Full wwPDB EM Validation Report (i)

Oct 5, 2026 – 03:31 PM EDT

PDB ID	:	12DU / pdb_000012du
EMDB ID	:	EMD-76347
Title	:	In situ cryo-EM structure of the flagellar export gate in complex with the FliF RBM12 ring in Borrelia burgdorferi
Authors	:	Yue, J.; Liu, J.
Deposited on	:	2026-03-30
Resolution	:	3.87 Å(reported)

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

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

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

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

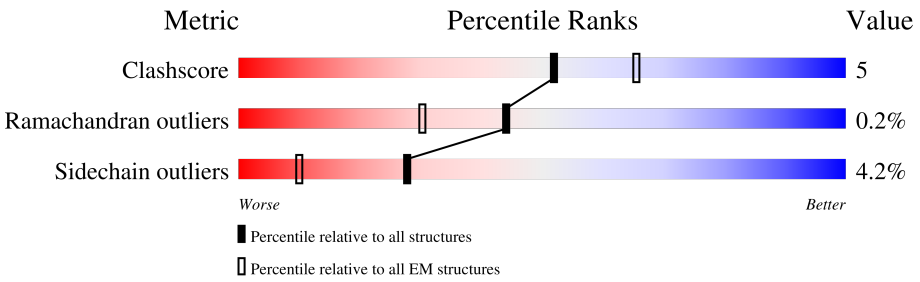
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

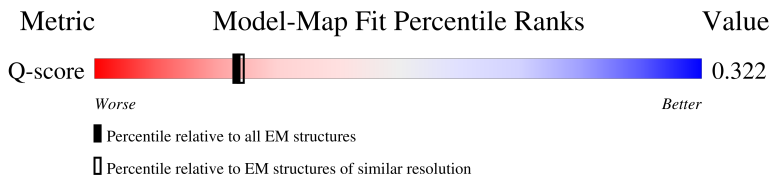
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.87 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	8831 (3.37 - 4.37)

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	c	569	14% 25% 6% 69%
1	d	569	16% 26% 5% • 69%
1	e	569	15% 26% 5% 69%
1	f	569	13% 25% 5% • 69%

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Mol	Chain	Length	Quality of chain
1	g	569	14% 27% 69%
1	h	569	15% 26% 5% 69%
1	i	569	14% 28% 69%
1	j	569	14% 25% 6% 69%
1	k	569	14% 25% 6% 69%
1	l	569	14% 27% 69%
1	m	569	16% 27% 69%
1	n	569	12% 27% 5% 69%
1	o	569	14% 27% 5% 69%
1	p	569	14% 25% 5% 69%
1	q	569	17% 25% 6% 69%
1	r	569	15% 26% 5% 69%
1	s	569	14% 26% 5% 69%
1	t	569	15% 24% 7% 69%
1	u	569	16% 23% 7% 70%
1	v	569	18% 25% 5% 70%
1	w	569	15% 27% 5% 69%
1	x	569	17% 24% 7% 69%
1	y	569	16% 26% 5% 69%
2	A	372	25% 57% 8% 35%
3	F	254	7% 63% 20% 18%
3	G	254	66% 15% 18%
3	H	254	5% 67% 15% 18%
3	I	254	10% 66% 15% 18%
3	J	254	7% 63% 19% 18%

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Mol	Chain	Length	Quality of chain
4	K	269	12% 72% 23%
5	L	111	54% 9% 37%
5	M	111	54% 8% 37%
5	N	111	55% 7% 37%
5	O	111	54% 7% 37%
5	P	111	50% 12% 37%
5	Q	111	5% 28% 6% 64%
6	R	135	7% 75% 8% 17%
6	S	135	5% 76% 7% 17%
6	T	135	6% 73% 10% 17%
6	U	135	7% 73% 9% 17%
6	V	135	7% 73% 9% 17%
7	W	152	12% 77% 12% 11%
7	X	152	9% 93% 7%
7	Y	152	11% 80% 9% 11%
7	Z	152	9% 92% 8%
7	a	152	11% 88% 12%
7	b	152	9% 95%
8	1	87	10% 69% 25% 6%
8	2	87	9% 79% 20%
8	3	87	8% 76% 24%
8	z	87	18% 72% 25%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 61305 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
			Total	C	N	O	S		
1	c	179	1397	891	240	264	2	0	0
1	d	179	1383	880	238	263	2	0	0
1	e	179	1391	885	240	264	2	0	0
1	f	178	1390	885	240	263	2	0	0
1	g	177	1381	879	238	262	2	0	0
1	h	178	1374	875	238	259	2	0	0
1	i	179	1392	885	241	264	2	0	0
1	j	179	1387	884	240	261	2	0	0
1	k	179	1388	882	240	264	2	0	0
1	l	179	1385	884	238	261	2	0	0
1	m	179	1397	892	241	262	2	0	0
1	n	179	1375	876	238	259	2	0	0
1	o	179	1387	886	236	263	2	0	0
1	p	179	1385	882	237	264	2	0	0
1	q	179	1391	886	240	263	2	0	0
1	r	179	1401	894	241	264	2	0	0
1	s	179	1401	894	241	264	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	t	179	1391	885	240	264	2	0	0
1	u	173	1347	859	231	255	2	0	0
1	v	173	1349	860	233	254	2	0	0
1	w	179	1383	880	238	263	2	0	0
1	x	179	1372	873	238	259	2	0	0
1	y	179	1393	889	240	262	2	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	209	1665	1118	255	277	15	0	0
3	G	209	1656	1114	252	275	15	0	0
3	H	209	1657	1116	252	274	15	0	0
3	I	209	1666	1119	255	277	15	0	0
3	J	209	1676	1128	256	277	15	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	70	542	342	94	104	2	0	0
5	M	70	542	342	94	104	2	0	0
5	N	70	542	342	94	104	2	0	0
5	O	70	530	333	91	104	2	0	0
5	P	70	542	342	94	104	2	0	0
5	Q	40	308	193	55	58	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	R	112	920	577	161	177	5	0	0
6	S	112	920	577	161	177	5	0	0
6	T	112	920	577	161	177	5	0	0
6	U	112	920	577	161	177	5	0	0
6	V	112	920	577	161	177	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	W	136	1030	639	187	200	4	0	0
7	X	152	1153	724	201	224	4	0	0
7	Y	136	1034	641	188	201	4	0	0
7	Z	152	1169	732	208	225	4	0	0
7	a	152	1169	732	208	225	4	0	0
7	b	152	1169	732	208	225	4	0	0

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

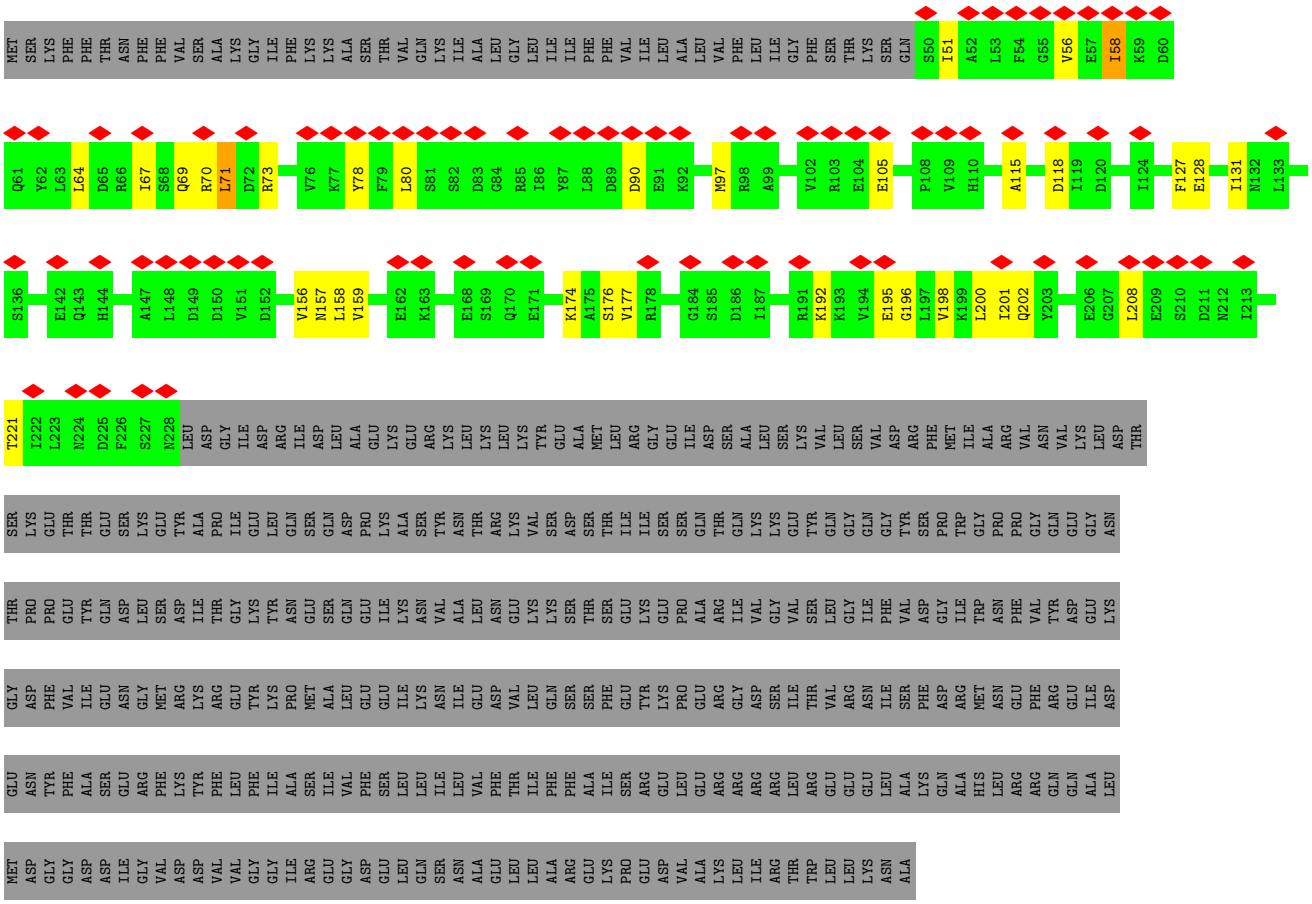
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	z	87	678	463	99	112	4	0	0
			Total	C	N	O	S		
8	1	87	682	465	100	113	4	0	0
			Total	C	N	O	S		
8	2	87	692	471	104	113	4	0	0
			Total	C	N	O	S		
8	3	87	692	471	104	113	4	0	0

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.

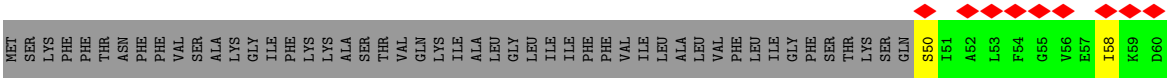
- Molecule 1: Flagellar M-ring protein

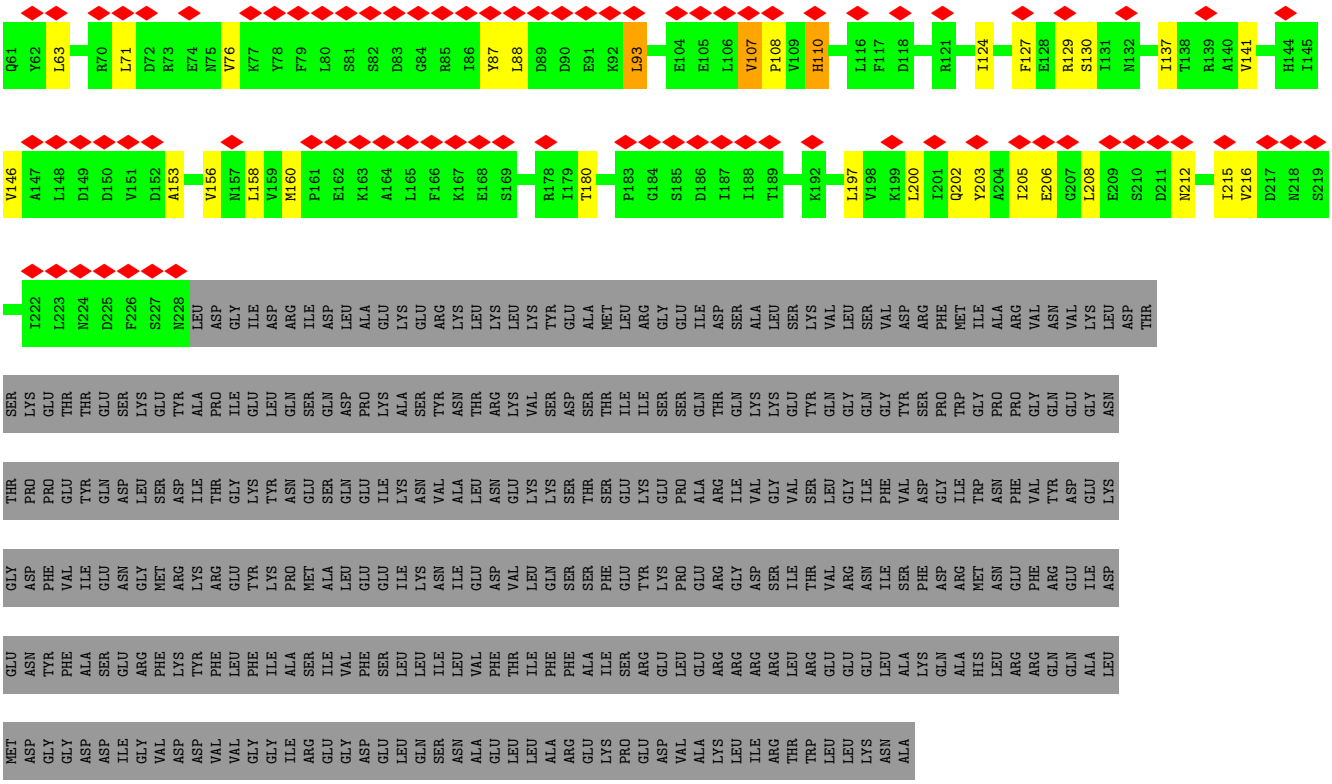
Chain c:



- Molecule 1: Flagellar M-ring protein

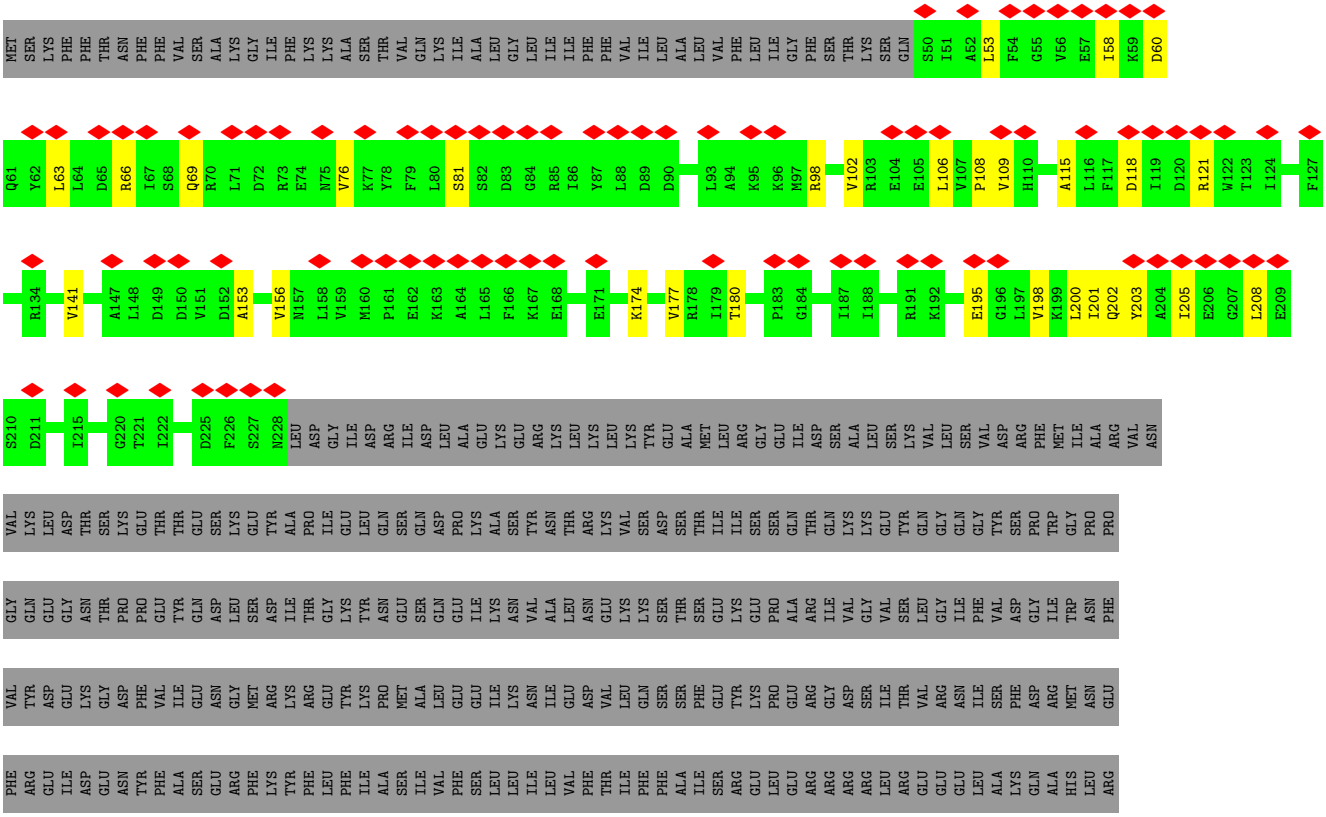
Chain d:





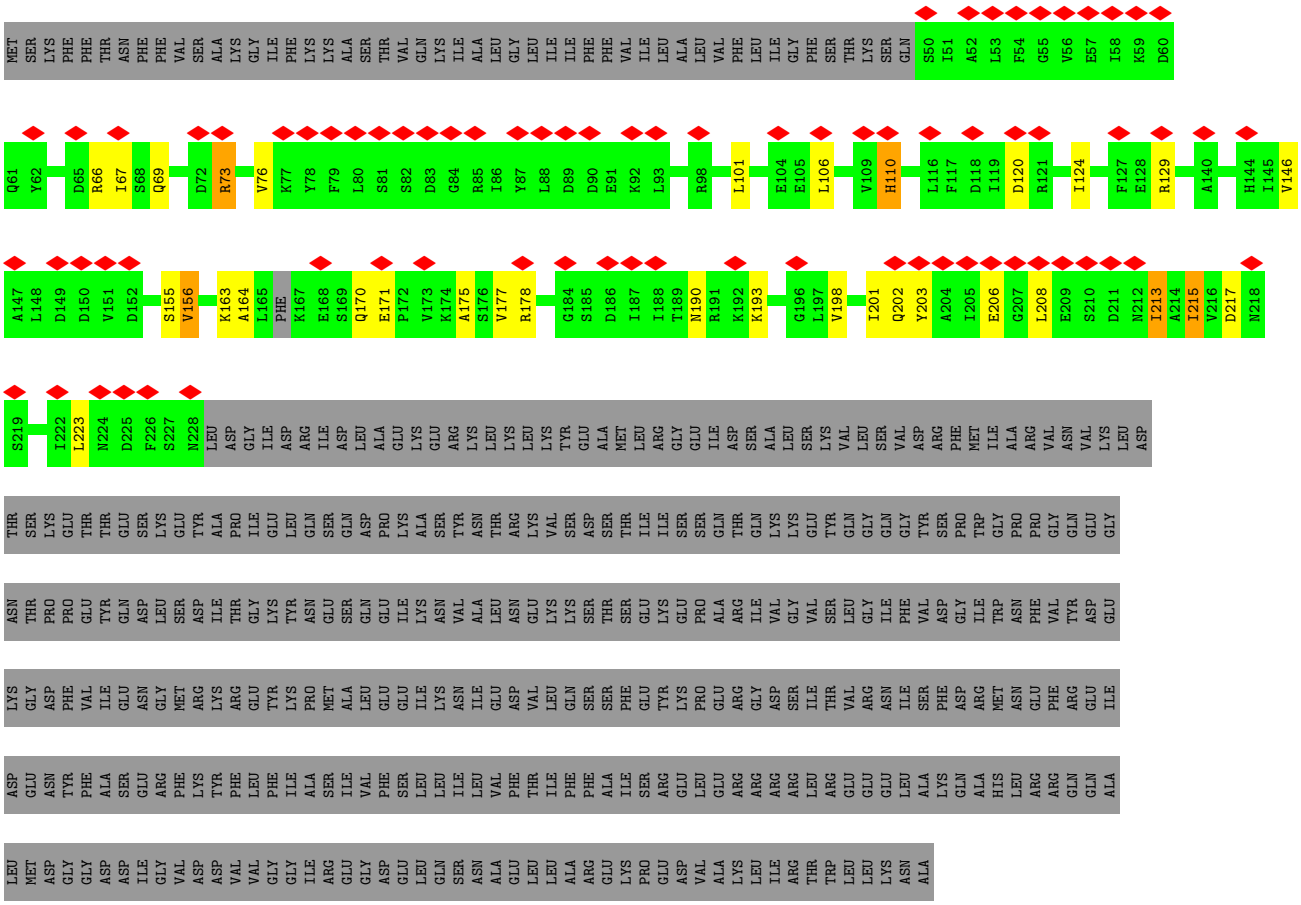
- Molecule 1: Flagellar M-ring protein

Chain e:



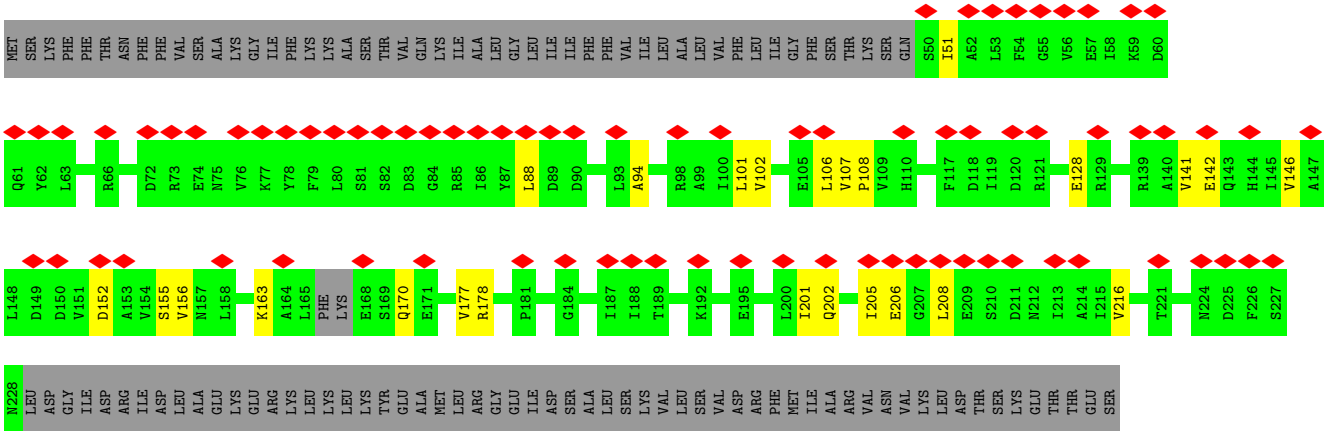
- Molecule 1: Flagellar M-ring protein

Chain f:



- Molecule 1: Flagellar M-ring protein

Chain g:



LYS GLU TYR ALA PRO ILE GLU LEU GLN SER GLN ASP PRO LYS ALA SER TYR ASN THR ARG LYS VAL SER ASP SER THR ILE ILE SER SER GLN THR GLN LYS LYS GLU TYR GLN GLY GLN GLY TYR SER PRO TRP GLY PRO PRO GLY GLN GLU GLY ASN THR PRO PRO GLU TYR GLN ASP

LEU SER ASP ILE THR GLY LYS TYR ASN GLU SER GLN GLU ILE LYS ASN VAL ALA LEU ASN GLU LYS LYS SER THR SER GLU LYS GLU PRO ALA ARG ILE VAL GLY VAL SER LEU GLY ILE PHE VAL ASP GLY ILE TRP ASN PHE VAL TYR ASP GLU LYS GLY ASP PHE VAL ILE GLU ASN

GLY MET ARG LYS ARG GLU TYR LYS PRO MET ALA LEU GLU GLU ILE LYS ASN ILE GLU ASP VAL LEU GLU GLN SER SER SER PHE GLU TYR LYS PRO GLU ARG GLY ASP SER ILE THR VAL ARG ASN ILE SER PHE ASP ARG MET ASN GLU PHE ARG GLU ILE ASP GLU ASN TYR PHE ALA SER GLU

ARG PHE LYS TYR PHE LEU PHE ILE ALA SER ILE VAL PHE SER LEU LEU ILE LEU VAL PHE THR ILE PHE PHE ALA ILE SER ARG GLU LEU GLU ARG ARG ARG LEU ARG GLU GLU LEU ALA LYS GLN ALA HIS LEU ARG ARG GLN GLN ALA LEU MET ASP GLY GLY ASP ASP ILE

GLY VAL ASP ASP VAL VAL GLY GLY ILE ARG GLU GLY ASP GLU GLU LEU GLN SER ASN ALA GLU LEU LEU ALA ARG GLU LYS PRO GLU ASP VAL ALA LYS LEU ILE ARG THR TRP LEU LEU LYS ASN ALA

- Molecule 1: Flagellar M-ring protein

Chain h: 15% 26% 5% • 69%

MET SER LYS PHE PHE THR ASN PHE PHE VAL SER ALA LYS GLY ILE PHE LYS LYS ALA SER THR VAL GLN LYS ILE ALA LEU GLY LEU ILE ILE PHE PHE VAL ILE LEU ALA LEU VAL PHE LEU ILE GLY PHE SER THR LYS SER GLN S50 I51 A52 L53 F54 G55 V56 E57 I58 K59 D60

Q61 Y62 L63 L64 D65 R66 Q69 D72 R73 E74 N75 V76 K77 Y78 F79 L80 S81 S82 D83 G84 R85 I86 Y87 L88 D89 D90 E91 K92 L93 K96 I100 L101 V102 R103 E104 E105 L106 V107 P108 V109 H110 M111 D112 D118 I119 D120 R121 I124 T125 D126 F127 E128 R129

R134 R139 A140 V141 E142 D149 D150 V151 D152 A153 V154 S155 L158 V159 A164 L165 PHE K167 E168 S169 Q170 K174 A175 S176 V177 R178 G184 I188 T189 K192 K193 G196 L197 V198 K199 L200 I201 Q202 Y203 A204 I205 E206 G207 L208 E209 S210 D211 N212 I213 A214 I215

I222 L223 N224 D225 F226 S227 N228 LEU ASP GLY ILE ASP ARG ILE ASP LEU ALA GLU LYS GLU ARG LYS LEU LYS LEU LYS TYR GLU ALA MET LEU ARG GLY GLU ILE ASP SER ALA LEU SER LYS VAL LEU SER VAL ASP ARG PHE MET ILE ILE ALA ARG VAL ASN VAL LYS LEU ASP THR

SER LYS GLU THR THR GLU SER LYS GLU TYR ALA PRO ILE GLU LEU GLN SER GLN ASP PRO LYS ALA SER TYR ASN THR ARG LYS VAL SER ASP SER THR ILE ILE SER SER GLN THR GLN LYS LYS GLU TYR GLN GLY GLN GLY TYR SER PRO TRP GLY PRO PRO GLY GLN GLU GLU GLY ASN

THR PRO PRO GLU TYR GLN ASP LEU SER ASP ILE THR GLY LYS TYR ASN GLU SER GLN GLU ILE LYS ASN VAL ALA LEU ASN GLU LYS LYS SER THR SER GLU LYS GLU PRO ALA ARG ILE VAL GLY VAL SER LEU GLY ILE PHE VAL ASP GLY ILE TRP ASN PHE VAL TYR ASP GLU LYS

GLY ASP PHE VAL ILE GLU ASN GLY MET ARG LYS ARG GLU TYR LYS PRO MET ALA LEU GLU GLU ILE LYS ASN ILE GLU ASP VAL LEU GLN SER SER PHE GLU TYR LYS PRO GLU ARG GLY ASP SER ILE THR VAL ARG ASN ILE SER PHE ASP ARG MET ASN GLU PHE ARG GLU ILE ASP

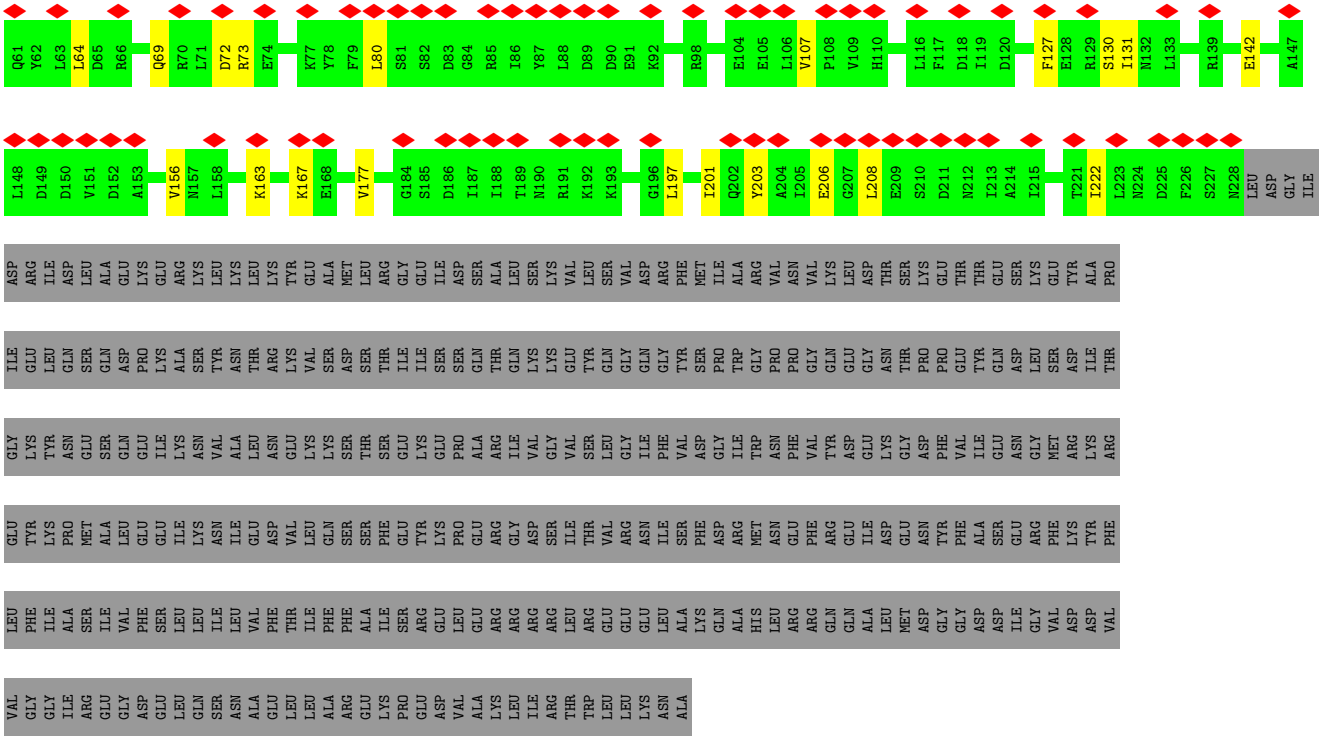
GLU ASN TYR PHE ALA SER GLU ARG PHE LYS TYR PHE LEU PHE ILE ALA SER ILE VAL PHE SER LEU LEU ILE LEU VAL PHE THR ILE PHE PHE ALA ILE SER ARG GLU LEU GLU ARG ARG ARG LEU ARG GLU GLU LEU ALA LYS GLN ALA HIS LEU ARG ARG GLN GLN ALA LEU

MET ASP GLY GLY ASP ASP ILE GLY VAL ASP ASP VAL VAL GLY GLY ILE ARG GLU GLY ASP GLU LEU GLN SER ASN ALA GLU LEU LEU ALA ARG GLU LYS PRO GLU ASP VAL ALA LYS LEU ILE ARG THR TRP LEU LEU LYS ASN ALA

- Molecule 1: Flagellar M-ring protein

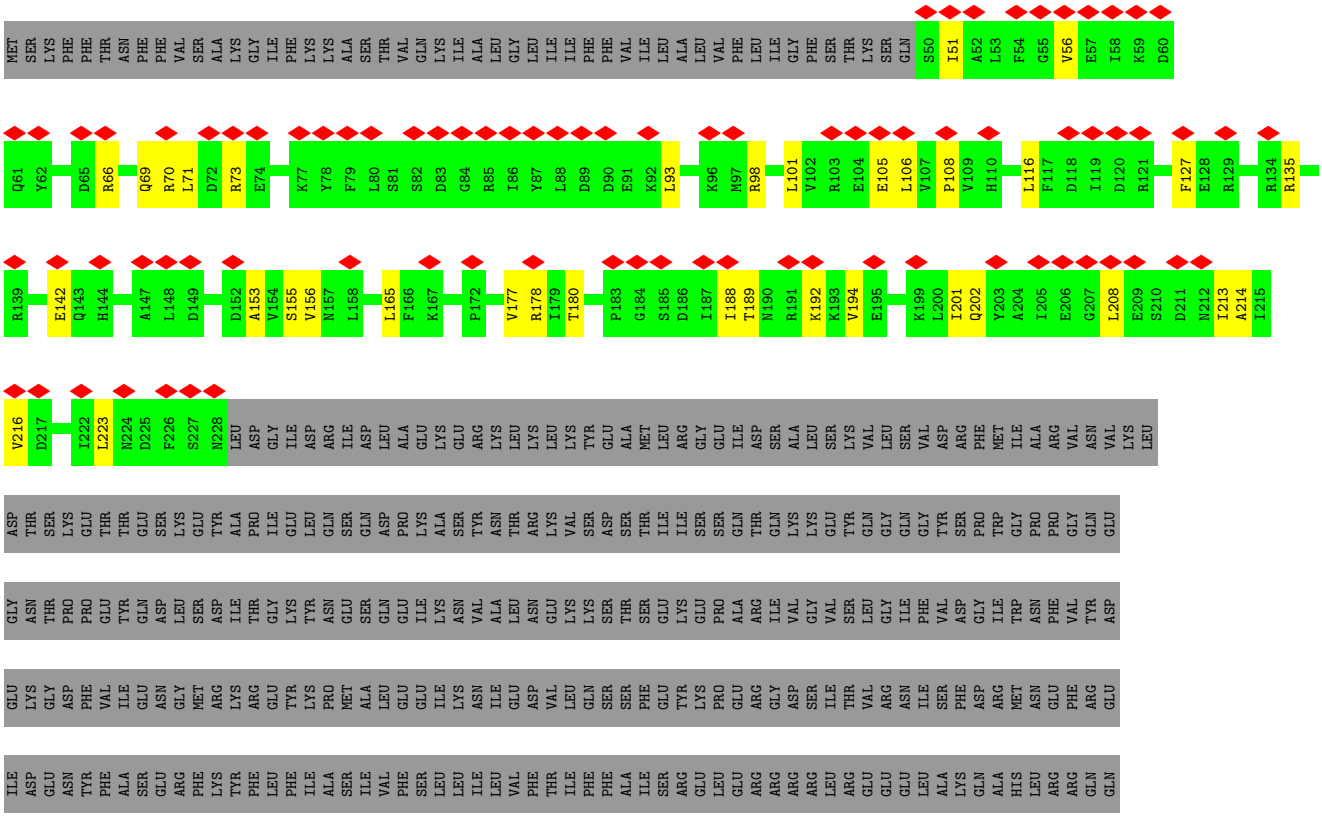
Chain i: 14% 28% • 69%

MET SER LYS PHE PHE THR ASN PHE PHE VAL SER ALA LYS GLY ILE PHE LYS LYS ALA SER THR VAL GLN LYS ILE ALA LEU GLY LEU ILE ILE PHE PHE VAL ILE LEU ALA LEU VAL PHE LEU ILE GLY PHE SER THR LYS SER GLN S50 I51 A52 L53 F54 G55 V56 E57 I58 K59 D60



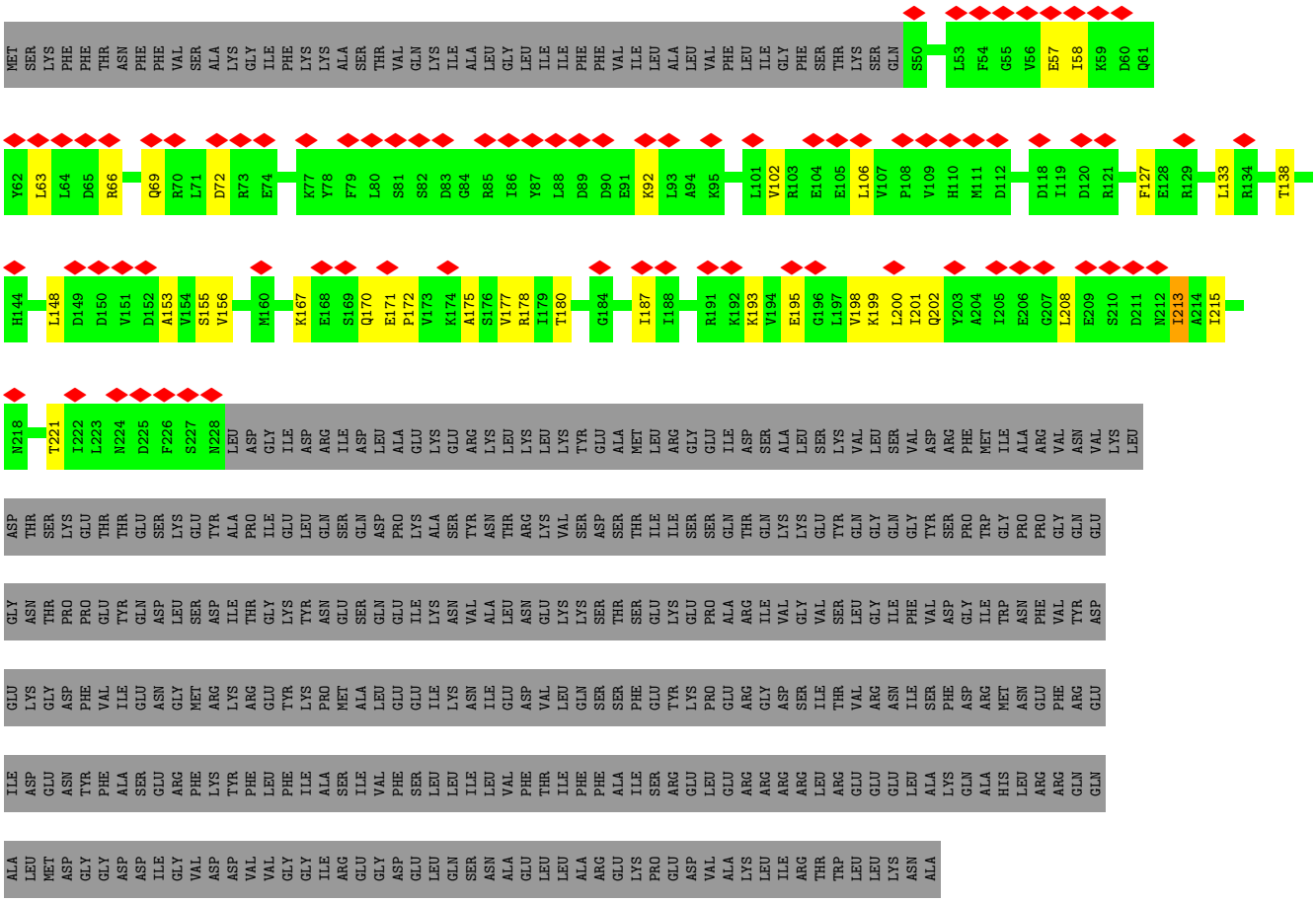
- Molecule 1: Flagellar M-ring protein

Chain j:



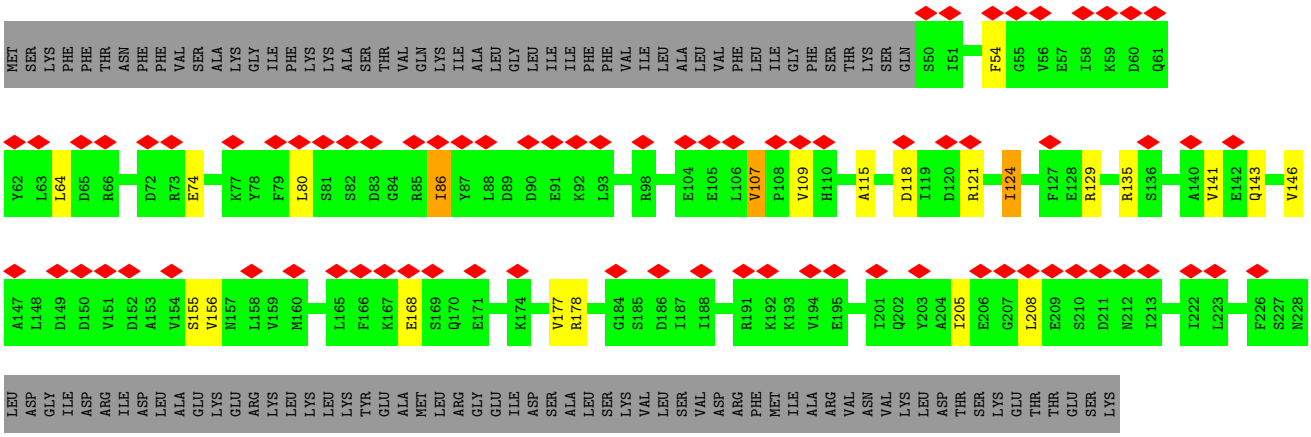
- Molecule 1: Flagellar M-ring protein

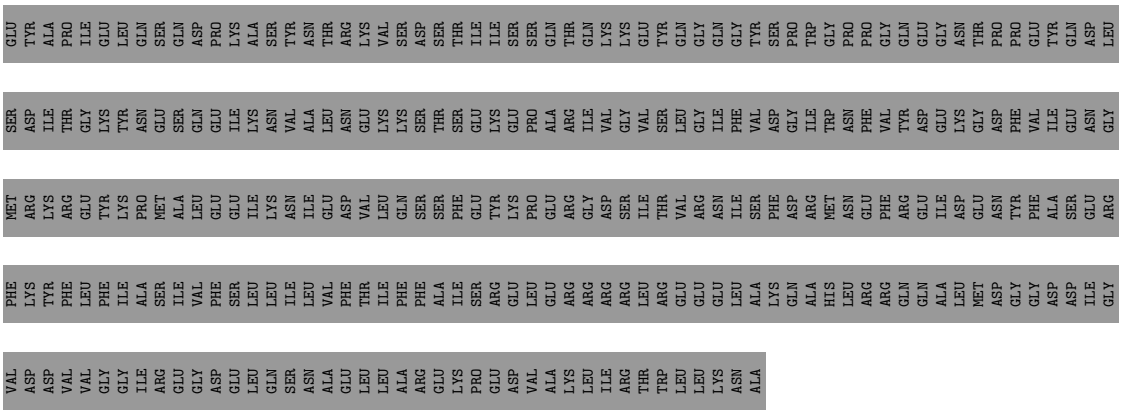
Chain k:



- Molecule 1: Flagellar M-ring protein

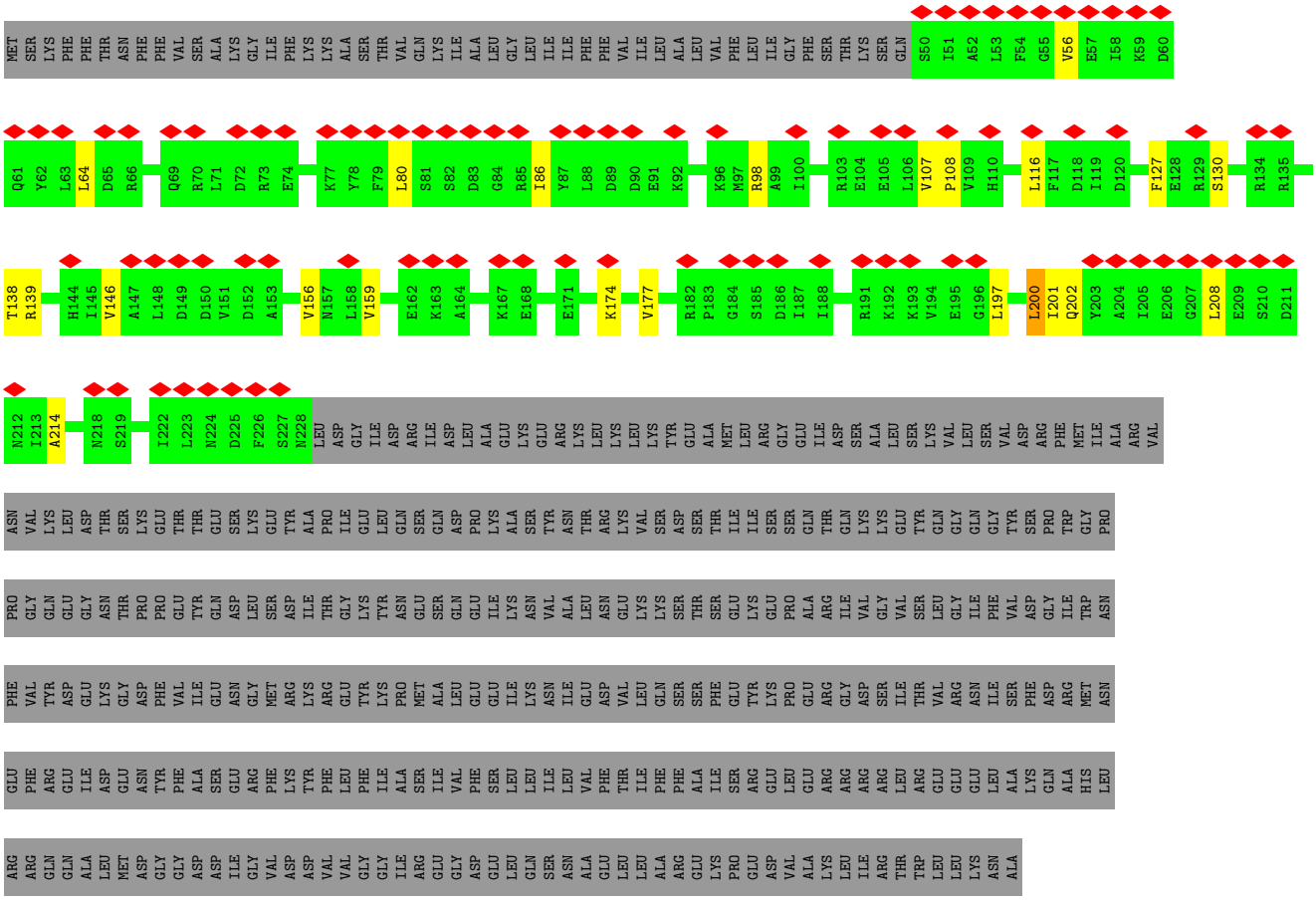
Chain l:





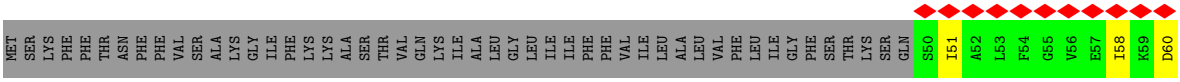
- Molecule 1: Flagellar M-ring protein

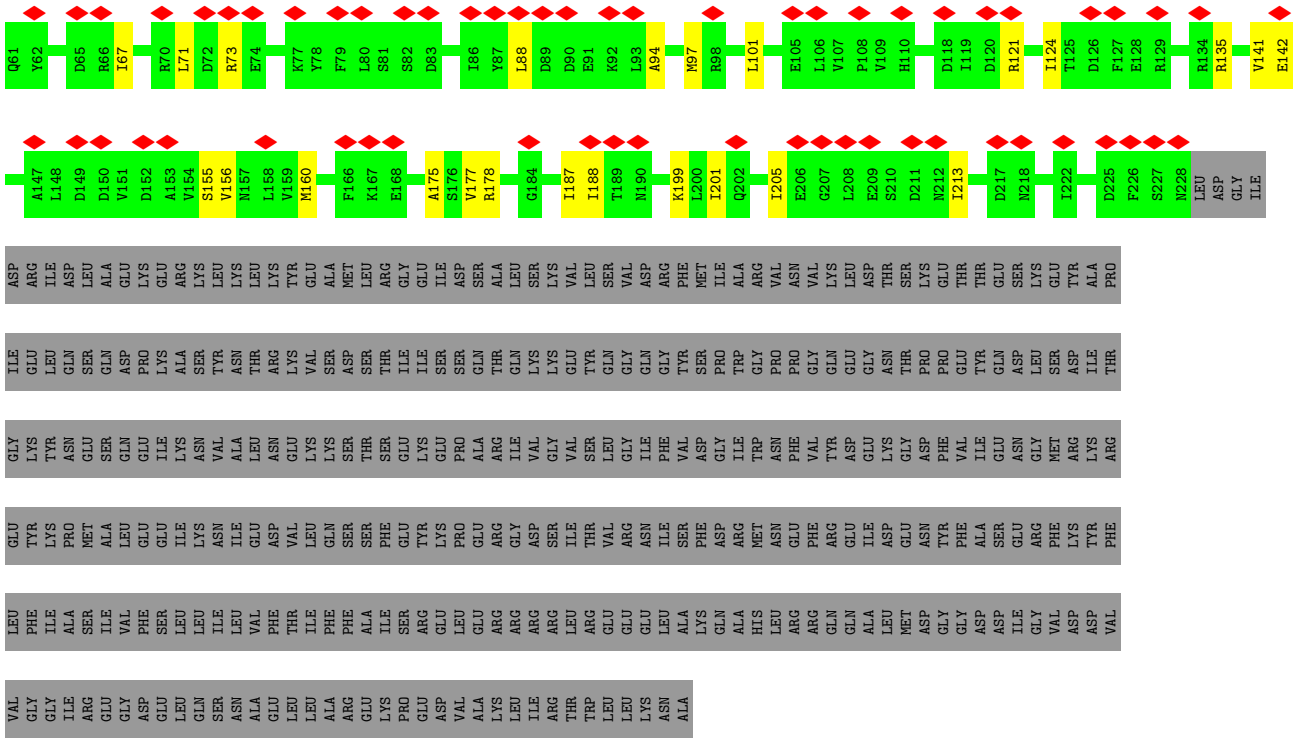
Chain m:



- Molecule 1: Flagellar M-ring protein

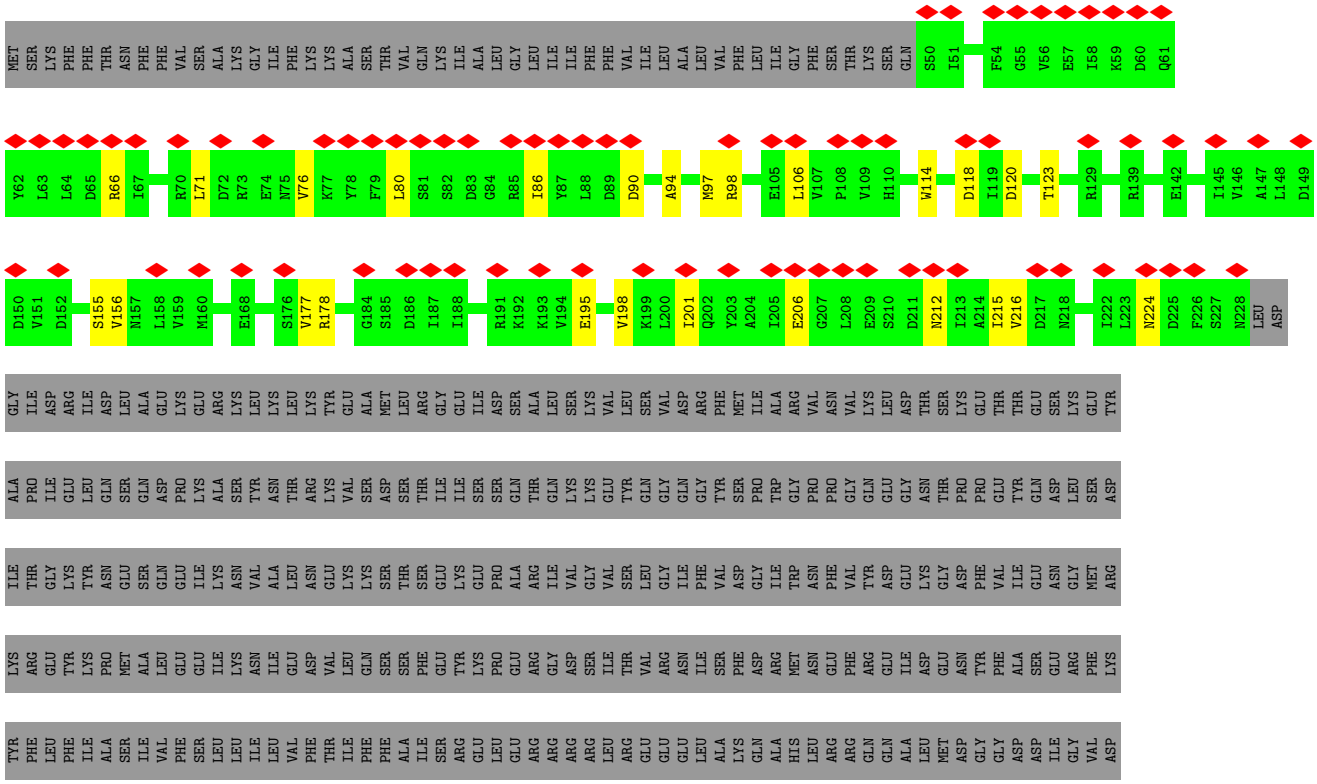
Chain n:

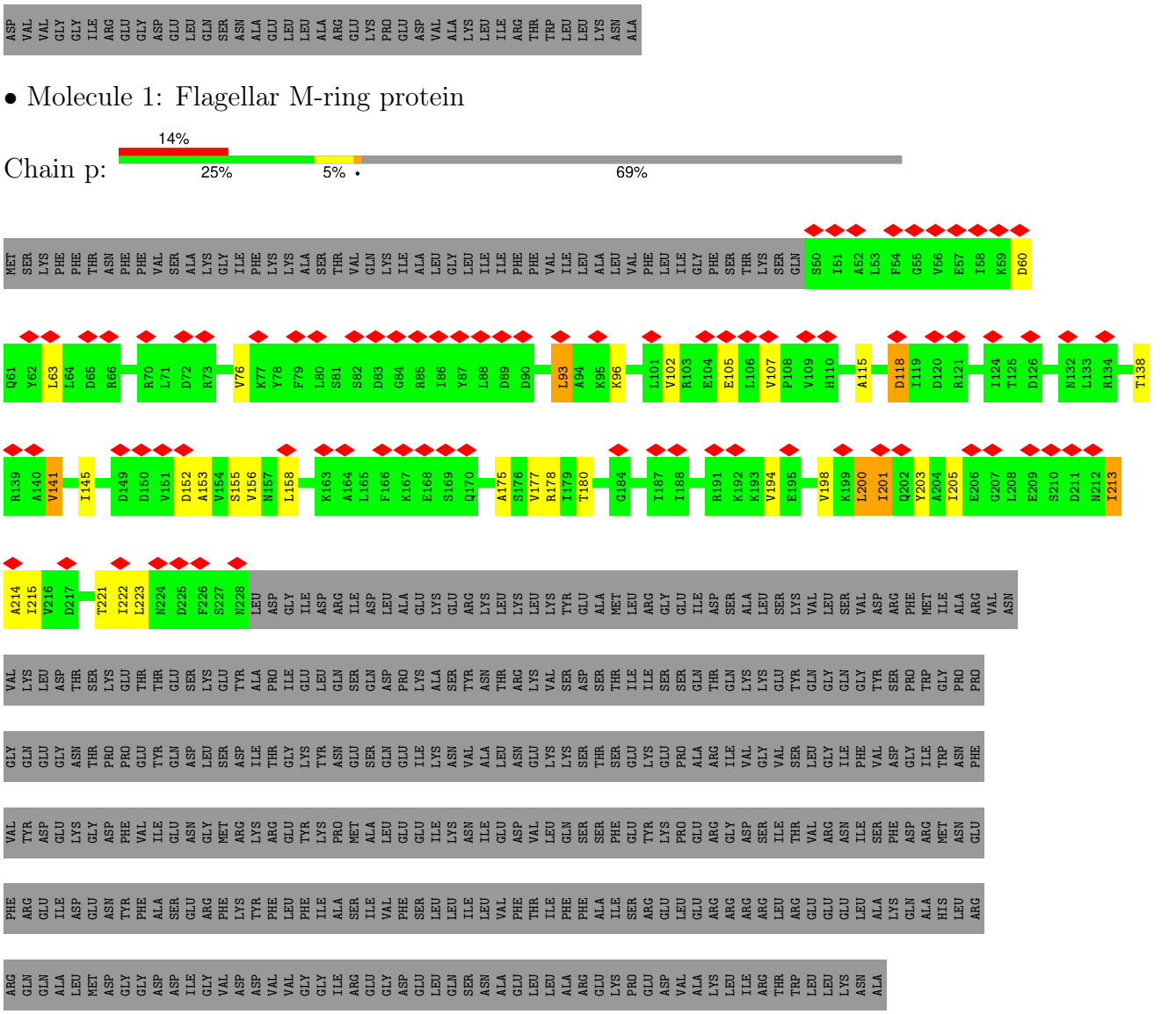


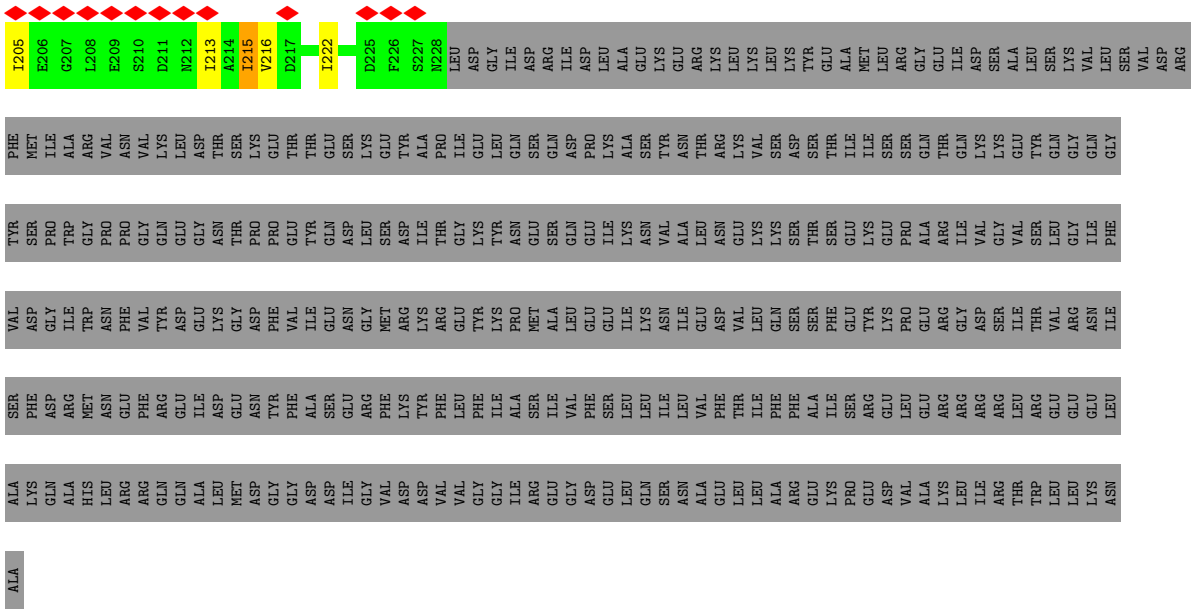


- Molecule 1: Flagellar M-ring protein

Chain o:

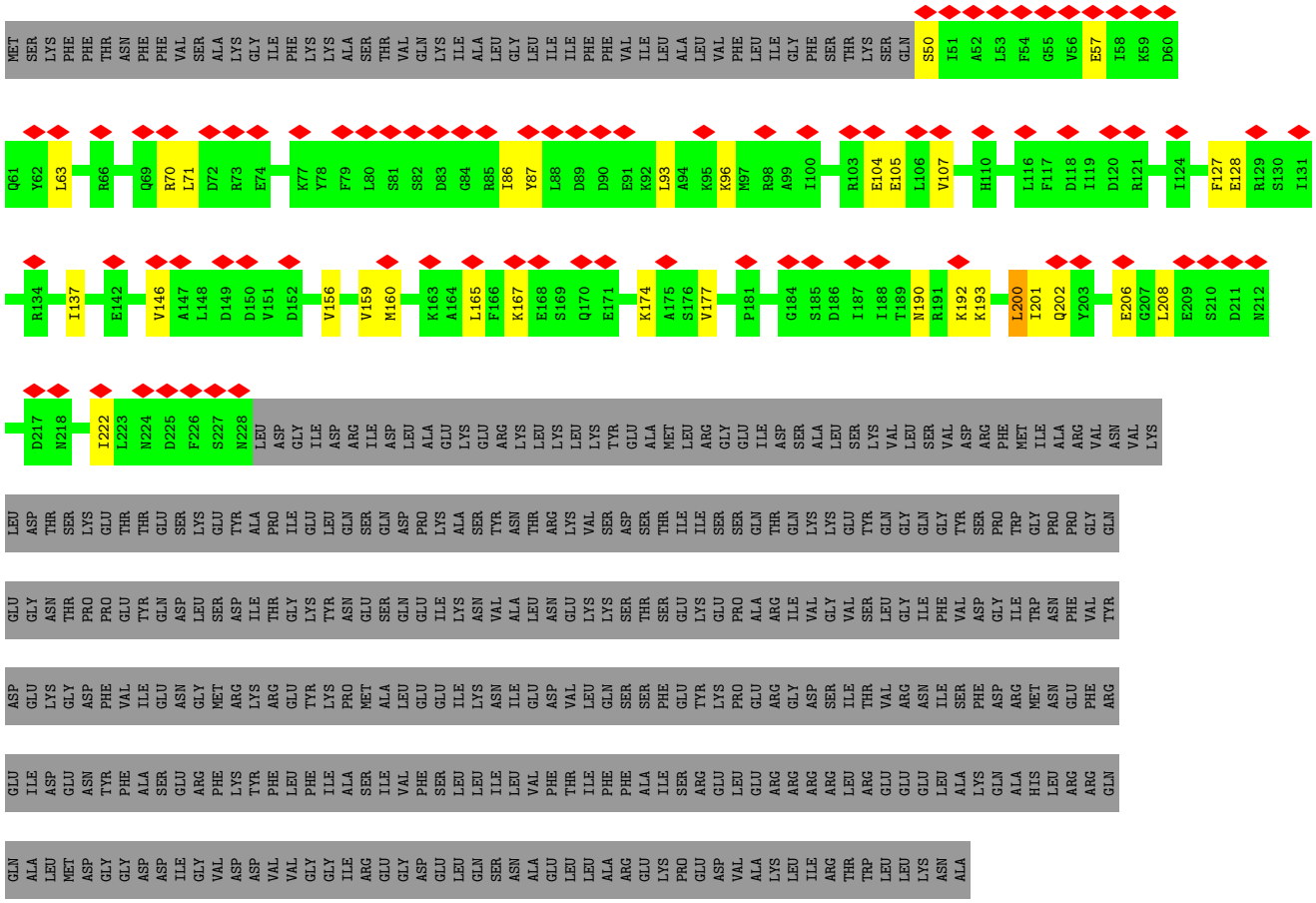



ASP VAL VAL GLY GLY ILE ARG GLU GLY ASP GLU LEU GLN SER ASN ALA GLU LEU LEU ALA ARG GLU LYS PRO GLU ASP VAL ALA LYS LEU ILE ARG THR TRP LEU LEU LYS ASN ALA
• Molecule 1: Flagellar M-ring protein
Chain p:
14%
25%
5%
69%
MET SER LYS PHE PHE THR ASN PHE PHE VAL SER ALA LYS GLY ILE PHE LYS LYS LYS ALA SER THR VAL GLN LYS ILE ALA LEU GLY LEU ILE ILE PHE PHE VAL ILE LEU ALA LEU VAL PHE LEU ILE GLY PHE SER THR LYS SER GLN S50 I51 A52 L53 F54 G55 V56 E57 I58 K59 D60
Q61 Y62 L63 L64 D65 R66 R70 L71 D72 R73 V76 K77 Y78 F79 L80 S81 S82 D83 G84 R85 I86 Y87 L88 D89 D90 L93 A94 K95 K96 L101 V102 R103 E104 E105 L106 V107 P108 V109 H110 A115 D118 I119 D120 R121 I124 T125 D126 N132 L133 R134 T138
R139 A140 V141 I145 D149 D150 V151 D152 A153 V154 S155 V156 N157 L158 K163 A164 L165 F166 K167 E168 S169 Q170 A175 S176 V177 R178 I179 T180 G184 I187 I188 R191 K192 K193 V194 E195 V198 K199 L200 I201 Q202 Y203 A204 I205 E206 G207 L208 E209 S210 D211 N212 I213
A214 I215 V216 D217 T221 I222 L223 N224 D225 F226 S227 N228 LEU ASP GLY ILE ASP ARG ILE ASP LEU ALA GLU LYS GLU ARG LYS LEU LYS LEU LYS TYR GLU ALA MET LEU ARG GLY GLU ILE ASP SER ALA LEU SER LYS VAL LEU SER VAL ASP ARG PHE MET ILE ALA ARG VAL ASN
VAL LYS LEU ASP THR SER LYS GLU THR THR GLU SER LYS GLU TYR ALA PRO ILE GLU LEU GLN SER GLN ASP PRO LYS ALA SER TYR ASN THR ARG LYS VAL SER ASP SER THR ILE ILE SER SER GLN THR GLN LYS LYS GLU TYR GLN GLY GLN GLY TYR SER PRO TRP GLY PRO PRO
GLY GLN GLU GLY ASN THR PRO PRO GLU TYR GLN ASP LEU SER ASP ILE THR GLY LYS TYR ASN GLU SER GLN GLU GLU ILE LYS ASN VAL ALA LEU ASN GLU LYS LYS SER THR SER GLU LYS GLU PRO ALA ARG ILE VAL GLY VAL SER LEU GLY ILE PHE VAL ASP GLY ILE TRP ASN PHE
VAL TYR ASP GLU LYS GLY ASP PHE VAL ILE GLU ASN GLY MET ARG LYS ARG GLU TYR LYS PRO MET ALA LEU GLU GLU ILE LYS ASN ILE GLU ASP VAL LEU GLN SER SER PHE GLU TYR LYS PRO GLU ARG GLY ASP SER ILE THR VAL ARG ASN ILE SER PHE ASP ARG MET ASN GLU
PHE ARG GLU ILE ASP GLU ASN TYR PHE ALA SER GLU ARG PHE LYS TYR PHE LEU PHE ILE ALA SER ILE VAL PHE SER LEU LEU ILE LEU VAL PHE THR ILE PHE PHE ALA ILE SER ARG GLU LEU GLU ARG ARG ARG ARG LEU ARG GLU GLU GLU LEU ALA LYS GLN ALA HIS LEU ARG
ARG GLN GLN ALA LEU MET ASP GLY GLY ASP ASP ILE GLY VAL ASP ASP VAL VAL GLY GLY ILE ARG GLU GLY ASP GLU LEU GLN SER ASN ALA GLU LEU ALA ARG GLU LYS PRO GLU ASP VAL ALA LYS LEU ILE ARG THR TRP LEU LEU LYS ASN ALA
• Molecule 1: Flagellar M-ring protein
Chain q:
17%
25%
6%
69%
MET SER LYS PHE PHE THR ASN PHE PHE VAL SER ALA LYS GLY ILE PHE LYS LYS LYS ALA SER THR VAL GLN LYS ILE ALA LEU GLY LEU ILE ILE PHE PHE VAL ILE LEU ALA LEU VAL PHE LEU ILE GLY PHE SER THR LYS SER GLN S50 I51 A52 L53 F54 G55 V56 E57 I58 K59 D60
Q61 Y62 L63 L64 D65 R66 I67 S68 Q69 R70 L71 D72 R73 E74 N75 V76 K77 Y78 F79 L80 S81 S82 D83 G84 R85 I86 Y87 L88 D89 D90 E91 K92 L93 A94 K95 R98 E104 E105 L106 V107 P108 V109 H110 M111 D112 A115 L116 F117 D118 I119 D120 R121 I124 T125 D126
R129 L133 V141 E142 Q143 H144 I145 V146 A147 L148 D149 D150 V151 D152 A153 V156 V159 M160 P161 E162 K163 A164 L165 F166 K167 E168 S169 Q170 E171 P172 V173 K174 A175 S176 V177 R178 G184 S185 D186 I187 I188 T189 N190 R191 E195 G196 L197 V198 K199 L200 I201 Q202 Y203 A204



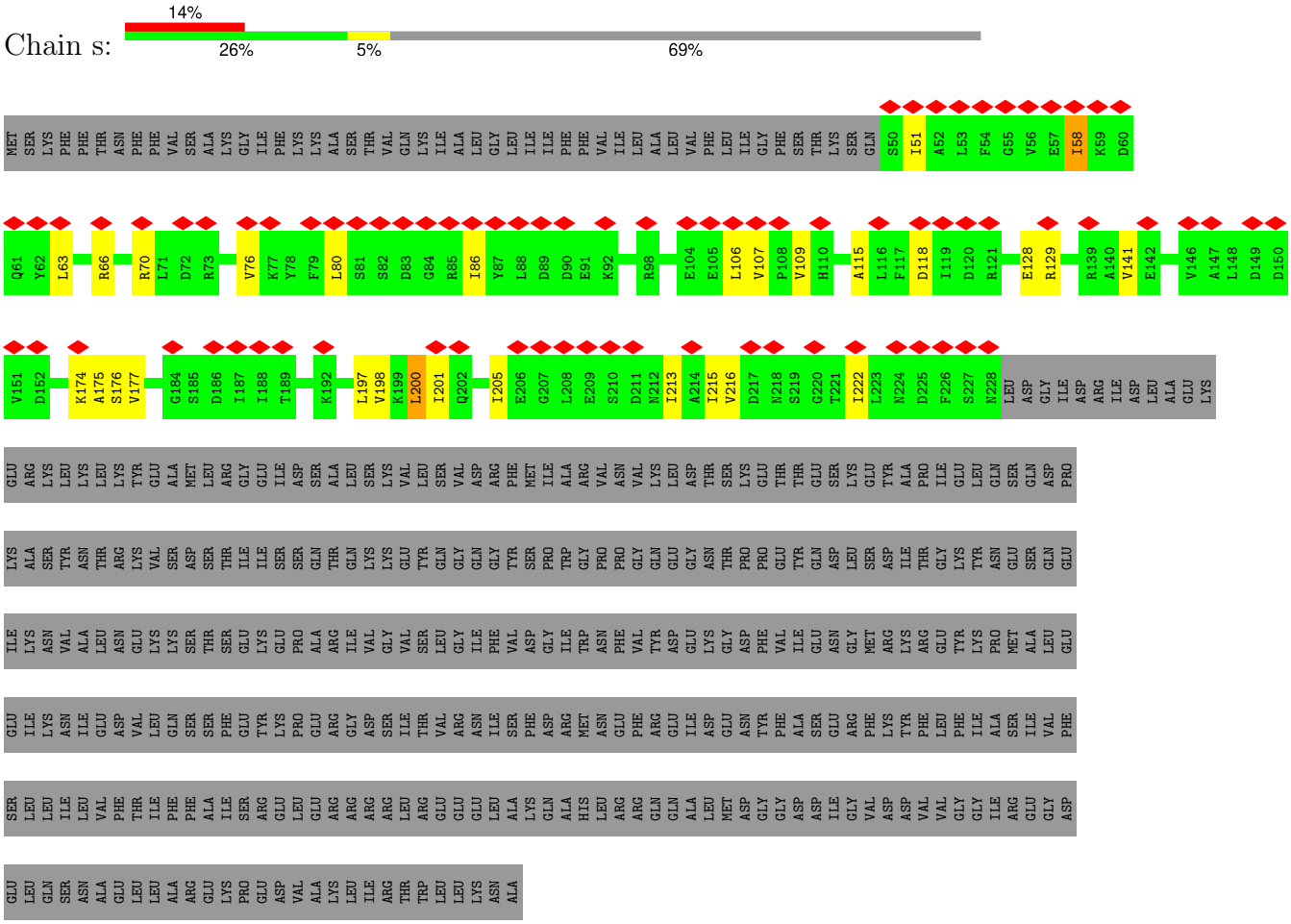
• Molecule 1: Flagellar M-ring protein

Chain r:



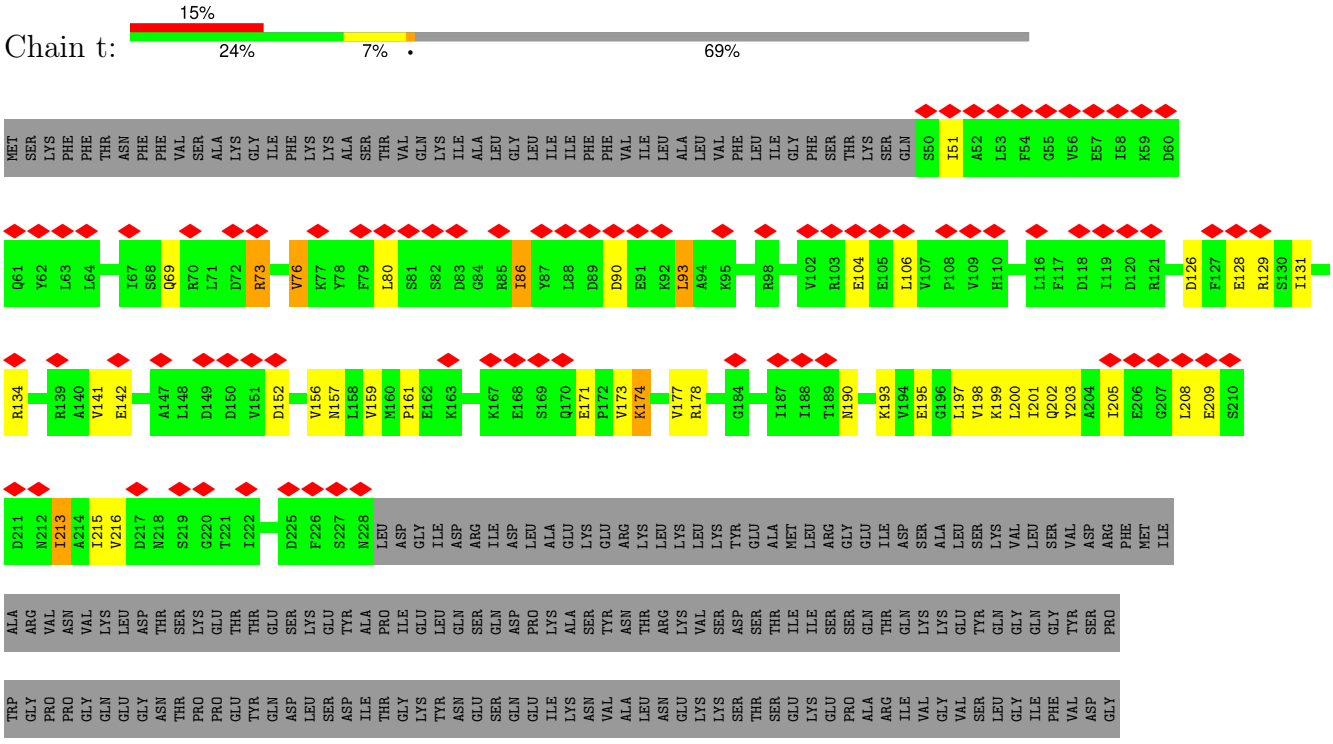
• Molecule 1: Flagellar M-ring protein

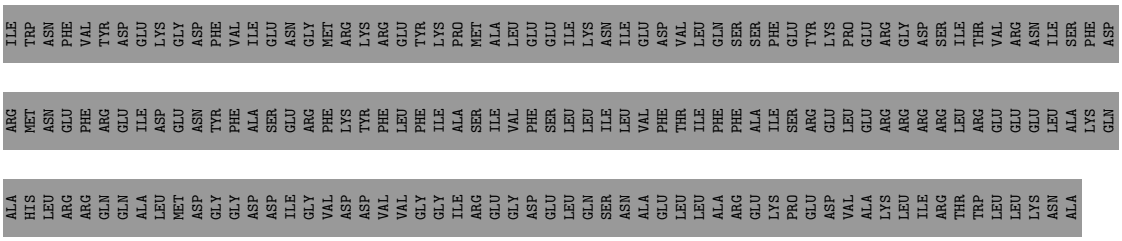
Chain s:



• Molecule 1: Flagellar M-ring protein

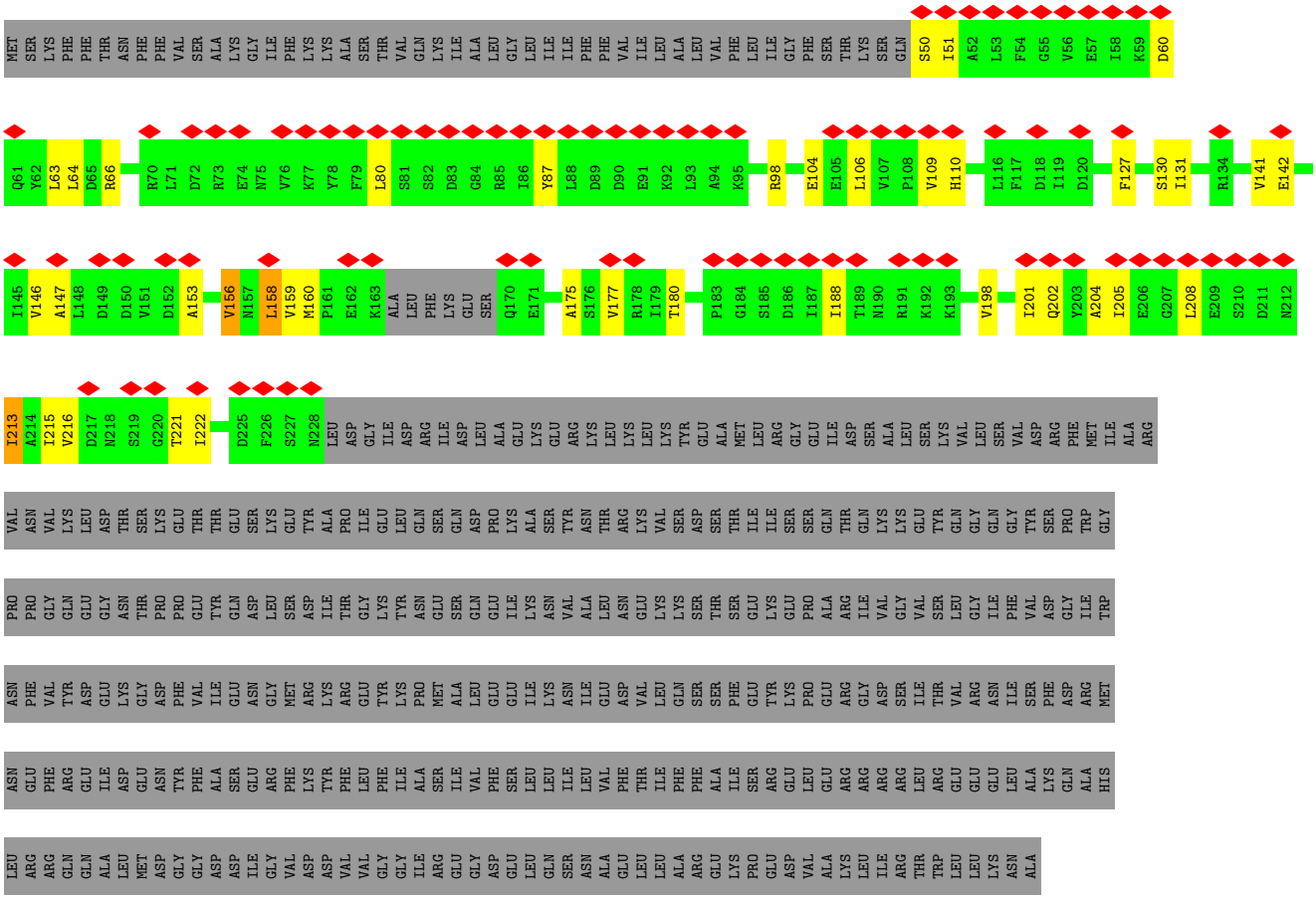
Chain t:





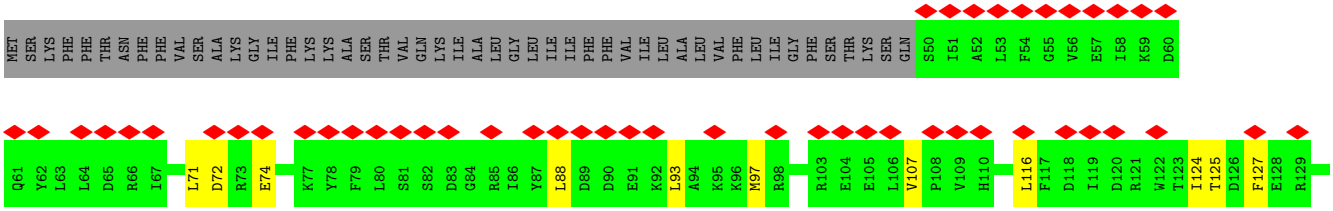
- Molecule 1: Flagellar M-ring protein

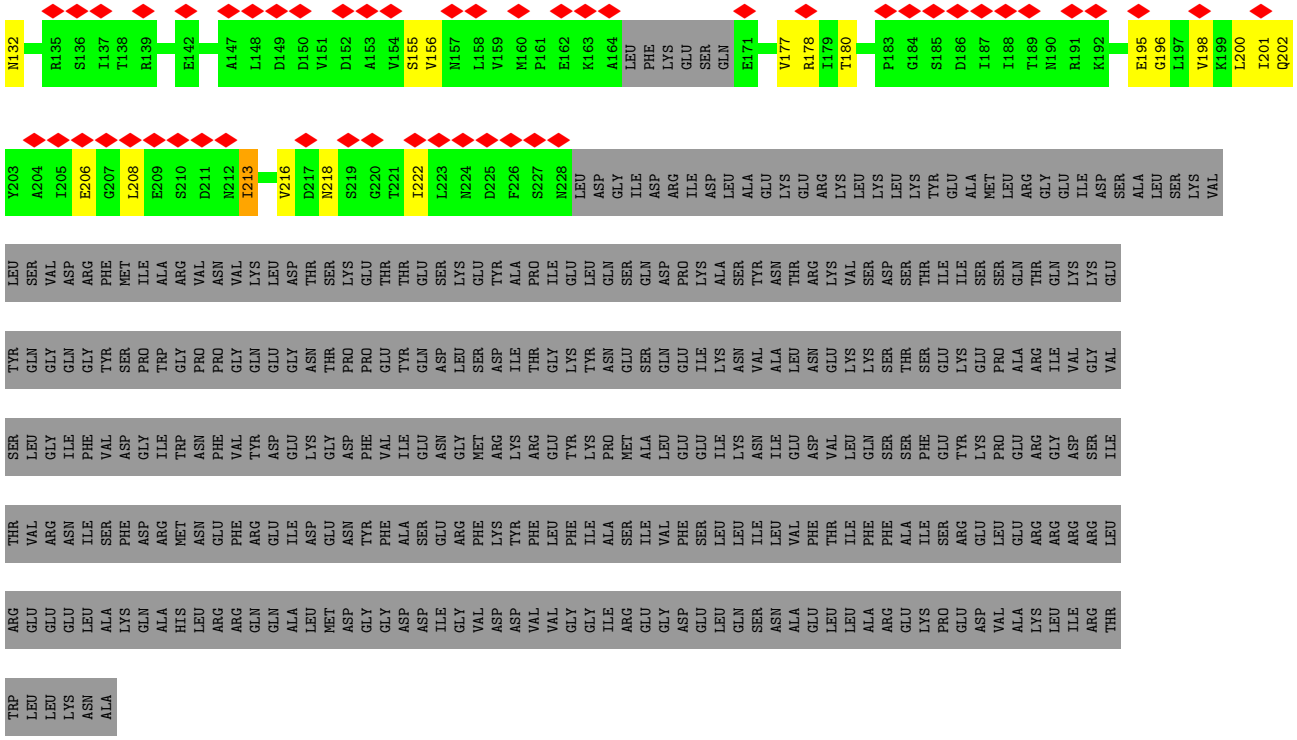
Chain u:



- Molecule 1: Flagellar M-ring protein

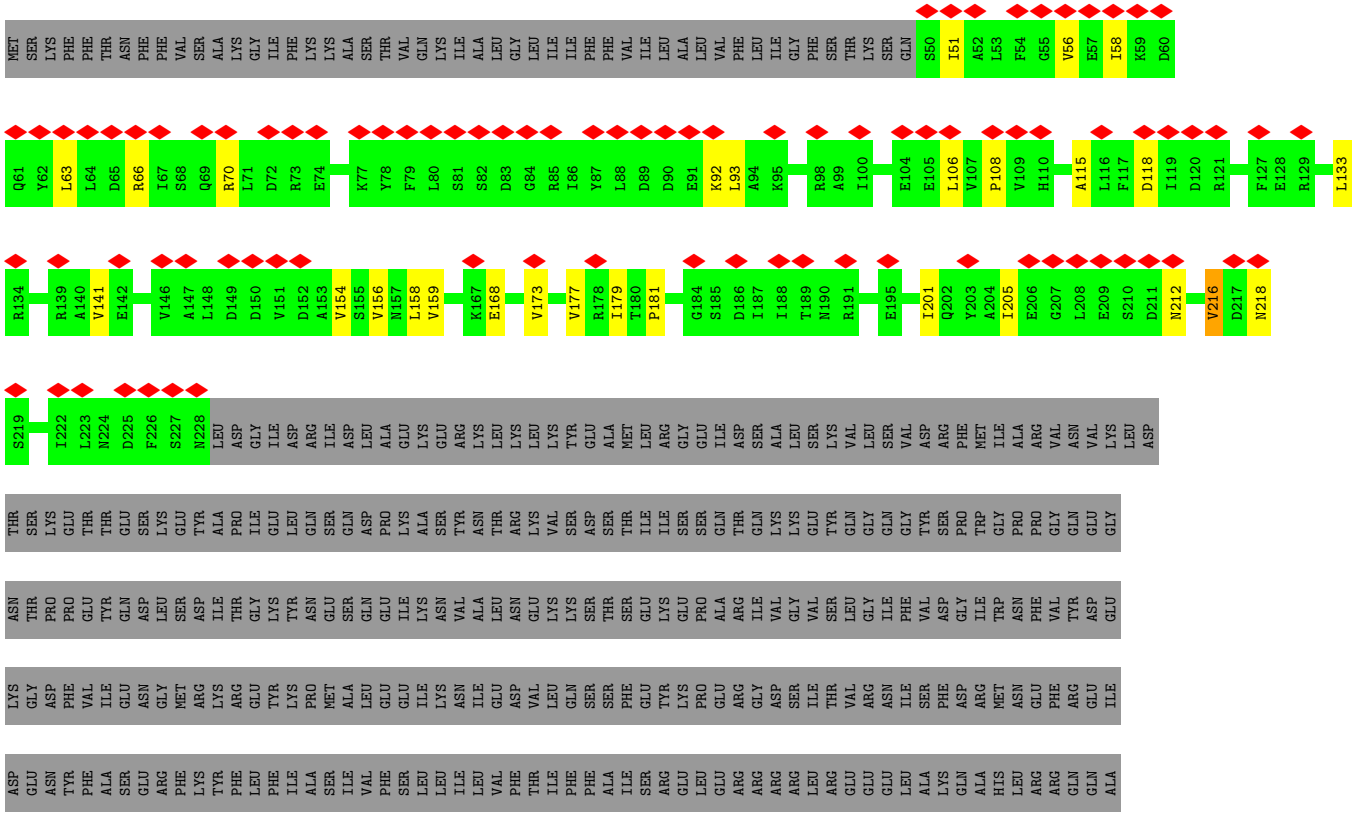
Chain v:





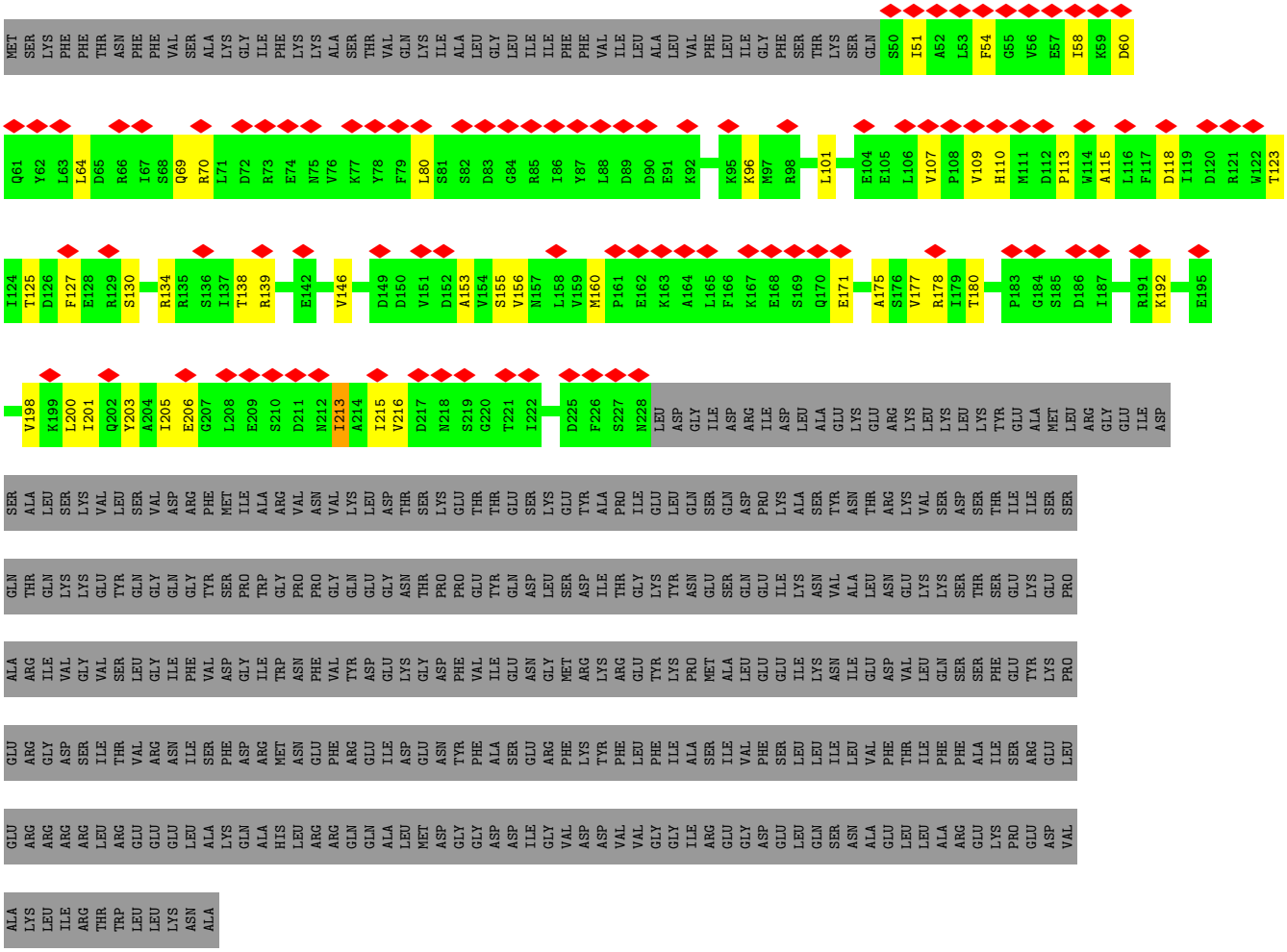
• Molecule 1: Flagellar M-ring protein

Chain w:



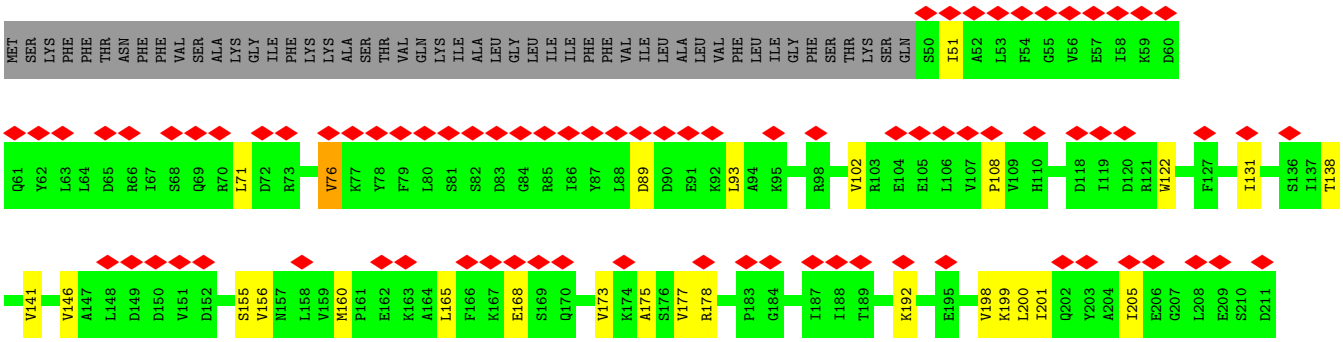
- Molecule 1: Flagellar M-ring protein

Chain x:



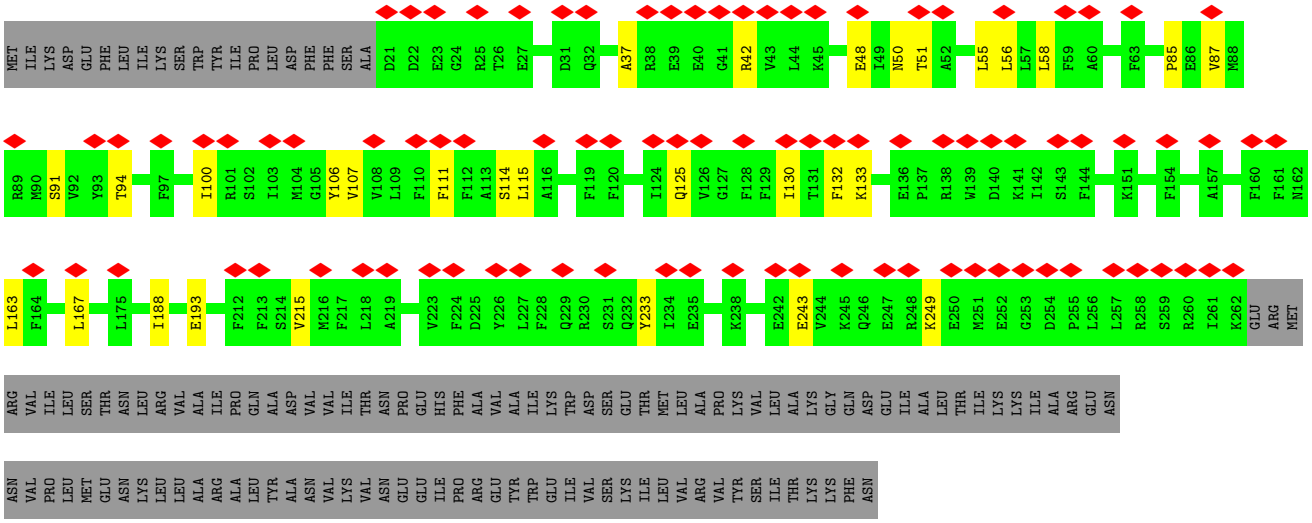
- Molecule 1: Flagellar M-ring protein

Chain y:



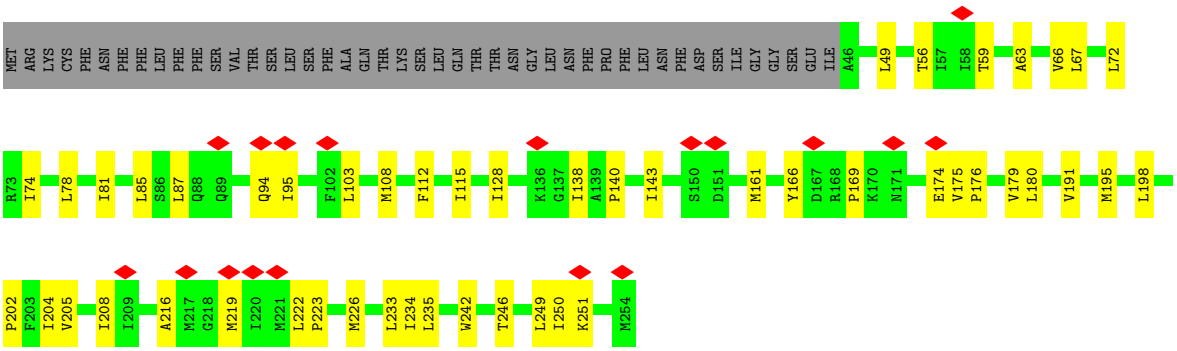
- Molecule 2: Flagellar biosynthetic protein FlhB

Chain A:



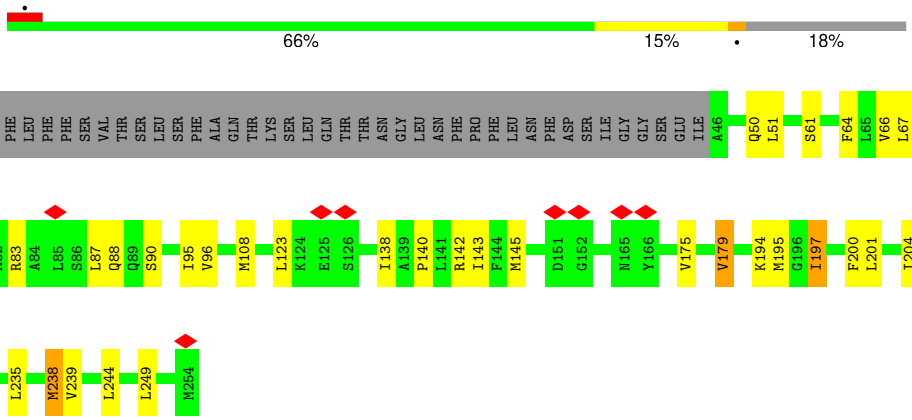
- Molecule 3: Flagellar biosynthetic protein FliP

Chain F:



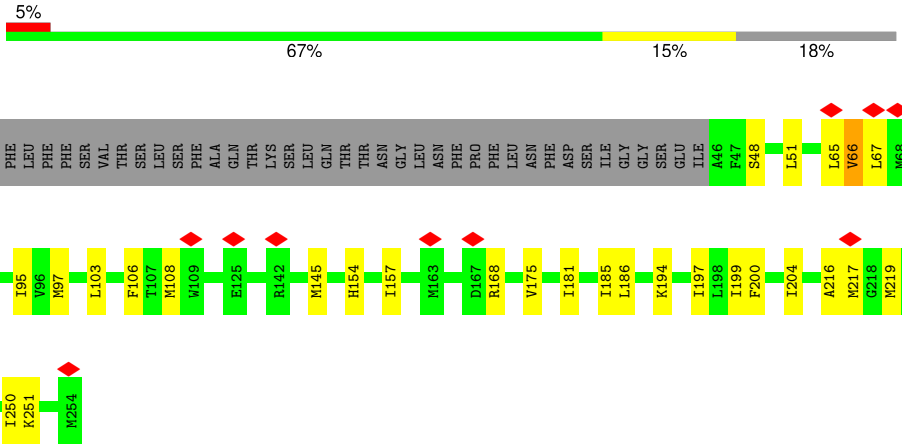
• Molecule 3: Flagellar biosynthetic protein FliP

Chain G:



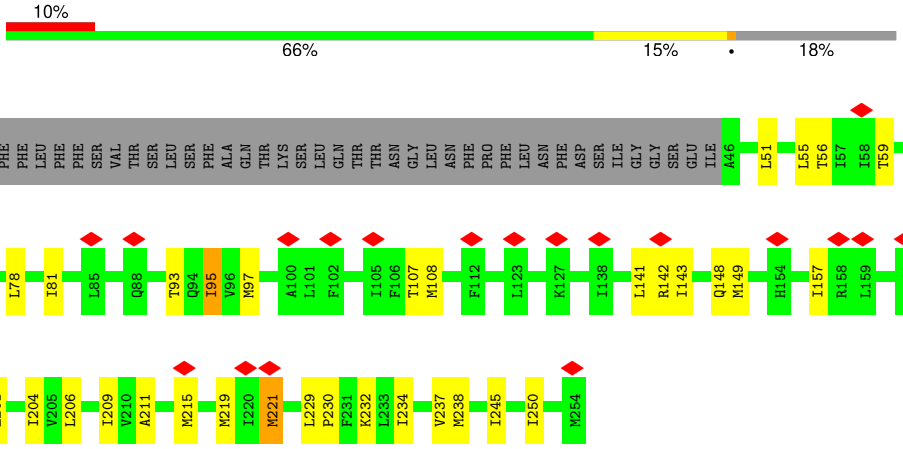
• Molecule 3: Flagellar biosynthetic protein FliP

Chain H:



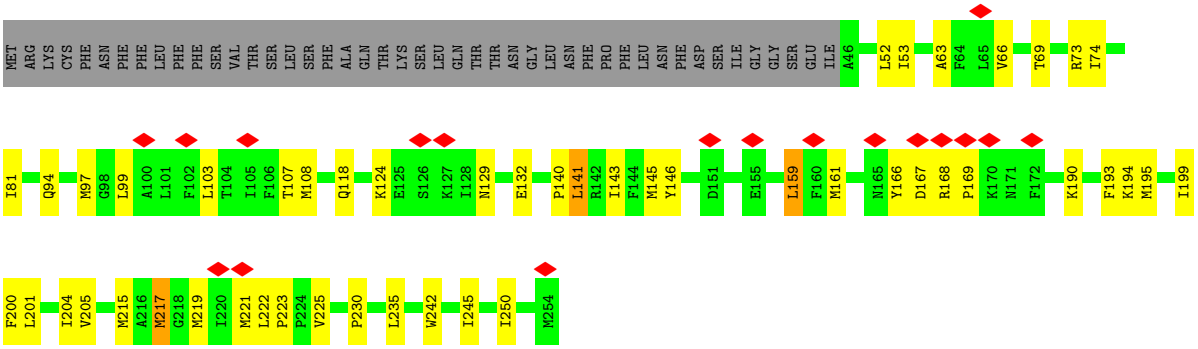
• Molecule 3: Flagellar biosynthetic protein FliP

Chain I:



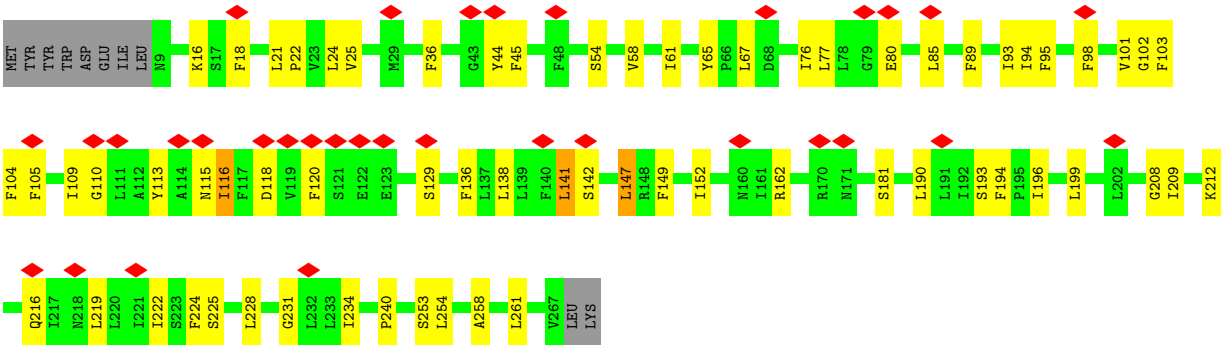
• Molecule 3: Flagellar biosynthetic protein FliP

Chain J:



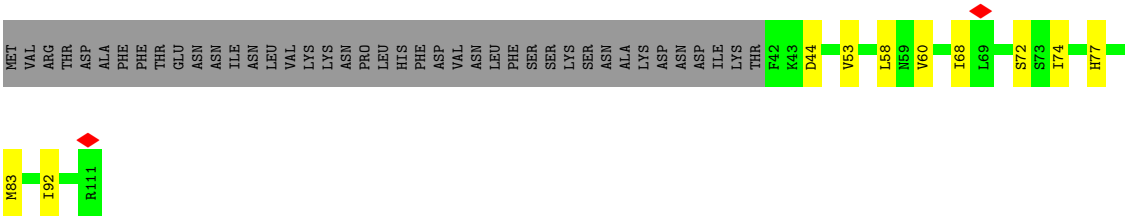
• Molecule 4: Flagellar biosynthetic protein FliR

Chain K:



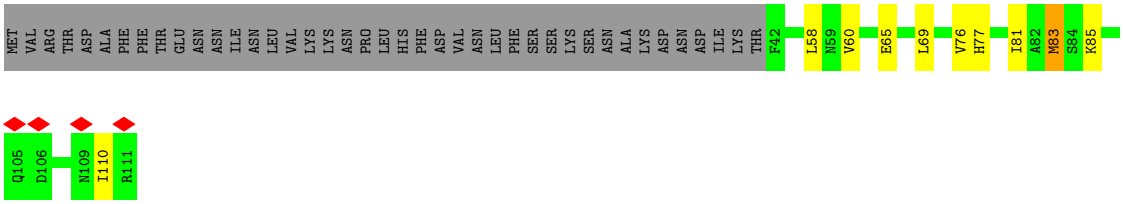
• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain L:



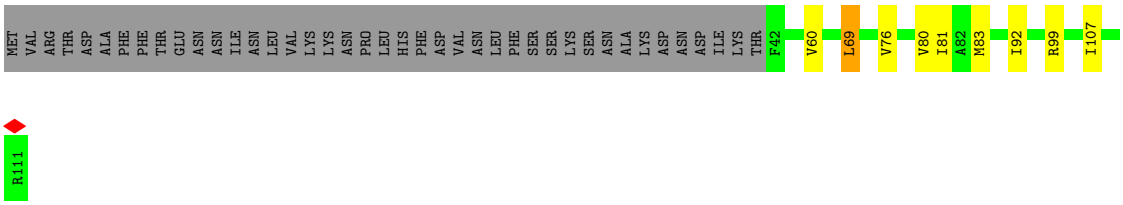
• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain M:



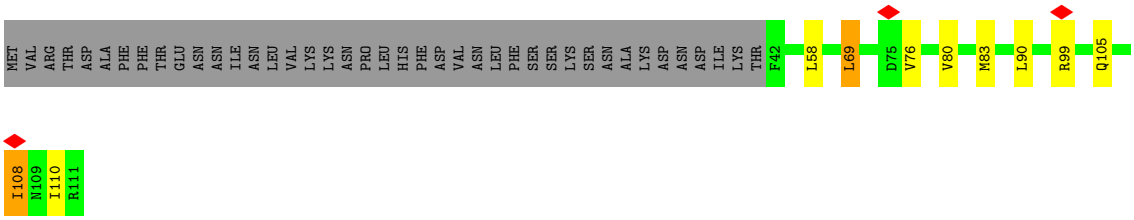
• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain N:



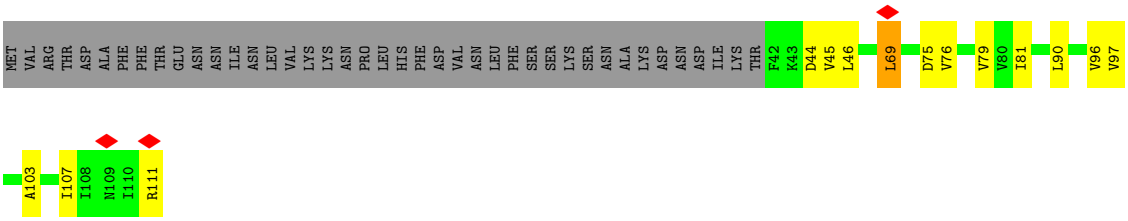
• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain O:



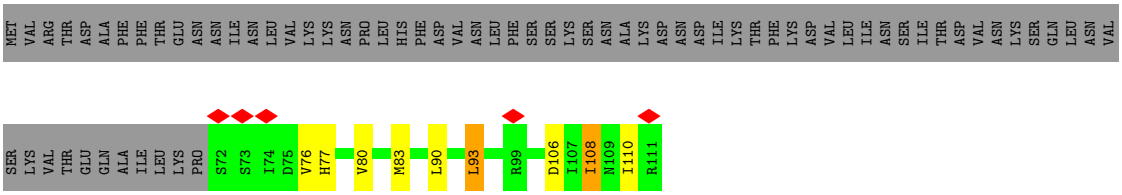
• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain P:



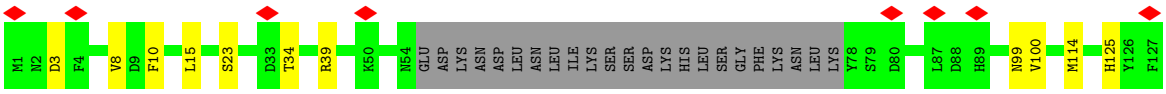
• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain Q:



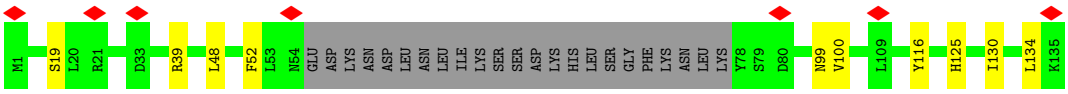
• Molecule 6: Flagellar basal body rod protein FlgB

Chain R:



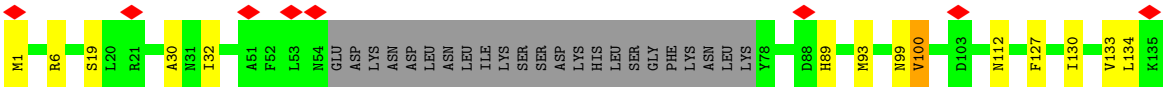
• Molecule 6: Flagellar basal body rod protein FlgB

Chain S:



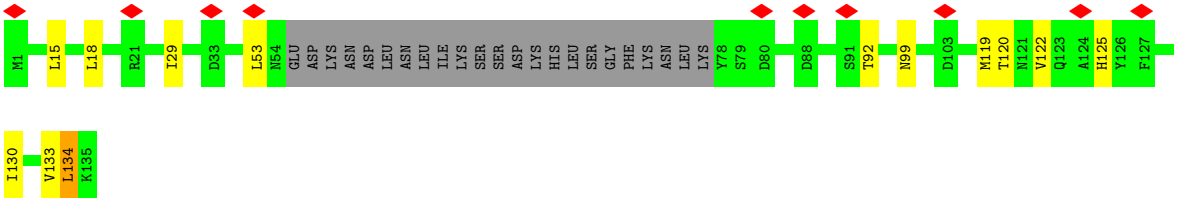
• Molecule 6: Flagellar basal body rod protein FlgB

Chain T:



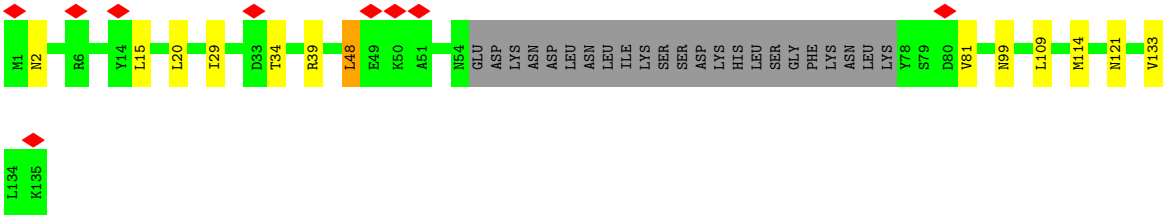
• Molecule 6: Flagellar basal body rod protein FlgB

Chain U:



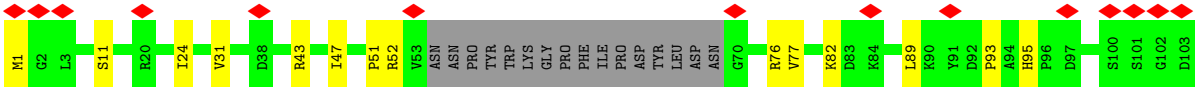
• Molecule 6: Flagellar basal body rod protein FlgB

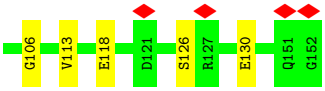
Chain V:



• Molecule 7: Flagellar basal-body rod protein FlgC

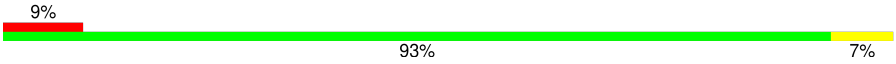
Chain W:

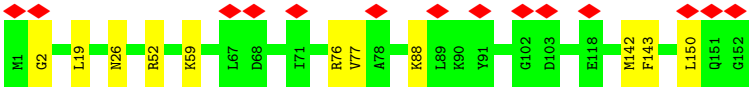




• Molecule 7: Flagellar basal-body rod protein FlgC

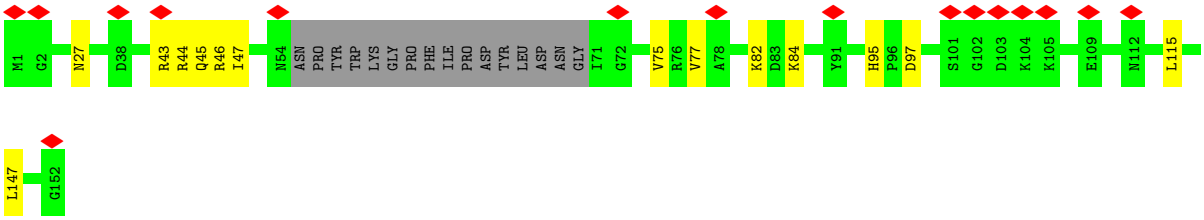
Chain X:





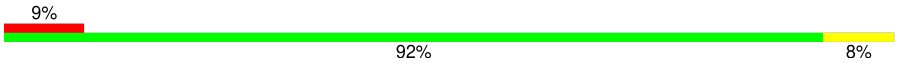
• Molecule 7: Flagellar basal-body rod protein FlgC

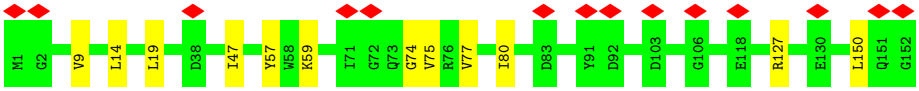
Chain Y:



• Molecule 7: Flagellar basal-body rod protein FlgC

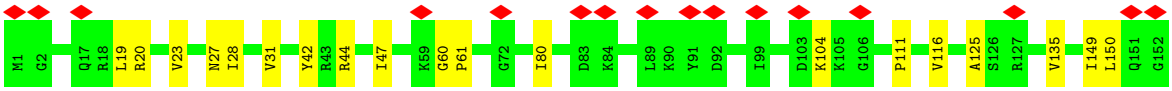
Chain Z:





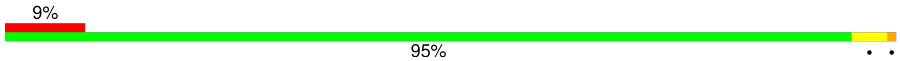
• Molecule 7: Flagellar basal-body rod protein FlgC

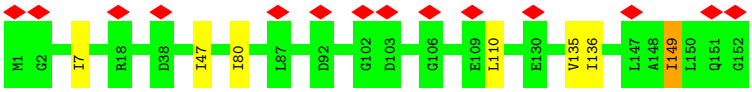
Chain a:



• Molecule 7: Flagellar basal-body rod protein FlgC

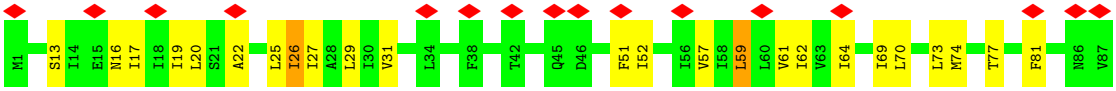
Chain b:





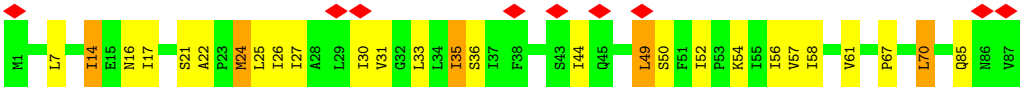
• Molecule 8: Flagellar biosynthetic protein FliQ

Chain z:



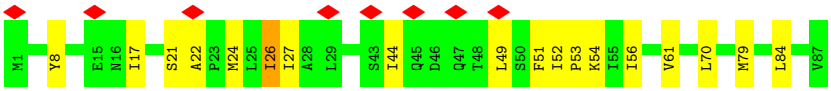
• Molecule 8: Flagellar biosynthetic protein FliQ

Chain 1:



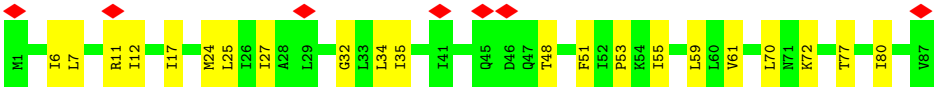
• Molecule 8: Flagellar biosynthetic protein FliQ

Chain 2:



• Molecule 8: Flagellar biosynthetic protein FliQ

Chain 3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37989	Depositor
Resolution determination method	FSC 0.143 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	0.578	Depositor
Minimum map value	-0.334	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	640.63995, 640.63995, 640.63995	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	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	c	0.17	0/1418	0.45	0/1924
1	d	0.17	0/1403	0.44	0/1906
1	e	0.17	0/1411	0.44	0/1915
1	f	0.17	0/1409	0.44	0/1909
1	g	0.16	0/1400	0.48	0/1898
1	h	0.17	0/1393	0.46	0/1891
1	i	0.17	0/1412	0.46	0/1915
1	j	0.18	0/1407	0.48	0/1909
1	k	0.17	0/1408	0.50	2/1911 (0.1%)
1	l	0.17	0/1406	0.47	0/1910
1	m	0.16	0/1418	0.43	0/1923
1	n	0.17	0/1395	0.45	0/1896
1	o	0.16	0/1408	0.43	0/1912
1	p	0.17	0/1405	0.42	0/1908
1	q	0.17	0/1411	0.45	1/1914 (0.1%)
1	r	0.16	0/1422	0.44	0/1928
1	s	0.17	0/1422	0.43	0/1928
1	t	0.16	0/1411	0.45	0/1915
1	u	0.15	0/1366	0.41	0/1853
1	v	0.15	0/1368	0.45	0/1855
1	w	0.16	0/1403	0.46	0/1906
1	x	0.16	0/1392	0.45	0/1892
1	y	0.16	0/1414	0.47	1/1919 (0.1%)
2	A	0.16	0/2033	0.37	0/2734
3	F	0.20	0/1706	0.42	0/2313
3	G	0.20	0/1696	0.43	0/2300
3	H	0.20	0/1697	0.40	0/2300
3	I	0.19	0/1706	0.44	0/2312
3	J	0.19	0/1717	0.40	0/2325
4	K	0.18	0/2135	0.40	0/2892
5	L	0.16	0/545	0.36	0/734
5	M	0.16	0/545	0.34	0/734
5	N	0.16	0/545	0.33	0/734
5	O	0.16	0/532	0.34	0/718

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	P	0.15	0/545	0.35	0/734
5	Q	0.15	0/309	0.32	0/414
6	R	0.17	0/936	0.33	0/1259
6	S	0.15	0/936	0.33	0/1259
6	T	0.16	0/936	0.31	0/1259
6	U	0.16	0/936	0.36	0/1259
6	V	0.16	0/936	0.33	0/1259
7	W	0.16	0/1043	0.33	0/1405
7	X	0.16	0/1175	0.34	0/1593
7	Y	0.15	0/1047	0.35	0/1411
7	Z	0.15	0/1191	0.34	0/1612
7	a	0.15	0/1191	0.35	0/1612
7	b	0.15	0/1191	0.33	0/1612
8	1	0.19	0/694	0.37	0/946
8	2	0.18	0/704	0.40	0/957
8	3	0.19	0/704	0.37	0/957
8	z	0.18	0/690	0.37	0/941
All	All	0.17	0/62323	0.42	4/84422 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	k	170	GLN	CA-C-N	6.57	129.81	120.49
1	k	170	GLN	C-N-CA	6.57	129.81	120.49
1	q	187	ILE	N-CA-C	-5.70	108.29	113.71
1	y	168	GLU	N-CA-C	-5.20	107.95	114.56

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	c	1397	0	1402	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	1383	0	1378	19	0
1	e	1391	0	1395	19	0
1	f	1390	0	1403	18	0
1	g	1381	0	1390	14	0
1	h	1374	0	1373	17	0
1	i	1392	0	1397	13	0
1	j	1387	0	1396	19	0
1	k	1388	0	1386	23	0
1	l	1385	0	1381	10	0
1	m	1397	0	1409	14	0
1	n	1375	0	1370	17	0
1	o	1387	0	1385	15	0
1	p	1385	0	1384	24	0
1	q	1391	0	1400	24	0
1	r	1401	0	1413	17	0
1	s	1401	0	1413	18	0
1	t	1391	0	1395	25	0
1	u	1347	0	1352	24	0
1	v	1349	0	1360	16	0
1	w	1383	0	1378	15	0
1	x	1372	0	1361	21	0
1	y	1393	0	1398	17	0
2	A	1988	0	2043	16	0
3	F	1665	0	1752	36	0
3	G	1656	0	1740	28	0
3	H	1657	0	1747	30	0
3	I	1666	0	1755	31	0
3	J	1676	0	1773	31	0
4	K	2083	0	2194	45	0
5	L	542	0	579	8	0
5	M	542	0	579	4	0
5	N	542	0	579	7	0
5	O	530	0	561	10	0
5	P	542	0	579	9	0
5	Q	308	0	327	6	0
6	R	920	0	896	6	0
6	S	920	0	896	6	0
6	T	920	0	896	9	0
6	U	920	0	896	14	0
6	V	920	0	896	8	0
7	W	1030	0	1055	11	0
7	X	1153	0	1150	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Y	1034	0	1058	9	0
7	Z	1169	0	1178	7	0
7	a	1169	0	1178	11	0
7	b	1169	0	1178	5	0
8	1	682	0	749	19	0
8	2	692	0	771	13	0
8	3	692	0	771	18	0
8	z	678	0	743	18	0
All	All	61305	0	62438	669	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 5.

All (669) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:107:VAL:HG22	1:q:69:GLN:HE22	1.52	0.75
1:m:80:LEU:H	1:m:86:ILE:HG23	1.51	0.75
8:1:27:ILE:HG21	8:1:61:VAL:HG21	1.71	0.72
8:2:27:ILE:HG21	8:2:61:VAL:HG21	1.72	0.71
3:J:168:ARG:HE	3:J:169:PRO:HD2	1.57	0.70
8:z:27:ILE:HG21	8:z:61:VAL:HG21	1.74	0.69
8:1:31:VAL:HG11	8:1:57:VAL:HG11	1.77	0.67
1:q:222:ILE:H	1:r:192:LYS:HZ1	1.43	0.67
6:V:29:ILE:HG21	7:b:135:VAL:HG21	1.78	0.66
1:c:73:ARG:HD3	1:y:102:VAL:HG21	1.78	0.66
1:n:121:ARG:HH21	1:o:120:ASP:HB2	1.61	0.65
1:g:202:GLN:HA	1:g:208:LEU:HD23	1.78	0.65
4:K:190:LEU:O	4:K:194:PHE:HB2	1.97	0.64
1:t:131:ILE:HD12	1:t:134:ARG:HH21	1.63	0.64
4:K:94:ILE:HD13	4:K:253:SER:HA	1.78	0.63
1:t:80:LEU:H	1:t:86:ILE:HG23	1.63	0.63
3:H:48:SER:HB2	6:T:133:VAL:HG21	1.80	0.63
3:G:83:ARG:HH12	3:H:87:LEU:HA	1.63	0.63
3:H:103:LEU:HD22	3:H:250:ILE:HD11	1.80	0.63
2:A:115:LEU:HB2	8:z:52:ILE:HG21	1.81	0.62
7:b:47:ILE:HG22	7:b:80:ILE:HG12	1.80	0.62
6:T:93:MET:H	6:T:99:ASN:HA	1.65	0.61
1:k:202:GLN:HA	1:k:208:LEU:HD23	1.82	0.61
3:G:51:LEU:HD11	5:L:92:ILE:HD11	1.81	0.61
7:Z:47:ILE:HG12	7:Z:80:ILE:HG12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:142:GLU:HG3	1:t:156:VAL:HG12	1.82	0.61
7:Y:27:ASN:HD21	7:Y:45:GLN:H	1.47	0.61
3:F:161:MET:HG3	3:F:166:TYR:HB2	1.81	0.61
7:X:19:LEU:HD23	7:X:77:VAL:HG21	1.83	0.61
1:d:216:VAL:HG21	1:e:200:LEU:HB3	1.83	0.60
3:I:81:ILE:HD11	3:I:245:ILE:HG21	1.83	0.60
3:J:217:MET:HE1	8:3:59:LEU:HG	1.83	0.60
7:a:47:ILE:HG12	7:a:80:ILE:HG12	1.82	0.60
1:j:188:ILE:HG13	1:j:189:THR:HG23	1.82	0.60
3:H:194:LYS:HA	3:H:197:ILE:HD12	1.83	0.60
6:U:29:ILE:HG21	7:a:135:VAL:HG21	1.82	0.60
5:L:92:ILE:HD13	6:S:134:LEU:HD21	1.84	0.60
1:m:156:VAL:HG12	1:m:177:VAL:HG22	1.84	0.60
1:x:177:VAL:HG21	1:x:201:ILE:HD13	1.83	0.60
2:A:55:LEU:HD13	4:K:212:LYS:HG2	1.84	0.60
7:a:27:ASN:HD21	7:a:44:ARG:HG3	1.66	0.60
1:q:152:ASP:HB3	1:r:104:GLU:HG2	1.83	0.60
1:f:177:VAL:HG21	1:f:201:ILE:HD13	1.83	0.60
4:K:199:LEU:HD22	4:K:234:ILE:HD11	1.83	0.60
3:F:169:PRO:HB3	3:F:174:GLU:HG2	1.84	0.59
3:H:78:LEU:HA	3:H:81:ILE:HD12	1.85	0.59
1:e:66:ARG:HB3	1:e:106:LEU:HD13	1.83	0.59
4:K:61:ILE:HG12	4:K:162:ARG:HH22	1.67	0.59
1:e:58:ILE:HG12	1:e:63:LEU:HD23	1.83	0.59
1:u:202:GLN:HA	1:u:208:LEU:HD23	1.83	0.59
1:x:58:ILE:HG22	1:x:60:ASP:H	1.66	0.59
3:G:201:LEU:HA	3:G:204:ILE:HD12	1.84	0.59
3:I:142:ARG:HH21	3:I:175:VAL:HG12	1.68	0.59
1:u:156:VAL:HG12	1:u:177:VAL:HG13	1.85	0.58
3:F:78:LEU:HA	3:F:81:ILE:HD12	1.86	0.58
1:f:156:VAL:HG12	1:f:177:VAL:HG22	1.85	0.58
3:H:157:ILE:HD11	3:H:175:VAL:HG11	1.86	0.58
6:S:39:ARG:HG2	6:S:99:ASN:HD21	1.68	0.58
1:t:190:ASN:HB3	1:t:193:LYS:HG2	1.86	0.58
1:d:58:ILE:HG12	1:d:63:LEU:HD22	1.85	0.58
1:g:152:ASP:HB3	1:h:104:GLU:HG2	1.84	0.58
1:g:102:VAL:HG21	1:h:73:ARG:HD3	1.85	0.58
1:t:177:VAL:HG21	1:t:201:ILE:HD13	1.86	0.57
1:q:198:VAL:HG12	1:q:215:ILE:HD13	1.85	0.57
1:v:177:VAL:HG21	1:v:201:ILE:HD13	1.84	0.57
3:F:216:ALA:HA	8:z:51:PHE:HZ	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:177:VAL:HG21	1:j:201:ILE:HD13	1.86	0.57
4:K:231:GLY:HA2	4:K:234:ILE:HD12	1.87	0.57
1:s:177:VAL:HG21	1:s:201:ILE:HD13	1.87	0.57
1:v:71:LEU:HD23	1:v:97:MET:HE3	1.87	0.57
1:s:222:ILE:HA	1:t:199:LYS:HZ3	1.67	0.57
8:2:22:ALA:O	8:2:26:ILE:HB	2.04	0.57
1:n:71:LEU:HD23	1:n:97:MET:HE2	1.85	0.57
1:w:181:PRO:HD2	1:w:218:ASN:HD22	1.69	0.57
3:G:195:MET:HE1	3:G:249:LEU:HD13	1.87	0.57
4:K:98:PHE:HA	4:K:101:VAL:HG12	1.86	0.57
3:F:103:LEU:HD22	3:F:250:ILE:HD11	1.86	0.56
1:o:71:LEU:HD23	1:o:97:MET:HE2	1.87	0.56
1:o:177:VAL:HG21	1:o:201:ILE:HD13	1.86	0.56
1:w:66:ARG:HB3	1:w:106:LEU:HD13	1.87	0.56
3:I:204:ILE:HD11	3:J:230:PRO:HG2	1.87	0.56
7:Z:19:LEU:HD23	7:Z:77:VAL:HG21	1.87	0.56
1:f:217:ASP:HB3	1:f:223:LEU:HD11	1.88	0.56
1:r:177:VAL:HG21	1:r:201:ILE:HD13	1.87	0.56
4:K:93:ILE:HG21	4:K:181:SER:HB3	1.88	0.56
7:W:24:ILE:HG23	7:W:118:GLU:HG3	1.88	0.56
1:q:175:ALA:HB3	1:q:213:ILE:HG23	1.86	0.56
6:U:122:VAL:HA	6:U:125:HIS:CD2	2.41	0.56
3:G:206:LEU:HD22	3:G:232:LYS:HG3	1.87	0.56
1:h:177:VAL:HG21	1:h:201:ILE:HD13	1.86	0.56
3:I:107:THR:HG22	3:I:250:ILE:HG23	1.88	0.56
1:c:156:VAL:HG23	1:c:177:VAL:HG22	1.88	0.55
3:J:107:THR:HG23	3:J:108:MET:HG3	1.88	0.55
1:k:187:ILE:HG13	1:k:193:LYS:HB3	1.87	0.55
1:o:123:THR:HG22	8:1:67:PRO:HG2	1.88	0.55
1:d:108:PRO:HA	1:e:69:GLN:HG3	1.88	0.55
1:p:158:LEU:HD11	1:p:205:ILE:HG21	1.87	0.55
1:m:98:ARG:HB3	1:n:73:ARG:HH12	1.72	0.55
1:w:115:ALA:HA	1:w:118:ASP:HB2	1.89	0.55
3:G:197:ILE:HD11	3:H:233:LEU:HB2	1.89	0.55
1:c:58:ILE:HG21	1:c:64:LEU:HD13	1.88	0.55
1:p:102:VAL:HG11	1:q:73:ARG:HE	1.71	0.55
1:p:153:ALA:HB3	1:p:180:THR:HB	1.88	0.55
1:j:98:ARG:HD3	1:k:72:ASP:HB3	1.89	0.54
1:u:98:ARG:HD3	1:v:72:ASP:HB3	1.89	0.54
1:i:107:VAL:HB	1:j:69:GLN:HE22	1.72	0.54
1:i:177:VAL:HG21	1:i:201:ILE:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:205:VAL:HA	8:3:17:ILE:HD11	1.90	0.54
1:n:121:ARG:HH12	1:o:118:ASP:HA	1.72	0.54
1:o:216:VAL:HG21	1:p:200:LEU:HB3	1.90	0.54
1:c:176:SER:HB2	1:d:200:LEU:HD12	1.89	0.54
1:c:192:LYS:HE2	1:y:221:THR:HA	1.90	0.54
1:j:116:LEU:HD21	1:j:135:ARG:HE	1.73	0.54
1:j:202:GLN:HA	1:j:208:LEU:HD23	1.89	0.54
1:o:80:LEU:H	1:o:86:ILE:HG23	1.72	0.54
1:s:175:ALA:HB3	1:s:213:ILE:HG23	1.90	0.54
6:T:89:HIS:HB2	7:Z:59:LYS:HE2	1.88	0.54
1:y:198:VAL:HG12	1:y:215:ILE:HD13	1.90	0.54
3:G:235:LEU:HD21	8:z:73:LEU:HB3	1.90	0.54
1:o:156:VAL:HG12	1:o:177:VAL:HG22	1.89	0.54
1:x:198:VAL:HG12	1:x:215:ILE:HD13	1.90	0.54
7:Z:9:VAL:HG13	7:Z:74:GLY:HA2	1.89	0.53
1:w:177:VAL:HG21	1:w:201:ILE:HD13	1.89	0.53
1:m:116:LEU:HG	1:m:139:ARG:HH22	1.71	0.53
4:K:115:ASN:HA	4:K:118:ASP:HB2	1.89	0.53
1:x:134:ARG:HH21	1:x:160:MET:HB2	1.74	0.53
3:H:251:LYS:HE2	8:1:85:GLN:HE22	1.73	0.53
6:U:130:ILE:O	6:U:134:LEU:HB2	2.08	0.53
8:1:25:LEU:HG	8:2:52:ILE:HD12	1.90	0.53
1:p:175:ALA:HB3	1:p:213:ILE:HG23	1.89	0.53
5:L:77:HIS:HE1	6:S:19:SER:HB2	1.73	0.53
5:O:83:MET:HG2	6:U:125:HIS:CD2	2.44	0.53
1:e:174:LYS:HE3	1:f:203:TYR:HA	1.91	0.53
1:k:58:ILE:HG21	1:k:63:LEU:HD22	1.90	0.53
1:u:60:ASP:HB3	1:u:63:LEU:HB2	1.91	0.53
2:A:56:LEU:HD13	2:A:215:VAL:HG11	1.88	0.53
3:F:219:MET:HE3	4:K:208:GLY:HA3	1.88	0.53
1:n:155:SER:HB3	1:n:178:ARG:HE	1.73	0.53
3:H:224:PRO:HD3	3:I:221:MET:HE1	1.89	0.53
1:x:115:ALA:HA	1:x:118:ASP:HB2	1.90	0.53
3:J:73:ARG:HD3	3:J:195:MET:HE1	1.90	0.53
8:2:53:PRO:HA	8:2:56:ILE:HG22	1.91	0.53
1:v:216:VAL:HG12	1:v:222:ILE:HG22	1.91	0.53
1:w:92:LYS:HG3	1:w:93:LEU:HD22	1.91	0.53
3:F:140:PRO:HA	3:F:143:ILE:HG12	1.91	0.53
1:c:127:PHE:HE2	1:d:129:ARG:HB2	1.75	0.52
1:r:159:VAL:HB	1:r:174:LYS:H	1.74	0.52
1:v:202:GLN:HA	1:v:208:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:101:VAL:HG23	4:K:193:SER:HB3	1.90	0.52
6:T:32:ILE:HA	6:T:100:VAL:HG11	1.91	0.52
1:s:58:ILE:HG12	1:s:63:LEU:HD22	1.91	0.52
3:I:93:THR:HG22	3:I:97:MET:HE2	1.90	0.52
3:J:190:LYS:HG3	4:K:141:LEU:HD12	1.91	0.52
1:l:141:VAL:HG21	1:l:205:ILE:HD11	1.90	0.52
1:w:58:ILE:HG12	1:w:63:LEU:HD23	1.91	0.52
3:I:62:PRO:HA	5:N:107:ILE:HD11	1.91	0.52
1:j:153:ALA:HB3	1:j:180:THR:HB	1.91	0.52
1:k:156:VAL:HG12	1:k:177:VAL:HG22	1.91	0.52
3:J:124:LYS:HD3	6:V:2:ASN:HD21	1.73	0.52
1:s:128:GLU:HG3	1:t:129:ARG:HD3	1.91	0.52
3:I:78:LEU:HD23	3:I:81:ILE:HD12	1.91	0.52
3:H:238:MET:HE1	8:1:70:LEU:HG	1.90	0.52
1:h:155:SER:HB3	1:h:178:ARG:HE	1.75	0.52
3:I:69:THR:HG22	3:I:108:MET:HE2	1.91	0.52
8:1:35:ILE:HD11	8:1:54:LYS:HZ2	1.74	0.52
1:c:159:VAL:HB	1:c:174:LYS:HB2	1.92	0.51
1:y:156:VAL:HG12	1:y:177:VAL:HG22	1.92	0.51
3:J:103:LEU:HD22	3:J:250:ILE:HD11	1.91	0.51
1:d:202:GLN:HA	1:d:208:LEU:HD22	1.92	0.51
3:H:194:LYS:HD3	3:I:237:VAL:HG11	1.92	0.51
5:M:77:HIS:HE1	6:T:19:SER:HB2	1.74	0.51
1:k:175:ALA:HB3	1:k:213:ILE:HG23	1.92	0.51
1:q:156:VAL:HG12	1:q:177:VAL:HG22	1.92	0.51
3:J:159:LEU:HB2	4:K:147:LEU:HD12	1.92	0.51
8:z:25:LEU:HG	8:1:52:ILE:HD12	1.93	0.51
1:c:177:VAL:HG21	1:c:201:ILE:HD13	1.93	0.51
1:e:156:VAL:HG12	1:e:177:VAL:HG22	1.91	0.51
1:j:127:PHE:HZ	1:k:133:LEU:HD22	1.76	0.51
1:t:104:GLU:HB3	1:t:106:LEU:HD13	1.91	0.51
1:o:94:ALA:HB1	1:o:98:ARG:HH21	1.76	0.51
4:K:105:PHE:HD1	4:K:196:ILE:HG21	1.75	0.51
7:Y:43:ARG:HD3	7:Y:82:LYS:HD3	1.93	0.51
1:e:141:VAL:HG21	1:e:205:ILE:HD11	1.93	0.51
1:g:108:PRO:HB3	1:h:69:GLN:HE22	1.76	0.51
1:s:109:VAL:HG23	1:t:69:GLN:HE22	1.74	0.51
3:J:235:LEU:HD11	8:3:77:THR:HG21	1.93	0.51
1:f:202:GLN:HA	1:f:208:LEU:HD23	1.93	0.51
1:m:202:GLN:HA	1:m:208:LEU:HD23	1.93	0.51
1:u:153:ALA:HB3	1:u:180:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:47:ILE:HG23	7:Z:77:VAL:HG13	1.93	0.51
8:z:22:ALA:O	8:z:26:ILE:HB	2.10	0.51
8:2:51:PHE:HA	8:2:54:LYS:HB2	1.92	0.51
3:H:81:ILE:HD11	3:H:245:ILE:HG21	1.92	0.51
3:I:73:ARG:HH22	3:I:148:GLN:HE21	1.59	0.51
8:z:31:VAL:HG11	8:z:57:VAL:HG11	1.93	0.51
1:g:163:LYS:HE2	1:g:170:GLN:HE21	1.76	0.51
1:m:116:LEU:HD11	1:m:139:ARG:HH12	1.76	0.50
1:u:142:GLU:HG3	1:u:156:VAL:HG22	1.92	0.50
5:P:103:ALA:HB1	5:Q:90:LEU:HD23	1.93	0.50
6:S:39:ARG:HB3	6:S:100:VAL:HG22	1.92	0.50
1:j:214:ALA:HB1	1:k:199:LYS:HE3	1.93	0.50
1:k:177:VAL:HG21	1:k:201:ILE:HD13	1.93	0.50
3:G:70:SER:H	3:G:108:MET:HE3	1.76	0.50
7:Y:47:ILE:HG23	7:Y:77:VAL:HG13	1.94	0.50
1:e:102:VAL:HG21	1:f:73:ARG:HE	1.77	0.50
1:e:153:ALA:HB3	1:e:180:THR:HB	1.94	0.50
1:n:177:VAL:HG21	1:n:201:ILE:HD13	1.94	0.50
1:v:156:VAL:HG12	1:v:177:VAL:HG22	1.94	0.50
6:R:34:THR:HG21	7:W:51:PRO:HD3	1.93	0.50
1:f:175:ALA:HB3	1:f:213:ILE:HG23	1.94	0.50
1:x:138:THR:HG23	1:x:156:VAL:HG23	1.93	0.50
1:y:175:ALA:HB3	1:y:213:ILE:HG23	1.94	0.50
3:J:222:LEU:HD12	3:J:223:PRO:HD2	1.93	0.50
1:c:115:ALA:HA	1:c:118:ASP:HB2	1.92	0.50
1:m:159:VAL:HB	1:m:174:LYS:HB2	1.94	0.49
1:n:142:GLU:HG3	1:n:156:VAL:HG22	1.93	0.49
1:q:159:VAL:HG11	1:r:206:GLU:HA	1.94	0.49
1:u:177:VAL:HG21	1:u:201:ILE:HD13	1.93	0.49
3:J:217:MET:HE2	8:3:55:ILE:HA	1.94	0.49
6:R:39:ARG:H	6:R:99:ASN:HD21	1.59	0.49
3:F:202:PRO:HA	3:F:205:VAL:HG12	1.93	0.49
3:G:206:LEU:HD12	3:G:235:LEU:HD22	1.94	0.49
4:K:95:PHE:HA	4:K:136:PHE:HE2	1.76	0.49
4:K:199:LEU:HD13	4:K:234:ILE:HG12	1.94	0.49
7:W:47:ILE:HG23	7:W:77:VAL:HG13	1.93	0.49
1:j:216:VAL:HG21	1:k:200:LEU:HD22	1.95	0.49
1:x:64:LEU:HD12	1:x:80:LEU:HD21	1.93	0.49
1:s:176:SER:HB2	1:t:200:LEU:HD12	1.94	0.49
4:K:109:ILE:HG21	4:K:228:LEU:HD13	1.94	0.49
5:M:83:MET:HG3	6:S:125:HIS:CG	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:156:VAL:HG12	1:n:177:VAL:HG13	1.94	0.49
1:v:116:LEU:HB3	1:v:132:ASN:HD21	1.77	0.49
1:v:155:SER:HB2	1:v:178:ARG:HH21	1.76	0.49
4:K:102:GLY:HA3	4:K:129:SER:HA	1.94	0.49
1:j:155:SER:HB3	1:j:178:ARG:HE	1.78	0.49
2:A:111:PHE:HD2	8:z:52:ILE:HG23	1.78	0.49
1:o:212:ASN:HA	1:p:203:TYR:HE2	1.77	0.49
3:F:87:LEU:HD11	4:K:104:PHE:HE1	1.78	0.49
3:G:87:LEU:HD13	3:G:90:SER:HB2	1.95	0.49
1:g:216:VAL:HG21	1:h:200:LEU:HB3	1.93	0.49
1:d:71:LEU:HD23	1:d:76:VAL:HG21	1.95	0.48
1:e:202:GLN:HA	1:e:208:LEU:HD23	1.94	0.48
1:o:155:SER:HB2	1:o:178:ARG:HH21	1.77	0.48
1:p:156:VAL:HG12	1:p:177:VAL:HG22	1.94	0.48
3:F:223:PRO:HB2	3:F:226:MET:HG2	1.95	0.48
8:z:61:VAL:HA	8:z:64:ILE:HG22	1.94	0.48
1:c:196:GLY:HA2	1:y:222:ILE:HD11	1.93	0.48
1:h:141:VAL:HG21	1:h:205:ILE:HD11	1.95	0.48
1:w:159:VAL:HG11	1:x:206:GLU:HA	1.95	0.48
1:h:58:ILE:HG21	1:h:63:LEU:HD22	1.95	0.48
3:I:186:LEU:HD22	3:J:242:TRP:HB3	1.94	0.48
7:b:7:ILE:HG23	7:b:136:ILE:HD11	1.94	0.48
8:1:36:SER:HB2	8:2:44:ILE:HG23	1.95	0.48
1:d:153:ALA:HB3	1:d:180:THR:HB	1.94	0.48
3:F:56:THR:HA	3:F:59:THR:HG22	1.95	0.48
3:F:72:LEU:HD13	3:G:95:ILE:HG12	1.95	0.48
3:J:221:MET:HE3	3:J:221:MET:H	1.79	0.48
5:P:90:LEU:HD21	6:V:133:VAL:HB	1.96	0.48
1:e:177:VAL:HG21	1:e:201:ILE:HD13	1.95	0.48
1:i:142:GLU:HG2	1:i:156:VAL:HG22	1.95	0.48
3:I:157:ILE:HD11	3:I:180:LEU:HA	1.95	0.48
1:d:50:SER:HA	1:d:87:TYR:HD1	1.77	0.48
1:e:115:ALA:HA	1:e:118:ASP:HB2	1.96	0.48
3:J:52:LEU:HD11	5:P:97:VAL:HG21	1.95	0.48
5:N:83:MET:HE3	5:N:83:MET:HB3	1.74	0.48
1:l:156:VAL:HG12	1:l:177:VAL:HG22	1.94	0.48
1:y:141:VAL:HG21	1:y:205:ILE:HD11	1.94	0.48
3:I:206:LEU:HD22	3:I:232:LYS:HG3	1.95	0.48
4:K:240:PRO:HD3	8:3:11:ARG:HH12	1.78	0.48
5:N:92:ILE:HG12	6:U:134:LEU:HD11	1.95	0.48
3:F:204:ILE:HG13	3:G:230:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:141:VAL:HG21	1:w:205:ILE:HD11	1.96	0.48
3:J:94:GLN:HE22	5:O:108:ILE:HB	1.79	0.47
5:Q:77:HIS:HA	5:Q:80:VAL:HG12	1.96	0.47
1:g:156:VAL:HG12	1:g:177:VAL:HG13	1.95	0.47
1:m:214:ALA:HA	1:n:199:LYS:HZ1	1.80	0.47
1:p:214:ALA:HB1	1:q:199:LYS:HE3	1.94	0.47
1:y:155:SER:HB2	1:y:178:ARG:HH21	1.79	0.47
3:G:140:PRO:HA	3:G:143:ILE:HG22	1.96	0.47
5:N:69:LEU:HD13	5:N:69:LEU:HA	1.77	0.47
1:y:89:ASP:H	1:y:93:LEU:HD23	1.79	0.47
5:L:72:SER:HA	7:X:2:GLY:HA2	1.96	0.47
6:R:23:SER:HB3	7:W:1:MET:HE2	1.96	0.47
1:f:67:ILE:HD12	1:f:101:LEU:HD13	1.97	0.47
1:w:156:VAL:HG12	1:w:177:VAL:HG22	1.97	0.47
1:y:177:VAL:HB	1:y:215:ILE:HG13	1.95	0.47
3:G:239:VAL:HG21	8:z:77:THR:HG21	1.97	0.47
4:K:138:LEU:HD21	8:3:6:ILE:HG23	1.97	0.47
4:K:222:ILE:HD11	8:3:32:GLY:HA3	1.96	0.47
1:t:141:VAL:HG21	1:t:205:ILE:HD11	1.96	0.47
1:t:156:VAL:HG23	1:t:177:VAL:HG22	1.96	0.47
1:f:198:VAL:HG12	1:f:215:ILE:HD13	1.95	0.47
1:s:66:ARG:HB3	1:s:106:LEU:HD13	1.97	0.47
1:s:222:ILE:HG23	1:t:199:LYS:HZ2	1.80	0.47
3:F:166:TYR:HE2	3:F:176:PRO:HG3	1.80	0.47
1:h:125:THR:HG21	8:2:8:TYR:HD1	1.80	0.47
1:k:153:ALA:HB3	1:k:180:THR:HB	1.96	0.47
1:o:195:GLU:HA	1:o:198:VAL:HG12	1.96	0.47
1:o:215:ILE:HD12	1:o:224:ASN:HB3	1.96	0.47
1:q:54:PHE:CZ	1:q:107:VAL:HG21	2.50	0.47
1:w:154:VAL:HG22	1:w:179:ILE:HG22	1.96	0.47
1:y:177:VAL:HG21	1:y:201:ILE:HD13	1.96	0.47
3:F:205:VAL:HA	3:F:208:ILE:HG22	1.96	0.47
3:I:211:ALA:HB1	3:J:219:MET:HE2	1.96	0.47
1:g:155:SER:HB3	1:g:178:ARG:HE	1.79	0.47
8:1:27:ILE:HA	8:1:30:ILE:HG22	1.96	0.47
8:3:27:ILE:HG21	8:3:61:VAL:HG21	1.95	0.47
1:r:137:ILE:HD12	1:r:160:MET:HE1	1.96	0.47
3:F:49:LEU:HD21	5:L:53:VAL:HG12	1.97	0.47
3:H:216:ALA:HB2	8:2:52:ILE:HD11	1.97	0.47
1:q:126:ASP:HA	1:q:129:ARG:HG2	1.97	0.47
5:N:92:ILE:HA	6:U:134:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:198:VAL:HG12	1:h:215:ILE:HD13	1.96	0.46
1:n:155:SER:HB2	1:n:178:ARG:HH21	1.79	0.46
1:q:177:VAL:HB	1:q:215:ILE:HG13	1.97	0.46
1:s:141:VAL:HG21	1:s:205:ILE:HD11	1.97	0.46
1:u:104:GLU:HB3	1:u:106:LEU:HD13	1.97	0.46
1:x:153:ALA:HB3	1:x:180:THR:HB	1.96	0.46
1:k:148:LEU:HD11	1:k:200:LEU:HD21	1.97	0.46
1:n:67:ILE:HD12	1:n:101:LEU:HD13	1.98	0.46
1:n:141:VAL:HG21	1:n:205:ILE:HD11	1.96	0.46
1:t:208:LEU:HD21	1:t:213:ILE:HG12	1.97	0.46
1:x:113:PRO:HB3	1:x:139:ARG:HB3	1.96	0.46
3:H:154:HIS:HB3	3:H:157:ILE:HG22	1.97	0.46
4:K:149:PHE:HA	4:K:254:LEU:HD11	1.98	0.46
5:O:83:MET:HE2	6:U:125:HIS:HB2	1.96	0.46
7:W:52:ARG:NE	7:W:76:ARG:HB2	2.31	0.46
1:g:177:VAL:HG21	1:g:201:ILE:HD13	1.97	0.46
1:q:177:VAL:HG21	1:q:201:ILE:HD13	1.97	0.46
4:K:258:ALA:HA	4:K:261:LEU:HD12	1.98	0.46
8:2:24:MET:HE2	8:2:24:MET:HB3	1.69	0.46
1:p:93:LEU:HA	1:p:96:LYS:HG2	1.98	0.46
1:x:160:MET:HE2	1:x:205:ILE:HG23	1.98	0.46
3:F:94:GLN:HA	5:Q:108:ILE:HG13	1.97	0.46
3:I:51:LEU:HD23	6:U:133:VAL:HG13	1.97	0.46
8:1:35:ILE:HD12	8:1:50:SER:HA	1.98	0.46
1:k:167:LYS:HE2	3:H:168:ARG:HD2	1.98	0.46
1:k:198:VAL:HG12	1:k:215:ILE:HD13	1.97	0.46
1:r:202:GLN:HA	1:r:208:LEU:HD23	1.97	0.46
3:H:229:LEU:HA	3:H:232:LYS:HD2	1.97	0.46
6:U:119:MET:HA	6:U:122:VAL:HG22	1.97	0.46
8:1:21:SER:HB2	8:1:25:LEU:HD13	1.98	0.46
1:p:178:ARG:NH2	1:q:147:ALA:HB3	2.31	0.46
1:y:71:LEU:HG	1:y:76:VAL:HG13	1.98	0.46
3:H:66:VAL:HG13	3:I:95:ILE:HG22	1.97	0.46
5:O:110:ILE:HA	5:P:111:ARG:HH22	1.79	0.46
1:e:108:PRO:HA	1:f:69:GLN:HG3	1.98	0.46
1:i:163:LYS:HD3	1:i:167:LYS:HZ3	1.81	0.46
1:p:198:VAL:HA	1:p:201:ILE:HG22	1.97	0.46
1:x:123:THR:HG21	1:y:122:TRP:CD1	2.51	0.46
3:F:63:ALA:O	3:F:67:LEU:HB2	2.16	0.46
1:t:76:VAL:HG21	1:t:93:LEU:HD21	1.98	0.46
3:J:63:ALA:HA	4:K:44:TYR:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:105:PHE:CD1	4:K:196:ILE:HG21	2.51	0.46
8:1:22:ALA:O	8:1:26:ILE:HB	2.15	0.46
1:x:175:ALA:HB3	1:x:213:ILE:HG23	1.97	0.45
3:G:238:MET:HE1	8:z:74:MET:HG2	1.98	0.45
3:I:56:THR:HA	3:I:59:THR:HG22	1.97	0.45
6:V:121:ASN:HD22	7:Y:147:LEU:HD22	1.80	0.45
1:d:137:ILE:HG23	1:d:158:LEU:HD21	1.98	0.45
1:u:198:VAL:HG12	1:u:215:ILE:HD13	1.97	0.45
1:v:127:PHE:HZ	1:w:133:LEU:HD22	1.81	0.45
3:F:195:MET:HE2	3:F:195:MET:HB3	1.81	0.45
7:a:23:VAL:HG11	7:a:47:ILE:HG13	1.99	0.45
8:z:20:LEU:HD22	8:z:69:ILE:HG23	1.98	0.45
1:f:163:LYS:HA	1:f:170:GLN:HE22	1.81	0.45
1:j:101:LEU:O	1:j:105:GLU:HA	2.15	0.45
1:m:177:VAL:HG21	1:m:201:ILE:HD13	1.99	0.45
3:H:69:THR:HG22	3:H:108:MET:HE2	1.97	0.45
3:H:204:ILE:HG13	3:I:230:PRO:HG2	1.98	0.45
1:d:141:VAL:HG21	1:d:205:ILE:HD11	1.99	0.45
1:n:135:ARG:HD3	1:o:114:TRP:HB2	1.99	0.45
2:A:58:LEU:HD21	2:A:114:SER:HA	1.98	0.45
3:F:161:MET:HE1	3:F:175:VAL:HG13	1.98	0.45
3:I:64:PHE:O	3:I:68:MET:CB	2.64	0.45
3:I:149:MET:HE3	3:I:149:MET:HB3	1.92	0.45
4:K:110:GLY:HA3	4:K:224:PHE:CZ	2.52	0.45
6:U:122:VAL:HA	6:U:125:HIS:NE2	2.32	0.45
1:h:159:VAL:HG13	1:i:206:GLU:HG2	1.98	0.45
1:k:155:SER:HB2	1:k:178:ARG:HH21	1.82	0.45
1:l:54:PHE:CZ	1:l:107:VAL:HG11	2.51	0.45
1:p:138:THR:HG23	1:p:156:VAL:HG23	1.99	0.45
3:F:191:VAL:O	3:F:195:MET:HG2	2.17	0.45
1:c:69:GLN:HG3	1:y:108:PRO:HA	1.99	0.45
3:G:179:VAL:HA	3:H:106:PHE:HZ	1.81	0.45
3:I:238:MET:HE2	8:2:70:LEU:HD21	1.99	0.45
4:K:22:PRO:HB3	4:K:80:GLU:HG3	1.97	0.45
1:i:64:LEU:HD11	1:i:80:LEU:HD11	1.99	0.45
3:F:74:ILE:HA	3:F:249:LEU:HD21	1.98	0.45
1:c:174:LYS:HE3	1:d:203:TYR:HA	1.99	0.45
1:i:69:GLN:O	1:i:73:ARG:HG2	2.17	0.45
1:n:187:ILE:HG23	1:n:188:ILE:HD12	1.99	0.45
4:K:109:ILE:HD12	4:K:228:LEU:HA	1.99	0.45
6:T:1:MET:HE1	6:T:6:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:30:ALA:HB1	7:Z:75:VAL:HG12	1.99	0.45
8:3:24:MET:HE3	8:3:24:MET:HB2	1.86	0.45
1:m:197:LEU:HA	1:m:200:LEU:HD23	1.99	0.45
1:u:158:LEU:HD13	1:u:160:MET:HE3	1.99	0.45
3:J:215:MET:HE3	3:J:215:MET:HB3	1.76	0.45
4:K:21:LEU:HD22	5:Q:93:LEU:HD22	1.99	0.45
7:a:20:ARG:HD3	7:a:125:ALA:HB2	1.99	0.45
7:a:27:ASN:ND2	7:a:44:ARG:HG3	2.32	0.45
1:v:208:LEU:HD21	1:v:213:ILE:HB	1.98	0.44
7:a:28:ILE:HA	7:a:31:VAL:HG23	1.99	0.44
1:d:127:PHE:HA	1:d:130:SER:HB3	1.98	0.44
1:l:115:ALA:HA	1:l:118:ASP:HB2	1.99	0.44
1:q:115:ALA:HA	1:q:118:ASP:HB2	1.98	0.44
1:w:216:VAL:HG21	1:x:200:LEU:HB3	1.99	0.44
2:A:100:ILE:HG23	8:z:59:LEU:HD12	1.99	0.44
3:J:52:LEU:HD21	5:P:97:VAL:HG21	1.99	0.44
6:V:109:LEU:HD22	7:b:135:VAL:HG22	1.99	0.44
1:g:141:VAL:HG21	1:g:205:ILE:HD11	1.99	0.44
1:n:175:ALA:HB3	1:n:213:ILE:HG23	1.99	0.44
1:q:169:SER:HB3	1:r:167:LYS:HZ2	1.81	0.44
1:r:93:LEU:HD13	1:r:96:LYS:HD3	2.00	0.44
2:A:249:LYS:HE3	2:A:249:LYS:HB3	1.83	0.44
1:l:80:LEU:HD12	1:l:86:ILE:HD12	2.00	0.44
3:G:244:LEU:HD23	8:z:81:PHE:HD2	1.83	0.44
3:I:55:LEU:HD22	5:N:99:ARG:HD2	2.00	0.44
4:K:240:PRO:HD3	8:3:11:ARG:NH1	2.33	0.44
7:X:59:LYS:HD2	7:X:59:LYS:HA	1.78	0.44
1:f:66:ARG:HB3	1:f:106:LEU:HD13	1.98	0.44
1:v:180:THR:HA	1:v:218:ASN:HB3	2.00	0.44
3:H:145:MET:HE1	3:H:181:ILE:HG12	1.99	0.44
5:O:69:LEU:HD13	5:O:69:LEU:HA	1.79	0.44
1:t:157:ASN:HD22	1:u:204:ALA:HB1	1.83	0.44
3:H:51:LEU:HD21	6:T:134:LEU:HD13	1.99	0.44
1:j:156:VAL:HG12	1:j:177:VAL:HG13	1.99	0.44
1:s:198:VAL:HG12	1:s:215:ILE:HD13	1.99	0.44
3:G:77:VAL:O	3:G:81:ILE:HG12	2.18	0.44
5:O:80:VAL:HG11	7:b:149:ILE:HG23	1.99	0.44
5:P:96:VAL:HG23	5:Q:83:MET:HE3	1.99	0.44
7:W:95:HIS:HA	7:Y:46:ARG:NH2	2.32	0.44
7:Y:147:LEU:HD23	7:Y:147:LEU:HA	1.84	0.44
1:e:58:ILE:HG13	1:e:60:ASP:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:58:ILE:HG22	1:n:60:ASP:H	1.82	0.44
1:q:92:LYS:HG3	1:q:93:LEU:HD22	1.98	0.44
1:r:128:GLU:HG3	1:s:129:ARG:HH22	1.82	0.44
5:L:83:MET:HG2	6:R:125:HIS:CG	2.53	0.44
5:M:85:LYS:HE3	5:M:85:LYS:HB2	1.84	0.44
3:G:206:LEU:HA	3:G:209:ILE:HG22	2.00	0.44
3:G:238:MET:HE3	3:G:238:MET:HB3	1.66	0.44
3:J:194:LYS:HE2	4:K:142:SER:HB3	2.00	0.44
8:1:14:ILE:HA	8:1:17:ILE:HD12	2.00	0.44
1:h:175:ALA:HB3	1:h:213:ILE:HG23	2.00	0.43
1:k:195:GLU:HA	1:k:198:VAL:HG22	2.00	0.43
1:v:195:GLU:HA	1:v:198:VAL:HG12	2.00	0.43
1:w:108:PRO:HG3	1:x:69:GLN:HE22	1.83	0.43
1:c:70:ARG:HG3	1:c:97:MET:HE1	2.00	0.43
1:c:159:VAL:HG13	1:d:206:GLU:HB3	2.00	0.43
1:l:155:SER:HB2	1:l:178:ARG:HH21	1.82	0.43
1:v:88:LEU:HD23	1:v:93:LEU:HG	1.99	0.43
3:J:140:PRO:HA	3:J:143:ILE:HG12	2.00	0.43
4:K:89:PHE:O	4:K:93:ILE:HG13	2.18	0.43
7:W:31:VAL:HG12	7:W:113:VAL:HG11	2.00	0.43
8:3:27:ILE:HG13	8:3:61:VAL:HG21	2.00	0.43
1:t:198:VAL:HG12	1:t:215:ILE:HD13	1.99	0.43
2:A:188:ILE:HG21	4:K:199:LEU:HD12	2.00	0.43
3:I:238:MET:HB3	3:I:238:MET:HE3	1.81	0.43
5:O:83:MET:HG2	6:U:125:HIS:CG	2.52	0.43
7:Z:127:ARG:HA	7:Z:127:ARG:HD2	1.83	0.43
1:k:127:PHE:HE2	1:l:129:ARG:HB3	1.84	0.43
3:F:85:LEU:HD22	3:F:233:LEU:HD23	1.99	0.43
3:F:138:ILE:HD12	3:F:138:ILE:HA	1.92	0.43
3:G:142:ARG:HA	3:G:145:MET:HE3	2.00	0.43
3:G:197:ILE:HD13	3:G:197:ILE:HA	1.67	0.43
5:P:81:ILE:HD13	7:W:11:SER:HB2	2.00	0.43
7:a:104:LYS:HA	7:a:104:LYS:HD3	1.84	0.43
8:1:24:MET:HE2	8:1:24:MET:HB3	1.83	0.43
8:2:79:MET:HE3	8:2:79:MET:HB3	1.88	0.43
1:h:202:GLN:HA	1:h:208:LEU:HD23	2.00	0.43
1:p:60:ASP:HB3	1:p:63:LEU:HB2	2.00	0.43
1:p:198:VAL:HG12	1:p:215:ILE:HD13	2.00	0.43
7:X:88:LYS:HD3	7:X:88:LYS:HA	1.82	0.43
1:m:80:LEU:HA	1:m:86:ILE:HG12	2.01	0.43
1:o:66:ARG:HB3	1:o:106:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:s:197:LEU:HA	1:s:200:LEU:HD23	2.00	0.43
3:G:61:SER:HA	3:G:64:PHE:HB3	1.99	0.43
5:L:68:ILE:HG21	6:R:10:PHE:CE1	2.54	0.43
6:U:120:THR:HG22	7:a:149:ILE:HD11	2.00	0.43
6:V:39:ARG:HG2	6:V:99:ASN:HD22	1.84	0.43
1:t:126:ASP:C	1:t:128:GLU:H	2.27	0.43
3:F:176:PRO:HG2	3:F:179:VAL:HG12	2.00	0.43
8:3:48:THR:HA	8:3:51:PHE:HB2	1.99	0.43
1:f:124:ILE:HG23	1:f:129:ARG:HE	1.83	0.43
1:n:88:LEU:HD22	1:n:94:ALA:HA	2.01	0.43
1:r:50:SER:HA	1:r:87:TYR:HD1	1.83	0.43
1:s:80:LEU:H	1:s:86:ILE:HG23	1.84	0.43
4:K:65:TYR:HE1	4:K:76:ILE:HG21	1.84	0.43
1:g:155:SER:HB2	1:g:178:ARG:HH21	1.83	0.43
1:p:152:ASP:HB3	1:q:104:GLU:HG2	2.00	0.43
1:q:141:VAL:HG21	1:q:205:ILE:HD11	2.00	0.43
1:t:73:ARG:HA	1:t:73:ARG:HH11	1.84	0.43
1:t:159:VAL:HB	1:t:174:LYS:HG3	2.00	0.43
1:u:141:VAL:HG21	1:u:205:ILE:HD11	2.01	0.43
2:A:58:LEU:HD23	2:A:58:LEU:HA	1.90	0.43
2:A:107:VAL:O	2:A:111:PHE:HB2	2.19	0.43
1:h:126:ASP:C	1:h:128:GLU:H	2.27	0.43
2:A:132:PHE:HE2	2:A:133:LYS:HE2	1.84	0.43
7:W:93:PRO:HA	7:W:106:GLY:HA2	2.01	0.43
1:d:88:LEU:HD23	1:d:93:LEU:HD23	2.01	0.42
1:e:121:ARG:HH11	1:f:120:ASP:HB2	1.84	0.42
1:w:70:ARG:HH11	1:w:70:ARG:HA	1.83	0.42
7:Y:95:HIS:CE1	7:Y:97:ASP:HB2	2.53	0.42
1:j:66:ARG:HB3	1:j:106:LEU:HD13	2.00	0.42
1:q:195:GLU:HA	1:q:198:VAL:HG22	2.01	0.42
3:J:69:THR:HB	3:J:108:MET:SD	2.59	0.42
3:J:193:PHE:CG	4:K:36:PHE:HE1	2.37	0.42
4:K:225:SER:HB2	8:3:25:LEU:HD22	2.00	0.42
8:3:70:LEU:HD23	8:3:70:LEU:HA	1.85	0.42
8:3:72:LYS:HE3	8:3:72:LYS:HB3	1.84	0.42
1:e:109:VAL:HB	1:f:66:ARG:HH12	1.84	0.42
1:s:115:ALA:HA	1:s:118:ASP:HB2	2.02	0.42
3:G:205:VAL:HA	8:z:17:ILE:HD11	2.00	0.42
6:R:114:MET:HE3	7:X:143:PHE:CG	2.55	0.42
1:c:202:GLN:HA	1:c:208:LEU:HD23	2.00	0.42
1:m:107:VAL:HG23	1:m:108:PRO:HD3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:219:MET:HE3	3:J:219:MET:HB3	1.81	0.42
8:z:29:LEU:HD11	8:1:49:LEU:HD23	2.02	0.42
3:G:72:LEU:HD23	3:H:95:ILE:HD13	2.01	0.42
1:d:160:MET:HE3	1:d:160:MET:HB2	1.83	0.42
1:r:190:ASN:HB3	1:r:193:LYS:HB2	2.02	0.42
2:A:42:ARG:HE	2:A:233:TYR:HE1	1.67	0.42
3:I:234:ILE:O	3:I:238:MET:HB2	2.19	0.42
7:W:126:SER:O	7:W:130:GLU:HG2	2.19	0.42
1:m:138:THR:HG23	1:m:156:VAL:HG23	2.02	0.42
1:p:115:ALA:HA	1:p:118:ASP:HB2	2.02	0.42
1:p:141:VAL:HG21	1:p:205:ILE:HD11	2.02	0.42
3:F:180:LEU:HD12	3:F:180:LEU:HA	1.78	0.42
3:F:234:ILE:HG12	4:K:190:LEU:HD21	2.02	0.42
3:J:161:MET:HE1	3:J:166:TYR:HB2	2.01	0.42
1:u:66:ARG:HB3	1:u:106:LEU:HD23	2.01	0.42
1:u:216:VAL:HG21	1:v:200:LEU:HB3	2.02	0.42
6:V:48:LEU:HD12	6:V:81:VAL:HG11	2.00	0.42
1:c:128:GLU:HA	1:c:131:ILE:HG22	2.01	0.42
1:d:124:ILE:HD12	1:d:124:ILE:HA	1.88	0.42
1:f:155:SER:HB3	1:f:178:ARG:HE	1.85	0.42
1:f:164:ALA:H	1:f:170:GLN:HE22	1.67	0.42
1:h:58:ILE:HG22	1:h:60:ASP:H	1.84	0.42
1:k:66:ARG:HB2	1:k:106:LEU:HD21	2.01	0.42
1:s:174:LYS:HE2	1:t:203:TYR:HA	2.00	0.42
1:u:177:VAL:HB	1:u:215:ILE:HG13	2.01	0.42
1:j:70:ARG:NH1	1:j:73:ARG:HG2	2.35	0.42
1:u:127:PHE:HA	1:u:130:SER:HB3	2.01	0.42
1:x:127:PHE:HA	1:x:130:SER:HB3	2.01	0.42
3:F:95:ILE:HD11	4:K:93:ILE:HG12	2.02	0.42
3:G:138:ILE:HD12	3:G:138:ILE:HA	1.95	0.42
1:e:53:LEU:HD22	1:e:98:ARG:HG3	2.01	0.41
1:f:190:ASN:HB3	1:f:193:LYS:HB2	2.02	0.41
1:g:88:LEU:HD22	1:g:94:ALA:HA	2.02	0.41
1:x:54:PHE:CE1	1:x:107:VAL:HG11	2.54	0.41
1:y:138:THR:HG23	1:y:156:VAL:HG23	2.01	0.41
4:K:54:SER:O	4:K:58:VAL:HB	2.20	0.41
5:O:105:GLN:O	5:O:108:ILE:HG13	2.19	0.41
1:r:165:LEU:HD23	1:r:165:LEU:HA	1.92	0.41
2:A:48:GLU:HA	2:A:51:THR:HG22	2.02	0.41
3:F:166:TYR:CE2	3:F:176:PRO:HG3	2.55	0.41
3:F:242:TRP:O	3:F:246:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:97:MET:HE1	5:M:110:ILE:HB	2.02	0.41
1:j:108:PRO:HA	1:k:69:GLN:HG3	2.01	0.41
1:j:194:VAL:HG11	1:j:223:LEU:HB3	2.02	0.41
1:q:51:ILE:H	1:q:88:LEU:H	1.67	0.41
1:u:175:ALA:HB3	1:u:213:ILE:HG23	2.02	0.41
1:x:70:ARG:HD2	1:x:70:ARG:HA	1.88	0.41
3:F:108:MET:HE2	3:F:108:MET:HB3	1.90	0.41
8:1:52:ILE:O	8:1:56:ILE:HG12	2.19	0.41
1:l:143:GLN:HA	1:l:146:VAL:HG12	2.01	0.41
1:t:195:GLU:HA	1:t:198:VAL:HG22	2.02	0.41
1:u:63:LEU:HD13	1:u:63:LEU:HA	1.95	0.41
1:u:131:ILE:HD13	1:u:131:ILE:HA	1.84	0.41
1:y:160:MET:HA	1:y:173:VAL:HG22	2.02	0.41
2:A:85:PRO:HG2	3:F:251:LYS:HE3	2.03	0.41
8:2:26:ILE:HD12	8:2:26:ILE:HA	1.86	0.41
1:u:50:SER:HA	1:u:87:TYR:HD2	1.84	0.41
3:H:217:MET:HG3	8:1:58:ILE:HG21	2.03	0.41
6:V:114:MET:HE3	6:V:114:MET:HB2	1.94	0.41
8:z:16:ASN:HA	8:z:19:ILE:HG22	2.01	0.41
1:k:171:GLU:HA	1:k:172:PRO:HD3	1.95	0.41
1:l:121:ARG:HE	1:l:124:ILE:HB	1.85	0.41
3:F:198:LEU:HD23	3:F:198:LEU:HA	1.95	0.41
3:G:50:GLN:HG2	3:G:123:LEU:HG	2.02	0.41
3:I:64:PHE:O	3:I:68:MET:HB3	2.21	0.41
3:I:143:ILE:HD12	3:I:143:ILE:HA	1.94	0.41
5:P:69:LEU:HD13	5:P:69:LEU:HA	1.82	0.41
5:P:75:ASP:O	5:P:79:VAL:HG13	2.21	0.41
7:Y:44:ARG:HH12	7:Y:46:ARG:NH1	2.19	0.41
1:k:66:ARG:HB3	1:k:106:LEU:HD11	2.03	0.41
2:A:37:ALA:HB1	2:A:42:ARG:HG3	2.02	0.41
4:K:16:LYS:HD3	4:K:16:LYS:HA	1.90	0.41
4:K:116:ILE:H	4:K:116:ILE:HG12	1.64	0.41
5:O:90:LEU:HD21	6:U:133:VAL:HB	2.03	0.41
5:O:99:ARG:HD3	5:O:99:ARG:HA	1.87	0.41
5:Q:106:ASP:O	5:Q:110:ILE:HG13	2.21	0.41
1:c:67:ILE:HG12	1:c:71:LEU:HD23	2.02	0.41
1:i:131:ILE:HD13	1:i:131:ILE:HA	1.89	0.41
1:j:142:GLU:HG2	1:j:156:VAL:HG22	2.02	0.41
1:p:145:ILE:HD11	1:p:201:ILE:HD13	2.03	0.41
1:t:161:PRO:HD2	1:t:173:VAL:HG22	2.03	0.41
1:t:178:ARG:HH12	1:u:147:ALA:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:188:ILE:HD11	1:u:221:THR:HG21	2.03	0.41
1:w:212:ASN:HA	1:x:203:TYR:HE2	1.85	0.41
3:F:95:ILE:HD12	4:K:89:PHE:CE1	2.56	0.41
6:S:116:TYR:CD2	7:X:142:MET:HG3	2.55	0.41
7:W:43:ARG:HB2	7:W:82:LYS:HD3	2.03	0.41
1:c:78:TYR:CE2	1:c:80:LEU:HB2	2.56	0.41
1:d:212:ASN:HA	1:e:203:TYR:HE2	1.86	0.41
1:g:101:LEU:HD22	1:g:106:LEU:HD11	2.02	0.41
1:h:69:GLN:HE21	1:h:69:GLN:HB3	1.62	0.41
1:l:208:LEU:HD23	1:l:208:LEU:HA	1.86	0.41
1:m:127:PHE:HA	1:m:130:SER:HB3	2.03	0.41
1:q:216:VAL:HG21	1:r:200:LEU:HB3	2.02	0.41
1:r:127:PHE:HD1	1:s:129:ARG:HH11	1.69	0.41
1:r:222:ILE:HD13	1:r:222:ILE:HA	1.96	0.41
1:u:222:ILE:HD11	1:v:196:GLY:HA2	2.02	0.41
1:x:96:LYS:HE2	1:x:96:LYS:HB3	1.86	0.41
3:F:78:LEU:HD23	3:F:81:ILE:HD12	2.02	0.41
3:H:200:PHE:CD1	3:I:230:PRO:HG3	2.56	0.41
3:I:206:LEU:HA	3:I:209:ILE:HG22	2.03	0.41
6:T:127:PHE:HA	6:T:130:ILE:HG22	2.03	0.41
6:U:92:THR:HA	6:U:99:ASN:HB3	2.03	0.41
7:a:42:TYR:HB3	7:a:111:PRO:HG3	2.03	0.41
8:3:35:ILE:HD11	8:3:53:PRO:HB2	2.03	0.41
1:y:131:ILE:HD13	1:y:131:ILE:HA	1.89	0.41
3:H:186:LEU:HD23	3:H:186:LEU:HA	1.91	0.41
3:I:201:LEU:HD23	3:I:204:ILE:HD12	2.03	0.41
5:N:80:VAL:HA	5:N:83:MET:HE3	2.03	0.41
7:a:60:GLY:HA2	7:a:61:PRO:HD3	1.95	0.41
8:2:54:LYS:HE2	8:3:48:THR:HG21	2.03	0.41
8:3:12:ILE:HD12	8:3:12:ILE:HA	1.94	0.41
1:d:107:VAL:HG23	1:d:108:PRO:HD3	2.03	0.40
1:j:93:LEU:HD13	1:j:93:LEU:HA	1.95	0.40
1:p:201:ILE:HG23	1:p:213:ILE:HD13	2.03	0.40
1:s:70:ARG:HD2	1:s:70:ARG:HA	1.90	0.40
3:I:219:MET:HE2	3:I:219:MET:HB2	1.80	0.40
3:J:141:LEU:HD13	3:J:141:LEU:HA	1.91	0.40
4:K:25:VAL:HG21	4:K:77:LEU:HD22	2.03	0.40
1:i:222:ILE:HD13	1:i:222:ILE:HA	1.87	0.40
1:u:159:VAL:HG11	1:v:206:GLU:HA	2.04	0.40
3:G:88:GLN:HG3	4:K:120:PHE:HA	2.04	0.40
3:H:67:LEU:HD22	3:H:185:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:81:ILE:HG13	3:H:199:ILE:HD13	2.02	0.40
5:L:92:ILE:HD13	5:L:92:ILE:HA	1.93	0.40
7:X:52:ARG:HG2	7:X:76:ARG:HB2	2.03	0.40
1:h:174:LYS:HD2	1:i:203:TYR:HA	2.03	0.40
1:q:160:MET:HE2	1:q:160:MET:HB2	1.95	0.40
3:F:112:PHE:HA	3:F:115:ILE:HG12	2.03	0.40
3:J:74:ILE:HD13	3:J:103:LEU:HB3	2.04	0.40
1:k:138:THR:HG23	1:k:156:VAL:HG23	2.03	0.40
1:p:141:VAL:HG12	1:p:156:VAL:HG21	2.03	0.40
1:p:155:SER:HB3	1:p:178:ARG:HE	1.87	0.40
1:p:222:ILE:HD11	1:q:196:GLY:HA2	2.02	0.40
1:r:70:ARG:HA	1:r:70:ARG:HH11	1.86	0.40
1:t:202:GLN:HE21	1:t:209:GLU:HA	1.85	0.40
2:A:50:ASN:N	2:A:125:GLN:HE22	2.19	0.40
3:J:201:LEU:HD23	3:J:201:LEU:HA	1.93	0.40
8:1:26:ILE:HD12	8:1:26:ILE:HA	1.90	0.40
1:c:195:GLU:HA	1:c:198:VAL:HG12	2.03	0.40
1:e:195:GLU:HA	1:e:198:VAL:HG22	2.03	0.40
1:g:142:GLU:HG3	1:g:156:VAL:HG22	2.03	0.40
1:i:58:ILE:H	1:i:58:ILE:HG12	1.69	0.40
1:i:127:PHE:HA	1:i:130:SER:HB3	2.03	0.40
1:i:156:VAL:HG12	1:i:177:VAL:HG22	2.02	0.40
1:k:92:LYS:HE2	1:k:92:LYS:HB2	1.97	0.40
1:p:194:VAL:HG22	1:p:223:LEU:HD13	2.03	0.40
1:x:155:SER:HB2	1:x:178:ARG:HH21	1.87	0.40
3:H:65:LEU:HD23	3:H:69:THR:HG21	2.04	0.40
3:J:81:ILE:HD13	3:J:199:ILE:HG21	2.03	0.40
7:Y:43:ARG:HH21	7:Y:84:LYS:HA	1.85	0.40
8:z:59:LEU:HD13	8:z:59:LEU:HA	1.86	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	c	177/569 (31%)	164 (93%)	12 (7%)	1 (1%)	21	55
1	d	177/569 (31%)	160 (90%)	16 (9%)	1 (1%)	21	55
1	e	177/569 (31%)	161 (91%)	16 (9%)	0	100	100
1	f	174/569 (31%)	160 (92%)	13 (8%)	1 (1%)	21	55
1	g	173/569 (30%)	162 (94%)	11 (6%)	0	100	100
1	h	174/569 (31%)	158 (91%)	15 (9%)	1 (1%)	21	55
1	i	177/569 (31%)	164 (93%)	13 (7%)	0	100	100
1	j	177/569 (31%)	159 (90%)	18 (10%)	0	100	100
1	k	177/569 (31%)	158 (89%)	19 (11%)	0	100	100
1	l	177/569 (31%)	163 (92%)	12 (7%)	2 (1%)	11	43
1	m	177/569 (31%)	165 (93%)	12 (7%)	0	100	100
1	n	177/569 (31%)	161 (91%)	16 (9%)	0	100	100
1	o	177/569 (31%)	166 (94%)	10 (6%)	1 (1%)	21	55
1	p	177/569 (31%)	161 (91%)	16 (9%)	0	100	100
1	q	177/569 (31%)	162 (92%)	15 (8%)	0	100	100
1	r	177/569 (31%)	160 (90%)	17 (10%)	0	100	100
1	s	177/569 (31%)	164 (93%)	13 (7%)	0	100	100
1	t	177/569 (31%)	167 (94%)	8 (4%)	2 (1%)	11	43
1	u	169/569 (30%)	160 (95%)	8 (5%)	1 (1%)	21	55
1	v	169/569 (30%)	159 (94%)	10 (6%)	0	100	100
1	w	177/569 (31%)	162 (92%)	14 (8%)	1 (1%)	21	55
1	x	177/569 (31%)	162 (92%)	13 (7%)	2 (1%)	11	43
1	y	177/569 (31%)	162 (92%)	15 (8%)	0	100	100
2	A	240/372 (64%)	231 (96%)	8 (3%)	1 (0%)	30	64
3	F	207/254 (82%)	205 (99%)	2 (1%)	0	100	100
3	G	207/254 (82%)	199 (96%)	8 (4%)	0	100	100
3	H	207/254 (82%)	202 (98%)	5 (2%)	0	100	100
3	I	207/254 (82%)	201 (97%)	6 (3%)	0	100	100
3	J	207/254 (82%)	206 (100%)	1 (0%)	0	100	100
4	K	257/269 (96%)	246 (96%)	11 (4%)	0	100	100
5	L	68/111 (61%)	66 (97%)	2 (3%)	0	100	100
5	M	68/111 (61%)	68 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	N	68/111 (61%)	68 (100%)	0	0	100	100
5	O	68/111 (61%)	68 (100%)	0	0	100	100
5	P	68/111 (61%)	66 (97%)	2 (3%)	0	100	100
5	Q	38/111 (34%)	38 (100%)	0	0	100	100
6	R	108/135 (80%)	108 (100%)	0	0	100	100
6	S	108/135 (80%)	108 (100%)	0	0	100	100
6	T	108/135 (80%)	108 (100%)	0	0	100	100
6	U	108/135 (80%)	106 (98%)	2 (2%)	0	100	100
6	V	108/135 (80%)	103 (95%)	5 (5%)	0	100	100
7	W	132/152 (87%)	132 (100%)	0	0	100	100
7	X	150/152 (99%)	146 (97%)	4 (3%)	0	100	100
7	Y	132/152 (87%)	130 (98%)	2 (2%)	0	100	100
7	Z	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
7	a	150/152 (99%)	148 (99%)	2 (1%)	0	100	100
7	b	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
8	1	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
8	2	85/87 (98%)	85 (100%)	0	0	100	100
8	3	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
8	z	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
All	All	7699/17599 (44%)	7301 (95%)	384 (5%)	14 (0%)	44	74

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	h	76	VAL
1	l	109	VAL
1	c	90	ASP
1	f	110	HIS
1	d	110	HIS
1	t	171	GLU
1	x	171	GLU
2	A	91	SER
1	l	168	GLU
1	t	90	ASP
1	w	168	GLU

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Mol	Chain	Res	Type
1	o	90	ASP
1	u	109	VAL
1	x	109	VAL

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	c	151/506 (30%)	142 (94%)	9 (6%)	17	44
1	d	148/506 (29%)	141 (95%)	7 (5%)	23	48
1	e	150/506 (30%)	148 (99%)	2 (1%)	61	71
1	f	151/506 (30%)	142 (94%)	9 (6%)	17	44
1	g	150/506 (30%)	145 (97%)	5 (3%)	33	56
1	h	147/506 (29%)	137 (93%)	10 (7%)	14	41
1	i	150/506 (30%)	147 (98%)	3 (2%)	48	65
1	j	149/506 (29%)	143 (96%)	6 (4%)	28	51
1	k	149/506 (29%)	145 (97%)	4 (3%)	39	59
1	l	148/506 (29%)	142 (96%)	6 (4%)	27	51
1	m	151/506 (30%)	147 (97%)	4 (3%)	40	60
1	n	146/506 (29%)	143 (98%)	3 (2%)	47	64
1	o	149/506 (29%)	147 (99%)	2 (1%)	61	71
1	p	149/506 (29%)	140 (94%)	9 (6%)	17	44
1	q	150/506 (30%)	144 (96%)	6 (4%)	28	51
1	r	152/506 (30%)	143 (94%)	9 (6%)	18	44
1	s	152/506 (30%)	146 (96%)	6 (4%)	28	52
1	t	150/506 (30%)	140 (93%)	10 (7%)	15	41
1	u	146/506 (29%)	138 (94%)	8 (6%)	19	46
1	v	146/506 (29%)	141 (97%)	5 (3%)	32	55
1	w	148/506 (29%)	143 (97%)	5 (3%)	32	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	145/506 (29%)	137 (94%)	8 (6%)	19	46
1	y	150/506 (30%)	143 (95%)	7 (5%)	23	48
2	A	217/335 (65%)	209 (96%)	8 (4%)	30	53
3	F	187/232 (81%)	183 (98%)	4 (2%)	47	64
3	G	185/232 (80%)	175 (95%)	10 (5%)	20	46
3	H	185/232 (80%)	183 (99%)	2 (1%)	65	73
3	I	187/232 (81%)	182 (97%)	5 (3%)	39	59
3	J	189/232 (82%)	172 (91%)	17 (9%)	9	31
4	K	236/249 (95%)	222 (94%)	14 (6%)	18	44
5	L	64/103 (62%)	60 (94%)	4 (6%)	16	42
5	M	64/103 (62%)	57 (89%)	7 (11%)	6	24
5	N	64/103 (62%)	60 (94%)	4 (6%)	16	42
5	O	62/103 (60%)	58 (94%)	4 (6%)	15	42
5	P	64/103 (62%)	58 (91%)	6 (9%)	8	29
5	Q	35/103 (34%)	32 (91%)	3 (9%)	10	33
6	R	107/129 (83%)	103 (96%)	4 (4%)	30	53
6	S	107/129 (83%)	104 (97%)	3 (3%)	38	59
6	T	107/129 (83%)	105 (98%)	2 (2%)	50	66
6	U	107/129 (83%)	103 (96%)	4 (4%)	30	53
6	V	107/129 (83%)	103 (96%)	4 (4%)	30	53
7	W	115/130 (88%)	114 (99%)	1 (1%)	70	75
7	X	127/130 (98%)	125 (98%)	2 (2%)	55	68
7	Y	116/130 (89%)	114 (98%)	2 (2%)	53	67
7	Z	130/130 (100%)	127 (98%)	3 (2%)	44	63
7	a	130/130 (100%)	127 (98%)	3 (2%)	44	63
7	b	130/130 (100%)	128 (98%)	2 (2%)	57	69
8	1	78/80 (98%)	69 (88%)	9 (12%)	5	22
8	2	80/80 (100%)	75 (94%)	5 (6%)	16	42
8	3	80/80 (100%)	77 (96%)	3 (4%)	29	52
8	z	77/80 (96%)	72 (94%)	5 (6%)	15	42
All	All	6764/15745 (43%)	6481 (96%)	283 (4%)	28	50

All (283) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	51	ILE
1	c	56	VAL
1	c	58	ILE
1	c	71	LEU
1	c	105	GLU
1	c	157	ASN
1	c	158	LEU
1	c	200	LEU
1	c	221	THR
1	d	93	LEU
1	d	107	VAL
1	d	110	HIS
1	d	146	VAL
1	d	156	VAL
1	d	197	LEU
1	d	215	ILE
1	e	76	VAL
1	e	81	SER
1	f	73	ARG
1	f	76	VAL
1	f	110	HIS
1	f	146	VAL
1	f	156	VAL
1	f	171	GLU
1	f	206	GLU
1	f	213	ILE
1	f	215	ILE
1	g	51	ILE
1	g	107	VAL
1	g	128	GLU
1	g	146	VAL
1	g	206	GLU
1	h	56	VAL
1	h	64	LEU
1	h	73	ARG
1	h	76	VAL
1	h	80	LEU
1	h	86	ILE
1	h	107	VAL
1	h	124	ILE
1	h	158	LEU
1	h	213	ILE

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Mol	Chain	Res	Type
1	i	72	ASP
1	i	197	LEU
1	i	208	LEU
1	j	51	ILE
1	j	56	VAL
1	j	71	LEU
1	j	165	LEU
1	j	192	LYS
1	j	213	ILE
1	k	57	GLU
1	k	102	VAL
1	k	213	ILE
1	k	221	THR
1	l	64	LEU
1	l	74	GLU
1	l	86	ILE
1	l	107	VAL
1	l	124	ILE
1	l	135	ARG
1	m	56	VAL
1	m	64	LEU
1	m	146	VAL
1	m	200	LEU
1	n	51	ILE
1	n	124	ILE
1	n	160	MET
1	o	76	VAL
1	o	206	GLU
1	p	76	VAL
1	p	93	LEU
1	p	105	GLU
1	p	118	ASP
1	p	141	VAL
1	p	200	LEU
1	p	201	ILE
1	p	213	ILE
1	p	221	THR
1	q	78	TYR
1	q	124	ILE
1	q	146	VAL
1	q	160	MET
1	q	171	GLU

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Mol	Chain	Res	Type
1	q	215	ILE
1	r	57	GLU
1	r	63	LEU
1	r	71	LEU
1	r	86	ILE
1	r	105	GLU
1	r	107	VAL
1	r	146	VAL
1	r	156	VAL
1	r	200	LEU
1	s	51	ILE
1	s	58	ILE
1	s	76	VAL
1	s	107	VAL
1	s	200	LEU
1	s	216	VAL
1	t	51	ILE
1	t	73	ARG
1	t	76	VAL
1	t	86	ILE
1	t	93	LEU
1	t	152	ASP
1	t	174	LYS
1	t	197	LEU
1	t	213	ILE
1	t	216	VAL
1	u	51	ILE
1	u	64	LEU
1	u	80	LEU
1	u	110	HIS
1	u	146	VAL
1	u	156	VAL
1	u	158	LEU
1	u	213	ILE
1	v	74	GLU
1	v	107	VAL
1	v	124	ILE
1	v	125	THR
1	v	213	ILE
1	w	51	ILE
1	w	56	VAL
1	w	158	LEU

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Mol	Chain	Res	Type
1	w	173	VAL
1	w	216	VAL
1	x	51	ILE
1	x	101	LEU
1	x	110	HIS
1	x	125	THR
1	x	146	VAL
1	x	192	LYS
1	x	213	ILE
1	x	216	VAL
1	y	51	ILE
1	y	76	VAL
1	y	146	VAL
1	y	165	LEU
1	y	192	LYS
1	y	199	LYS
1	y	200	LEU
2	A	87	VAL
2	A	94	THR
2	A	106	TYR
2	A	130	ILE
2	A	163	LEU
2	A	167	LEU
2	A	193	GLU
2	A	243	GLU
3	F	66	VAL
3	F	128	ILE
3	F	222	LEU
3	F	235	LEU
3	G	66	VAL
3	G	67	LEU
3	G	72	LEU
3	G	96	VAL
3	G	175	VAL
3	G	179	VAL
3	G	194	LYS
3	G	197	ILE
3	G	200	PHE
3	G	238	MET
3	H	66	VAL
3	H	219	MET
3	I	95	ILE

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Mol	Chain	Res	Type
3	I	141	LEU
3	I	215	MET
3	I	221	MET
3	I	229	LEU
3	J	53	ILE
3	J	66	VAL
3	J	97	MET
3	J	99	LEU
3	J	118	GLN
3	J	129	ASN
3	J	132	GLU
3	J	141	LEU
3	J	145	MET
3	J	146	TYR
3	J	159	LEU
3	J	167	ASP
3	J	200	PHE
3	J	204	ILE
3	J	217	MET
3	J	225	VAL
3	J	245	ILE
4	K	18	PHE
4	K	24	LEU
4	K	45	PHE
4	K	67	LEU
4	K	85	LEU
4	K	103	PHE
4	K	113	TYR
4	K	116	ILE
4	K	141	LEU
4	K	147	LEU
4	K	152	ILE
4	K	209	ILE
4	K	216	GLN
4	K	219	LEU
5	L	44	ASP
5	L	58	LEU
5	L	60	VAL
5	L	74	ILE
5	M	58	LEU
5	M	60	VAL
5	M	65	GLU

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Mol	Chain	Res	Type
5	M	69	LEU
5	M	76	VAL
5	M	81	ILE
5	M	83	MET
5	N	60	VAL
5	N	69	LEU
5	N	76	VAL
5	N	81	ILE
5	O	58	LEU
5	O	69	LEU
5	O	76	VAL
5	O	108	ILE
5	P	44	ASP
5	P	45	VAL
5	P	46	LEU
5	P	69	LEU
5	P	76	VAL
5	P	107	ILE
5	Q	76	VAL
5	Q	93	LEU
5	Q	108	ILE
6	R	3	ASP
6	R	8	VAL
6	R	15	LEU
6	R	100	VAL
6	S	48	LEU
6	S	52	PHE
6	S	130	ILE
6	T	100	VAL
6	T	112	ASN
6	U	15	LEU
6	U	18	LEU
6	U	53	LEU
6	U	134	LEU
6	V	15	LEU
6	V	20	LEU
6	V	34	THR
6	V	48	LEU
7	W	89	LEU
7	X	26	ASN
7	X	150	LEU
7	Y	75	VAL

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Mol	Chain	Res	Type
7	Y	115	LEU
7	Z	14	LEU
7	Z	57	TYR
7	Z	150	LEU
7	a	19	LEU
7	a	116	VAL
7	a	150	LEU
7	b	110	LEU
7	b	149	ILE
8	z	13	SER
8	z	26	ILE
8	z	59	LEU
8	z	62	ILE
8	z	70	LEU
8	1	7	LEU
8	1	14	ILE
8	1	16	ASN
8	1	24	MET
8	1	33	LEU
8	1	35	ILE
8	1	44	ILE
8	1	49	LEU
8	1	70	LEU
8	2	17	ILE
8	2	21	SER
8	2	26	ILE
8	2	49	LEU
8	2	84	LEU
8	3	7	LEU
8	3	34	LEU
8	3	80	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	d	157	ASN
1	d	228	ASN
1	e	228	ASN
1	f	157	ASN
1	f	170	GLN
1	f	218	ASN
1	g	224	ASN

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Mol	Chain	Res	Type
1	g	228	ASN
1	h	69	GLN
1	i	69	GLN
1	i	110	HIS
1	i	170	GLN
1	j	69	GLN
1	k	69	GLN
1	l	224	ASN
1	m	69	GLN
1	m	212	ASN
1	m	228	ASN
1	n	190	ASN
1	o	61	GLN
1	o	212	ASN
1	o	224	ASN
1	o	228	ASN
1	p	61	GLN
1	p	202	GLN
1	q	144	HIS
1	q	228	ASN
1	r	170	GLN
1	s	157	ASN
1	t	69	GLN
1	t	132	ASN
1	t	143	GLN
1	u	61	GLN
1	u	110	HIS
1	w	202	GLN
1	w	218	ASN
1	x	61	GLN
1	y	144	HIS
2	A	80	GLN
2	A	118	ASN
2	A	125	GLN
3	G	148	GLN
3	H	88	GLN
3	J	88	GLN
3	J	94	GLN
3	J	118	GLN
4	K	96	ASN
4	K	115	ASN
5	L	89	ASN

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Mol	Chain	Res	Type
5	M	54	ASN
5	M	57	GLN
5	M	59	ASN
5	M	109	ASN
5	O	57	GLN
5	O	66	GLN
5	Q	109	ASN
6	R	121	ASN
6	S	36	ASN
6	V	2	ASN
6	V	121	ASN
7	W	26	ASN
7	W	73	GLN
7	X	137	ASN
7	Y	27	ASN
7	Y	73	GLN
7	Y	95	HIS
7	Z	112	ASN
7	a	55	ASN
7	a	73	GLN
7	b	17	GLN
7	b	26	ASN
7	b	45	GLN
8	z	45	GLN
8	1	16	ASN
8	1	45	GLN
8	1	85	GLN
8	2	39	GLN
8	2	45	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

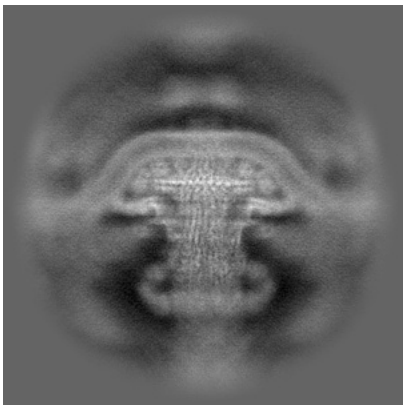
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-76347. These allow visual inspection of the internal detail of the map and identification of artifacts.

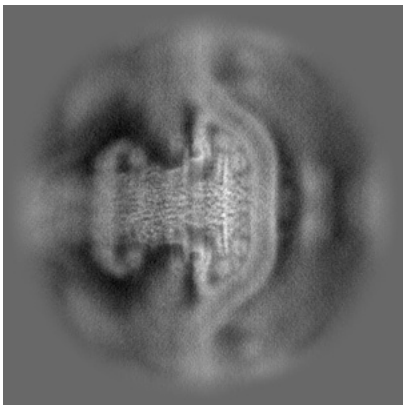
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

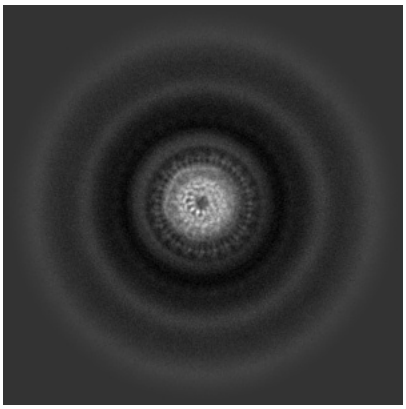
6.1.1 Primary map



X

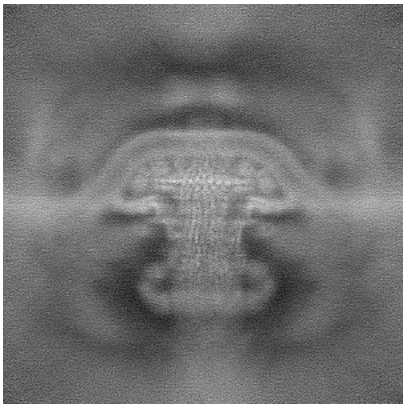


Y

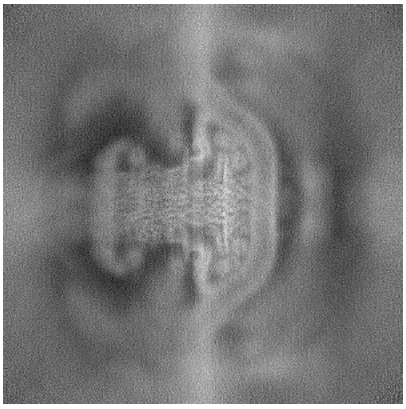


Z

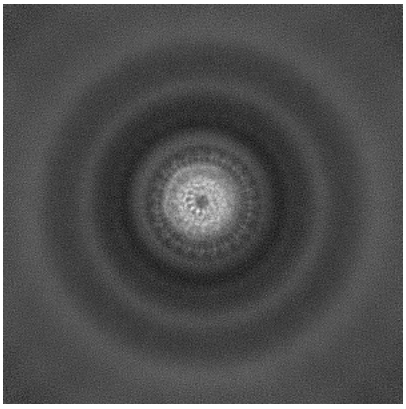
6.1.2 Raw map



X



Y

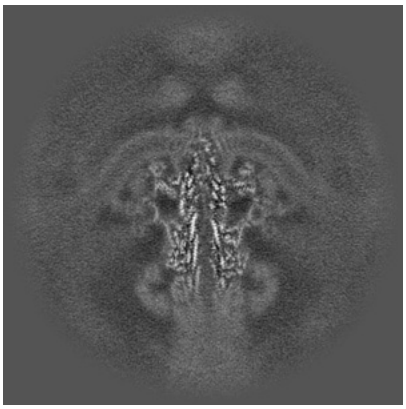


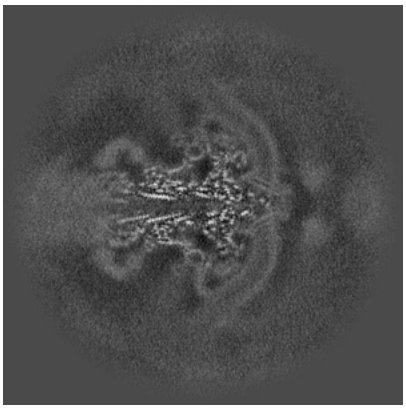
Z

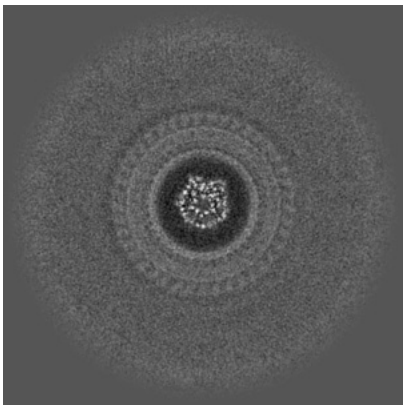
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

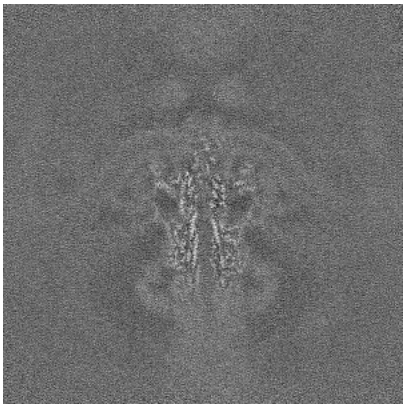
6.2.1 Primary map

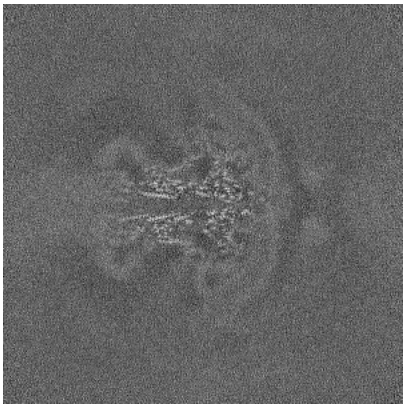

X Index: 224

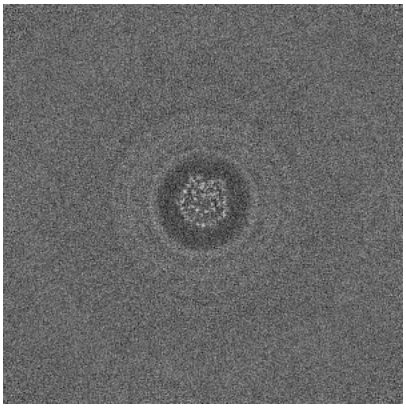

Y Index: 224


Z Index: 224

6.2.2 Raw map


X Index: 224

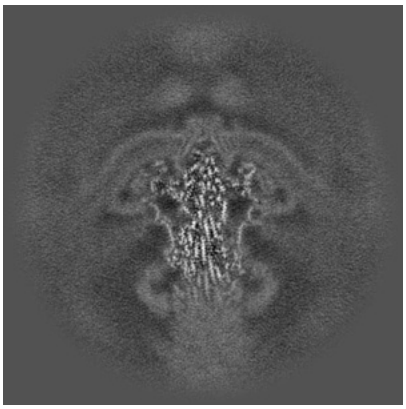

Y Index: 224


Z Index: 224

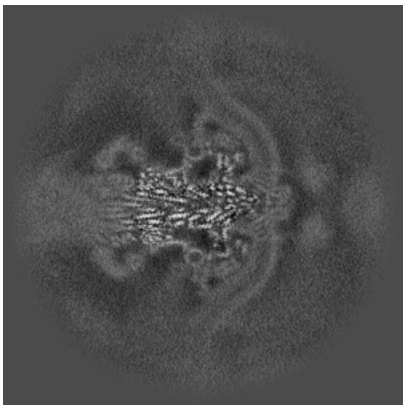
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

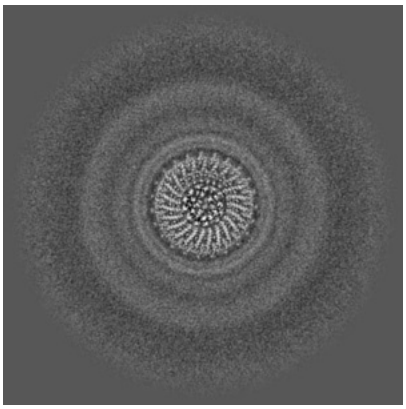
6.3.1 Primary map



X Index: 233

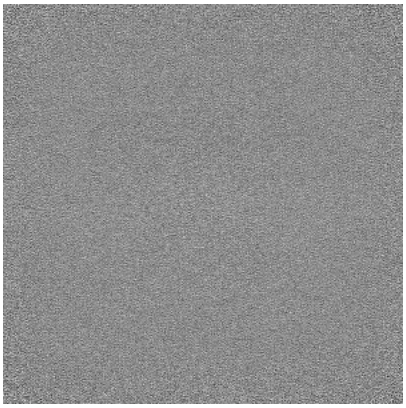


Y Index: 218

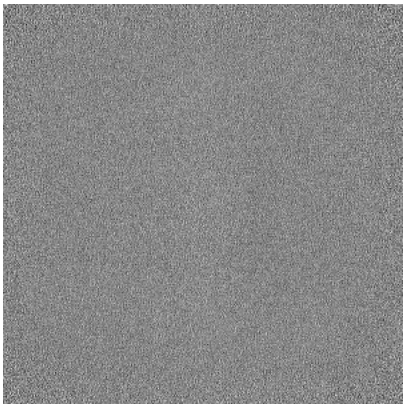


Z Index: 249

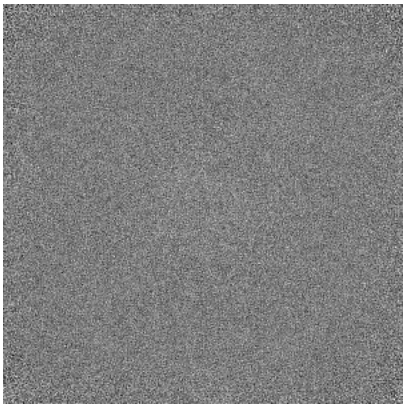
6.3.2 Raw map



X Index: 0



Y Index: 0

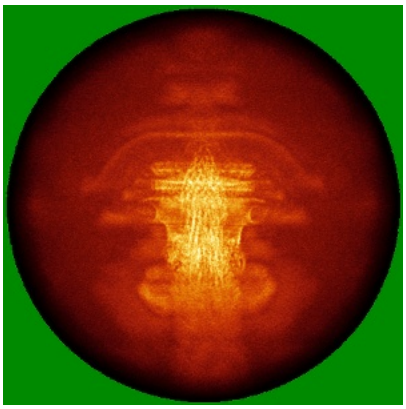


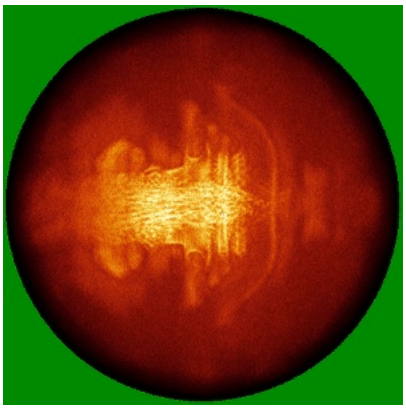
Z Index: 447

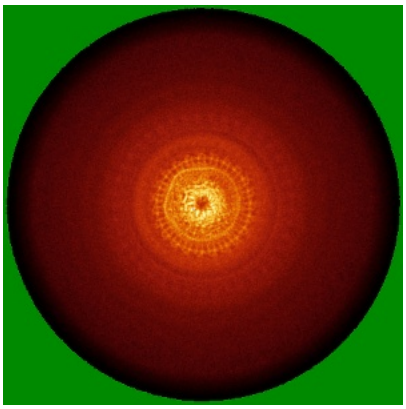
The images above show the largest variance slices of the map in three orthogonal directions.

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

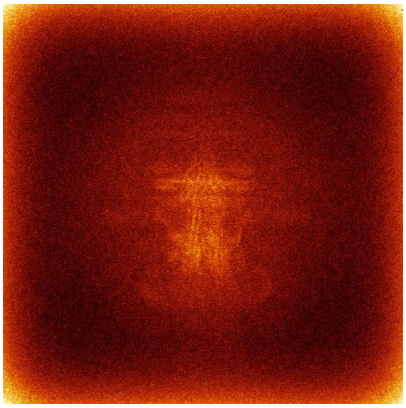
6.4.1 Primary map

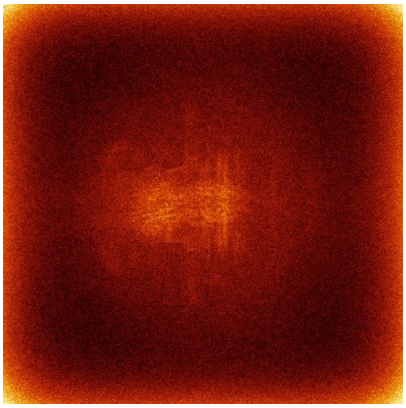

X

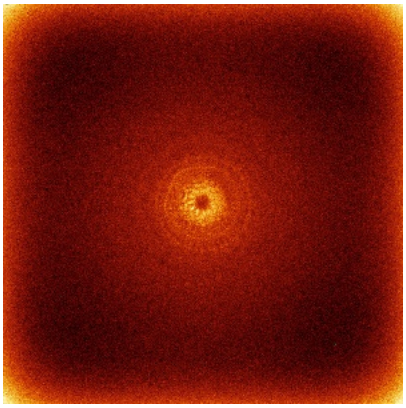

Y


Z

6.4.2 Raw map


X

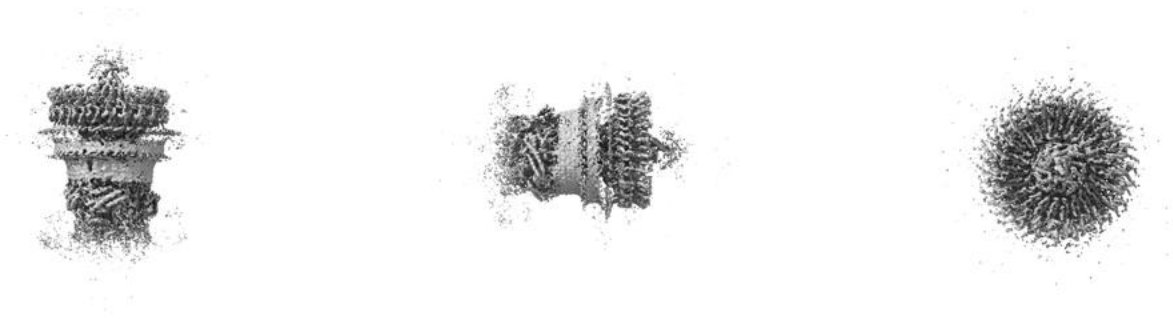

Y


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.

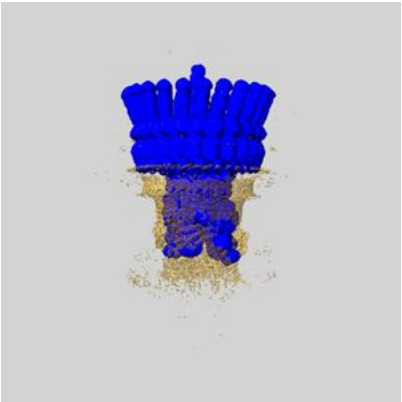
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

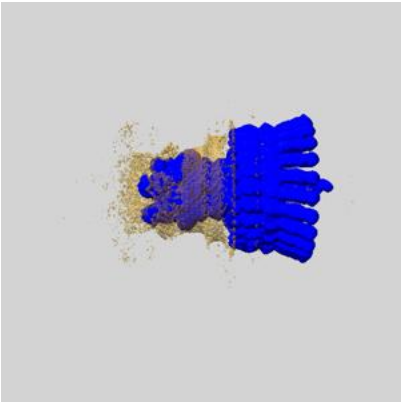
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

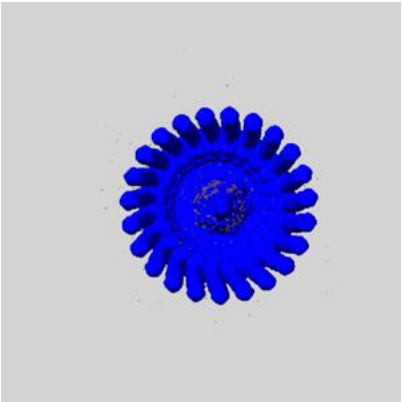
6.6.1 emd_76347_msk_1.map (i)



X



Y

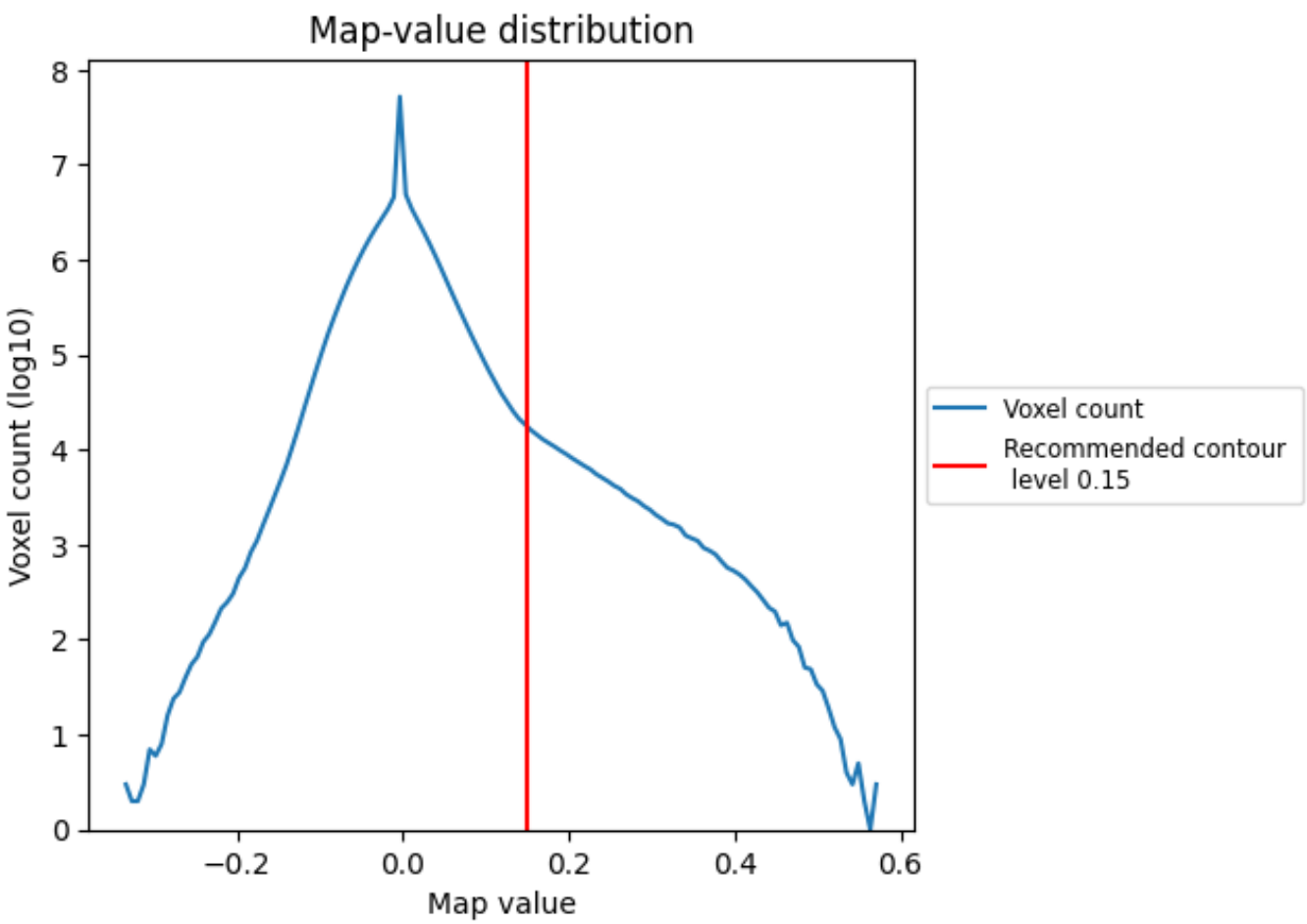


Z

7 Map analysis (i)

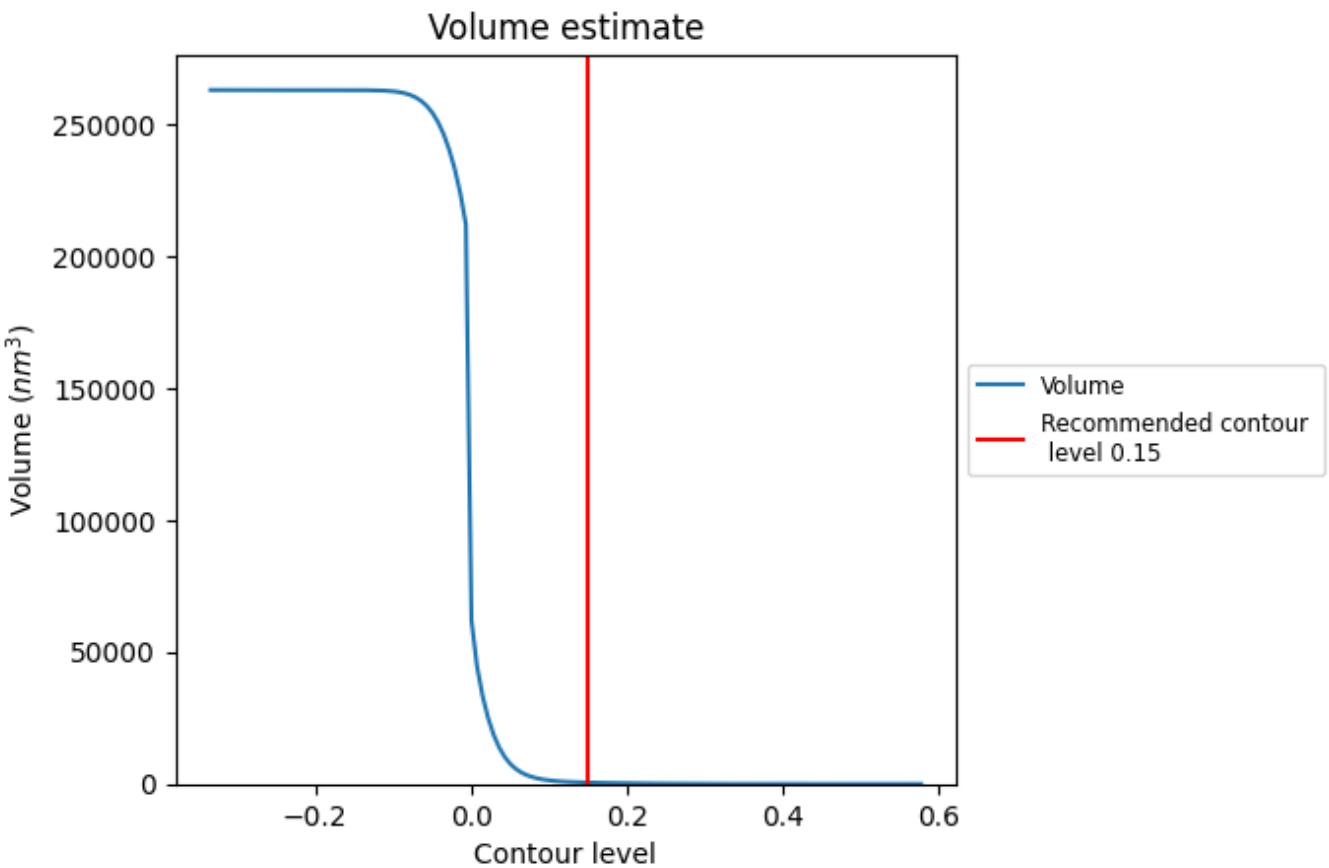
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

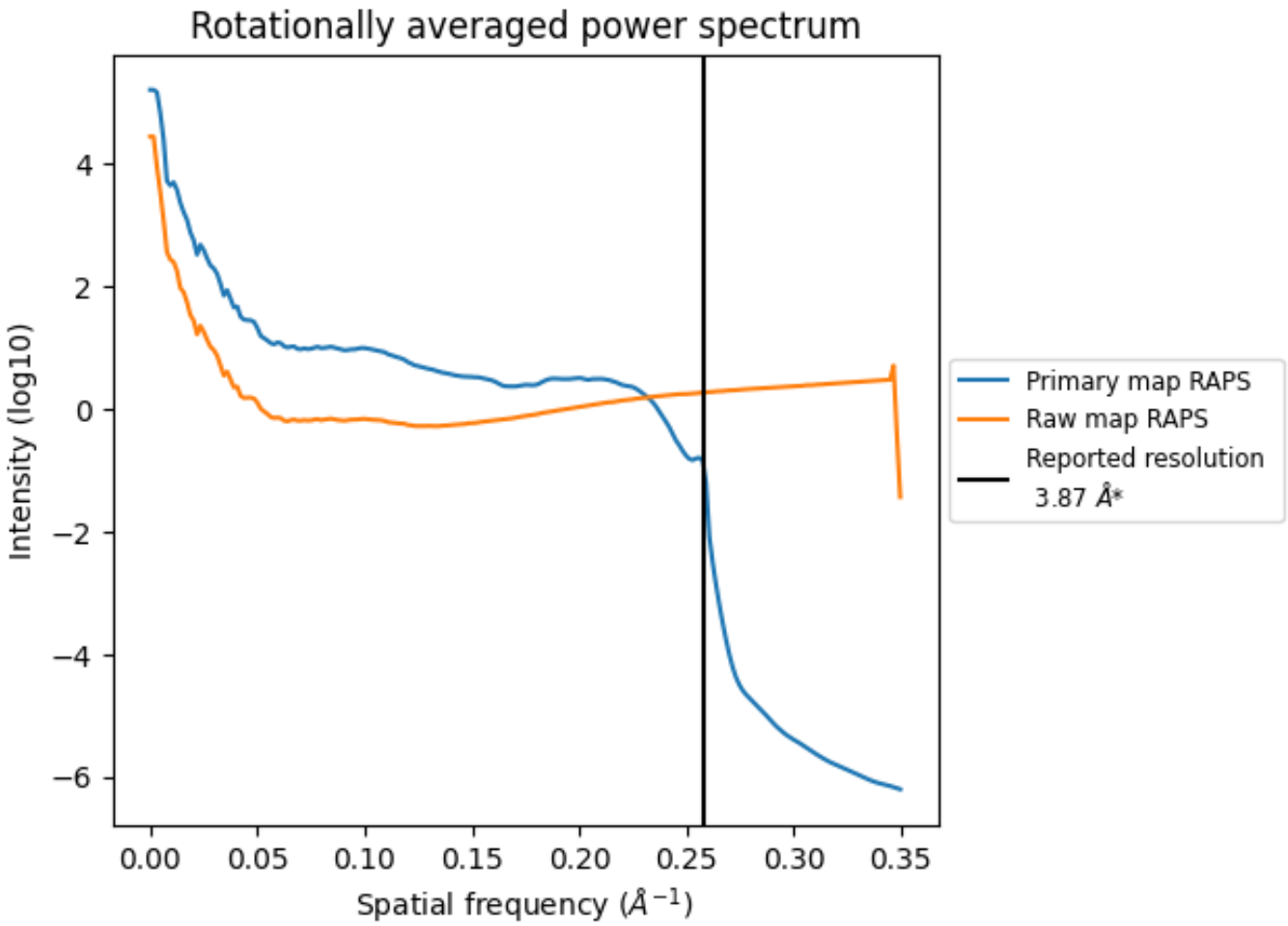
7.2 Volume estimate (i)



The volume at the recommended contour level is 529 nm^3; this corresponds to an approximate mass of 478 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)

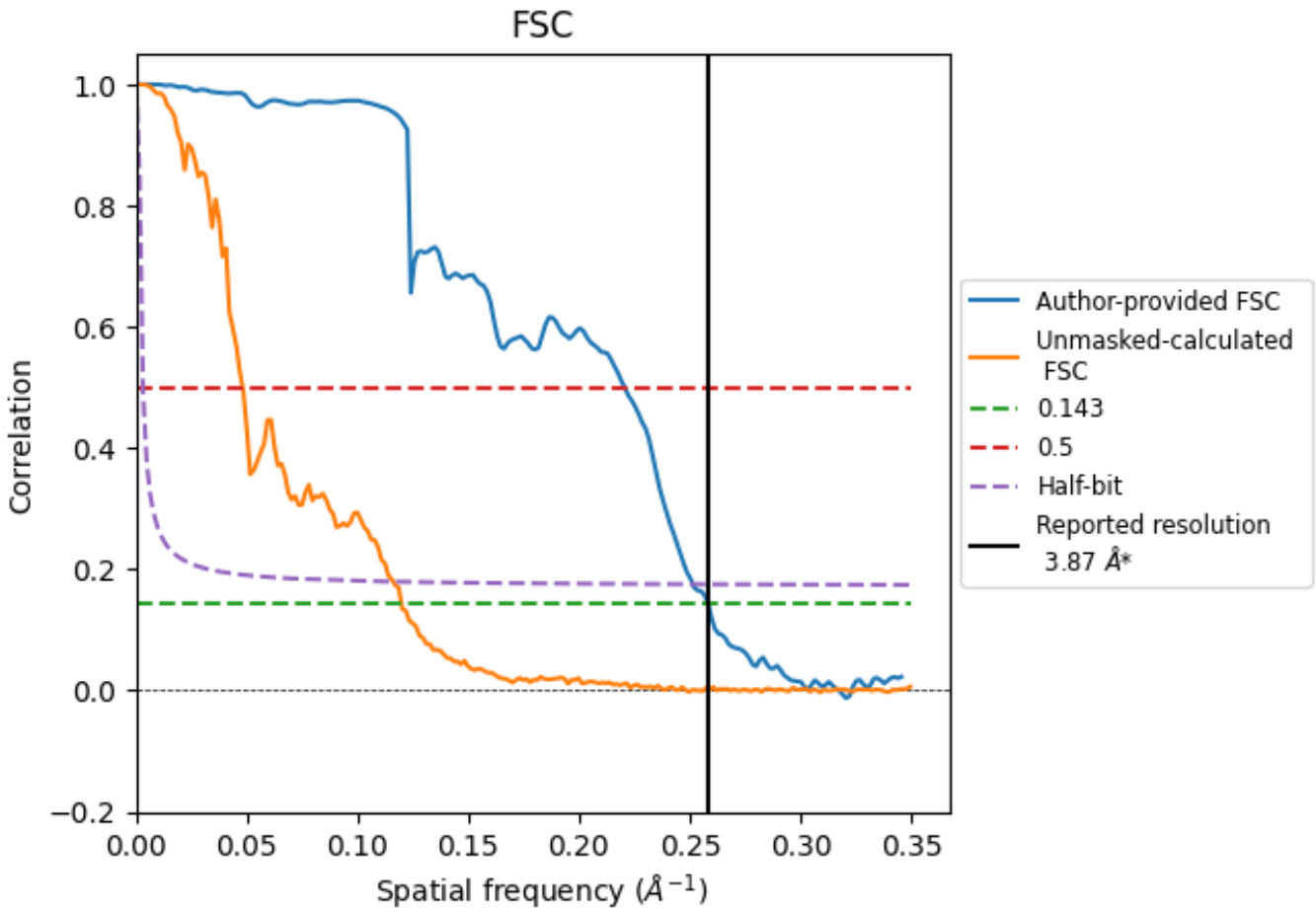


*Reported resolution corresponds to spatial frequency of 0.258 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.258 Å^{-1}

8.2 Resolution estimates (i)

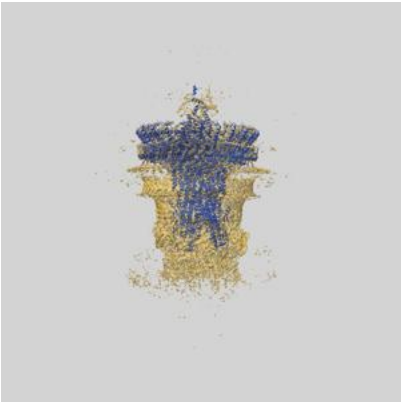
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.87	-	-
Author-provided FSC curve	3.87	4.53	3.98
Unmasked-calculated*	8.35	20.79	8.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.35 differs from the reported value 3.87 by more than 10 %

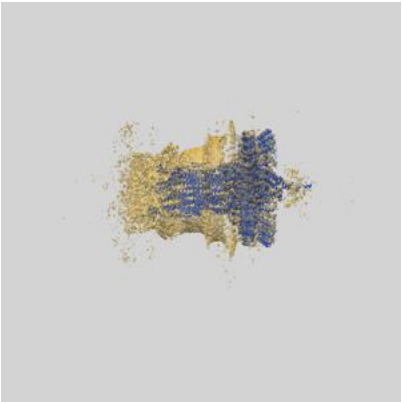
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-76347 and PDB model 12DU. Per-residue inclusion information can be found in section 3 on page 9.

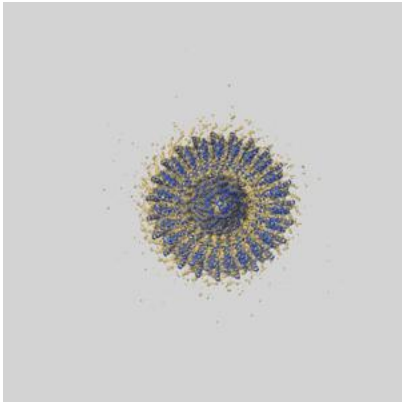
9.1 Map-model overlay (i)



X



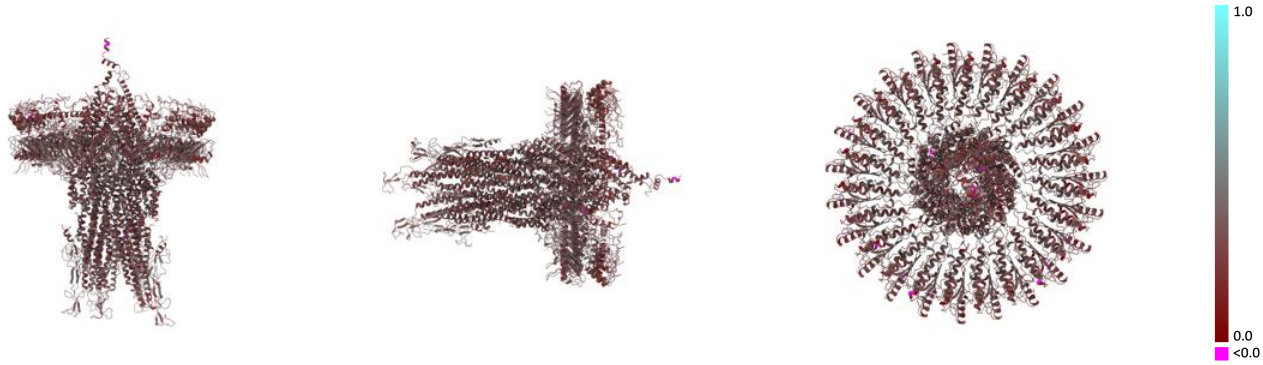
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 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.

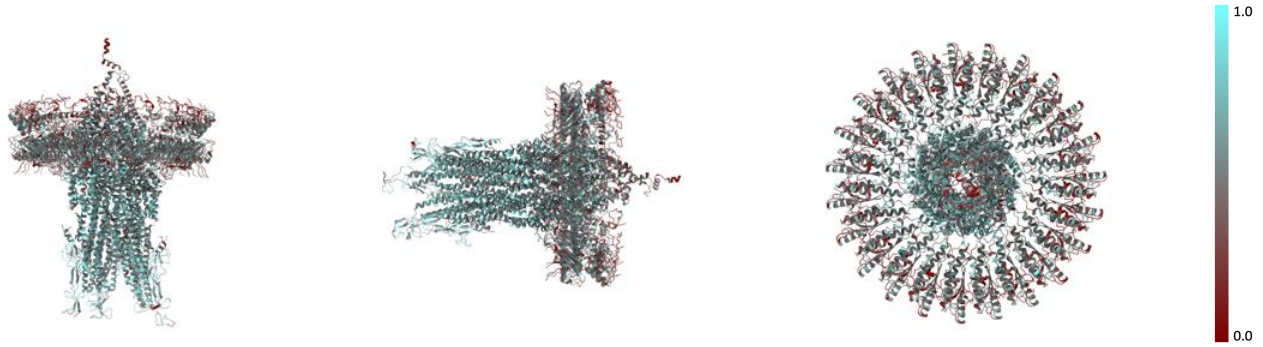
9.2 Q-score mapped to coordinate model (i)



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.

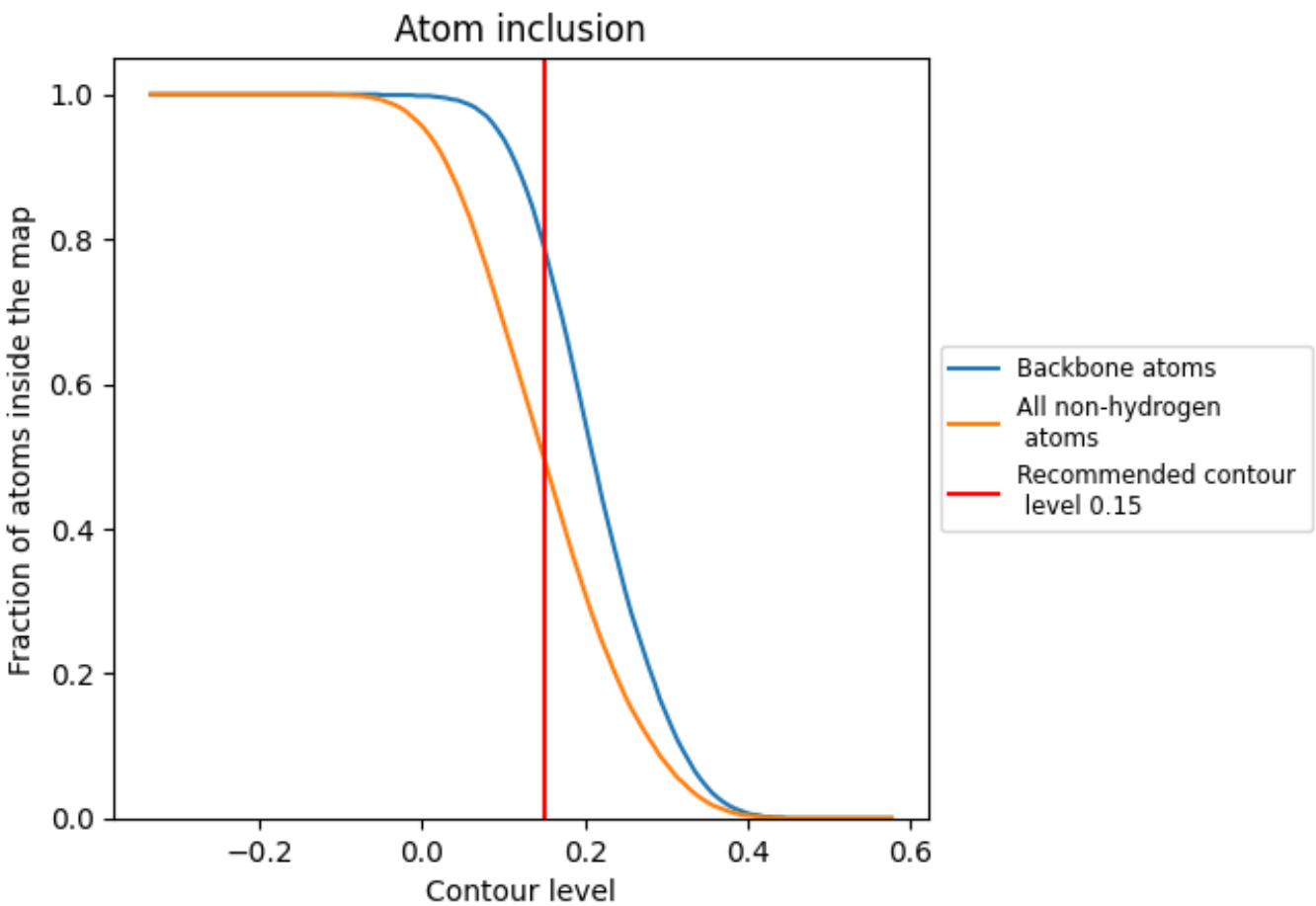
9.3 Atom inclusion mapped to coordinate model (i)



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, 79% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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

Chain	Atom inclusion	Q-score
All	0.4970	0.3220
1	0.5690	0.3240
2	0.5780	0.3120
3	0.5570	0.3160
A	0.4470	0.2770
F	0.6070	0.3390
G	0.6070	0.3280
H	0.6100	0.3430
I	0.5900	0.3310
J	0.5940	0.3300
K	0.5610	0.3140
L	0.6390	0.3330
M	0.6200	0.3300
N	0.6350	0.3320
O	0.6320	0.3160
P	0.6110	0.3200
Q	0.5480	0.3090
R	0.6160	0.3330
S	0.6320	0.3360
T	0.5960	0.3380
U	0.6100	0.3280
V	0.6120	0.3320
W	0.6040	0.3200
X	0.6430	0.3540
Y	0.5820	0.3210
Z	0.6300	0.3520
a	0.6300	0.3520
b	0.6240	0.3560
c	0.4190	0.3230
d	0.3900	0.3190
e	0.3960	0.3210
f	0.4210	0.3180
g	0.4230	0.3190
h	0.4040	0.3170
i	0.4160	0.3160

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	0.4280	0.3190
k	0.4410	0.3220
l	0.4210	0.3220
m	0.4120	0.3120
n	0.4280	0.3160
o	0.4400	0.3210
p	0.4180	0.3260
q	0.3880	0.3190
r	0.4050	0.3090
s	0.4110	0.3190
t	0.4090	0.3150
u	0.3830	0.3160
v	0.3630	0.3100
w	0.3880	0.3070
x	0.3820	0.3050
y	0.3970	0.3140
z	0.5330	0.3010