Ae	64/103 (62%)	60 (94%)	4 (6%)	16	37
5	Af	64/103 (62%)	59 (92%)	5 (8%)	11	32
5	Ag	64/103 (62%)	59 (92%)	5 (8%)	11	32
5	Ah	62/103 (60%)	58 (94%)	4 (6%)	15	37
5	Ai	64/103 (62%)	62 (97%)	2 (3%)	35	56
5	Aj	35/103 (34%)	32 (91%)	3 (9%)	10	29
6	Ak	107/129 (83%)	104 (97%)	3 (3%)	38	60
6	Al	107/129 (83%)	104 (97%)	3 (3%)	38	60
6	Am	107/129 (83%)	105 (98%)	2 (2%)	50	67
6	An	107/129 (83%)	103 (96%)	4 (4%)	30	51
6	Ao	107/129 (83%)	106 (99%)	1 (1%)	70	79
7	Ap	115/130 (88%)	115 (100%)	0	100	100
7	Aq	127/130 (98%)	125 (98%)	2 (2%)	55	70
7	Ar	116/130 (89%)	115 (99%)	1 (1%)	70	79
7	As	130/130 (100%)	128 (98%)	2 (2%)	57	72
7	At	130/130 (100%)	128 (98%)	2 (2%)	57	72
7	Au	130/130 (100%)	129 (99%)	1 (1%)	73	80
8	AU	78/80 (98%)	71 (91%)	7 (9%)	9	27
8	AV	80/80 (100%)	75 (94%)	5 (6%)	16	37
8	AW	80/80 (100%)	75 (94%)	5 (6%)	16	37
8	Av	77/80 (96%)	74 (96%)	3 (4%)	28	49
9	A1	619/619 (100%)	605 (98%)	14 (2%)	44	64
9	A2	619/619 (100%)	604 (98%)	15 (2%)	43	64
9	A3	619/619 (100%)	604 (98%)	15 (2%)	43	64
9	A4	619/619 (100%)	605 (98%)	14 (2%)	44	64
9	A5	619/619 (100%)	605 (98%)	14 (2%)	44	64
9	Aw	619/619 (100%)	604 (98%)	15 (2%)	43	64
9	Ax	619/619 (100%)	605 (98%)	14 (2%)	44	64
9	Ay	619/619 (100%)	604 (98%)	15 (2%)	43	64
9	Az	619/619 (100%)	604 (98%)	15 (2%)	43	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	25492/51170 (50%)	24718 (97%)	774 (3%)	37 57

All (774) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	LEU
1	A	293	ILE
1	A	306	THR
1	A	383	VAL
1	A	385	LEU
1	B	237	LEU
1	B	306	THR
1	B	364	VAL
1	B	383	VAL
1	B	385	LEU
1	C	237	LEU
1	C	293	ILE
1	C	306	THR
1	C	383	VAL
1	C	388	PHE
1	D	293	ILE
1	D	306	THR
1	D	314	ILE
1	D	383	VAL
1	D	460	ASP
1	E	237	LEU
1	E	293	ILE
1	E	306	THR
1	E	383	VAL
1	E	385	LEU
1	F	293	ILE
1	F	306	THR
1	F	383	VAL
1	G	293	ILE
1	G	306	THR
1	G	383	VAL
1	H	293	ILE
1	H	306	THR
1	H	364	VAL
1	H	383	VAL
1	I	237	LEU
1	I	293	ILE

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Mol	Chain	Res	Type
1	I	364	VAL
1	I	383	VAL
1	J	237	LEU
1	J	293	ILE
1	J	306	THR
1	J	383	VAL
1	J	385	LEU
1	K	237	LEU
1	K	293	ILE
1	K	299	ASP
1	K	306	THR
1	K	314	ILE
1	K	364	VAL
1	K	383	VAL
1	L	237	LEU
1	L	293	ILE
1	L	306	THR
1	L	383	VAL
1	M	293	ILE
1	M	306	THR
1	M	383	VAL
1	M	385	LEU
1	N	293	ILE
1	N	306	THR
1	N	314	ILE
1	N	383	VAL
1	O	293	ILE
1	O	306	THR
1	O	383	VAL
1	P	293	ILE
1	P	306	THR
1	P	383	VAL
1	Q	233	ASP
1	Q	293	ILE
1	Q	306	THR
1	Q	383	VAL
1	Q	385	LEU
1	R	237	LEU
1	R	306	THR
1	R	383	VAL
1	S	234	ARG
1	S	293	ILE

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Mol	Chain	Res	Type
1	S	306	THR
1	S	383	VAL
1	T	237	LEU
1	T	306	THR
1	T	383	VAL
1	U	293	ILE
1	U	306	THR
1	U	364	VAL
1	U	383	VAL
1	V	293	ILE
1	V	306	THR
1	V	364	VAL
1	V	383	VAL
1	W	237	LEU
1	W	293	ILE
1	W	306	THR
1	W	314	ILE
1	W	383	VAL
1	X	237	LEU
1	X	306	THR
1	X	383	VAL
1	Y	237	LEU
1	Y	293	ILE
1	Y	306	THR
1	Y	364	VAL
1	Y	383	VAL
1	Z	293	ILE
1	Z	306	THR
1	Z	383	VAL
1	Z	385	LEU
1	Z	388	PHE
1	a	237	LEU
1	a	293	ILE
1	a	306	THR
1	a	383	VAL
1	b	258	SER
1	b	293	ILE
1	b	306	THR
1	b	314	ILE
1	b	383	VAL
1	c	293	ILE
1	c	306	THR

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Mol	Chain	Res	Type
1	c	383	VAL
1	d	237	LEU
1	d	306	THR
1	d	364	VAL
1	d	383	VAL
1	e	293	ILE
1	e	305	ASN
1	e	306	THR
1	e	383	VAL
1	f	293	ILE
1	f	306	THR
1	f	383	VAL
1	f	385	LEU
1	g	237	LEU
1	g	306	THR
1	g	314	ILE
1	g	370	LYS
1	g	383	VAL
1	g	385	LEU
1	h	237	LEU
1	h	306	THR
1	h	383	VAL
1	i	293	ILE
1	i	306	THR
1	i	383	VAL
1	i	385	LEU
1	j	293	ILE
1	j	306	THR
1	j	383	VAL
1	j	388	PHE
1	k	293	ILE
1	k	362	LYS
1	k	383	VAL
1	l	306	THR
1	l	383	VAL
1	m	251	MET
1	m	293	ILE
1	m	306	THR
1	m	314	ILE
1	m	319	THR
1	m	383	VAL
1	m	385	LEU

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Mol	Chain	Res	Type
1	n	288	LYS
1	n	314	ILE
1	n	383	VAL
1	o	237	LEU
1	o	293	ILE
1	o	306	THR
1	o	383	VAL
1	p	51	ILE
1	p	56	VAL
1	p	79	PHE
1	p	87	TYR
1	p	93	LEU
1	p	146	VAL
1	p	158	LEU
1	p	197	LEU
1	p	208	LEU
1	p	213	ILE
1	p	215	ILE
1	p	228	ASN
1	q	51	ILE
1	q	56	VAL
1	q	79	PHE
1	q	87	TYR
1	q	93	LEU
1	q	146	VAL
1	q	197	LEU
1	q	208	LEU
1	q	213	ILE
1	q	215	ILE
1	r	51	ILE
1	r	56	VAL
1	r	79	PHE
1	r	87	TYR
1	r	93	LEU
1	r	146	VAL
1	r	197	LEU
1	r	208	LEU
1	r	215	ILE
1	s	51	ILE
1	s	56	VAL
1	s	79	PHE
1	s	87	TYR

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Mol	Chain	Res	Type
1	s	93	LEU
1	s	146	VAL
1	s	158	LEU
1	s	197	LEU
1	s	208	LEU
1	s	213	ILE
1	s	215	ILE
1	t	51	ILE
1	t	56	VAL
1	t	79	PHE
1	t	87	TYR
1	t	93	LEU
1	t	146	VAL
1	t	197	LEU
1	t	208	LEU
1	t	213	ILE
1	t	215	ILE
1	u	51	ILE
1	u	56	VAL
1	u	79	PHE
1	u	87	TYR
1	u	93	LEU
1	u	146	VAL
1	u	158	LEU
1	u	197	LEU
1	u	208	LEU
1	u	213	ILE
1	u	215	ILE
1	u	228	ASN
1	v	51	ILE
1	v	56	VAL
1	v	79	PHE
1	v	87	TYR
1	v	93	LEU
1	v	106	LEU
1	v	146	VAL
1	v	197	LEU
1	v	208	LEU
1	v	213	ILE
1	v	215	ILE
1	w	51	ILE
1	w	56	VAL

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Mol	Chain	Res	Type
1	w	79	PHE
1	w	87	TYR
1	w	93	LEU
1	w	146	VAL
1	w	158	LEU
1	w	197	LEU
1	w	208	LEU
1	w	213	ILE
1	w	215	ILE
1	x	51	ILE
1	x	56	VAL
1	x	79	PHE
1	x	87	TYR
1	x	93	LEU
1	x	146	VAL
1	x	197	LEU
1	x	208	LEU
1	x	213	ILE
1	x	215	ILE
1	y	51	ILE
1	y	56	VAL
1	y	79	PHE
1	y	87	TYR
1	y	93	LEU
1	y	124	ILE
1	y	146	VAL
1	y	197	LEU
1	y	208	LEU
1	y	215	ILE
1	z	51	ILE
1	z	56	VAL
1	z	79	PHE
1	z	87	TYR
1	z	93	LEU
1	z	146	VAL
1	z	197	LEU
1	z	208	LEU
1	z	213	ILE
1	z	215	ILE
1	z	228	ASN
1	1	51	ILE
1	1	56	VAL

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Mol	Chain	Res	Type
1	1	79	PHE
1	1	87	TYR
1	1	93	LEU
1	1	106	LEU
1	1	124	ILE
1	1	146	VAL
1	1	158	LEU
1	1	197	LEU
1	1	208	LEU
1	1	213	ILE
1	1	215	ILE
1	2	51	ILE
1	2	56	VAL
1	2	79	PHE
1	2	87	TYR
1	2	93	LEU
1	2	146	VAL
1	2	158	LEU
1	2	197	LEU
1	2	208	LEU
1	2	213	ILE
1	2	215	ILE
1	3	51	ILE
1	3	56	VAL
1	3	79	PHE
1	3	87	TYR
1	3	93	LEU
1	3	146	VAL
1	3	197	LEU
1	3	208	LEU
1	3	213	ILE
1	3	215	ILE
1	4	51	ILE
1	4	56	VAL
1	4	79	PHE
1	4	87	TYR
1	4	93	LEU
1	4	146	VAL
1	4	197	LEU
1	4	208	LEU
1	4	213	ILE
1	5	51	ILE

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Mol	Chain	Res	Type
1	5	56	VAL
1	5	79	PHE
1	5	87	TYR
1	5	93	LEU
1	5	146	VAL
1	5	158	LEU
1	5	197	LEU
1	5	208	LEU
1	5	213	ILE
1	5	215	ILE
1	5	228	ASN
1	6	51	ILE
1	6	56	VAL
1	6	79	PHE
1	6	87	TYR
1	6	93	LEU
1	6	146	VAL
1	6	158	LEU
1	6	197	LEU
1	6	208	LEU
1	6	213	ILE
1	6	215	ILE
1	6	228	ASN
1	7	51	ILE
1	7	56	VAL
1	7	79	PHE
1	7	87	TYR
1	7	93	LEU
1	7	146	VAL
1	7	197	LEU
1	7	208	LEU
1	7	213	ILE
1	8	51	ILE
1	8	56	VAL
1	8	79	PHE
1	8	87	TYR
1	8	93	LEU
1	8	124	ILE
1	8	146	VAL
1	8	197	LEU
1	8	208	LEU
1	8	213	ILE

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Mol	Chain	Res	Type
1	8	215	ILE
1	9	51	ILE
1	9	56	VAL
1	9	79	PHE
1	9	87	TYR
1	9	93	LEU
1	9	146	VAL
1	9	197	LEU
1	9	208	LEU
1	9	213	ILE
1	9	215	ILE
1	0	51	ILE
1	0	56	VAL
1	0	79	PHE
1	0	87	TYR
1	0	93	LEU
1	0	146	VAL
1	0	158	LEU
1	0	197	LEU
1	0	208	LEU
1	0	213	ILE
1	0	215	ILE
1	AA	51	ILE
1	AA	56	VAL
1	AA	79	PHE
1	AA	87	TYR
1	AA	93	LEU
1	AA	106	LEU
1	AA	146	VAL
1	AA	197	LEU
1	AA	208	LEU
1	AA	213	ILE
1	AA	215	ILE
1	AA	228	ASN
1	AB	51	ILE
1	AB	56	VAL
1	AB	79	PHE
1	AB	87	TYR
1	AB	93	LEU
1	AB	146	VAL
1	AB	197	LEU
1	AB	208	LEU

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Mol	Chain	Res	Type
1	AB	213	ILE
1	AB	215	ILE
1	AC	23	GLN
1	AC	49	GLN
1	AC	51	ILE
1	AC	53	LEU
1	AC	154	VAL
1	AC	159	VAL
1	AD	23	GLN
1	AD	49	GLN
1	AD	51	ILE
1	AD	154	VAL
1	AD	159	VAL
1	AE	23	GLN
1	AE	49	GLN
1	AE	51	ILE
1	AE	109	VAL
1	AE	154	VAL
1	AE	159	VAL
1	AE	168	GLU
1	AF	49	GLN
1	AF	51	ILE
1	AF	53	LEU
1	AF	109	VAL
1	AF	154	VAL
1	AF	159	VAL
1	AG	23	GLN
1	AG	49	GLN
1	AG	51	ILE
1	AG	154	VAL
1	AG	159	VAL
1	AH	23	GLN
1	AH	49	GLN
1	AH	51	ILE
1	AH	53	LEU
1	AH	62	TYR
1	AH	109	VAL
1	AH	154	VAL
1	AH	159	VAL
1	AI	23	GLN
1	AI	49	GLN
1	AI	51	ILE

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Mol	Chain	Res	Type
1	AI	154	VAL
1	AI	159	VAL
1	AJ	49	GLN
1	AJ	51	ILE
1	AJ	154	VAL
1	AJ	159	VAL
1	AK	49	GLN
1	AK	51	ILE
1	AK	154	VAL
1	AK	159	VAL
1	AL	49	GLN
1	AL	51	ILE
1	AL	154	VAL
1	AL	159	VAL
1	AL	168	GLU
1	AM	23	GLN
1	AM	49	GLN
1	AM	51	ILE
1	AM	53	LEU
1	AM	109	VAL
1	AM	154	VAL
1	AM	159	VAL
1	AM	168	GLU
1	AN	23	GLN
1	AN	49	GLN
1	AN	51	ILE
1	AN	53	LEU
1	AN	154	VAL
1	AN	159	VAL
1	AO	23	GLN
1	AO	49	GLN
1	AO	51	ILE
1	AO	109	VAL
1	AO	154	VAL
1	AO	159	VAL
1	AO	166	PHE
1	AP	23	GLN
1	AP	49	GLN
1	AP	51	ILE
1	AP	109	VAL
1	AP	154	VAL
1	AP	159	VAL

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Mol	Chain	Res	Type
1	AQ	23	GLN
1	AQ	49	GLN
1	AQ	51	ILE
1	AQ	109	VAL
1	AQ	154	VAL
1	AQ	159	VAL
1	AR	49	GLN
1	AR	51	ILE
1	AR	53	LEU
1	AR	154	VAL
1	AR	159	VAL
1	AR	166	PHE
1	AS	23	GLN
1	AS	49	GLN
1	AS	51	ILE
1	AS	62	TYR
1	AS	109	VAL
1	AS	154	VAL
1	AS	159	VAL
1	AT	23	GLN
1	AT	49	GLN
1	AT	51	ILE
1	AT	154	VAL
1	AT	159	VAL
2	AX	87	VAL
2	AX	94	THR
2	AX	106	TYR
2	AX	107	VAL
2	AX	126	VAL
2	AX	130	ILE
2	AX	142	ILE
2	AX	193	GLU
2	AX	243	GLU
3	AY	66	VAL
3	AY	67	LEU
3	AY	95	ILE
3	AY	128	ILE
3	AY	235	LEU
3	AZ	66	VAL
3	AZ	72	LEU
3	AZ	89	GLN
3	AZ	162	SER

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Mol	Chain	Res	Type
3	AZ	175	VAL
3	AZ	179	VAL
3	Aa	66	VAL
3	Aa	159	LEU
3	Aa	219	MET
3	Aa	229	LEU
3	Ab	85	LEU
3	Ab	93	THR
3	Ab	95	ILE
3	Ab	141	LEU
3	Ab	151	ASP
3	Ab	221	MET
3	Ab	249	LEU
3	Ac	66	VAL
3	Ac	97	MET
3	Ac	99	LEU
3	Ac	118	GLN
3	Ac	146	TYR
3	Ac	159	LEU
3	Ac	167	ASP
3	Ac	175	VAL
3	Ac	200	PHE
4	Ad	24	LEU
4	Ad	42	ILE
4	Ad	45	PHE
4	Ad	57	VAL
4	Ad	85	LEU
4	Ad	94	ILE
4	Ad	113	TYR
4	Ad	116	ILE
4	Ad	127	ILE
4	Ad	128	ILE
4	Ad	147	LEU
4	Ad	185	LEU
4	Ad	209	ILE
4	Ad	216	GLN
4	Ad	219	LEU
4	Ad	232	LEU
5	Ae	60	VAL
5	Ae	74	ILE
5	Ae	76	VAL
5	Ae	110	ILE

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Mol	Chain	Res	Type
5	Af	65	GLU
5	Af	69	LEU
5	Af	76	VAL
5	Af	81	ILE
5	Af	106	ASP
5	Ag	60	VAL
5	Ag	63	VAL
5	Ag	69	LEU
5	Ag	76	VAL
5	Ag	83	MET
5	Ah	58	LEU
5	Ah	69	LEU
5	Ah	76	VAL
5	Ah	108	ILE
5	Ai	69	LEU
5	Ai	76	VAL
5	Aj	76	VAL
5	Aj	93	LEU
5	Aj	108	ILE
6	Ak	8	VAL
6	Ak	100	VAL
6	Ak	133	VAL
6	Al	48	LEU
6	Al	117	HIS
6	Al	130	ILE
6	Am	100	VAL
6	Am	112	ASN
6	An	15	LEU
6	An	18	LEU
6	An	53	LEU
6	An	134	LEU
6	Ao	34	THR
7	Aq	14	LEU
7	Aq	26	ASN
7	Ar	36	THR
7	As	57	TYR
7	As	150	LEU
7	At	19	LEU
7	At	116	VAL
7	Au	149	ILE
8	Av	26	ILE
8	Av	59	LEU

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Mol	Chain	Res	Type
8	Av	68	TRP
8	AU	7	LEU
8	AU	12	ILE
8	AU	24	MET
8	AU	33	LEU
8	AU	35	ILE
8	AU	49	LEU
8	AU	63	VAL
8	AV	17	ILE
8	AV	21	SER
8	AV	45	GLN
8	AV	49	LEU
8	AV	84	LEU
8	AW	7	LEU
8	AW	34	LEU
8	AW	63	VAL
8	AW	80	ILE
8	AW	87	VAL
9	Aw	70	PHE
9	Aw	75	THR
9	Aw	188	LEU
9	Aw	199	ASP
9	Aw	266	LEU
9	Aw	272	ILE
9	Aw	302	LEU
9	Aw	358	VAL
9	Aw	378	ASP
9	Aw	401	ILE
9	Aw	426	VAL
9	Aw	454	VAL
9	Aw	531	PHE
9	Aw	558	GLU
9	Aw	628	LEU
9	Ax	70	PHE
9	Ax	188	LEU
9	Ax	199	ASP
9	Ax	266	LEU
9	Ax	272	ILE
9	Ax	302	LEU
9	Ax	358	VAL
9	Ax	378	ASP
9	Ax	401	ILE

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Mol	Chain	Res	Type
9	Ax	426	VAL
9	Ax	454	VAL
9	Ax	531	PHE
9	Ax	558	GLU
9	Ax	628	LEU
9	Ay	70	PHE
9	Ay	75	THR
9	Ay	188	LEU
9	Ay	199	ASP
9	Ay	266	LEU
9	Ay	272	ILE
9	Ay	302	LEU
9	Ay	358	VAL
9	Ay	378	ASP
9	Ay	401	ILE
9	Ay	426	VAL
9	Ay	454	VAL
9	Ay	531	PHE
9	Ay	558	GLU
9	Ay	628	LEU
9	Az	70	PHE
9	Az	188	LEU
9	Az	199	ASP
9	Az	258	LEU
9	Az	266	LEU
9	Az	272	ILE
9	Az	302	LEU
9	Az	358	VAL
9	Az	378	ASP
9	Az	401	ILE
9	Az	426	VAL
9	Az	454	VAL
9	Az	531	PHE
9	Az	558	GLU
9	Az	628	LEU
9	A1	70	PHE
9	A1	188	LEU
9	A1	199	ASP
9	A1	266	LEU
9	A1	272	ILE
9	A1	302	LEU
9	A1	358	VAL

Continued on next page...

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Mol	Chain	Res	Type
9	A1	378	ASP
9	A1	401	ILE
9	A1	426	VAL
9	A1	454	VAL
9	A1	531	PHE
9	A1	558	GLU
9	A1	628	LEU
9	A2	37	PRO
9	A2	93	ARG
9	A2	188	LEU
9	A2	199	ASP
9	A2	266	LEU
9	A2	272	ILE
9	A2	302	LEU
9	A2	358	VAL
9	A2	378	ASP
9	A2	401	ILE
9	A2	426	VAL
9	A2	454	VAL
9	A2	531	PHE
9	A2	558	GLU
9	A2	628	LEU
9	A3	83	PHE
9	A3	85	LEU
9	A3	188	LEU
9	A3	199	ASP
9	A3	266	LEU
9	A3	272	ILE
9	A3	302	LEU
9	A3	358	VAL
9	A3	378	ASP
9	A3	401	ILE
9	A3	426	VAL
9	A3	454	VAL
9	A3	531	PHE
9	A3	558	GLU
9	A3	628	LEU
9	A4	188	LEU
9	A4	199	ASP
9	A4	249	ASP
9	A4	266	LEU
9	A4	272	ILE

Continued on next page...

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Mol	Chain	Res	Type
9	A4	302	LEU
9	A4	358	VAL
9	A4	378	ASP
9	A4	401	ILE
9	A4	426	VAL
9	A4	454	VAL
9	A4	531	PHE
9	A4	558	GLU
9	A4	628	LEU
9	A5	70	PHE
9	A5	188	LEU
9	A5	199	ASP
9	A5	266	LEU
9	A5	272	ILE
9	A5	302	LEU
9	A5	358	VAL
9	A5	378	ASP
9	A5	401	ILE
9	A5	426	VAL
9	A5	454	VAL
9	A5	531	PHE
9	A5	558	GLU
9	A5	628	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (232) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	GLN
1	A	363	ASN
1	D	298	GLN
1	F	363	ASN
1	G	298	GLN
1	H	298	GLN
1	H	363	ASN
1	I	462	ASN
1	L	367	ASN
1	L	462	ASN
1	M	298	GLN
1	N	298	GLN
1	O	298	GLN
1	O	356	ASN
1	O	367	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	O	447	ASN
1	Q	298	GLN
1	R	298	GLN
1	R	359	GLN
1	S	359	GLN
1	V	298	GLN
1	W	305	ASN
1	X	298	GLN
1	X	356	ASN
1	X	367	ASN
1	Y	298	GLN
1	a	359	GLN
1	a	462	ASN
1	b	298	GLN
1	b	447	ASN
1	c	298	GLN
1	d	298	GLN
1	e	275	ASN
1	e	298	GLN
1	g	298	GLN
1	i	356	ASN
1	i	394	ASN
1	j	298	GLN
1	k	298	GLN
1	n	298	GLN
1	n	447	ASN
1	o	298	GLN
1	p	49	GLN
1	p	144	HIS
1	p	157	ASN
1	p	228	ASN
1	q	49	GLN
1	q	157	ASN
1	q	228	ASN
1	r	49	GLN
1	s	49	GLN
1	t	49	GLN
1	t	157	ASN
1	t	228	ASN
1	u	49	GLN
1	u	228	ASN
1	v	49	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	v	202	GLN
1	v	228	ASN
1	w	49	GLN
1	w	144	HIS
1	x	49	GLN
1	y	49	GLN
1	y	144	HIS
1	z	49	GLN
1	1	49	GLN
1	1	144	HIS
1	1	228	ASN
1	2	49	GLN
1	2	157	ASN
1	3	49	GLN
1	4	49	GLN
1	4	157	ASN
1	5	49	GLN
1	6	49	GLN
1	6	144	HIS
1	7	49	GLN
1	7	144	HIS
1	8	49	GLN
1	8	69	GLN
1	8	228	ASN
1	9	49	GLN
1	9	228	ASN
1	0	49	GLN
1	AA	49	GLN
1	AA	144	HIS
1	AB	49	GLN
1	AC	23	GLN
1	AC	69	GLN
1	AC	202	GLN
1	AD	23	GLN
1	AD	69	GLN
1	AE	23	GLN
1	AE	69	GLN
1	AF	23	GLN
1	AF	69	GLN
1	AG	23	GLN
1	AG	69	GLN
1	AH	23	GLN

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Mol	Chain	Res	Type
1	AH	69	GLN
1	AI	23	GLN
1	AI	69	GLN
1	AJ	23	GLN
1	AJ	69	GLN
1	AJ	170	GLN
1	AK	23	GLN
1	AK	69	GLN
1	AL	23	GLN
1	AL	69	GLN
1	AL	170	GLN
1	AM	23	GLN
1	AM	69	GLN
1	AM	144	HIS
1	AN	23	GLN
1	AN	69	GLN
1	AN	144	HIS
1	AN	202	GLN
1	AO	23	GLN
1	AO	61	GLN
1	AO	69	GLN
1	AP	23	GLN
1	AP	69	GLN
1	AQ	23	GLN
1	AQ	69	GLN
1	AR	23	GLN
1	AR	69	GLN
1	AS	23	GLN
1	AS	69	GLN
1	AS	202	GLN
1	AT	23	GLN
1	AT	69	GLN
2	AX	118	ASN
3	AY	94	GLN
3	AY	148	GLN
3	AY	154	HIS
3	AY	187	HIS
3	AZ	148	GLN
3	Aa	148	GLN
3	Ab	50	GLN
3	Ac	94	GLN
3	Ac	118	GLN

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Mol	Chain	Res	Type
3	Ac	129	ASN
3	Ac	154	HIS
4	Ad	96	ASN
4	Ad	115	ASN
5	Ae	66	GLN
5	Ae	77	HIS
5	Ae	89	ASN
5	Af	54	ASN
5	Af	57	GLN
5	Af	109	ASN
5	Ag	87	ASN
5	Ah	57	GLN
5	Ah	66	GLN
5	Aj	109	ASN
6	Ak	121	ASN
6	Am	113	GLN
6	Am	117	HIS
6	Ao	125	HIS
7	Ap	26	ASN
7	Ap	73	GLN
7	Aq	112	ASN
7	Ar	27	ASN
7	Ar	73	GLN
7	Ar	95	HIS
7	As	17	GLN
7	As	30	ASN
7	As	45	GLN
7	As	112	ASN
7	At	26	ASN
7	At	45	GLN
7	At	55	ASN
7	At	73	GLN
7	Au	17	GLN
7	Au	26	ASN
7	Au	45	GLN
8	Av	45	GLN
8	Av	71	ASN
8	Av	86	ASN
8	AU	45	GLN
8	AU	85	GLN
8	AW	45	GLN
9	Aw	175	ASN

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Mol	Chain	Res	Type
9	Aw	186	ASN
9	Aw	219	ASN
9	Aw	584	GLN
9	Aw	644	GLN
9	Ax	175	ASN
9	Ax	186	ASN
9	Ax	219	ASN
9	Ax	254	GLN
9	Ax	584	GLN
9	Ax	644	GLN
9	Ay	175	ASN
9	Ay	186	ASN
9	Ay	219	ASN
9	Ay	254	GLN
9	Ay	584	GLN
9	Ay	644	GLN
9	Az	175	ASN
9	Az	186	ASN
9	Az	219	ASN
9	Az	254	GLN
9	Az	584	GLN
9	Az	644	GLN
9	A1	175	ASN
9	A1	186	ASN
9	A1	219	ASN
9	A1	254	GLN
9	A1	584	GLN
9	A1	644	GLN
9	A2	175	ASN
9	A2	186	ASN
9	A2	219	ASN
9	A2	510	GLN
9	A2	644	GLN
9	A3	175	ASN
9	A3	186	ASN
9	A3	219	ASN
9	A3	584	GLN
9	A3	644	GLN
9	A4	175	ASN
9	A4	186	ASN
9	A4	219	ASN
9	A4	254	GLN

Continued on next page...

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Mol	Chain	Res	Type
9	A4	584	GLN
9	A4	644	GLN
9	A5	175	ASN
9	A5	186	ASN
9	A5	219	ASN
9	A5	584	GLN
9	A5	644	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

This section contains visualisations of the EMDB entry EMD-76383. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

6.1.1 Primary map



X



Y

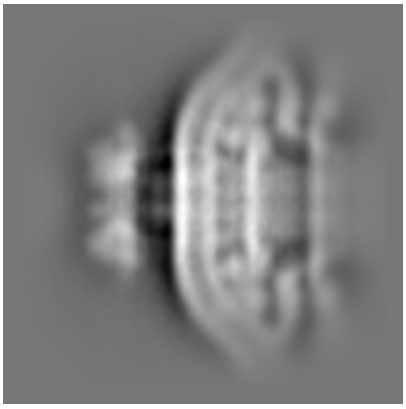


Z

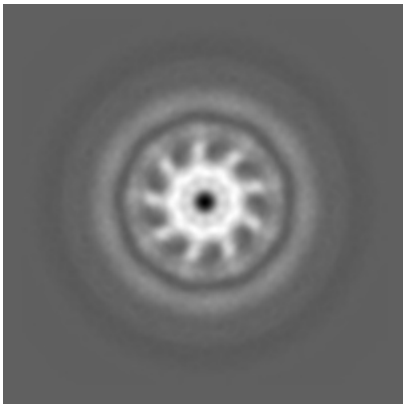
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 128



Y Index: 128

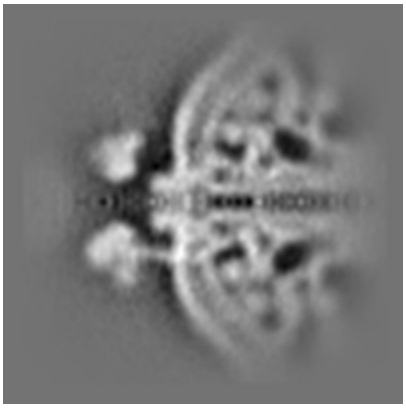


Z Index: 128

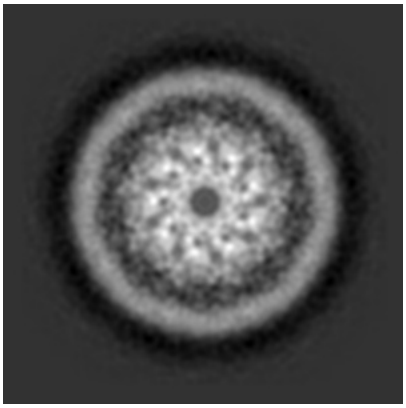
6.2.2 Raw map



X Index: 50



Y Index: 50



Z Index: 50

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: 138



Y Index: 116

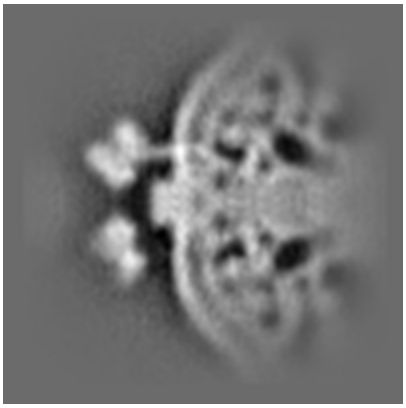


Z Index: 119

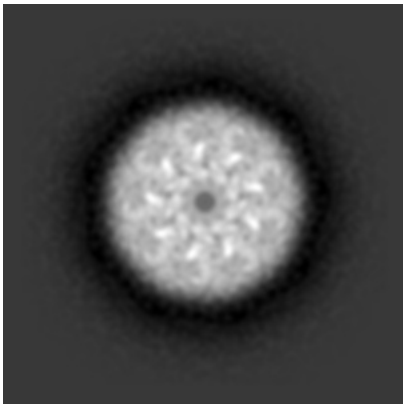
6.3.2 Raw map



X Index: 46



Y Index: 54

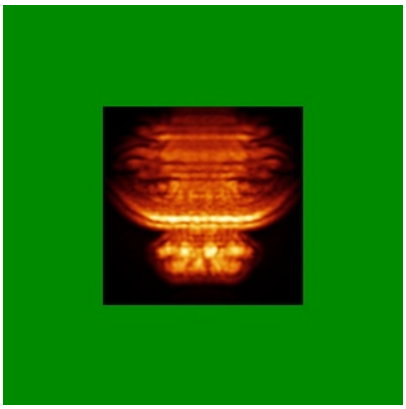


Z Index: 44

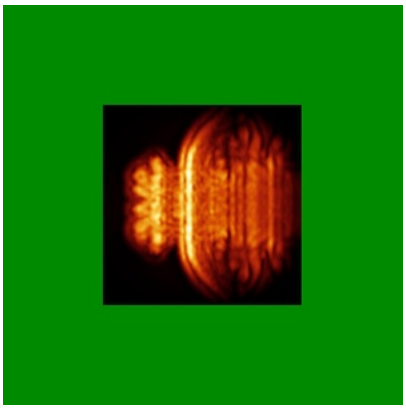
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

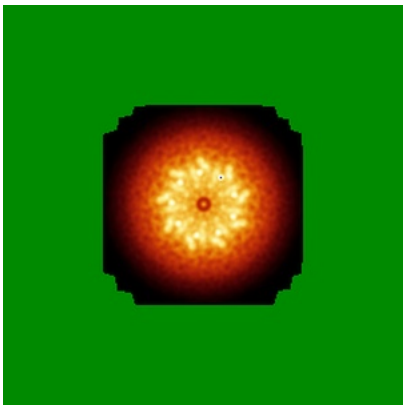
6.4.1 Primary map



X



Y

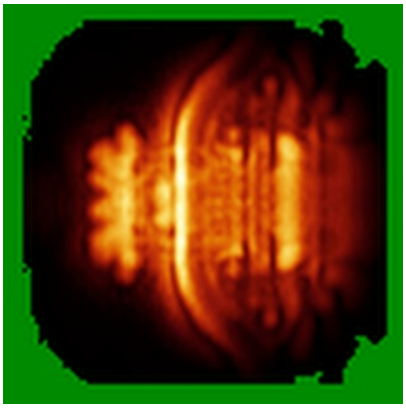


Z

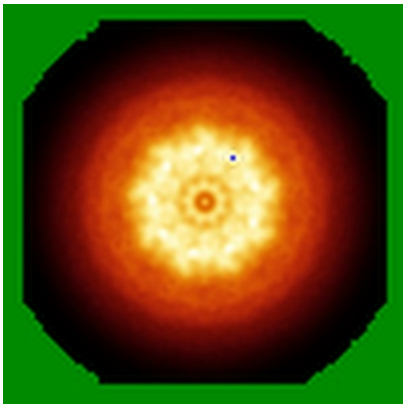
6.4.2 Raw map



X



Y

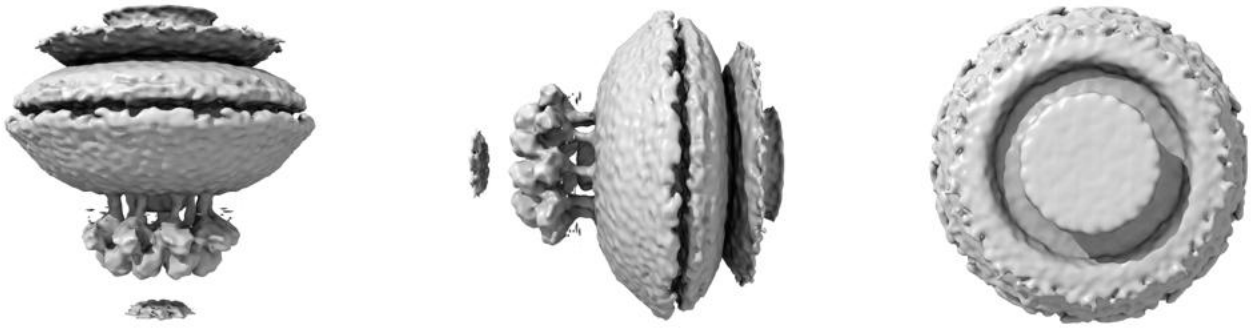


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

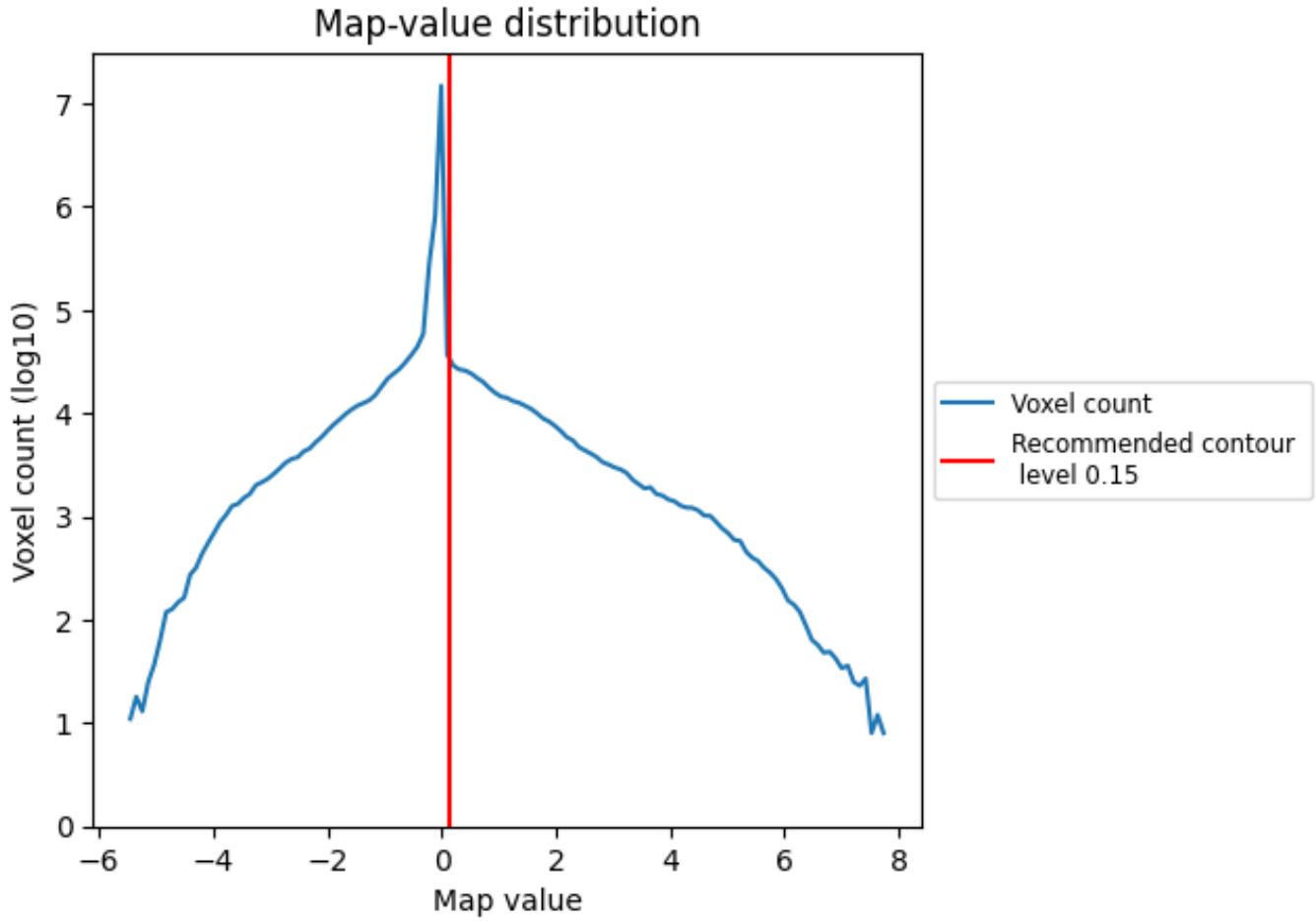
6.6 Mask visualisation (i)

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

7 Map analysis

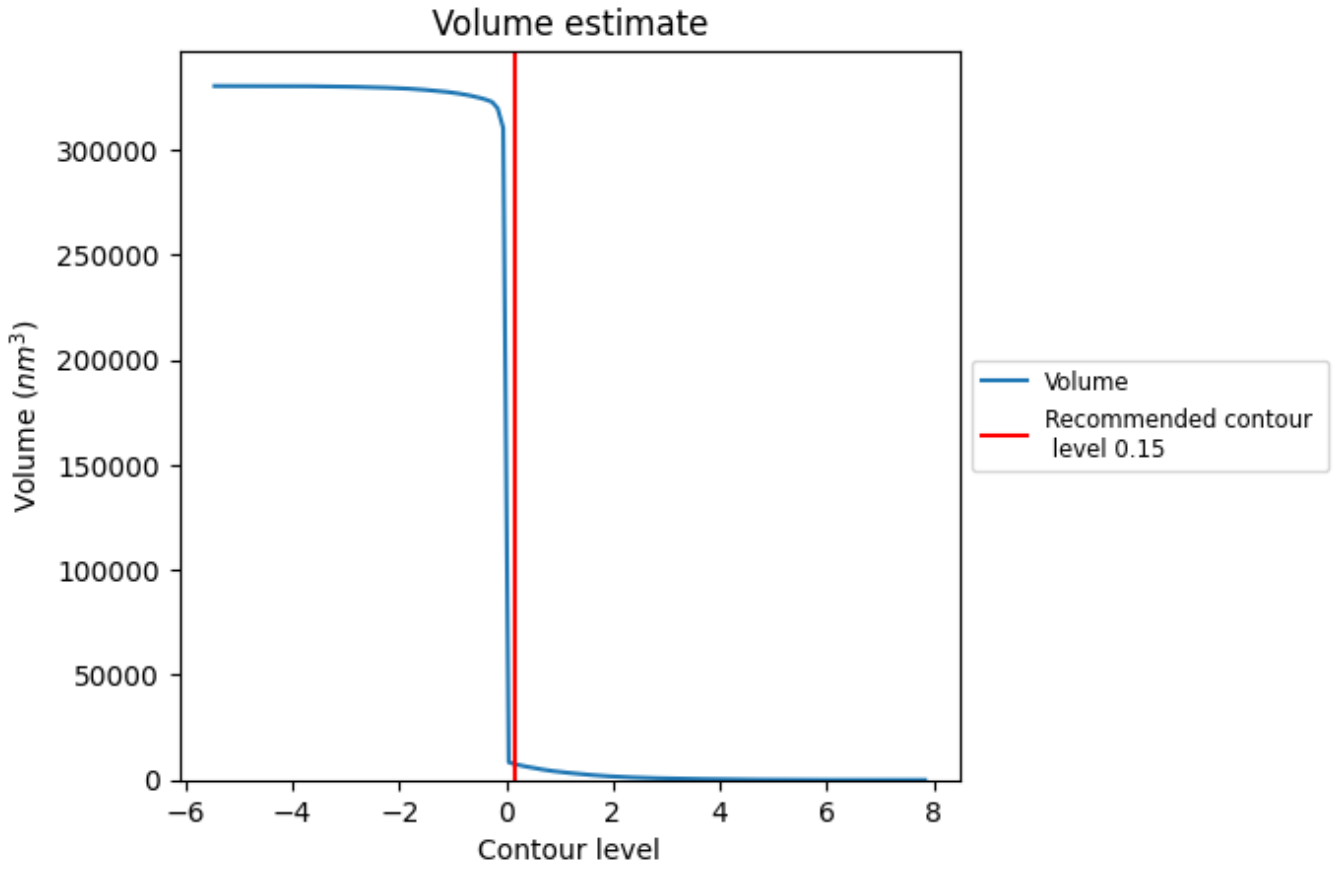
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

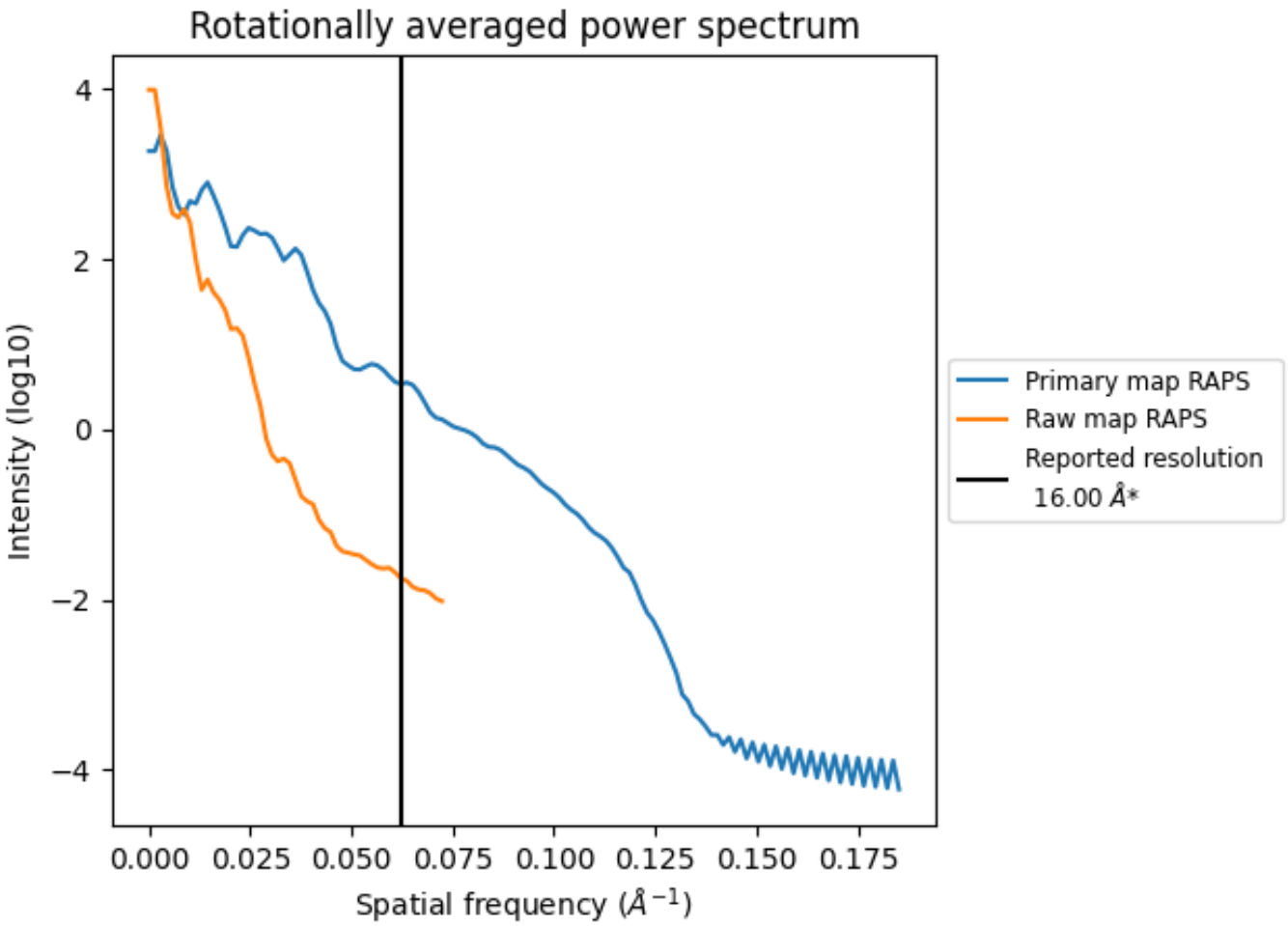
7.2 Volume estimate



The volume at the recommended contour level is 7631 nm^3; this corresponds to an approximate mass of 6894 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

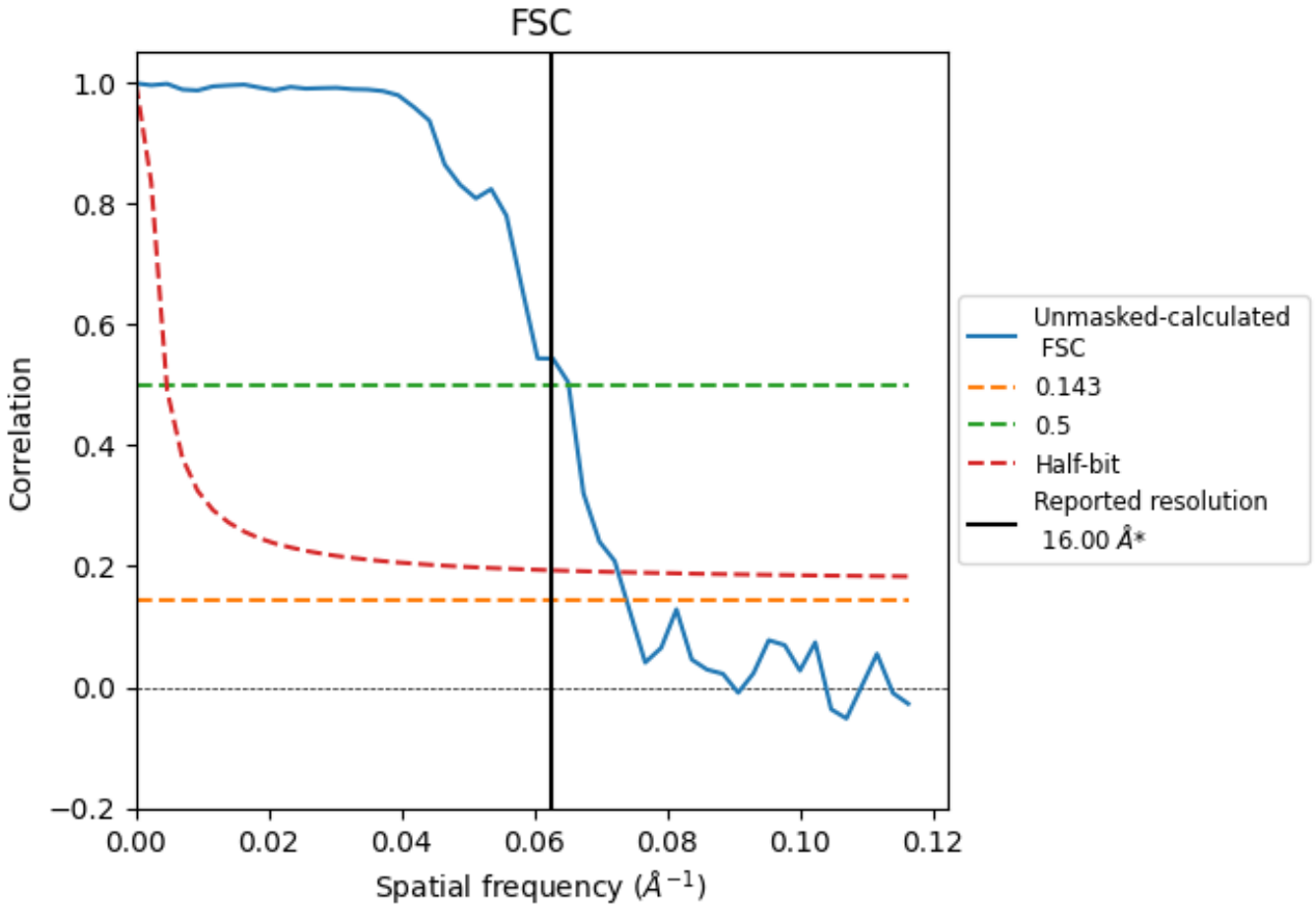


*Reported resolution corresponds to spatial frequency of 0.062 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.062 Å^{-1}

8.2 Resolution estimates (i)

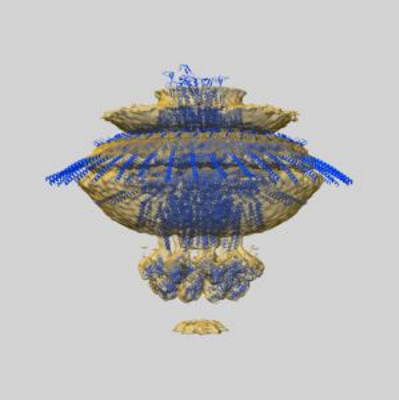
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	16.00	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	13.53	15.34	13.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

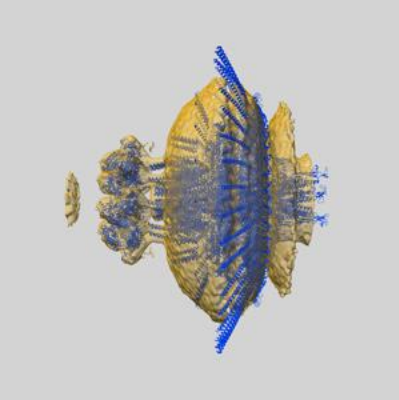
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76383 and PDB model 12EQ. Per-residue inclusion information can be found in section 3 on page 15.

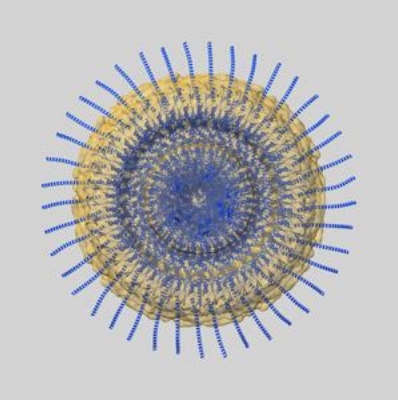
9.1 Map-model overlay



X



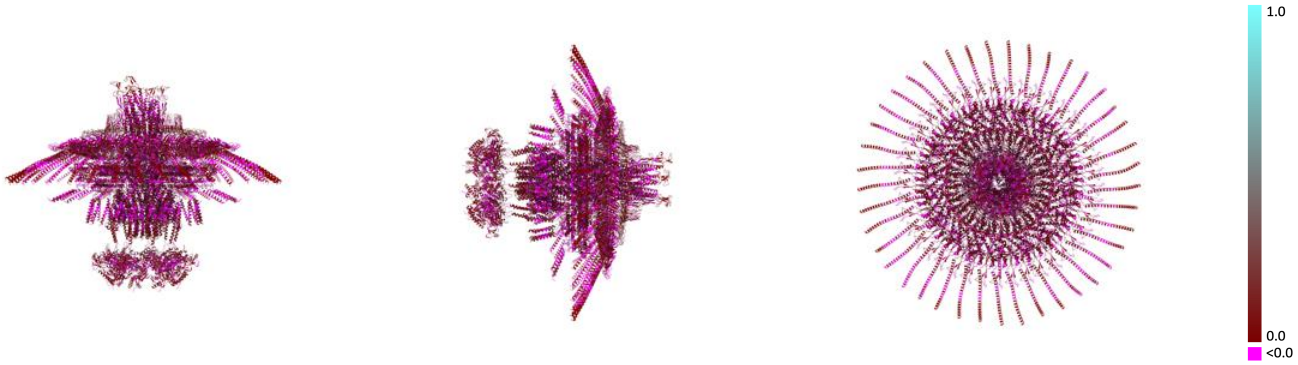
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

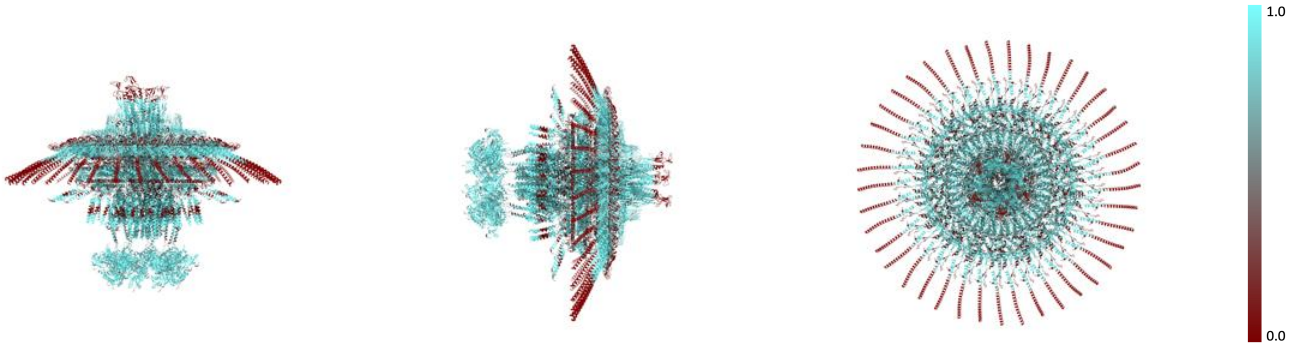
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

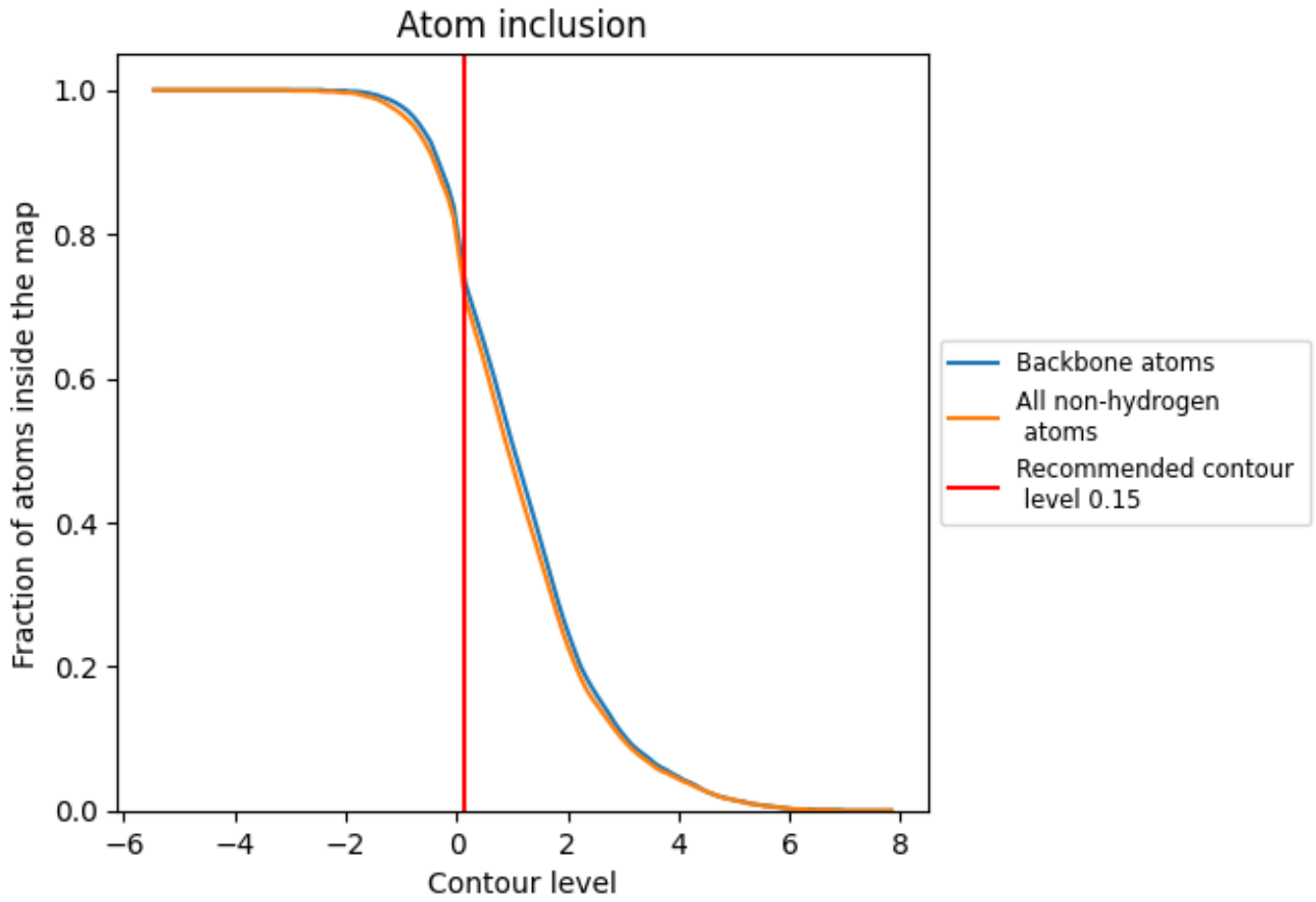
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7120	0.0410
0	0.7500	0.0450
1	0.7740	0.0480
2	0.7620	0.0550
3	0.7590	0.0470
4	0.7800	0.0570
5	0.7620	0.0530
6	0.7870	0.0520
7	0.7550	0.0580
8	0.7510	0.0470
9	0.7730	0.0530
A	0.6370	0.0450
A1	0.8910	0.0540
A2	0.8910	0.0540
A3	0.8910	0.0530
A4	0.8920	0.0530
A5	0.8910	0.0520
AA	0.7800	0.0550
AB	0.7710	0.0540
AC	0.5280	0.0170
AD	0.4740	0.0050
AE	0.5400	0.0180
AF	0.4780	0.0050
AG	0.5430	0.0150
AH	0.4820	0.0050
AI	0.5420	0.0190
AJ	0.4800	0.0100
AK	0.5350	0.0200
AL	0.4820	0.0050
AM	0.5270	0.0180
AN	0.4760	0.0090
AO	0.5230	0.0210
AP	0.4820	0.0060
AQ	0.5270	0.0150
AR	0.4750	0.0060



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Chain	Atom inclusion	Q-score
AS	0.5240	0.0160
AT	0.4800	0.0070
AU	0.7080	0.0040
AV	0.7180	0.0100
AW	0.7830	0.0030
AX	0.6200	0.0330
AY	0.8900	0.0330
AZ	0.9130	0.0320
Aa	0.8990	0.0470
Ab	0.8600	0.0170
Ac	0.8530	0.0330
Ad	0.9130	0.0370
Ae	0.8620	0.0510
Af	0.8510	0.0620
Ag	0.8530	0.0500
Ah	0.8050	0.0380
Ai	0.8160	0.0330
Aj	0.7760	0.0310
Ak	0.7970	0.0200
Al	0.8150	0.0210
Am	0.8210	0.0270
An	0.8330	0.0330
Ao	0.8690	0.0180
Ap	0.7690	0.0140
Aq	0.6510	-0.0060
Ar	0.4210	0.0000
As	0.5910	-0.0010
At	0.6010	0.0270
Au	0.5520	0.0100
Av	0.6520	0.0180
Aw	0.8920	0.0530
Ax	0.8930	0.0540
Ay	0.8930	0.0530
Az	0.8920	0.0530
B	0.6340	0.0490
C	0.6370	0.0480
D	0.6400	0.0440
E	0.6270	0.0380
F	0.6370	0.0390
G	0.6390	0.0510
H	0.6260	0.0470
I	0.6160	0.0440

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Chain	Atom inclusion	Q-score
J	0.6390	0.0470
K	0.6260	0.0500
L	0.6460	0.0480
M	0.6370	0.0430
N	0.6250	0.0410
O	0.6220	0.0400
P	0.6310	0.0490
Q	0.6220	0.0410
R	0.6280	0.0460
S	0.6060	0.0420
T	0.6290	0.0440
U	0.6450	0.0510
V	0.6380	0.0440
W	0.6240	0.0420
X	0.6280	0.0420
Y	0.6320	0.0520
Z	0.6280	0.0420
a	0.6250	0.0430
b	0.6310	0.0430
c	0.6290	0.0370
d	0.6450	0.0510
e	0.6370	0.0480
f	0.6310	0.0430
g	0.6400	0.0370
h	0.6360	0.0530
i	0.6290	0.0440
j	0.6260	0.0420
k	0.6290	0.0400
l	0.6330	0.0350
m	0.6450	0.0520
n	0.6420	0.0490
o	0.6210	0.0390
p	0.7710	0.0560
q	0.7700	0.0540
r	0.7450	0.0460
s	0.7740	0.0520
t	0.7940	0.0490
u	0.7760	0.0540
v	0.7790	0.0530
w	0.7430	0.0470
x	0.7660	0.0430
y	0.7850	0.0510

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Chain	Atom inclusion	Q-score
z	0.7720	0.0510