Full wwPDB EM Validation Report ⓘ

Oct 5, 2026 – 03:47 PM EDT

PDB ID	:	12DR / pdb_000012dr
EMDB ID	:	EMD-76344
Title	:	In situ cryo-EM structure of the MS ring RBM3 of the flagellar motor in Borrelia burgdorferi
Authors	:	Yue, J.; Liu, J.
Deposited on	:	2026-03-30
Resolution	:	3.37 Å(reported)

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

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

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

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

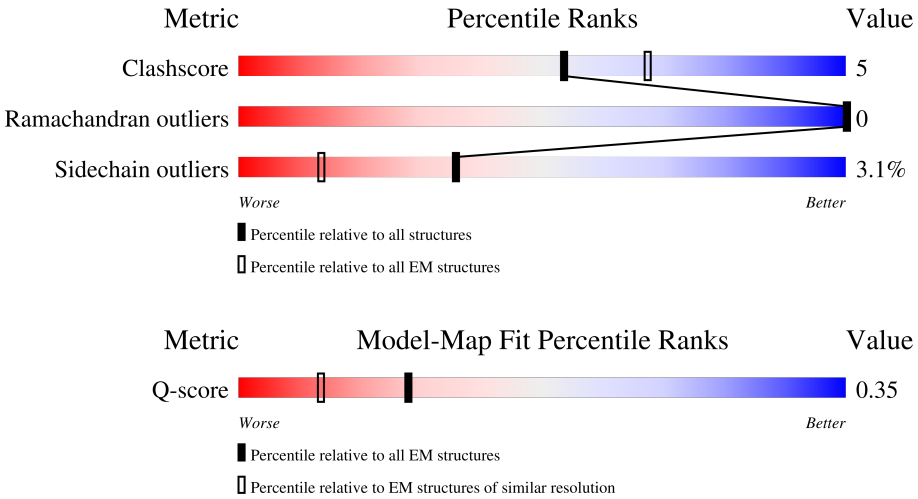
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.37 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	14287 (2.87 - 3.87)

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	A	569	9% 39% 7% 54%
1	B	569	10% 39% 6% • 54%
1	C	569	10% 37% 8% • 54%
1	D	569	10% 37% 9% 54%

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Mol	Chain	Length	Quality of chain
1	E	569	9% 38% 8% 54%
1	F	569	9% 38% 7% 54%
1	G	569	10% 39% 7% 54%
1	H	569	10% 39% 7% 54%
1	I	569	10% 39% 7% 54%
1	J	569	10% 40% 6% 54%
1	K	569	10% 40% 6% 54%
1	L	569	9% 40% 6% 54%
1	M	569	9% 38% 8% 54%
1	N	569	10% 37% 9% 54%
1	O	569	10% 38% 7% 54%
1	P	569	9% 39% 7% 54%
1	Q	569	10% 37% 8% 54%
1	R	569	9% 38% 7% 54%
1	S	569	11% 38% 7% 54%
1	T	569	10% 39% 7% 54%
1	U	569	10% 40% 5% 54%
1	V	569	10% 40% 6% 54%
1	W	569	10% 40% 6% 54%
1	X	569	10% 38% 8% 54%
1	Y	569	10% 39% 7% 54%
1	Z	569	10% 38% 8% 54%
1	a	569	9% 38% 8% 54%
1	b	569	10% 38% 8% 54%
1	c	569	10% 38% 7% 54%

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Mol	Chain	Length	Quality of chain
1	d	569	9% 40% 6% 54%
1	e	569	10% 38% 7% 54%
1	f	569	10% 40% 6% 54%
1	g	569	10% 39% 6% 54%
1	h	569	10% 38% 7% 54%
1	i	569	10% 38% 7% 54%
1	j	569	10% 38% 7% 54%
1	k	569	10% 37% 8% 54%
1	l	569	10% 38% 7% 54%
1	m	569	9% 38% 7% 54%
1	n	569	9% 39% 7% 54%
1	o	569	10% 39% 7% 54%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 86264 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flagellar M-ring protein.

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

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

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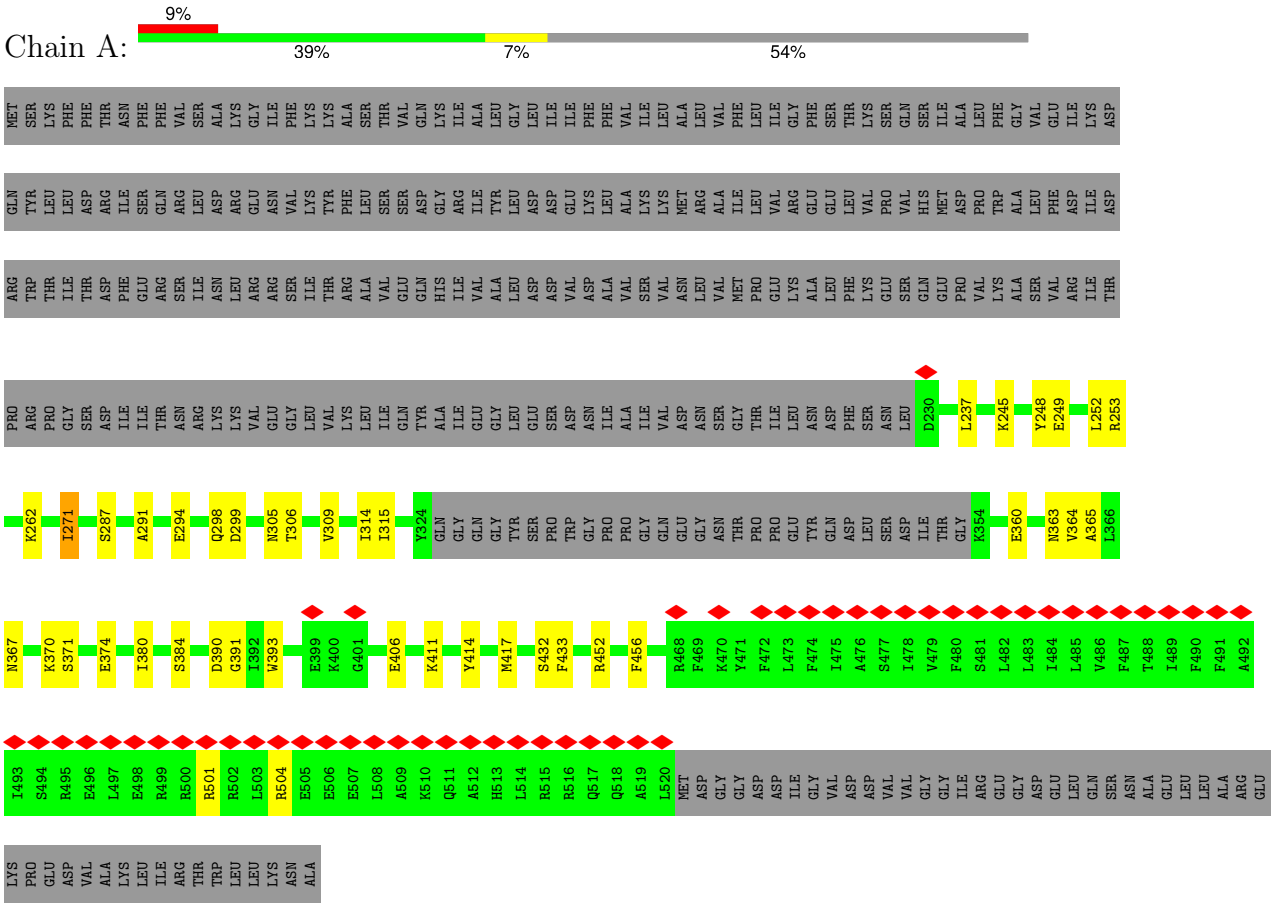
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	n	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		
1	o	262	Total	C	N	O	S	0	0
			2104	1328	365	406	5		

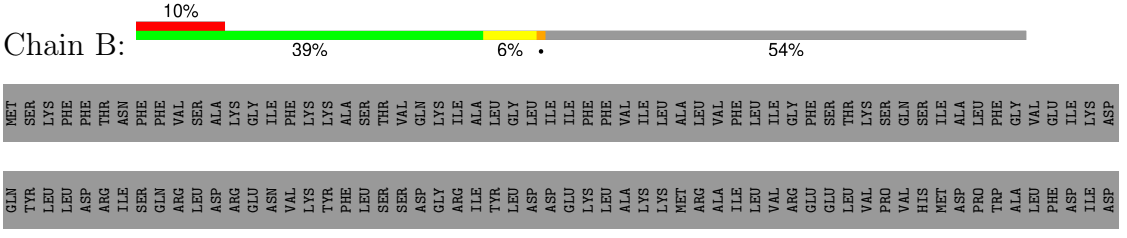
3 Residue-property plots (i)

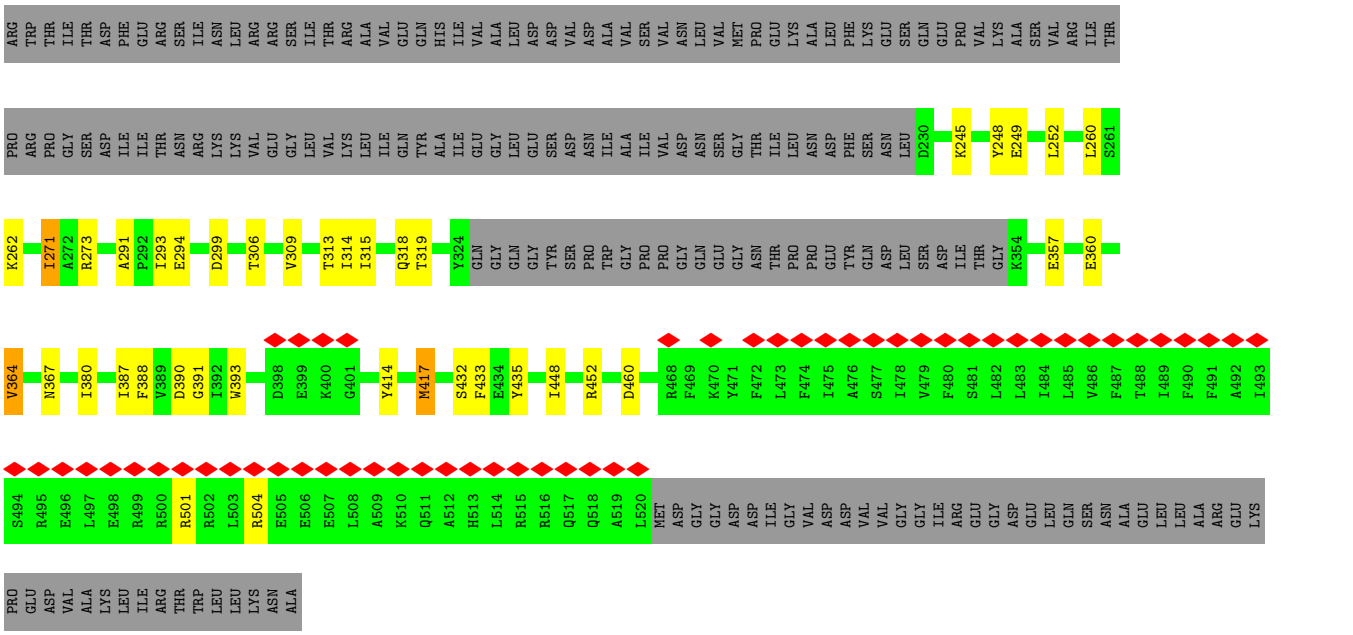
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



• Molecule 1: Flagellar M-ring protein

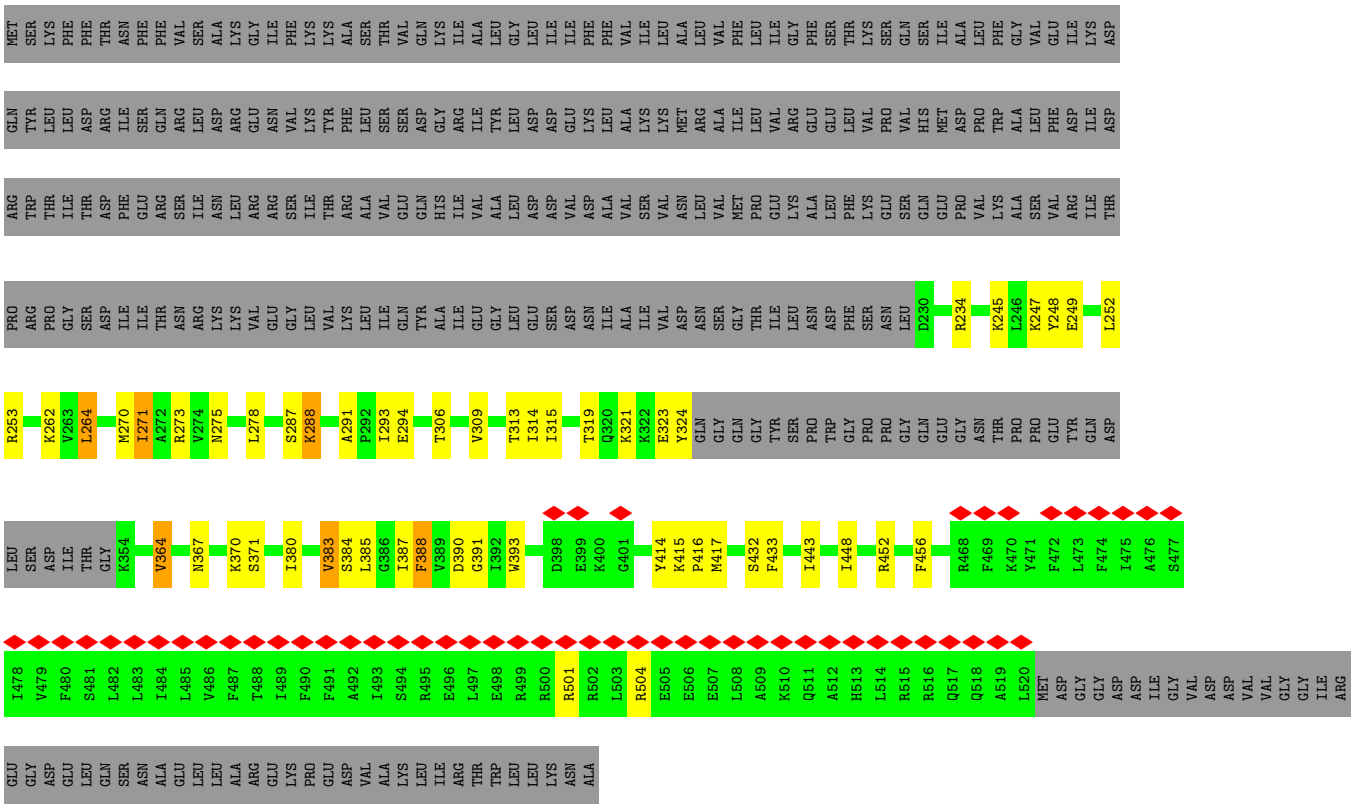




• Molecule 1: Flagellar M-ring protein

Chain C:

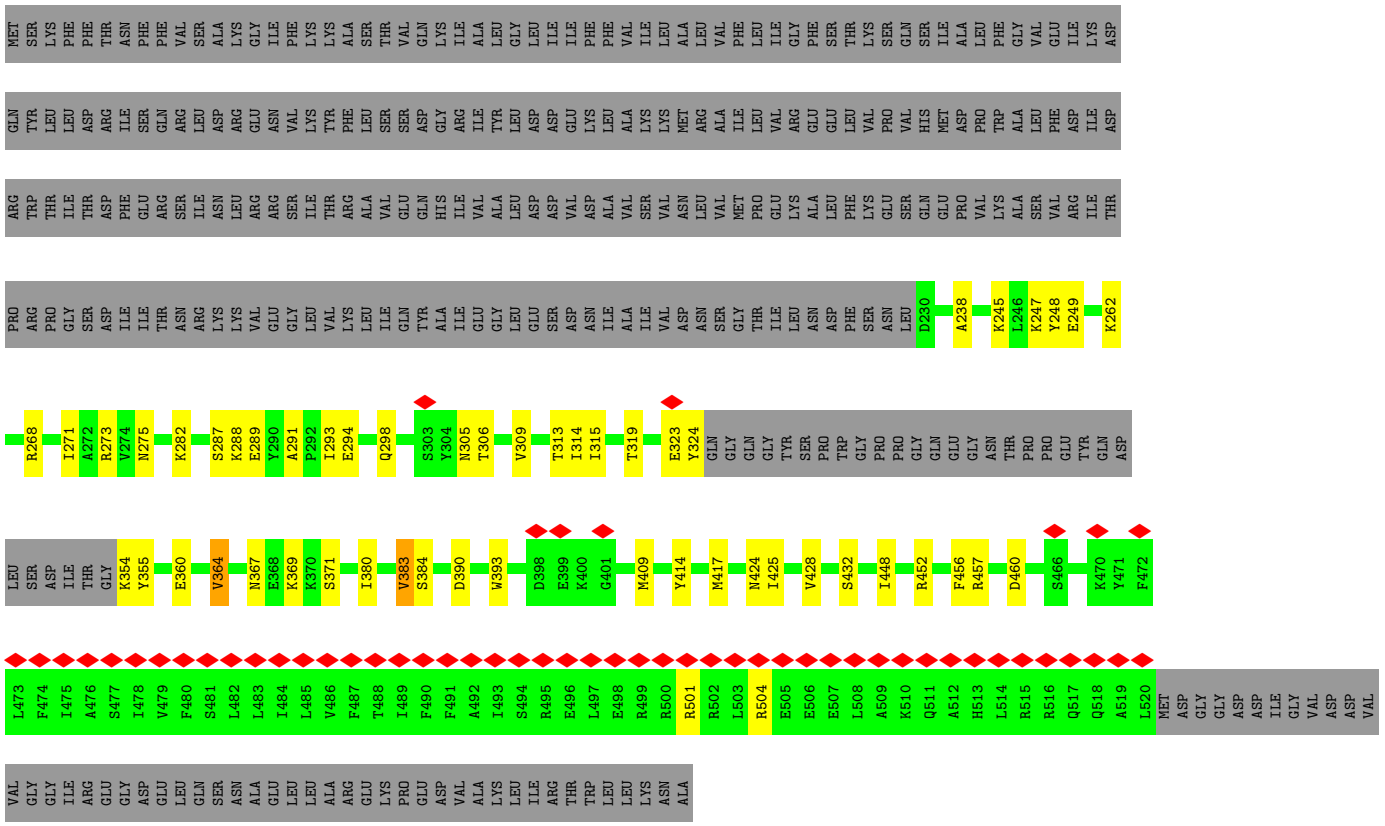




• Molecule 1: Flagellar M-ring protein

Chain D:

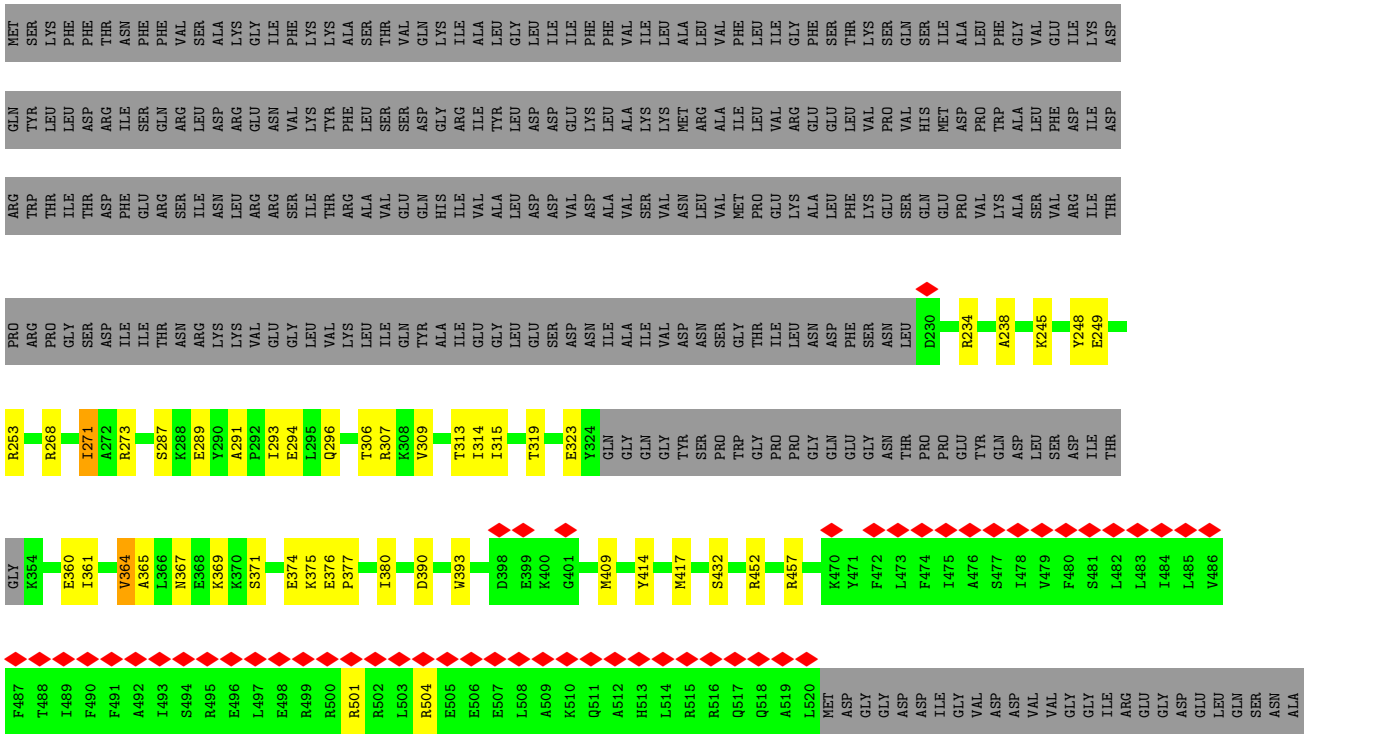




• Molecule 1: Flagellar M-ring protein

Chain E:



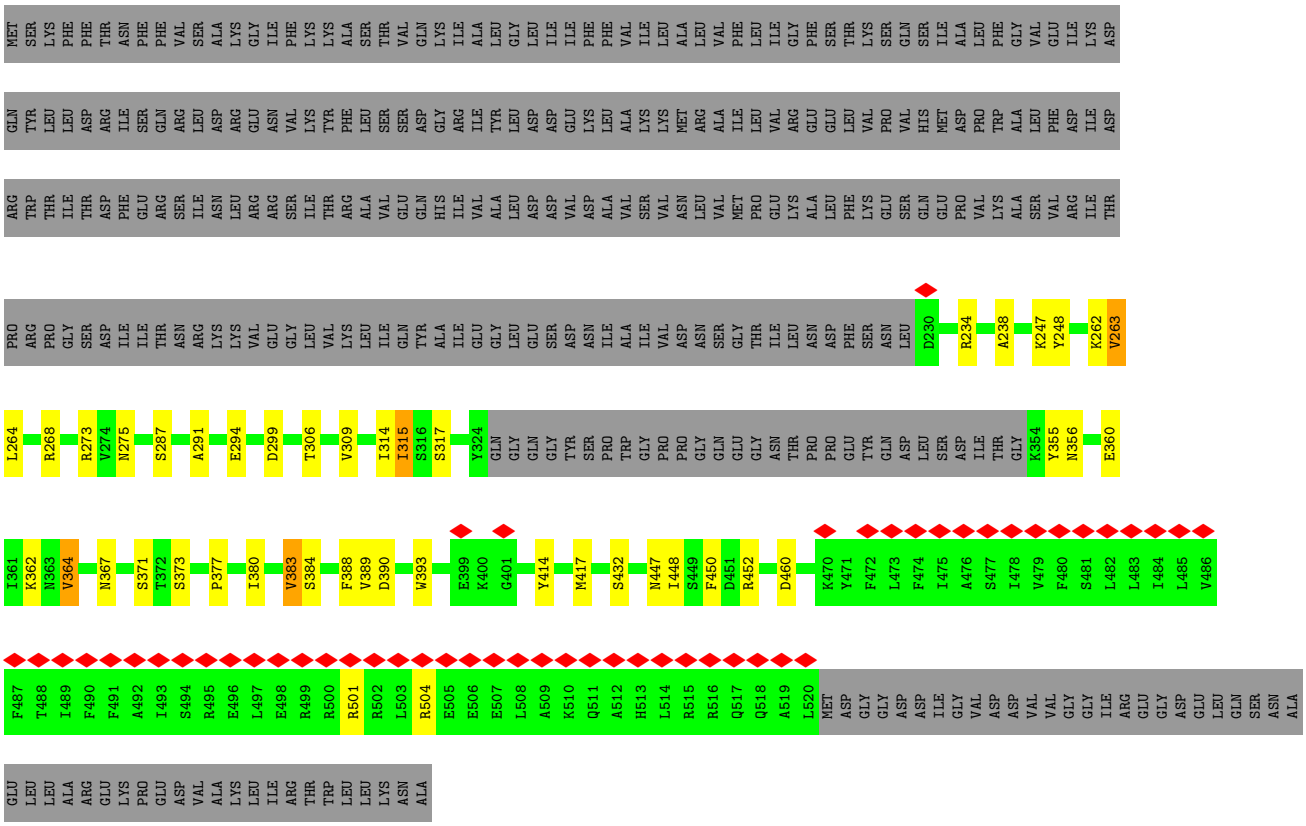




• Molecule 1: Flagellar M-ring protein

Chain F:

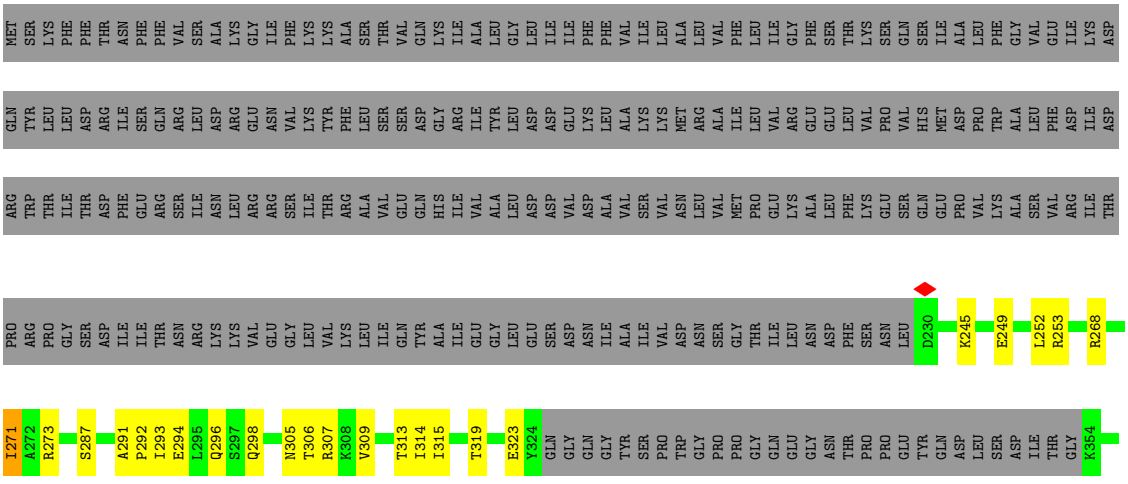


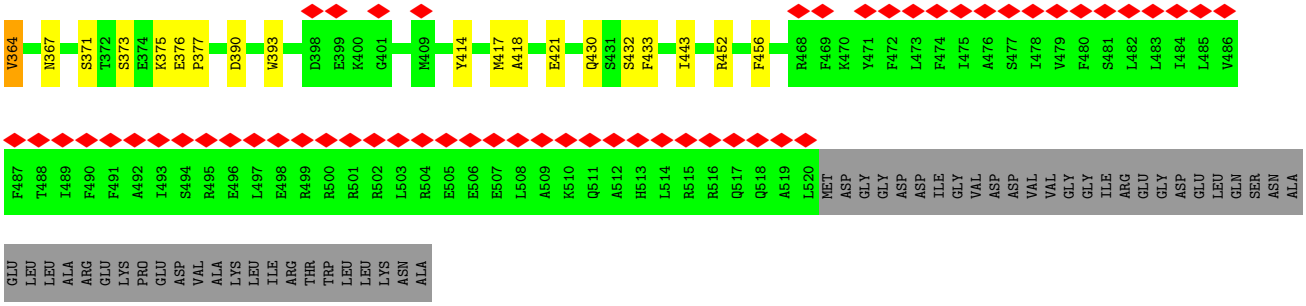


• Molecule 1: Flagellar M-ring protein

Chain G:



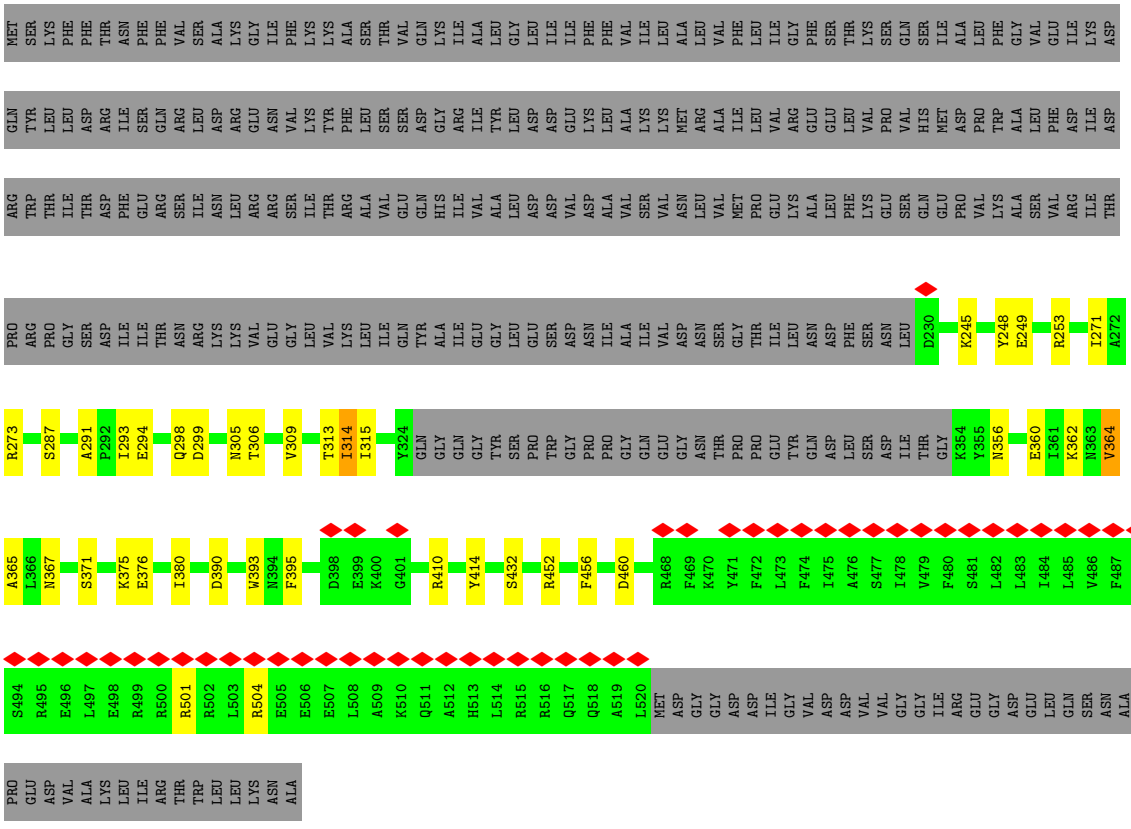




• Molecule 1: Flagellar M-ring protein

Chain H:

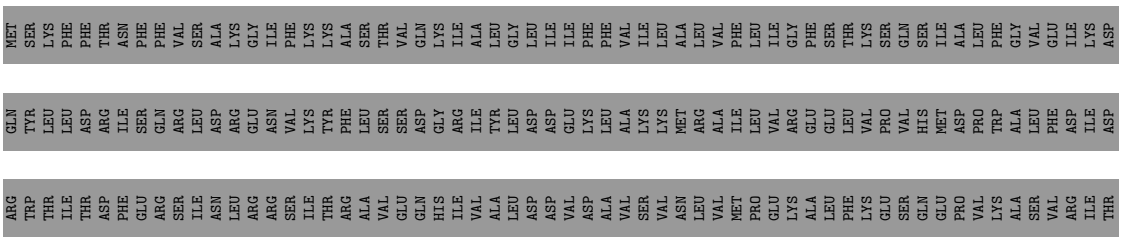


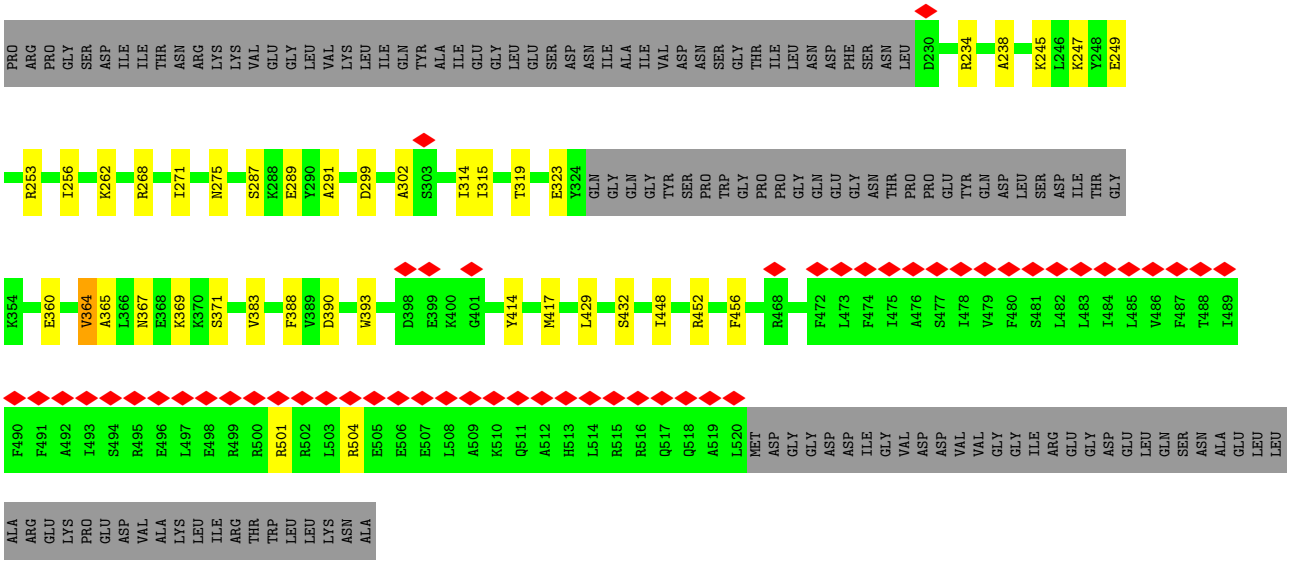


• Molecule 1: Flagellar M-ring protein

Chain I:



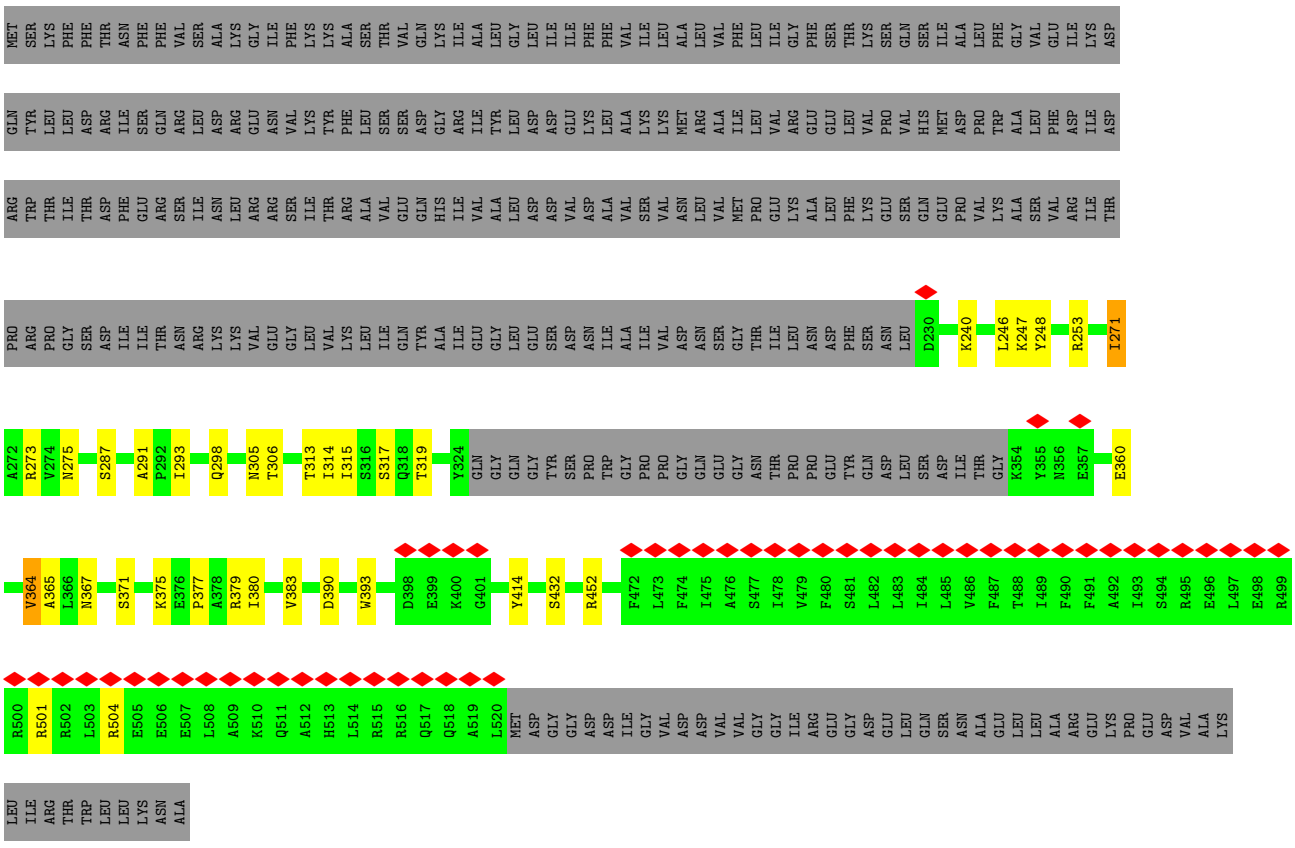




• Molecule 1: Flagellar M-ring protein

Chain J:





• Molecule 1: Flagellar M-ring protein

Chain K:

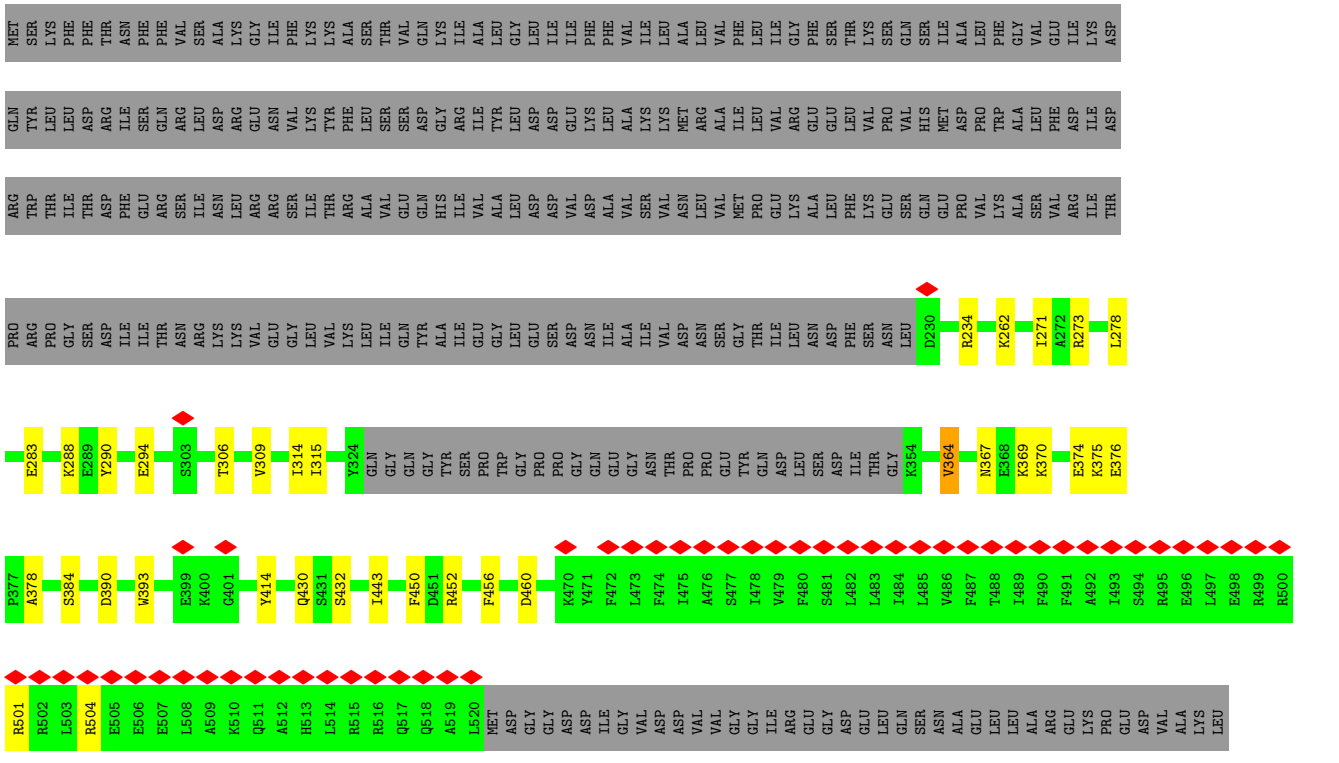




• Molecule 1: Flagellar M-ring protein

Chain L:



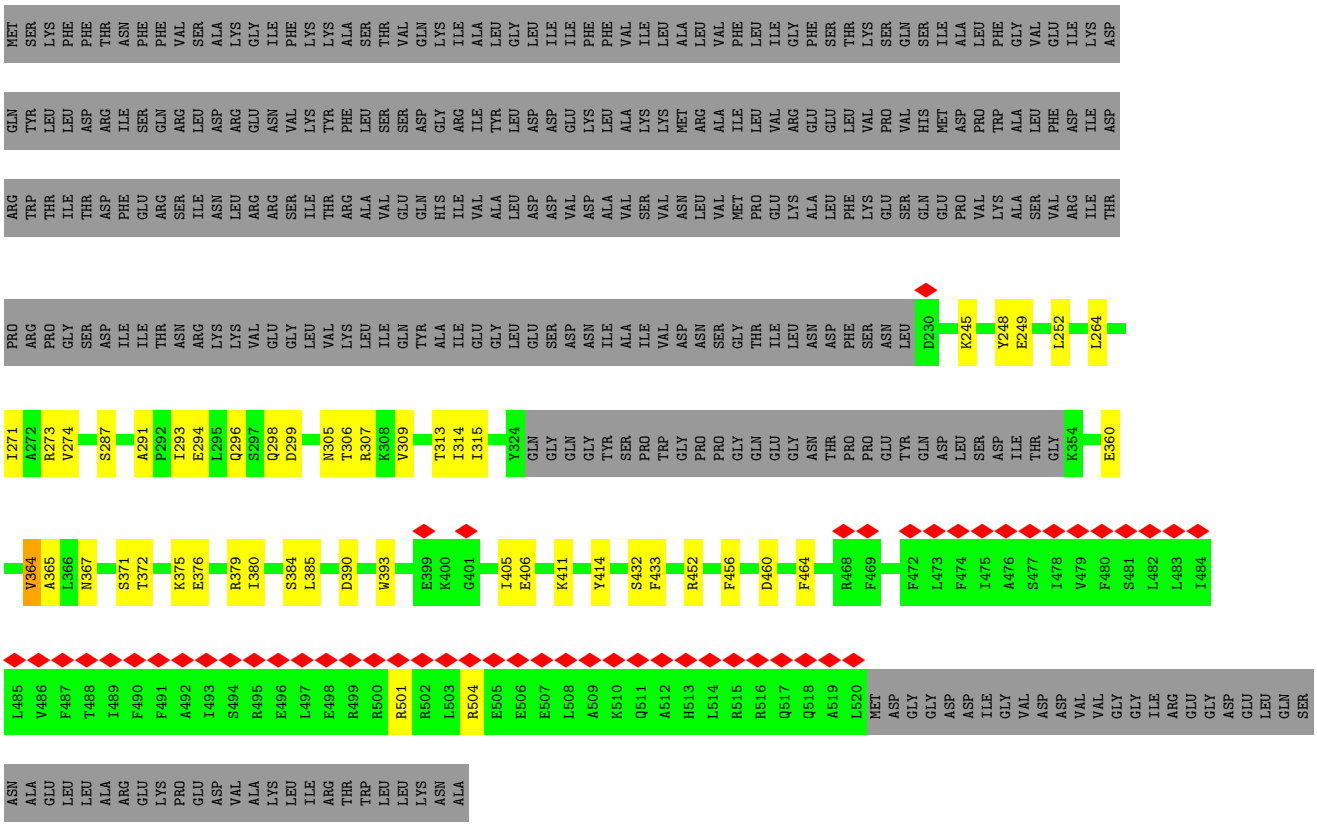




• Molecule 1: Flagellar M-ring protein

Chain M:

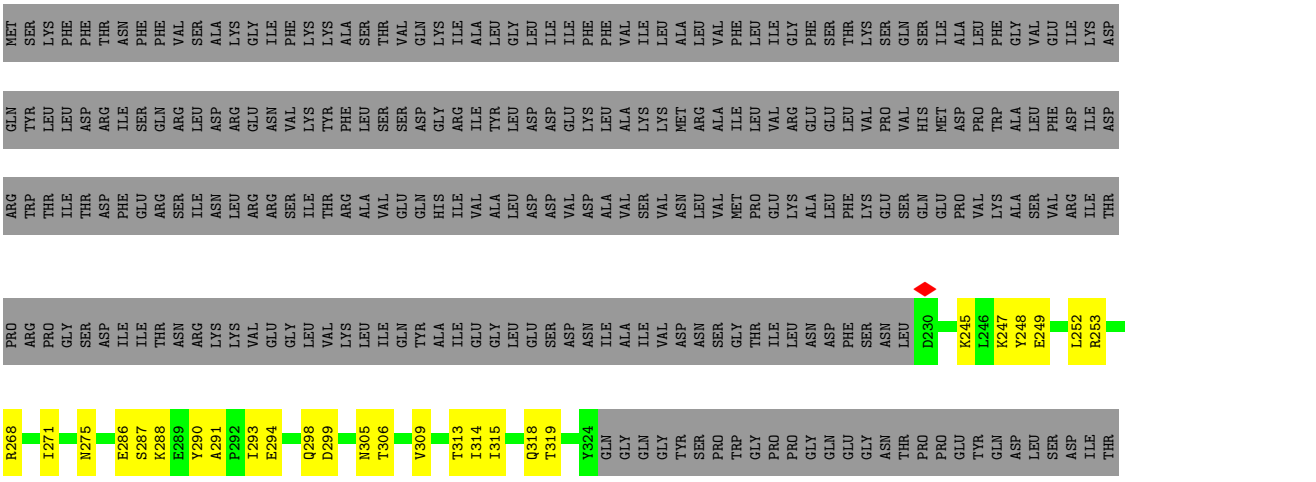


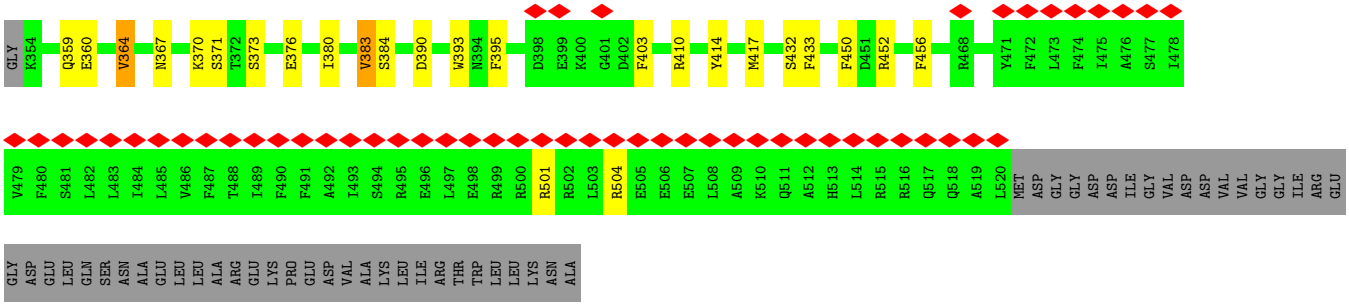


• Molecule 1: Flagellar M-ring protein

Chain N:



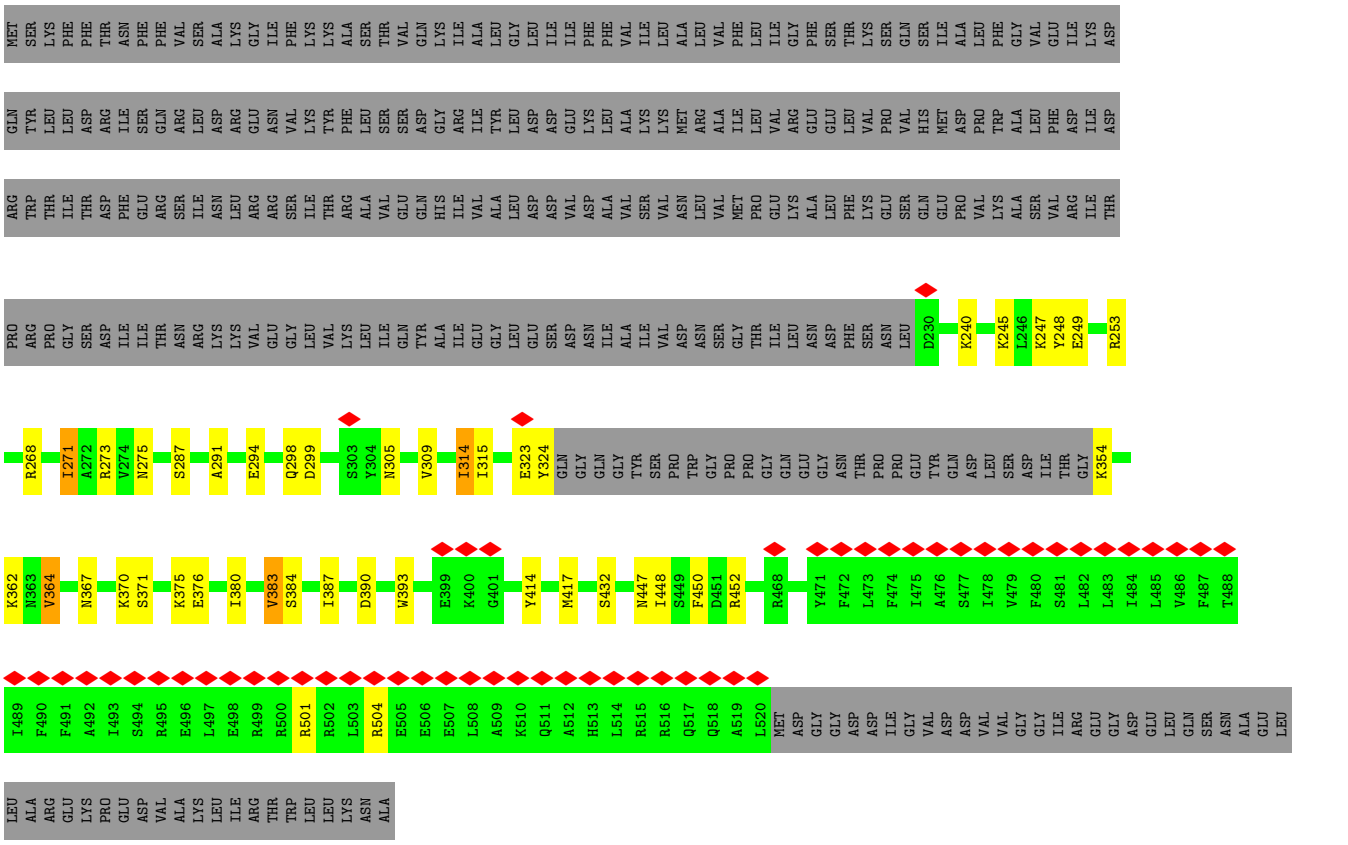




• Molecule 1: Flagellar M-ring protein

Chain O:

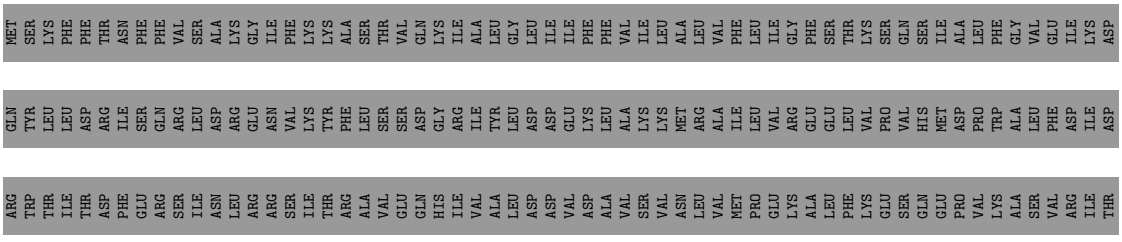


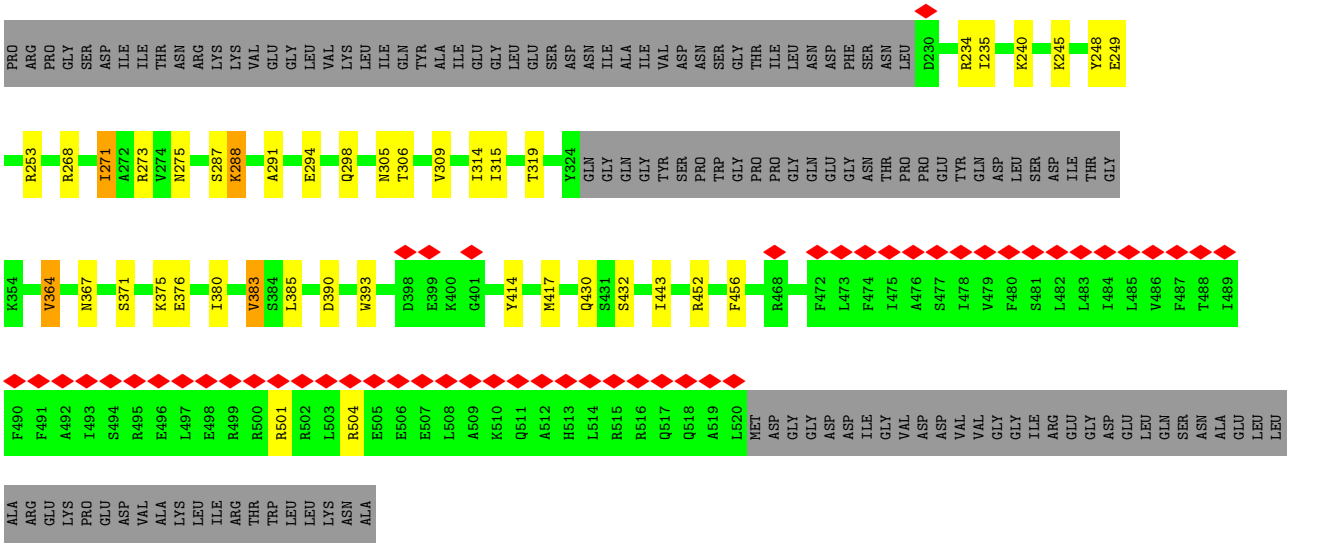


• Molecule 1: Flagellar M-ring protein

Chain P:



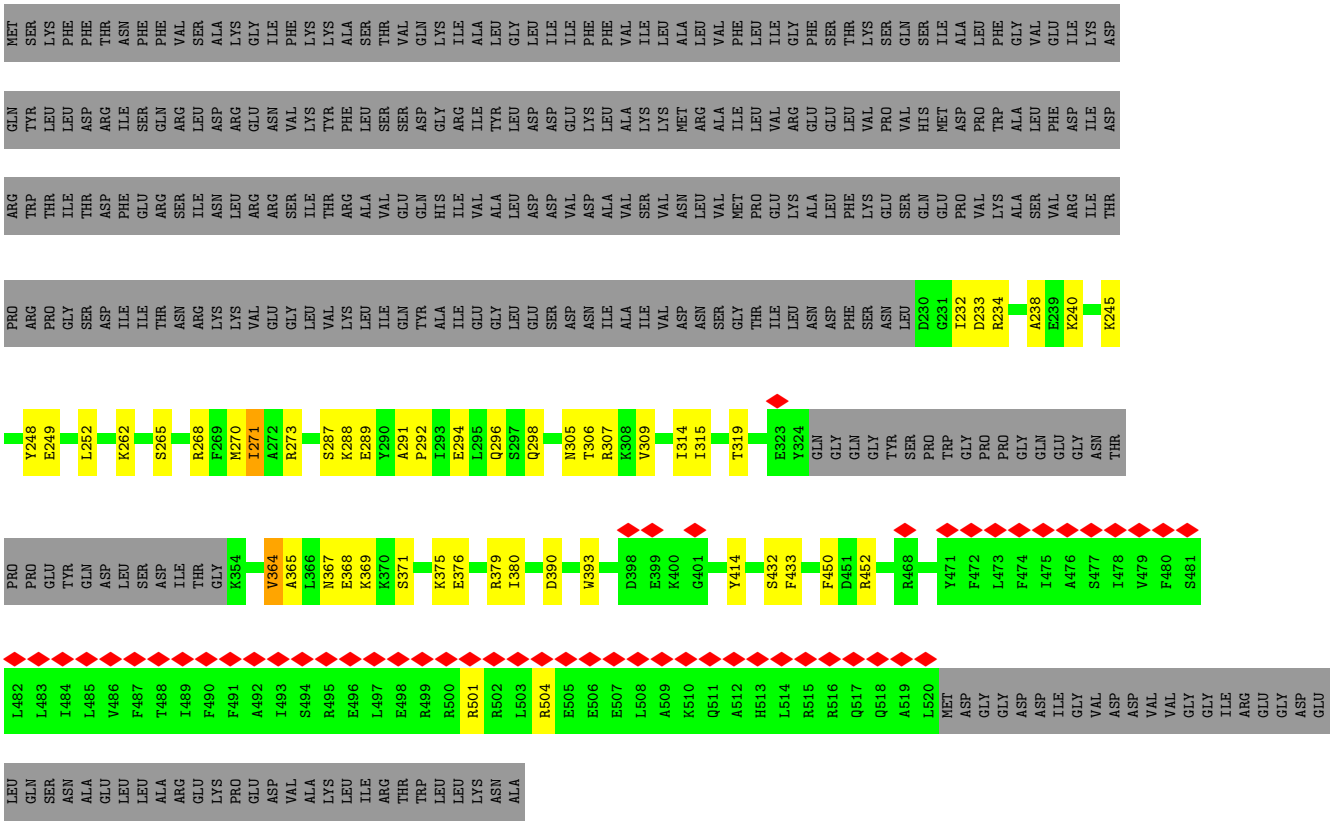




• Molecule 1: Flagellar M-ring protein

Chain Q:



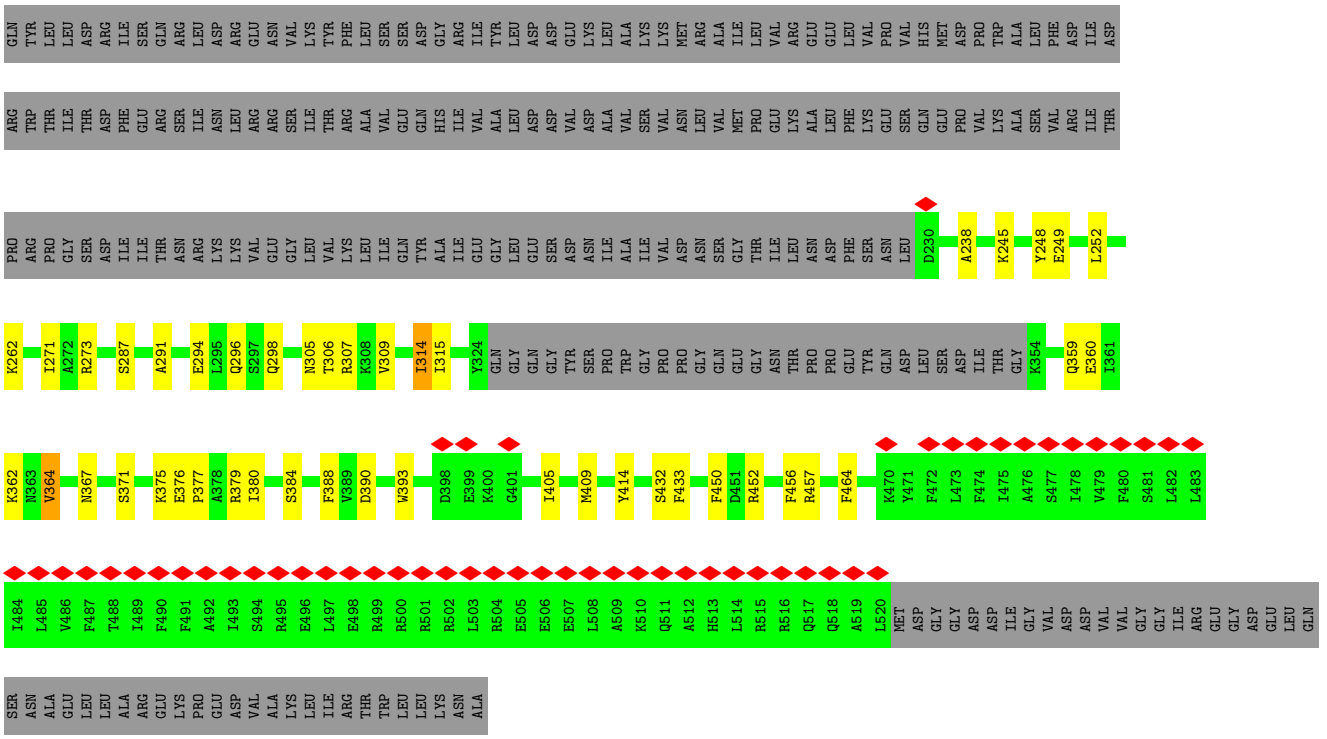


• Molecule 1: Flagellar M-ring protein

Chain R:



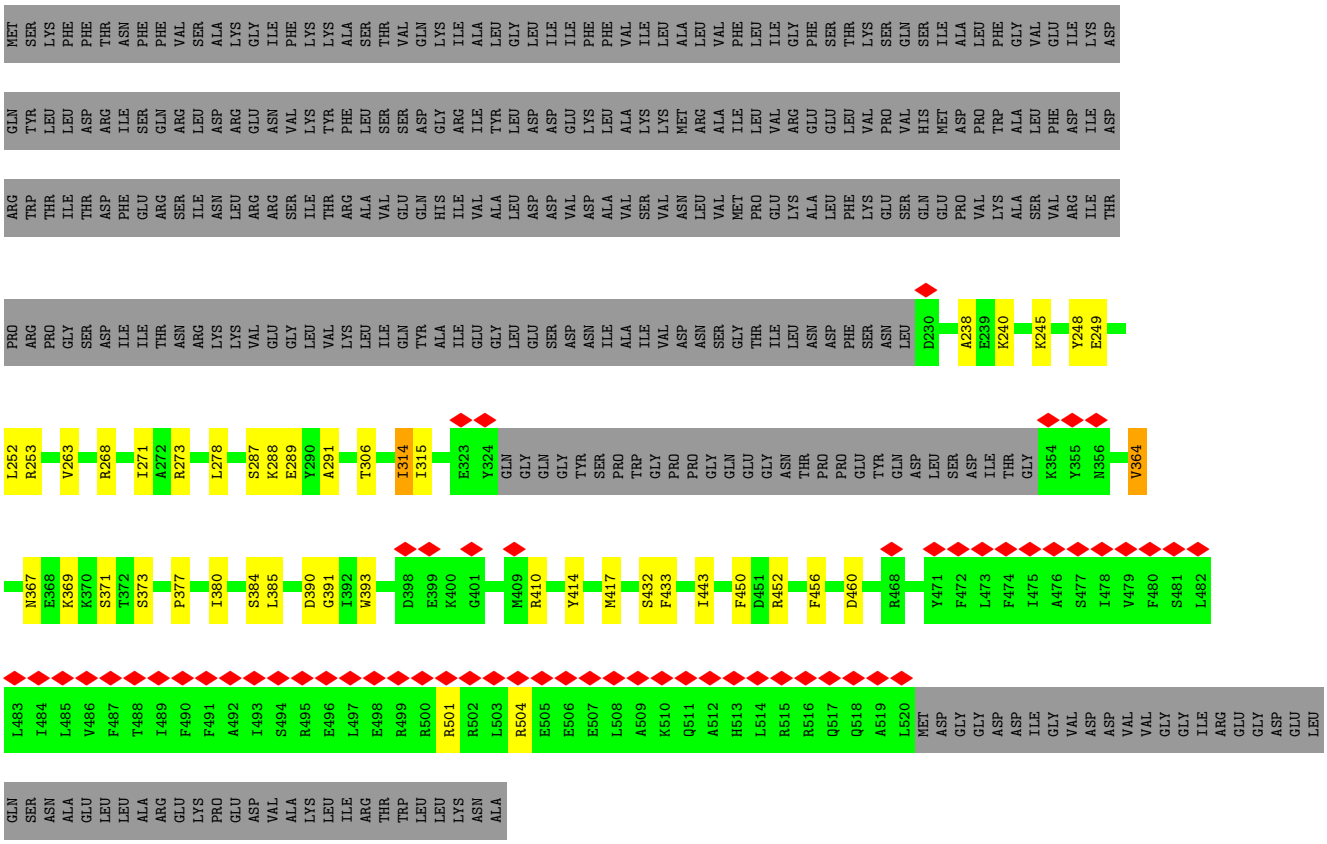




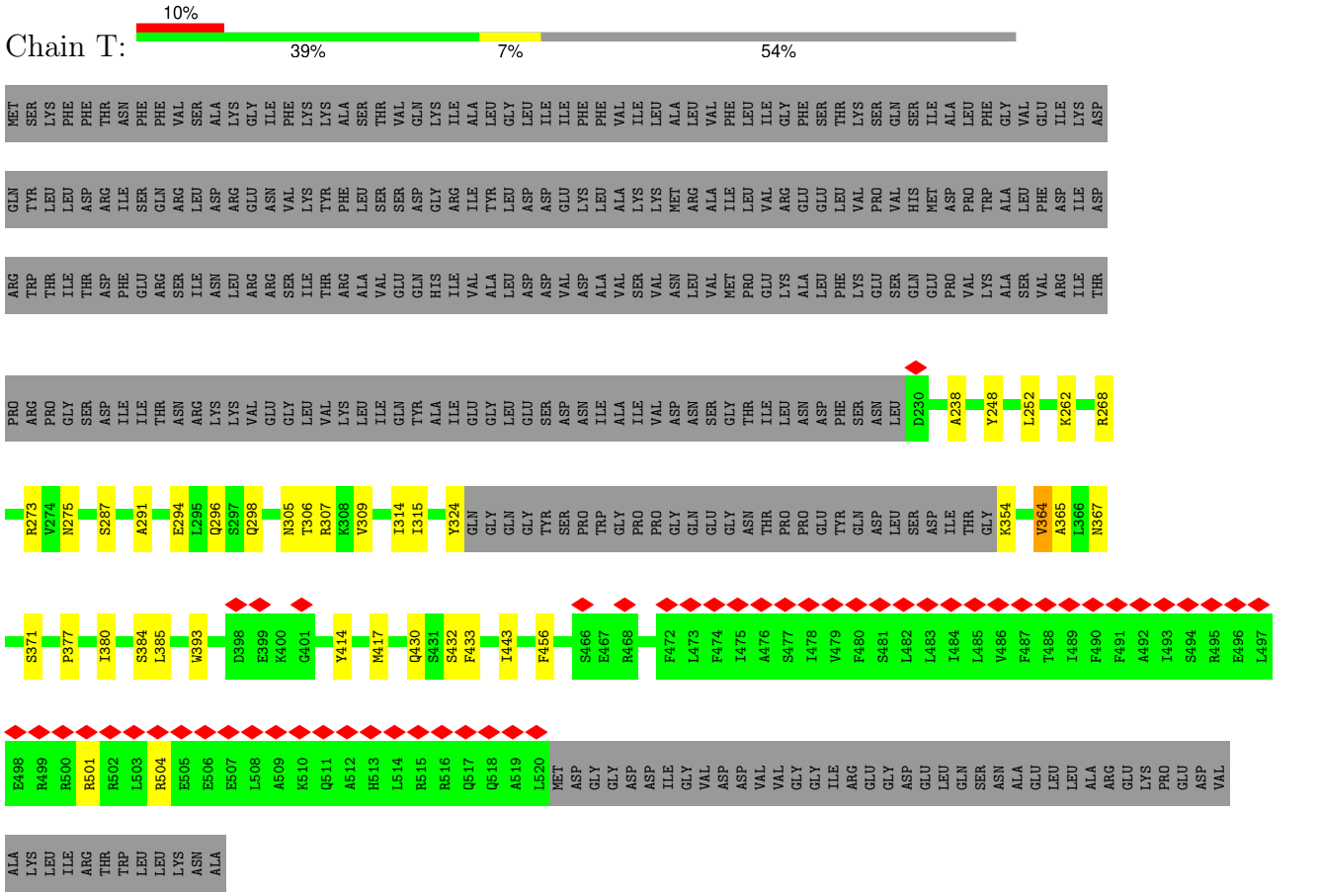
• Molecule 1: Flagellar M-ring protein

Chain S:

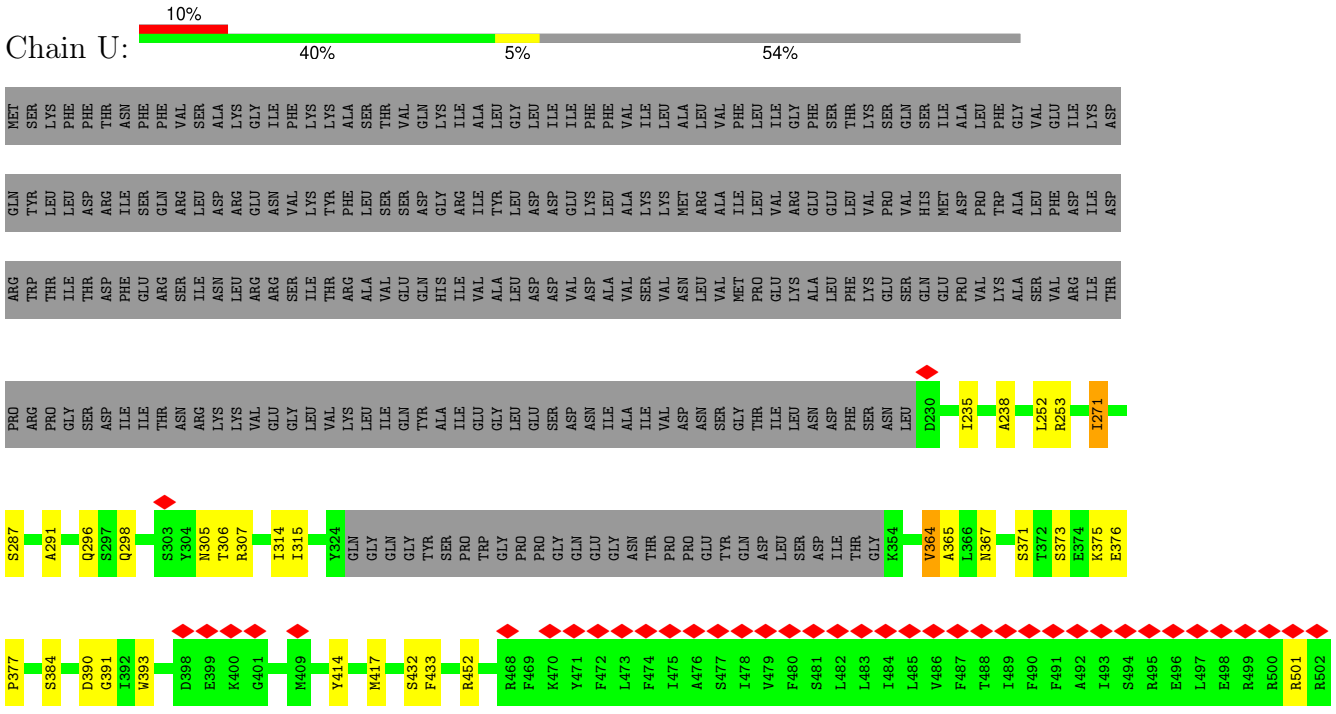


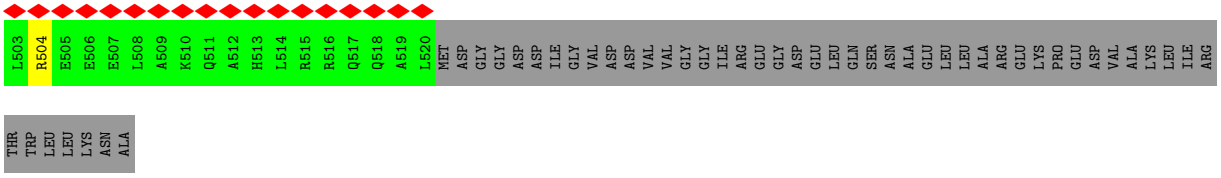


• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein

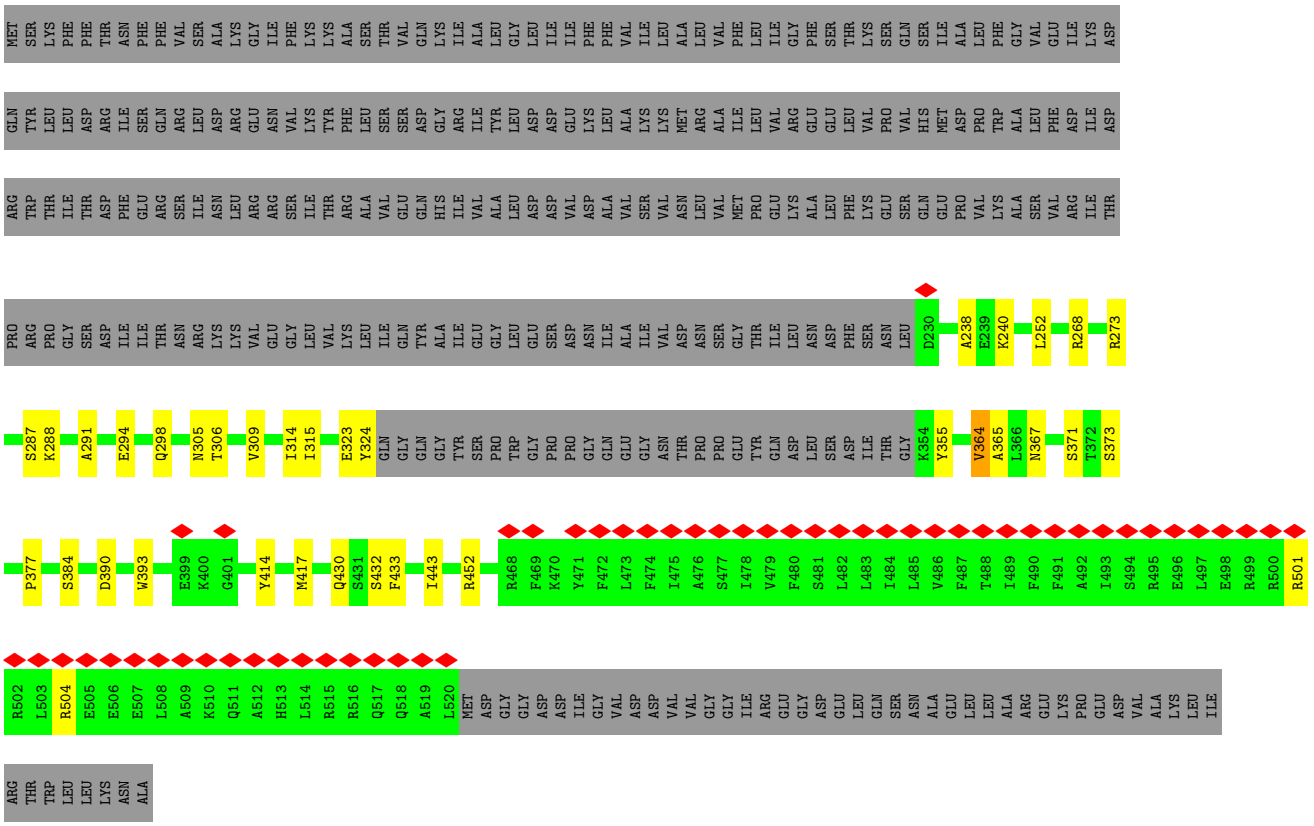




• Molecule 1: Flagellar M-ring protein

Chain V:

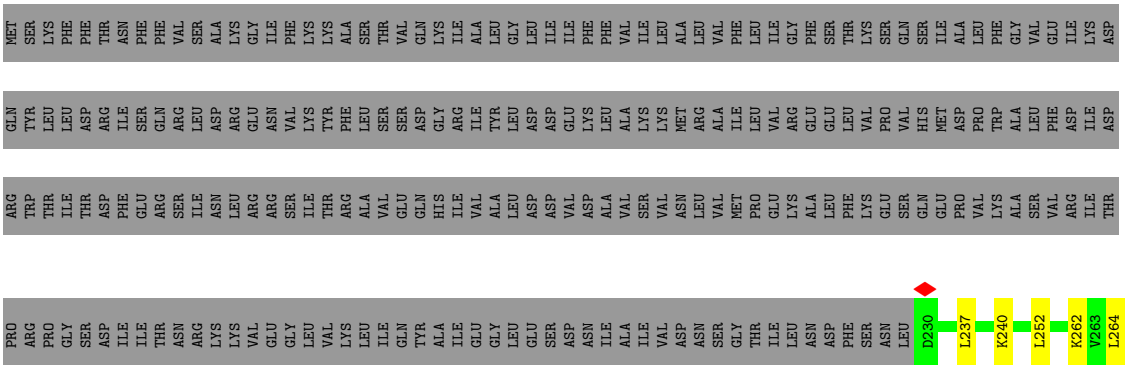


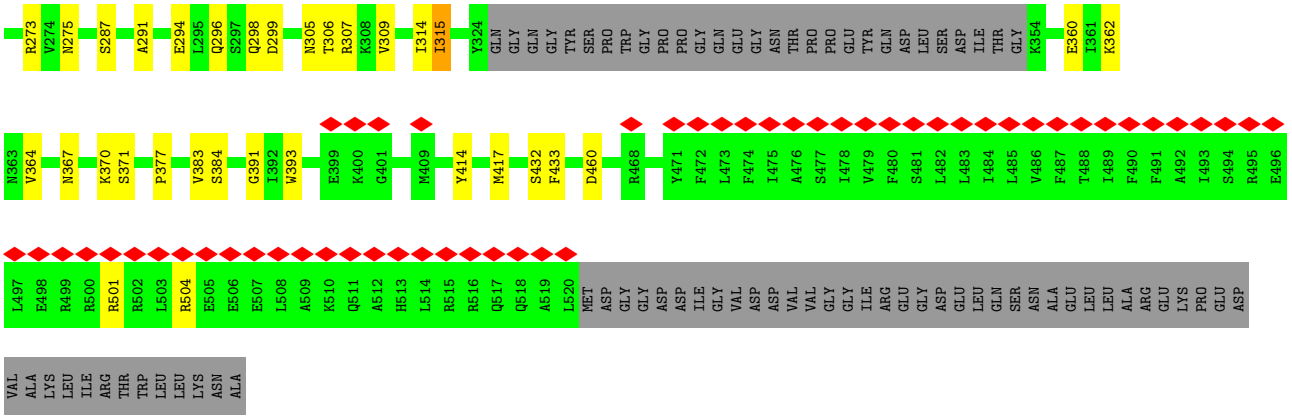


• Molecule 1: Flagellar M-ring protein

Chain W:



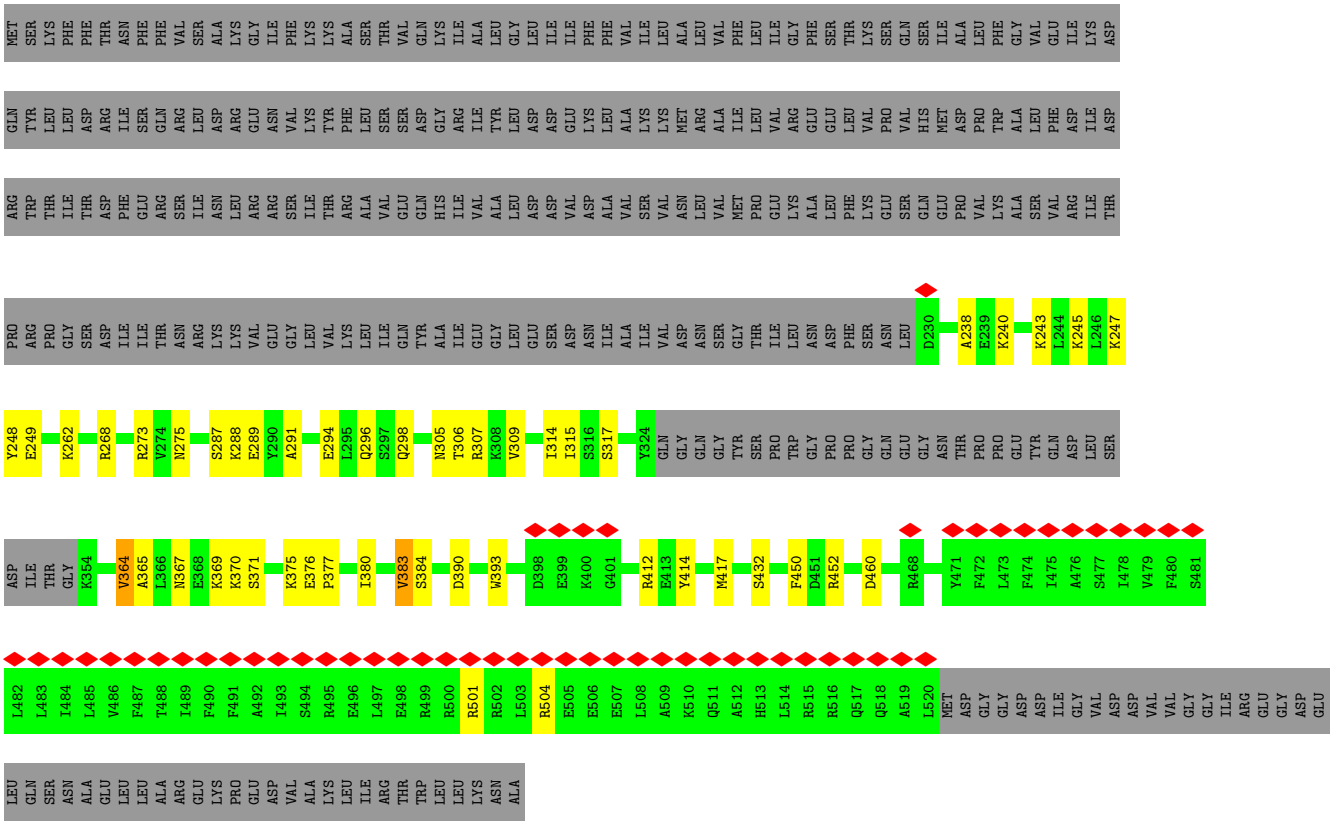




• Molecule 1: Flagellar M-ring protein

Chain X:

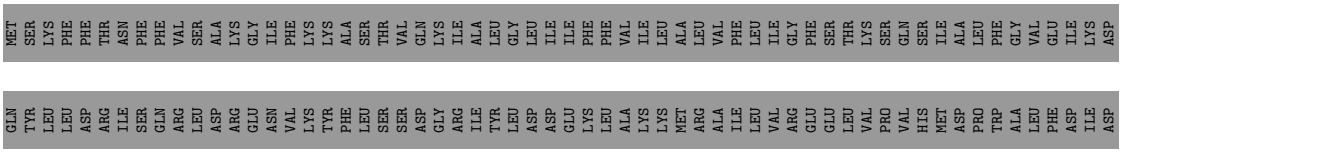


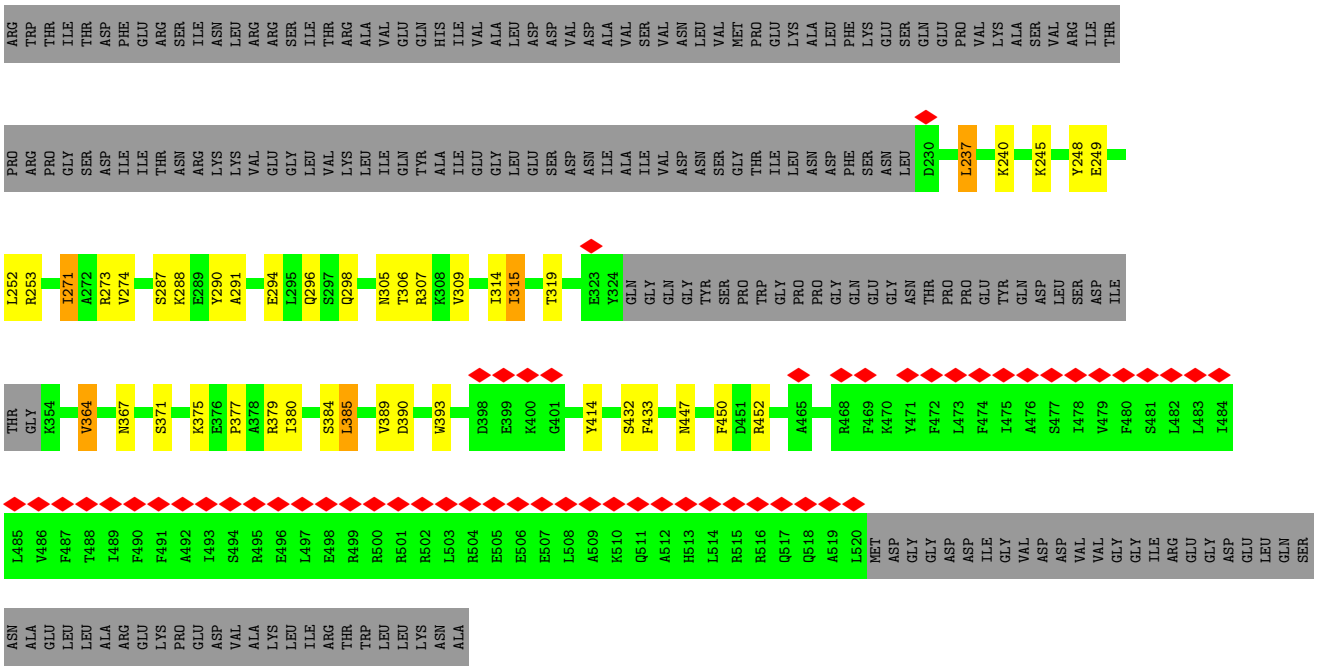


• Molecule 1: Flagellar M-ring protein

Chain Y:



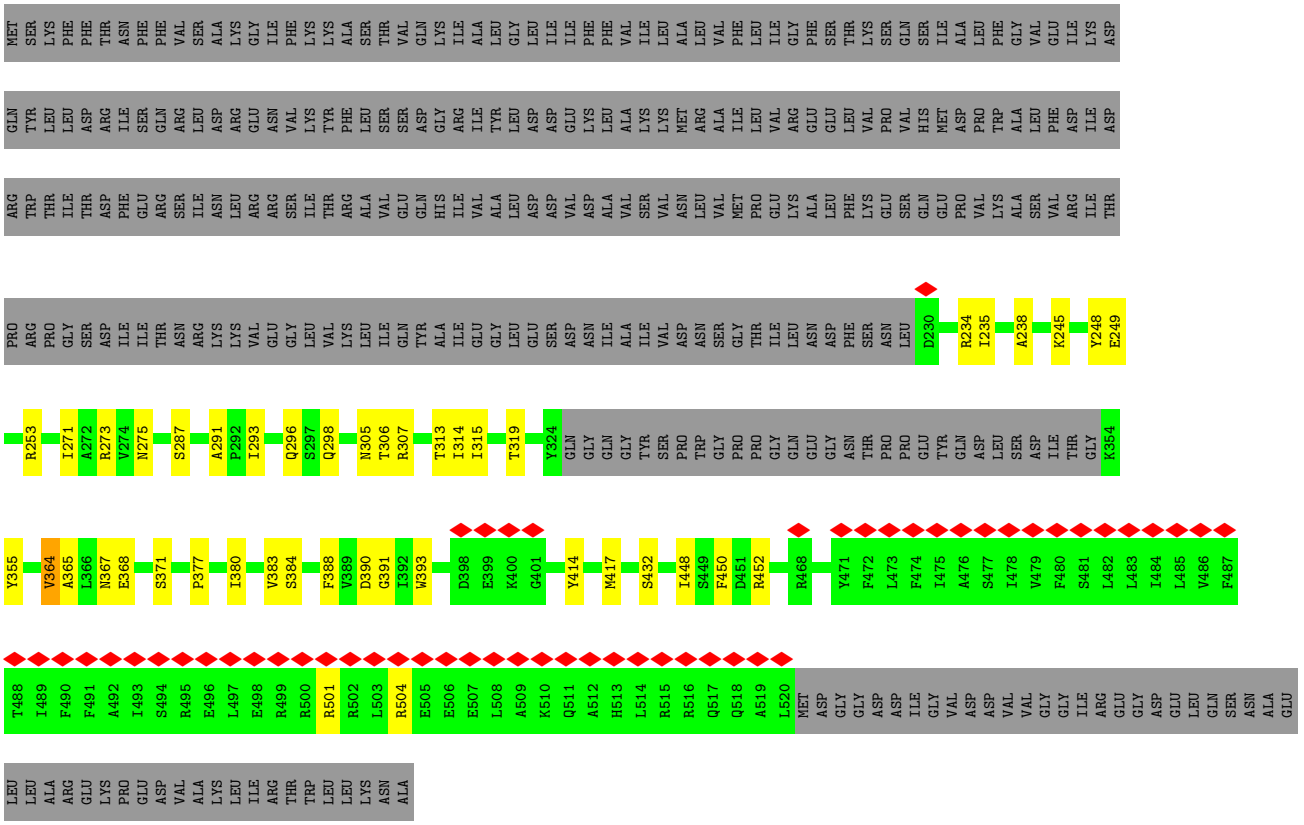




• Molecule 1: Flagellar M-ring protein

Chain Z:

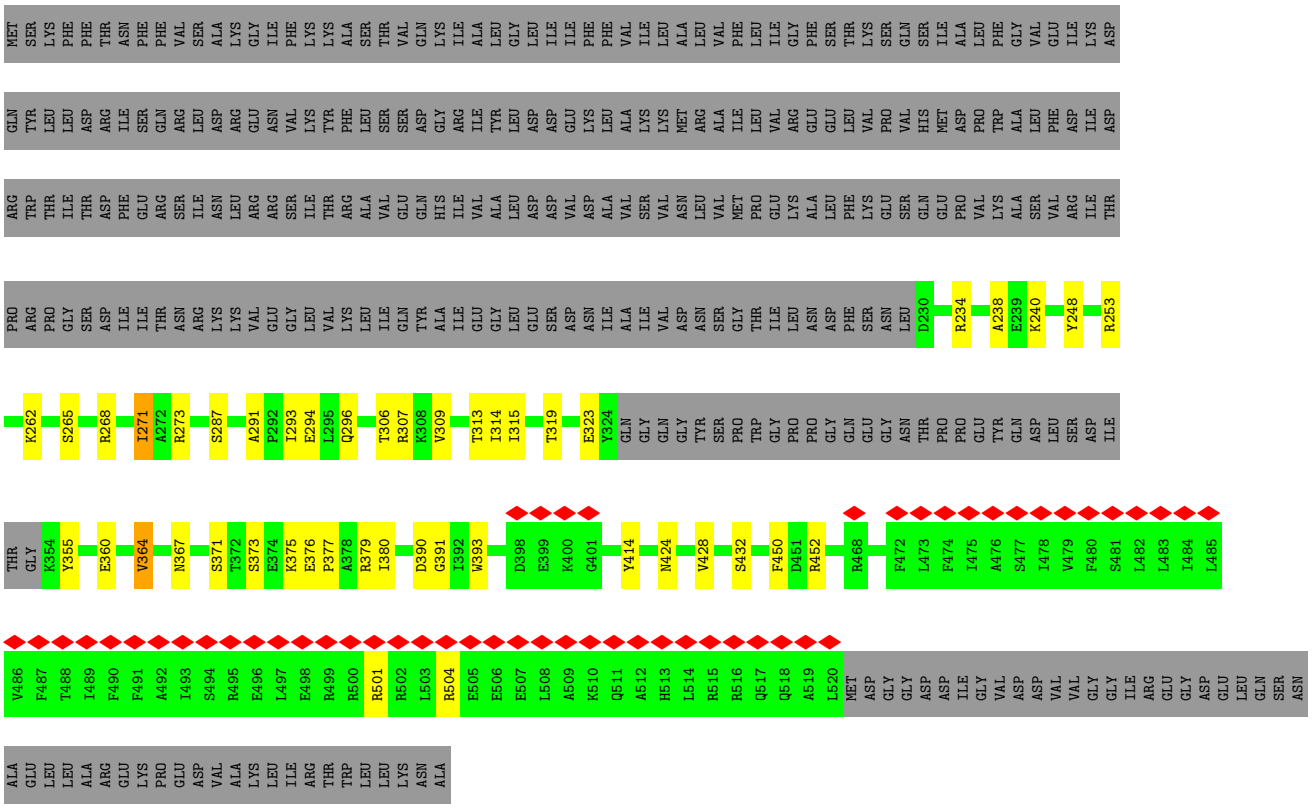




• Molecule 1: Flagellar M-ring protein

Chain a:

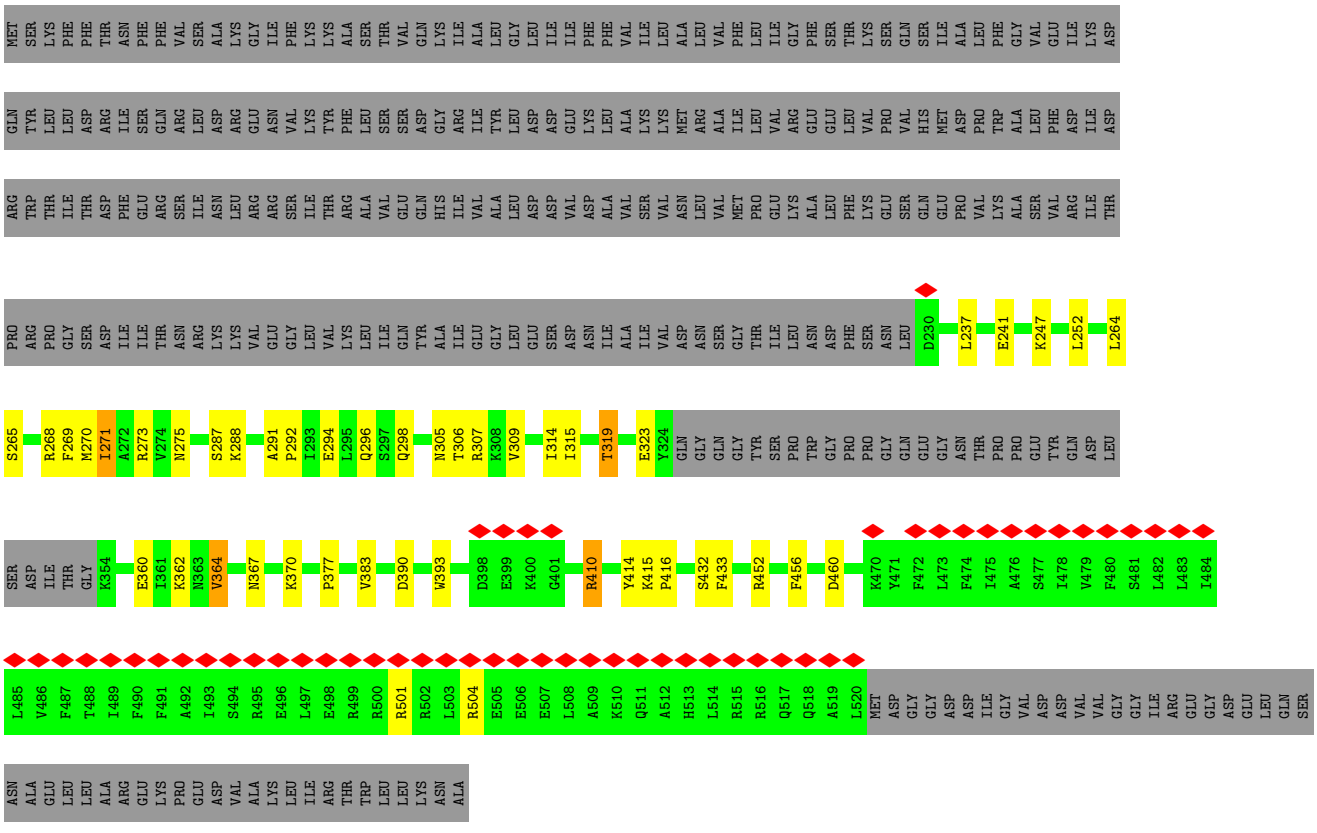




• Molecule 1: Flagellar M-ring protein

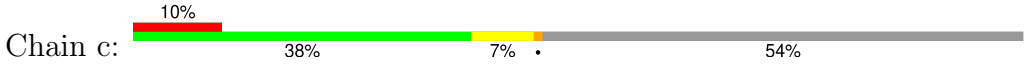
Chain b:

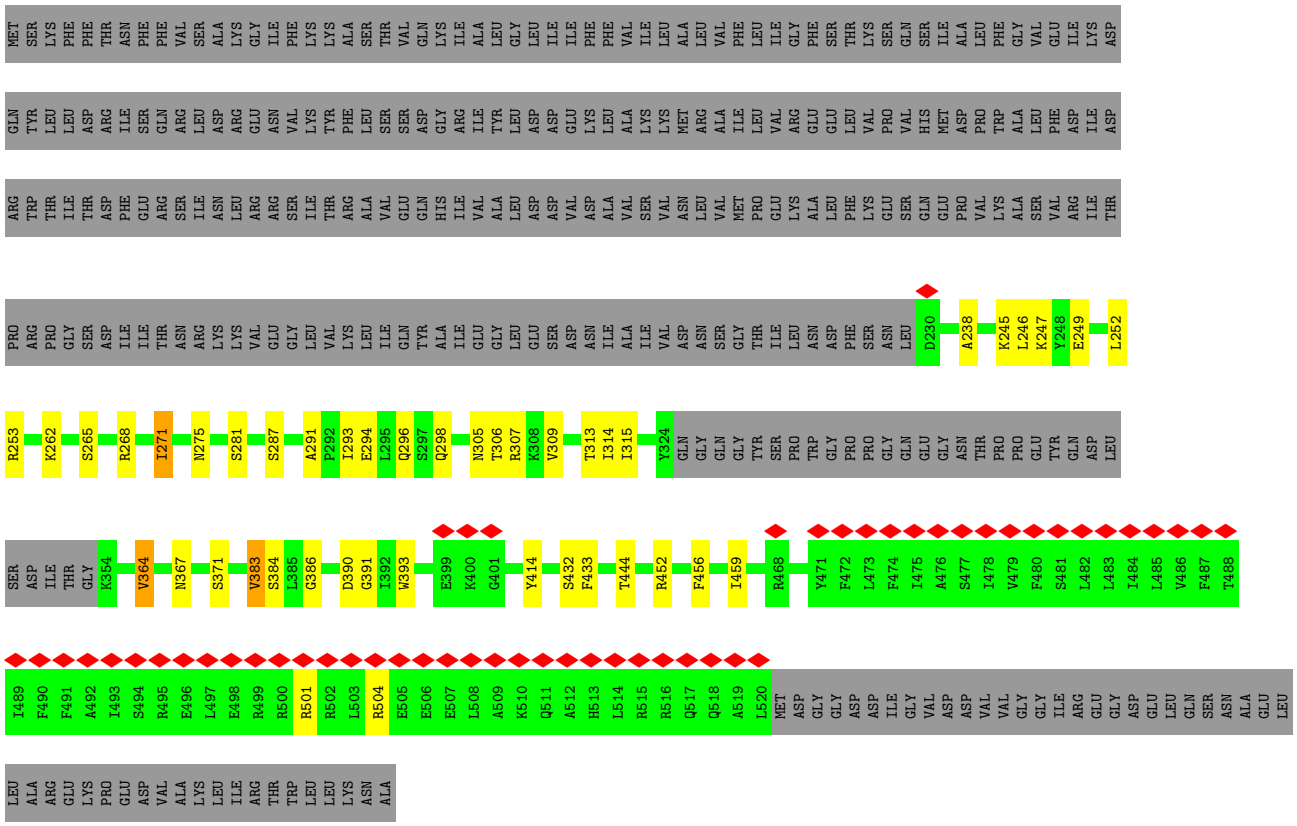




• Molecule 1: Flagellar M-ring protein

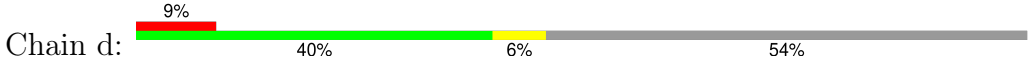
Chain c:

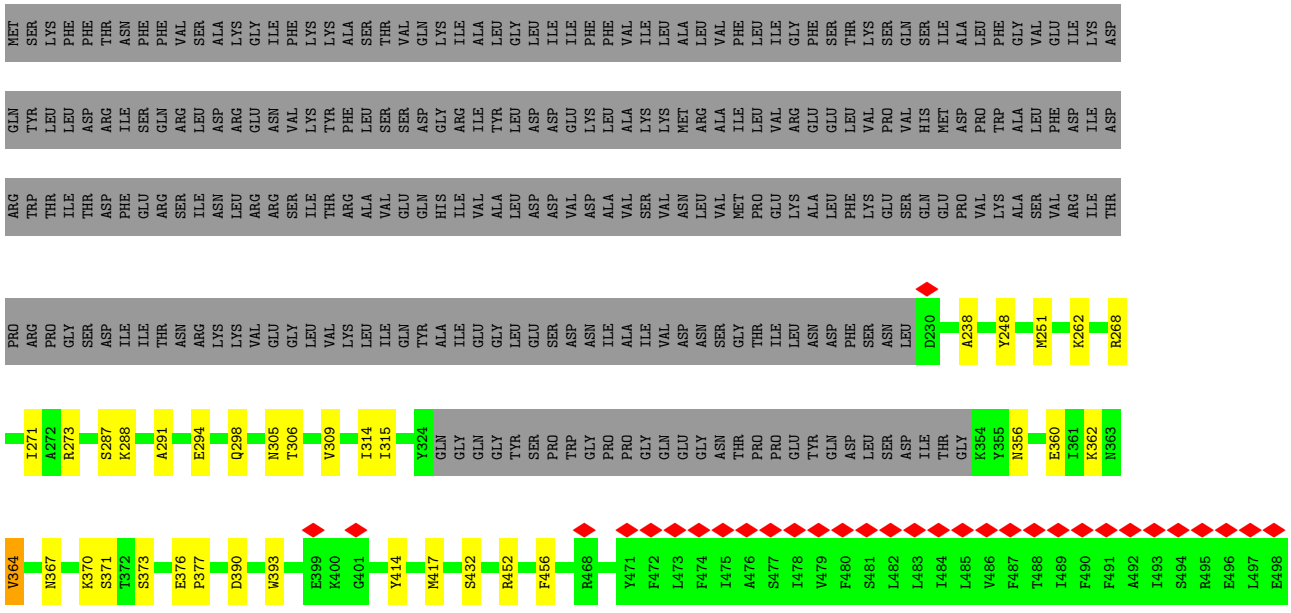


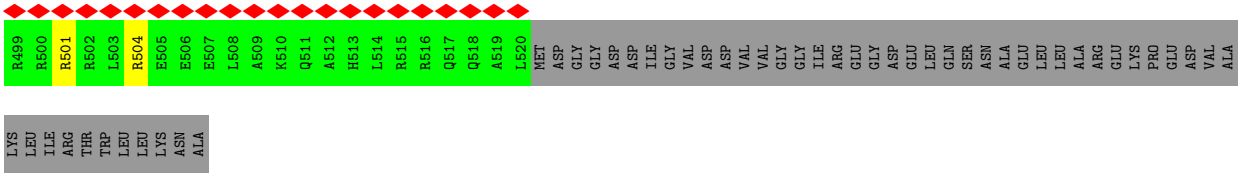


• Molecule 1: Flagellar M-ring protein

Chain d:



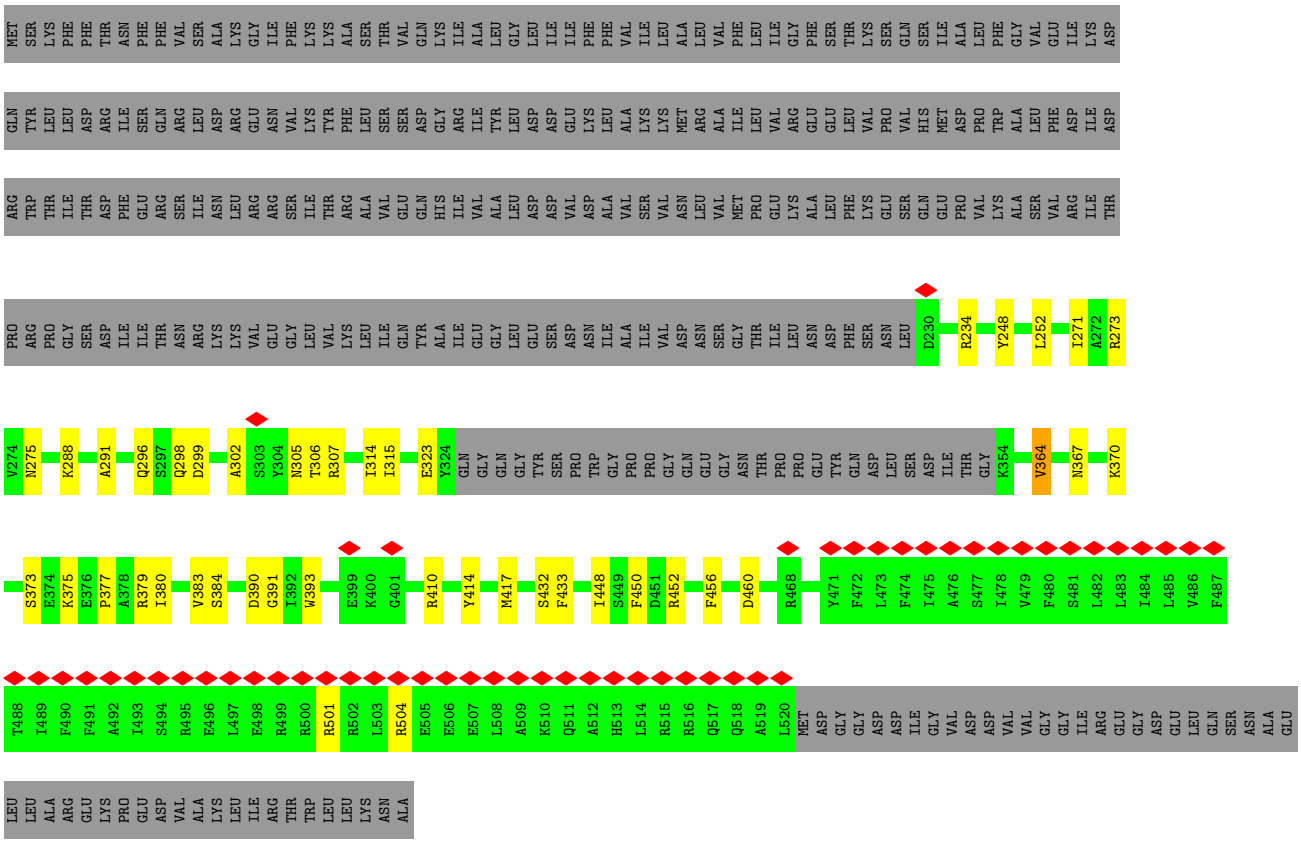




• Molecule 1: Flagellar M-ring protein

Chain e:

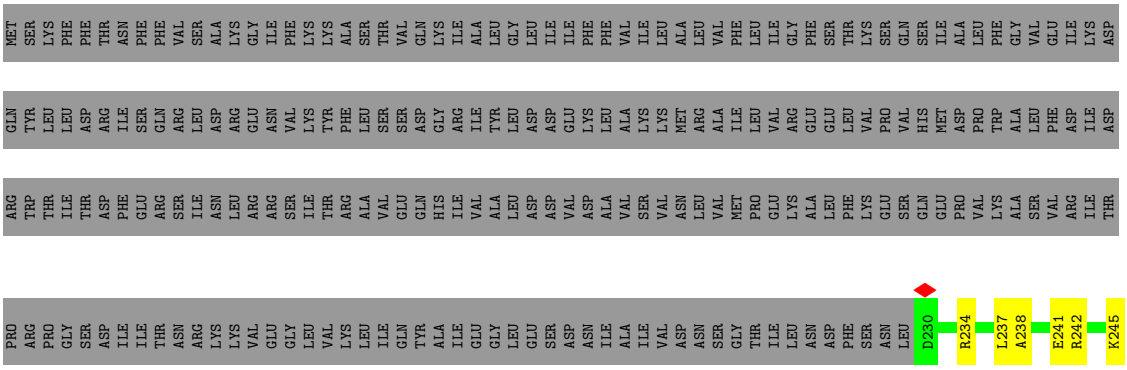


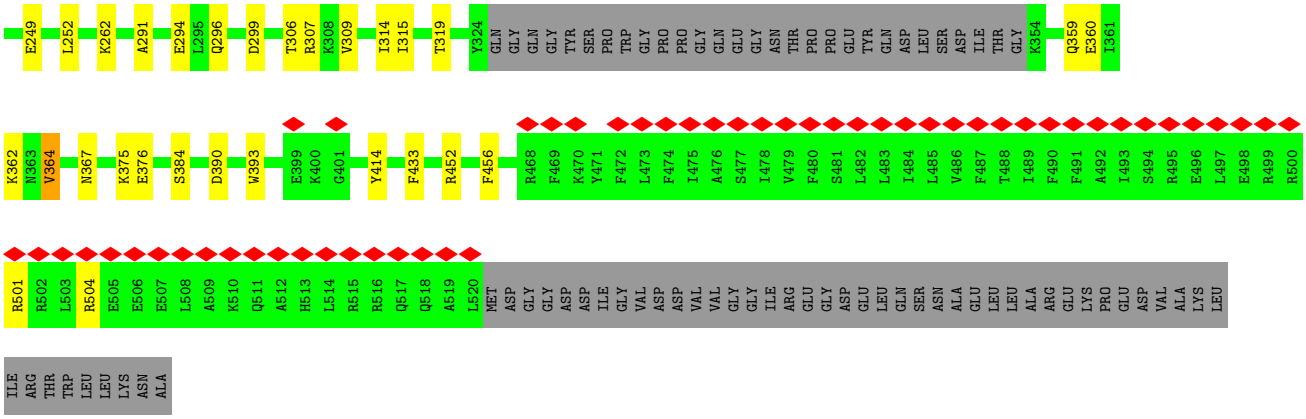


• Molecule 1: Flagellar M-ring protein

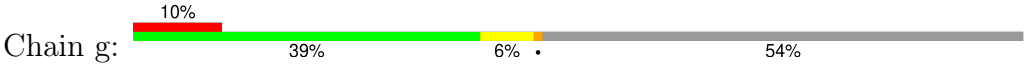
Chain f:

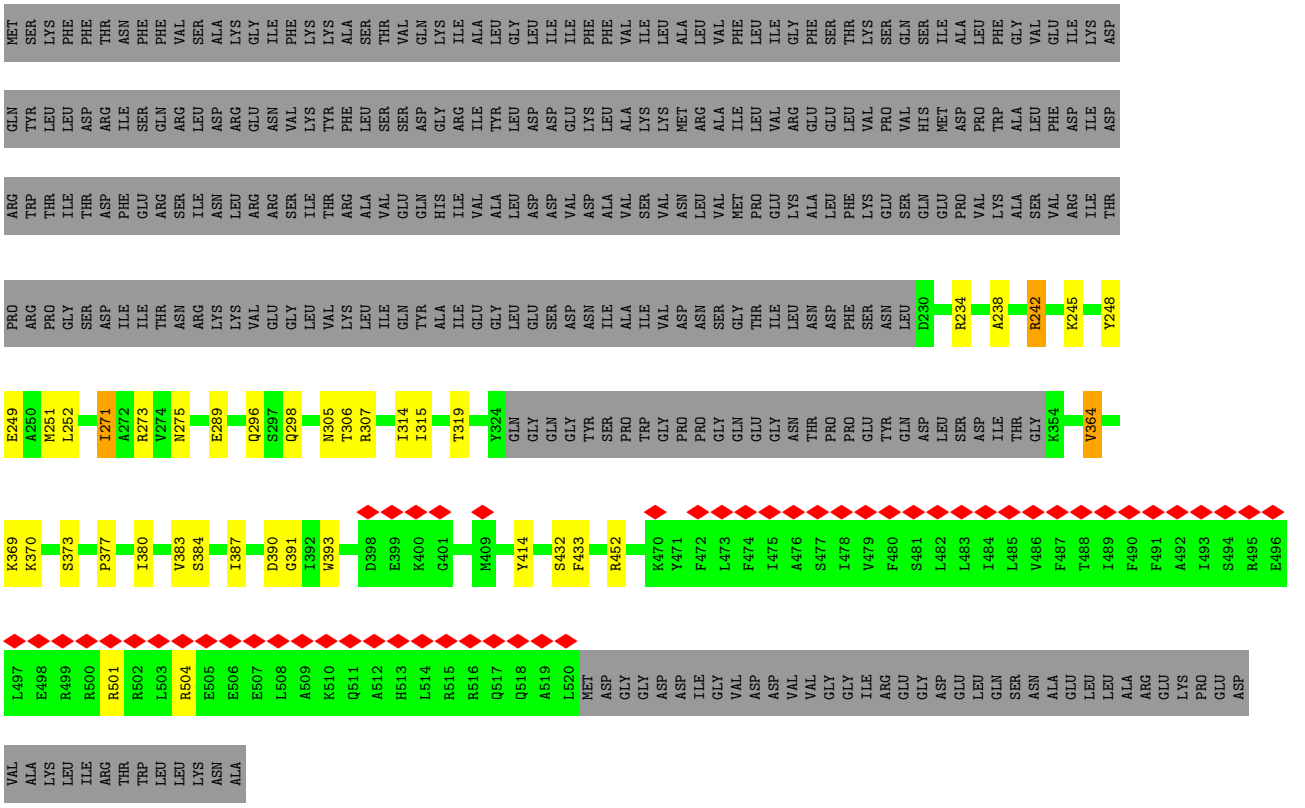




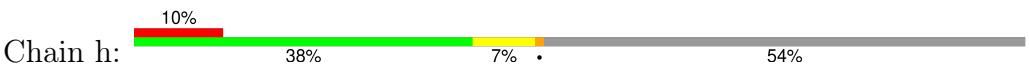


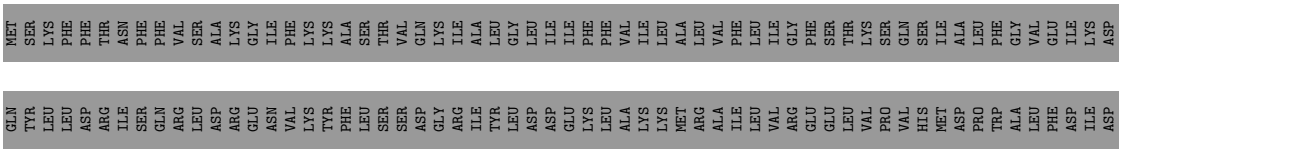
• Molecule 1: Flagellar M-ring protein

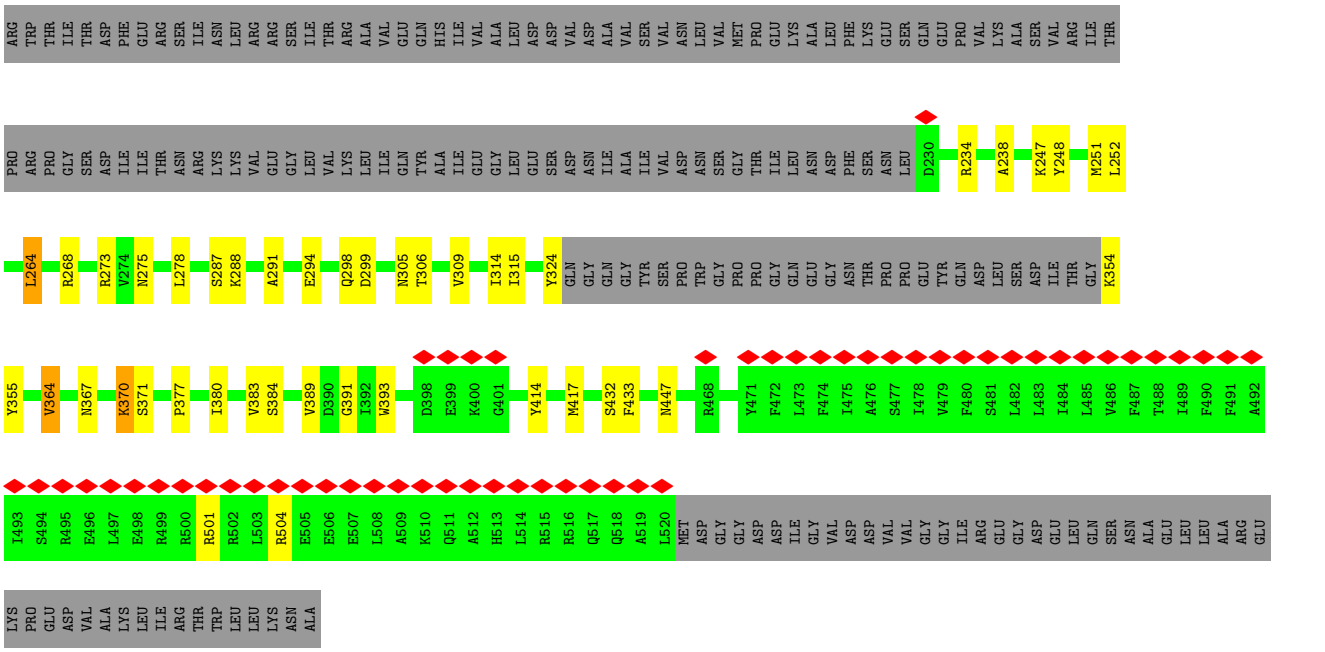




• Molecule 1: Flagellar M-ring protein



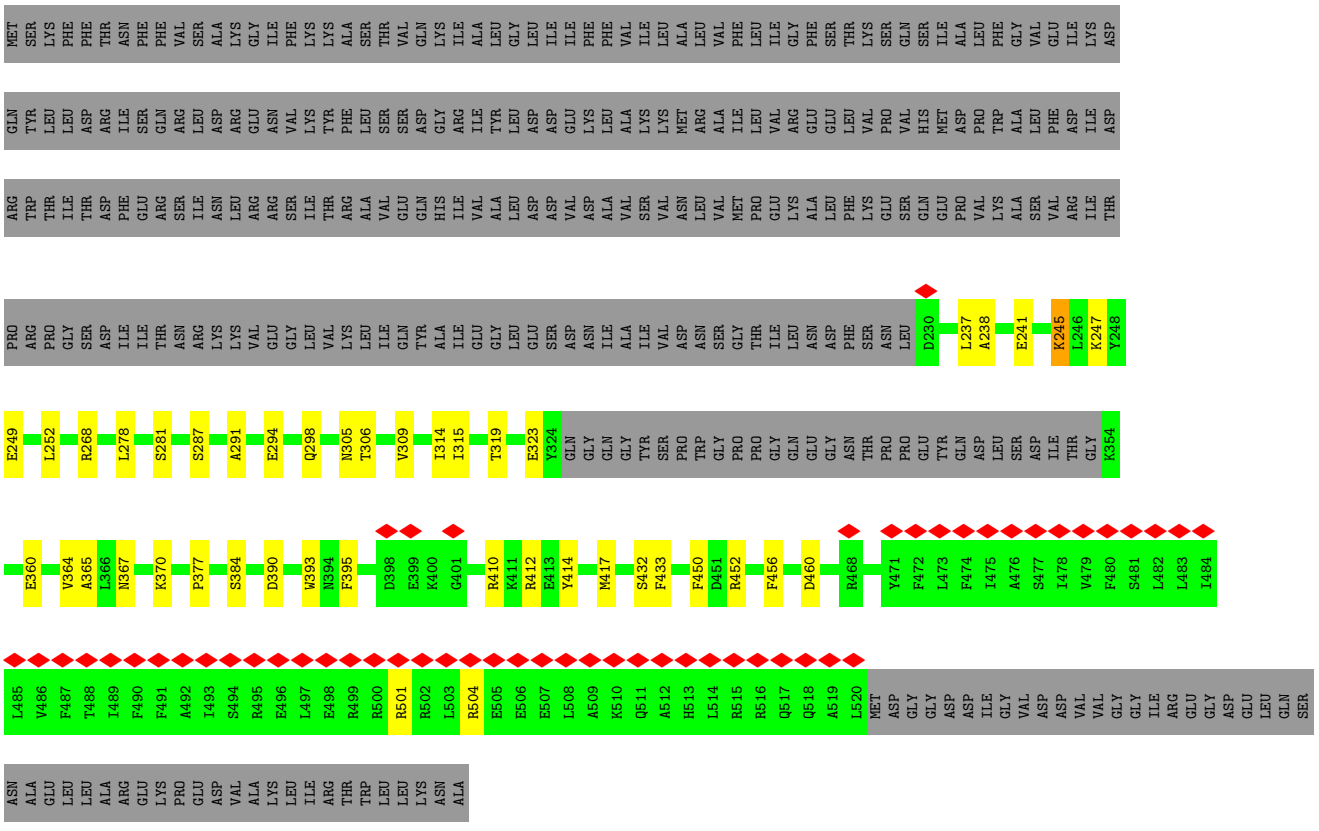




• Molecule 1: Flagellar M-ring protein

Chain i:

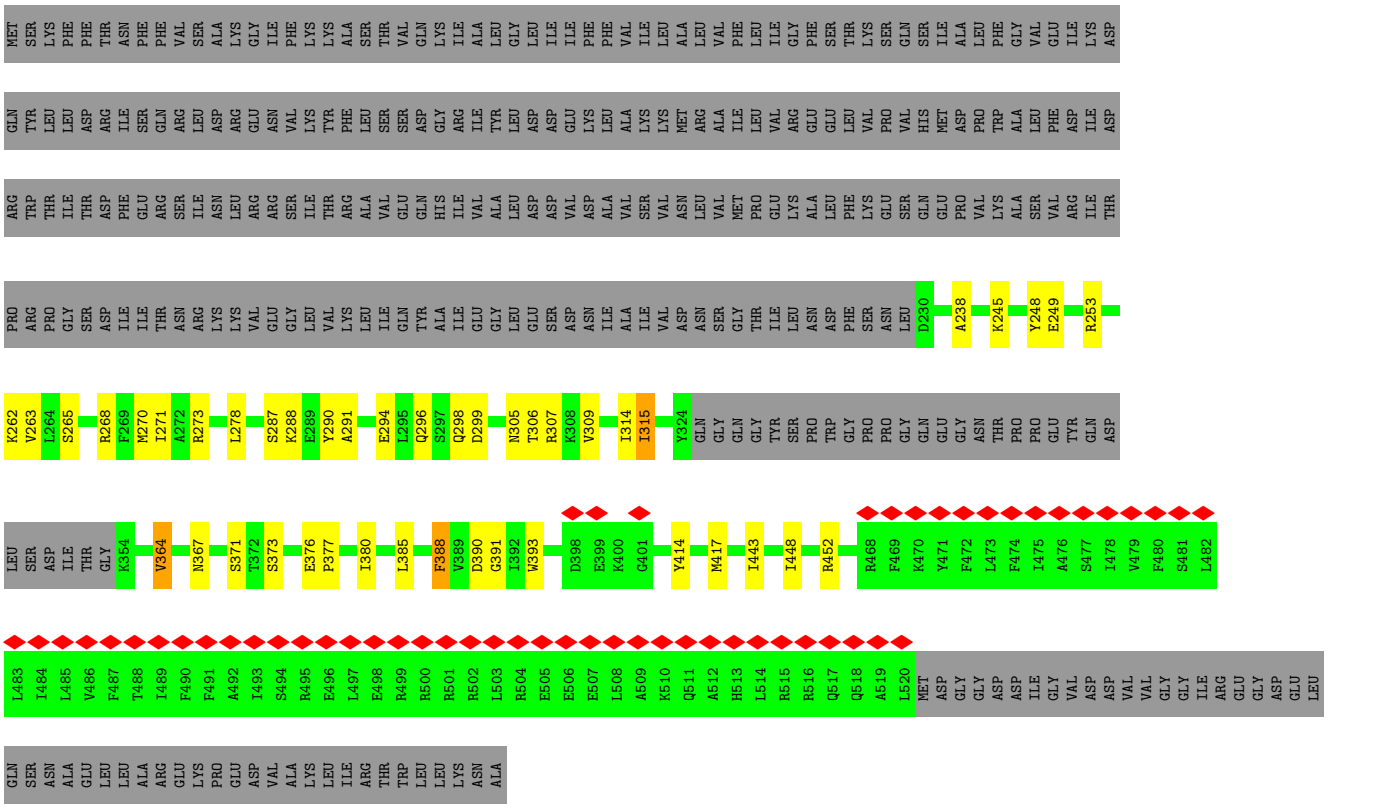




• Molecule 1: Flagellar M-ring protein

Chain j:

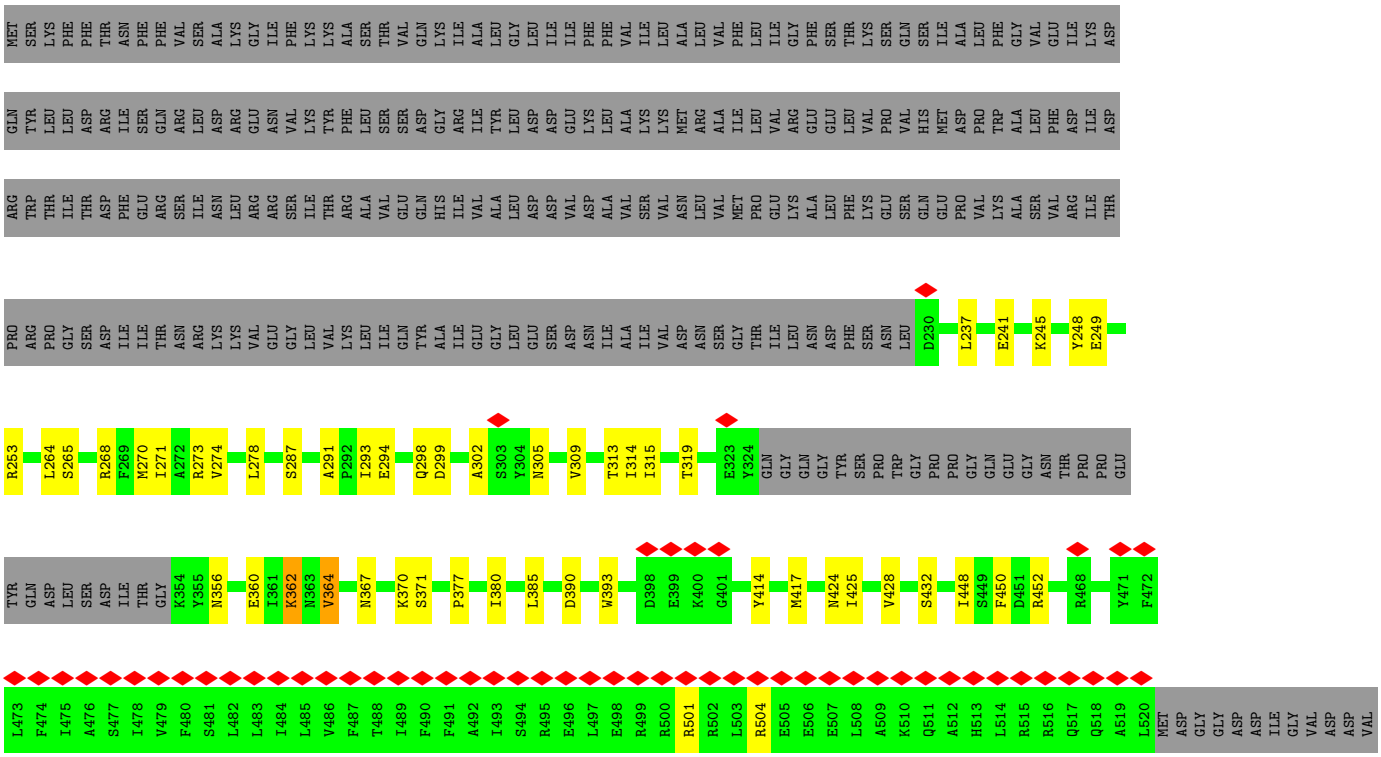




• Molecule 1: Flagellar M-ring protein

Chain k:



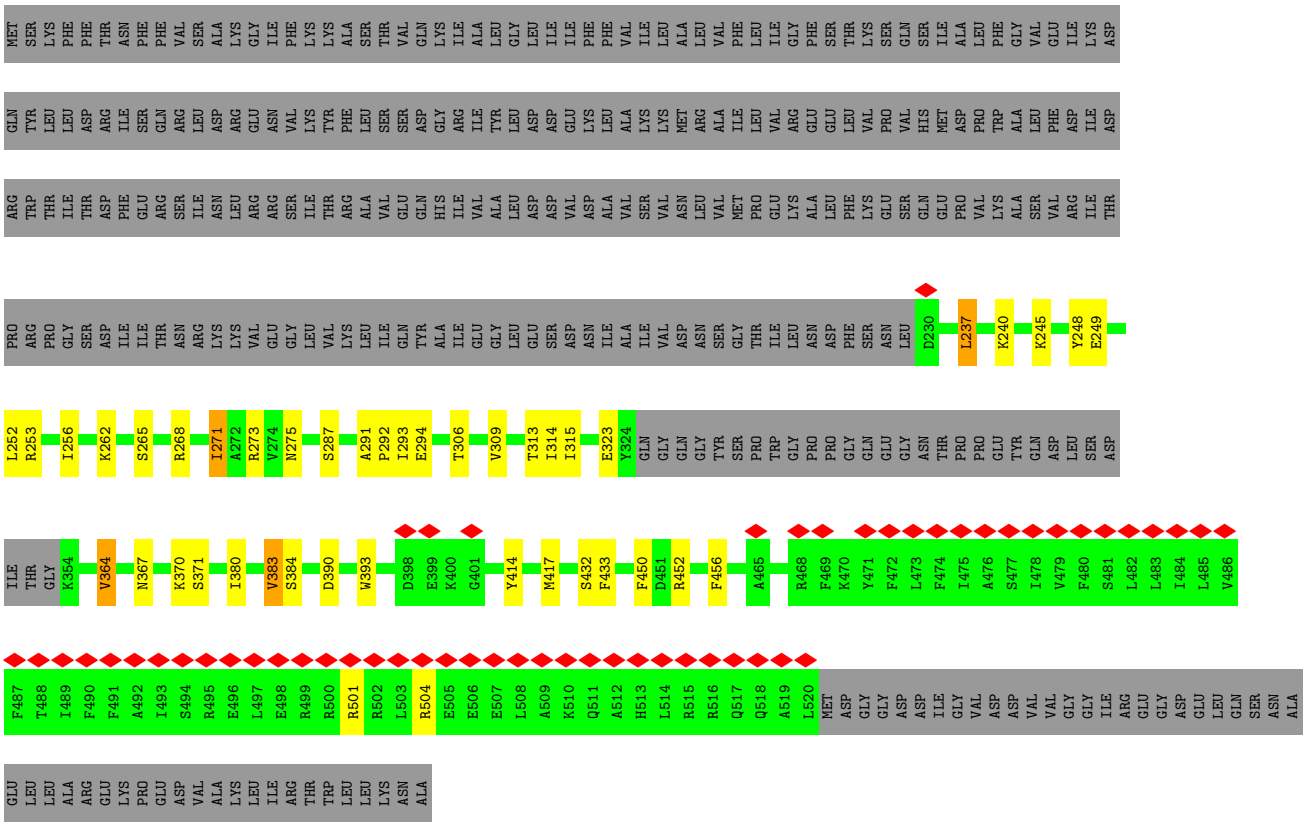




• Molecule 1: Flagellar M-ring protein

Chain l:

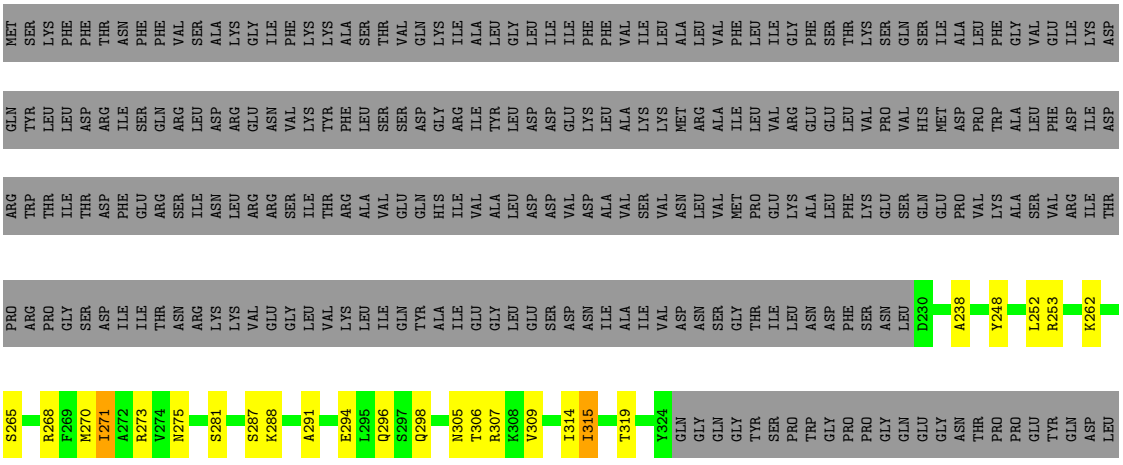


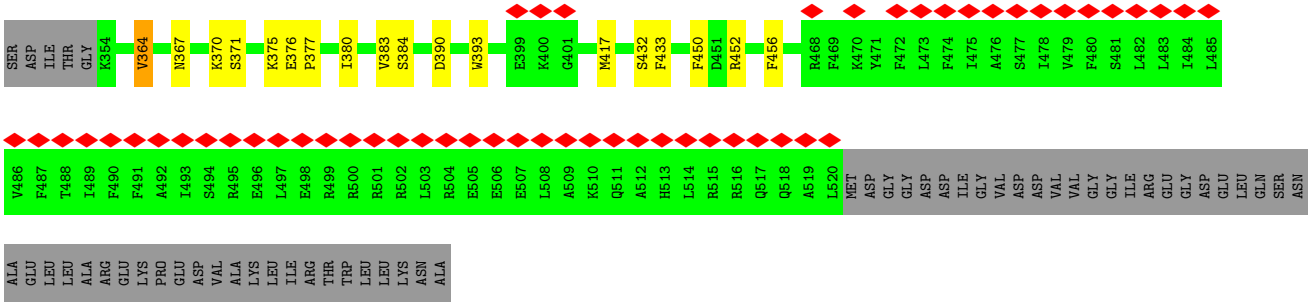


• Molecule 1: Flagellar M-ring protein

Chain m:



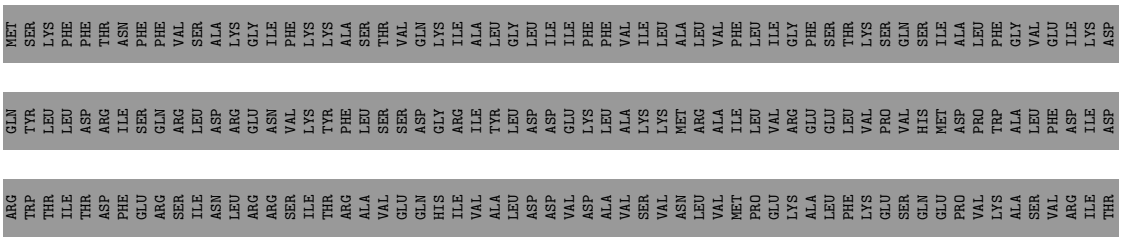


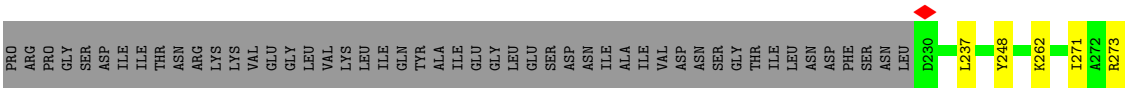


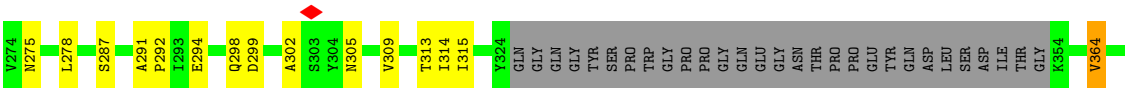
• Molecule 1: Flagellar M-ring protein

Chain n:

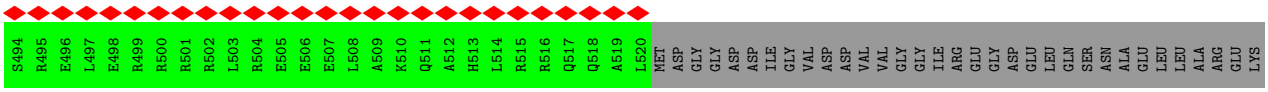










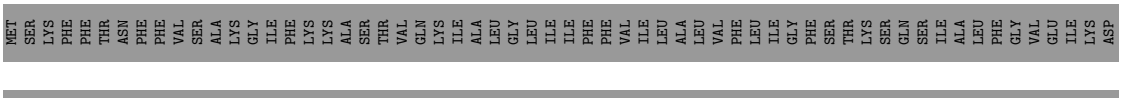


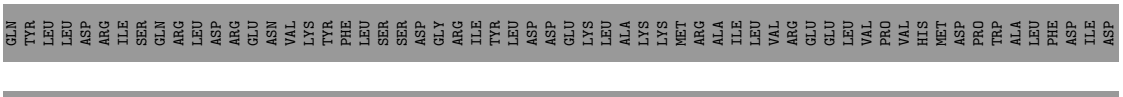


• Molecule 1: Flagellar M-ring protein

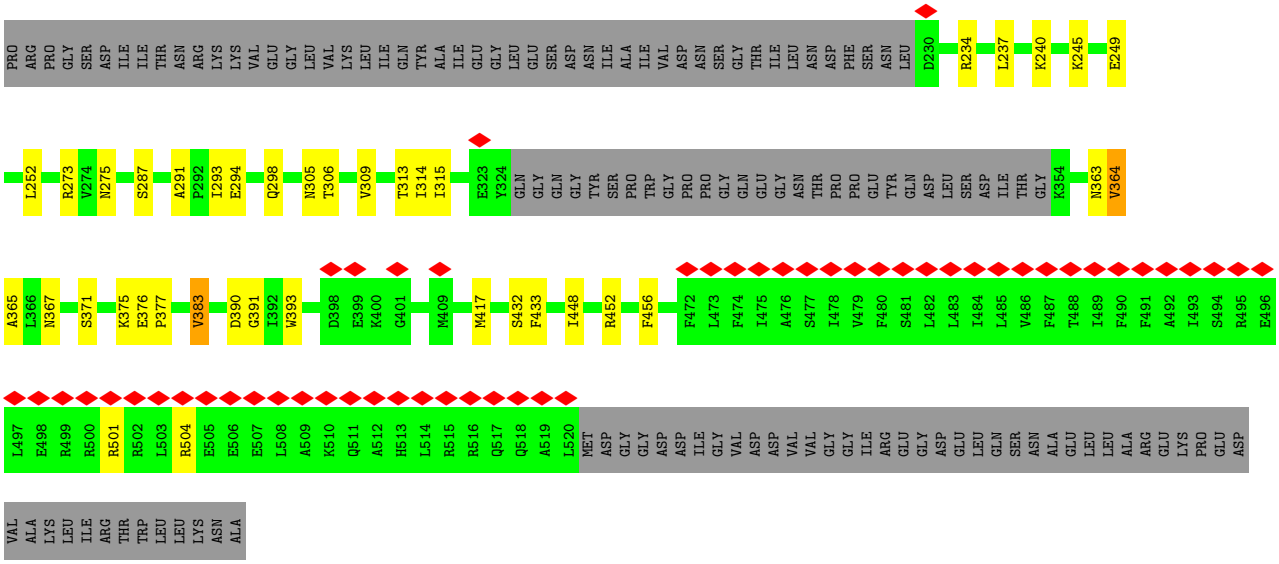
Chain o:










PRO ARG PRO GLY SER ASP ILE ILE THR ASN ARG LYS LYS VAL GLU GLY LEU VAL LYS LEU ILE GLN TYR ALA ILE GLU GLY LEU GLU SER ASP ASN ILE ALA ILE VAL ASP ASN SER GLY THR ILE LEU ASN ASP PHE SER ASN LEU D230 R234 L237 K240 K245 E249
L252 R273 W274 N275 S287 A291 P292 T293 E294 Q298 N305 T306 V309 T313 I314 I315 E323 Y324 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 K354 N363 V364
A365 L366 N367 S371 K375 E376 P377 V383 D390 G391 I392 W393 D398 E399 K400 G401 M409 M417 S432 F433 I448 R452 F456 F472 L473 F474 I475 A476 S477 I478 V479 F480 S481 L482 L483 I484 L485 V486 F487 T488 I489 F490 F491 A492 I493 S494 R495 E496
L497 E498 R499 R500 R501 R502 L503 R504 E505 E506 E507 L508 A509 K510 Q511 A512 H513 L514 R515 R516 Q517 Q518 A519 L520 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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40949	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	2.134	Depositor
Minimum map value	-1.694	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	640.8192, 640.8192, 640.8192	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4304, 1.4304, 1.4304	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.19	0/2132	0.29	0/2861
1	B	0.19	0/2132	0.29	0/2861
1	C	0.24	0/2132	0.33	0/2861
1	D	0.19	0/2132	0.29	0/2861
1	E	0.19	0/2132	0.30	0/2861
1	F	0.26	0/2132	0.33	0/2861
1	G	0.19	0/2132	0.28	0/2861
1	H	0.19	0/2132	0.29	0/2861
1	I	0.19	0/2132	0.29	0/2861
1	J	0.19	0/2132	0.30	0/2861
1	K	0.19	0/2132	0.28	0/2861
1	L	0.19	0/2132	0.29	0/2861
1	M	0.19	0/2132	0.28	0/2861
1	N	0.19	0/2132	0.29	0/2861
1	O	0.19	0/2132	0.29	0/2861
1	P	0.19	0/2132	0.29	0/2861
1	Q	0.19	0/2132	0.30	0/2861
1	R	0.25	0/2132	0.34	0/2861
1	S	0.19	0/2132	0.30	0/2861
1	T	0.19	0/2132	0.30	0/2861
1	U	0.19	0/2132	0.30	0/2861
1	V	0.23	0/2132	0.33	0/2861
1	W	0.19	0/2132	0.29	0/2861
1	X	0.19	0/2132	0.30	0/2861
1	Y	0.19	0/2132	0.29	0/2861
1	Z	0.20	0/2132	0.29	0/2861
1	a	0.19	0/2132	0.29	0/2861
1	b	0.19	0/2132	0.30	0/2861
1	c	0.19	0/2132	0.31	0/2861
1	d	0.19	0/2132	0.30	0/2861
1	e	0.20	0/2132	0.31	0/2861
1	f	0.19	0/2132	0.29	0/2861
1	g	0.19	0/2132	0.29	0/2861
1	h	0.19	0/2132	0.31	0/2861

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	i	0.19	0/2132	0.30	0/2861
1	j	0.19	0/2132	0.29	0/2861
1	k	0.19	0/2132	0.29	0/2861
1	l	0.19	0/2132	0.29	0/2861
1	m	0.19	0/2132	0.30	0/2861
1	n	0.19	0/2132	0.29	0/2861
1	o	0.19	0/2132	0.30	0/2861
All	All	0.20	0/87412	0.30	0/117301

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2104	0	2085	24	0
1	B	2104	0	2085	20	0
1	C	2104	0	2085	32	0
1	D	2104	0	2085	31	0
1	E	2104	0	2085	26	0
1	F	2104	0	2085	26	0
1	G	2104	0	2085	24	0
1	H	2104	0	2085	24	0
1	I	2104	0	2085	23	0
1	J	2104	0	2085	20	0
1	K	2104	0	2085	22	0
1	L	2104	0	2085	20	0
1	M	2104	0	2085	25	0
1	N	2104	0	2085	28	0
1	O	2104	0	2085	27	0
1	P	2104	0	2085	24	0
1	Q	2104	0	2085	30	0
1	R	2104	0	2085	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	2104	0	2085	26	0
1	T	2104	0	2085	23	0
1	U	2104	0	2085	18	0
1	V	2104	0	2085	19	0
1	W	2104	0	2085	23	0
1	X	2104	0	2085	29	0
1	Y	2104	0	2085	24	0
1	Z	2104	0	2085	27	0
1	a	2104	0	2085	29	0
1	b	2104	0	2085	29	0
1	c	2104	0	2085	28	0
1	d	2104	0	2085	21	0
1	e	2104	0	2085	23	0
1	f	2104	0	2085	19	0
1	g	2104	0	2085	22	0
1	h	2104	0	2085	26	0
1	i	2104	0	2085	28	0
1	j	2104	0	2085	28	0
1	k	2104	0	2085	31	0
1	l	2104	0	2085	28	0
1	m	2104	0	2085	27	0
1	n	2104	0	2085	25	0
1	o	2104	0	2085	22	0
All	All	86264	0	85485	884	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 (884) 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:C:324:TYR:CB	1:D:323:GLU:HG2	1.68	1.24
1:X:273:ARG:HB2	1:Y:432:SER:HB3	1.62	0.80
1:d:364:VAL:HG22	1:e:315:ILE:HA	1.64	0.80
1:l:364:VAL:HG22	1:m:315:ILE:HA	1.65	0.79
1:R:287:SER:HB2	1:R:371:SER:HB3	1.64	0.79
1:c:364:VAL:HG22	1:d:315:ILE:HA	1.66	0.77
1:R:273:ARG:HB2	1:S:432:SER:HB2	1.67	0.77
1:j:287:SER:HB3	1:j:371:SER:HB3	1.66	0.76
1:A:432:SER:HB2	1:o:273:ARG:HB2	1.67	0.76
1:A:364:VAL:HG22	1:B:315:ILE:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:273:ARG:HB2	1:X:432:SER:HB2	1.68	0.75
1:V:273:ARG:HB2	1:W:432:SER:HB2	1.67	0.75
1:O:364:VAL:HG22	1:P:315:ILE:HA	1.69	0.75
1:U:364:VAL:HG22	1:V:315:ILE:HA	1.67	0.75
1:J:364:VAL:HG22	1:K:315:ILE:HA	1.68	0.74
1:P:273:ARG:HB2	1:Q:432:SER:HB2	1.69	0.74
1:C:324:TYR:CB	1:D:323:GLU:CG	2.60	0.74
1:F:273:ARG:HB2	1:G:432:SER:HB2	1.70	0.74
1:K:273:ARG:HB2	1:L:432:SER:HB2	1.69	0.73
1:G:364:VAL:HG22	1:H:315:ILE:HA	1.71	0.73
1:I:364:VAL:HG22	1:J:315:ILE:HA	1.70	0.73
1:g:364:VAL:HG22	1:h:315:ILE:HA	1.70	0.73
1:N:291:ALA:HB3	1:N:367:ASN:HB2	1.71	0.73
1:a:273:ARG:HB2	1:b:432:SER:HB2	1.70	0.72
1:h:291:ALA:HB3	1:h:367:ASN:HB2	1.71	0.72
1:S:291:ALA:HB3	1:S:367:ASN:HB2	1.71	0.72
1:D:364:VAL:HG22	1:E:315:ILE:HA	1.69	0.72
1:b:273:ARG:HB2	1:c:432:SER:HB2	1.70	0.72
1:j:298:GLN:HE22	1:j:305:ASN:HA	1.55	0.72
1:S:364:VAL:HG22	1:T:315:ILE:HA	1.72	0.72
1:c:287:SER:HB2	1:c:371:SER:HB3	1.71	0.72
1:D:273:ARG:HB2	1:E:432:SER:HB2	1.71	0.72
1:J:273:ARG:HB2	1:K:432:SER:HB2	1.71	0.72
1:M:364:VAL:HG22	1:N:315:ILE:HA	1.72	0.71
1:m:364:VAL:HG22	1:n:315:ILE:HA	1.70	0.71
1:W:364:VAL:HG22	1:X:315:ILE:HA	1.73	0.71
1:k:273:ARG:HB2	1:l:432:SER:HB2	1.72	0.71
1:Z:364:VAL:HG22	1:a:315:ILE:HA	1.73	0.71
1:L:364:VAL:HG22	1:M:315:ILE:HA	1.72	0.71
1:Y:364:VAL:HG22	1:Z:315:ILE:HA	1.73	0.70
1:K:291:ALA:HB3	1:K:367:ASN:HB2	1.73	0.70
1:R:364:VAL:HG22	1:S:315:ILE:HA	1.73	0.70
1:B:364:VAL:HG22	1:C:315:ILE:HA	1.73	0.70
1:n:364:VAL:HG22	1:o:315:ILE:HA	1.74	0.70
1:H:273:ARG:HB2	1:I:432:SER:HB2	1.73	0.70
1:J:319:THR:HG22	1:J:360:GLU:HG3	1.72	0.70
1:G:273:ARG:HB2	1:H:432:SER:HB2	1.73	0.70
1:k:364:VAL:HG22	1:l:315:ILE:HA	1.73	0.70
1:h:273:ARG:HB2	1:i:432:SER:HB2	1.73	0.69
1:h:364:VAL:HG22	1:i:315:ILE:HA	1.72	0.69
1:Y:287:SER:HB2	1:Y:371:SER:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:273:ARG:HB2	1:m:432:SER:HB2	1.73	0.69
1:e:273:ARG:HH12	1:e:275:ASN:HD22	1.39	0.69
1:W:294:GLU:HA	1:W:309:VAL:HG12	1.74	0.69
1:C:294:GLU:HA	1:C:309:VAL:HG12	1.75	0.69
1:X:364:VAL:HG22	1:Y:315:ILE:HA	1.74	0.69
1:Y:273:ARG:HB2	1:Z:432:SER:HB2	1.74	0.69
1:b:364:VAL:HG22	1:c:315:ILE:HA	1.75	0.69
1:P:364:VAL:HG22	1:Q:315:ILE:HA	1.73	0.69
1:P:291:ALA:HB3	1:P:367:ASN:HB2	1.74	0.69
1:S:273:ARG:HB2	1:T:432:SER:HB2	1.75	0.68
1:Z:273:ARG:HB2	1:a:432:SER:HB2	1.74	0.68
1:f:364:VAL:HG22	1:g:315:ILE:HA	1.74	0.68
1:X:287:SER:HB2	1:X:371:SER:HB3	1.76	0.68
1:m:287:SER:HB3	1:m:371:SER:HB3	1.75	0.68
1:k:291:ALA:HB3	1:k:367:ASN:HB2	1.74	0.68
1:E:273:ARG:HB2	1:F:432:SER:HB2	1.74	0.68
1:L:273:ARG:HB2	1:M:432:SER:HB2	1.74	0.67
1:T:364:VAL:HG22	1:U:315:ILE:HA	1.75	0.67
1:B:273:ARG:HB2	1:C:432:SER:HB2	1.75	0.67
1:N:364:VAL:HG22	1:O:315:ILE:HA	1.75	0.67
1:j:273:ARG:HB2	1:k:432:SER:HB2	1.75	0.67
1:D:291:ALA:HB3	1:D:367:ASN:HB2	1.76	0.66
1:k:294:GLU:HA	1:k:309:VAL:HG12	1.77	0.66
1:C:364:VAL:HG22	1:D:315:ILE:HA	1.76	0.66
1:l:287:SER:HB2	1:l:371:SER:HB3	1.78	0.66
1:P:287:SER:HB2	1:P:371:SER:HB3	1.78	0.66
1:b:298:GLN:HE22	1:b:305:ASN:HA	1.61	0.66
1:g:273:ARG:HB2	1:h:432:SER:HB2	1.77	0.66
1:O:273:ARG:HB2	1:P:432:SER:HB2	1.77	0.65
1:n:294:GLU:HA	1:n:309:VAL:HG12	1.78	0.65
1:O:324:TYR:HA	1:O:354:LYS:HA	1.78	0.65
1:I:291:ALA:HB3	1:I:367:ASN:HB2	1.78	0.65
1:S:268:ARG:HH12	1:S:417:MET:HE3	1.61	0.65
1:V:291:ALA:HB3	1:V:367:ASN:HB2	1.79	0.65
1:A:287:SER:HB2	1:A:371:SER:HB3	1.78	0.65
1:Q:291:ALA:HB3	1:Q:367:ASN:HB2	1.78	0.65
1:n:273:ARG:HB2	1:o:432:SER:HB2	1.76	0.65
1:G:298:GLN:HE22	1:G:305:ASN:HA	1.61	0.65
1:k:298:GLN:HE22	1:k:305:ASN:HA	1.61	0.65
1:S:287:SER:HB3	1:S:371:SER:HB3	1.78	0.65
1:Z:355:TYR:HA	1:a:323:GLU:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:288:LYS:HD3	1:L:370:LYS:HD3	1.78	0.64
1:T:273:ARG:HB2	1:U:432:SER:HB2	1.79	0.64
1:U:291:ALA:HB3	1:U:367:ASN:HB2	1.78	0.64
1:P:268:ARG:HH12	1:P:417:MET:HE3	1.63	0.64
1:D:287:SER:HB2	1:D:371:SER:HB3	1.78	0.64
1:M:298:GLN:HE22	1:M:305:ASN:HA	1.63	0.64
1:b:501:ARG:HG2	1:b:504:ARG:HH21	1.63	0.63
1:Q:287:SER:HB2	1:Q:371:SER:HB3	1.80	0.63
1:N:298:GLN:HE22	1:N:305:ASN:HA	1.62	0.63
1:O:291:ALA:HB3	1:O:367:ASN:HB2	1.79	0.63
1:M:291:ALA:HB3	1:M:367:ASN:HB2	1.81	0.63
1:G:287:SER:HB2	1:G:371:SER:HB3	1.80	0.63
1:e:298:GLN:HE22	1:e:305:ASN:HA	1.64	0.63
1:d:294:GLU:HA	1:d:309:VAL:HG12	1.80	0.63
1:c:291:ALA:HB3	1:c:367:ASN:HB2	1.81	0.62
1:n:291:ALA:HB3	1:n:367:ASN:HB2	1.81	0.62
1:H:364:VAL:HG22	1:I:315:ILE:HA	1.81	0.62
1:H:291:ALA:HB3	1:H:367:ASN:HB2	1.81	0.62
1:X:291:ALA:HB3	1:X:367:ASN:HB2	1.82	0.62
1:Y:291:ALA:HB3	1:Y:367:ASN:HB2	1.82	0.62
1:M:273:ARG:HB2	1:N:432:SER:HB2	1.80	0.62
1:a:364:VAL:HG22	1:b:315:ILE:HA	1.82	0.62
1:j:294:GLU:HA	1:j:309:VAL:HG12	1.80	0.62
1:H:287:SER:HB2	1:H:371:SER:HB3	1.81	0.61
1:k:270:MET:HE3	1:l:262:LYS:HG3	1.81	0.61
1:R:298:GLN:HE22	1:R:305:ASN:HA	1.66	0.61
1:E:319:THR:HG22	1:E:360:GLU:HG3	1.83	0.61
1:i:291:ALA:HB3	1:i:367:ASN:HB2	1.83	0.61
1:T:291:ALA:HB3	1:T:367:ASN:HB2	1.82	0.61
1:d:291:ALA:HB3	1:d:367:ASN:HB2	1.82	0.61
1:F:287:SER:HB3	1:F:371:SER:HB3	1.83	0.60
1:o:291:ALA:HB3	1:o:367:ASN:HB2	1.83	0.60
1:Y:298:GLN:HE22	1:Y:305:ASN:HA	1.66	0.60
1:g:298:GLN:HE22	1:g:305:ASN:HA	1.66	0.60
1:M:294:GLU:HA	1:M:309:VAL:HG12	1.84	0.60
1:V:268:ARG:HH12	1:V:417:MET:HE3	1.67	0.60
1:n:298:GLN:HE22	1:n:305:ASN:HA	1.66	0.60
1:C:291:ALA:HB3	1:C:367:ASN:HB2	1.84	0.60
1:a:294:GLU:HA	1:a:309:VAL:HG12	1.83	0.60
1:e:364:VAL:HG22	1:f:315:ILE:HA	1.82	0.60
1:M:287:SER:HB2	1:M:371:SER:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:294:GLU:HA	1:O:309:VAL:HG12	1.84	0.60
1:o:294:GLU:HA	1:o:309:VAL:HG12	1.84	0.60
1:U:287:SER:HB2	1:U:371:SER:HB3	1.84	0.59
1:B:501:ARG:HG2	1:B:504:ARG:HH21	1.67	0.59
1:D:501:ARG:HG2	1:D:504:ARG:HH21	1.67	0.59
1:I:319:THR:HG22	1:I:360:GLU:HG3	1.84	0.59
1:N:287:SER:HB2	1:N:371:SER:HB3	1.83	0.59
1:P:294:GLU:HA	1:P:309:VAL:HG12	1.83	0.59
1:K:364:VAL:HG22	1:L:315:ILE:HA	1.84	0.59
1:Z:388:PHE:CE1	1:a:428:VAL:HG21	2.38	0.59
1:b:291:ALA:HB3	1:b:367:ASN:HB2	1.85	0.59
1:C:287:SER:HB2	1:C:371:SER:HB3	1.85	0.58
1:m:291:ALA:HB3	1:m:367:ASN:HB2	1.85	0.58
1:F:291:ALA:HB3	1:F:367:ASN:HB2	1.85	0.58
1:O:417:MET:H	1:O:447:ASN:HD21	1.50	0.58
1:U:501:ARG:HG2	1:U:504:ARG:HH21	1.68	0.58
1:P:253:ARG:HG3	1:P:271:ILE:HD12	1.86	0.58
1:Q:501:ARG:HG2	1:Q:504:ARG:HH21	1.69	0.58
1:F:364:VAL:HG22	1:G:315:ILE:HA	1.85	0.58
1:Y:390:ASP:HB2	1:Y:450:PHE:CD1	2.38	0.58
1:n:287:SER:HB2	1:n:371:SER:HB3	1.85	0.58
1:o:501:ARG:HG2	1:o:504:ARG:HH21	1.69	0.58
1:S:393:TRP:CE2	1:S:414:TYR:HB2	2.38	0.58
1:W:291:ALA:HB3	1:W:367:ASN:HB2	1.84	0.58
1:o:293:ILE:HD13	1:o:313:THR:HG21	1.84	0.58
1:V:298:GLN:HE22	1:V:305:ASN:HA	1.68	0.58
1:O:501:ARG:HG2	1:O:504:ARG:HH21	1.68	0.58
1:W:501:ARG:HG2	1:W:504:ARG:HH21	1.69	0.58
1:a:291:ALA:HB3	1:a:367:ASN:HB2	1.85	0.58
1:A:391:GLY:HA2	1:A:417:MET:HG2	1.85	0.58
1:B:293:ILE:HD13	1:B:313:THR:HG21	1.86	0.58
1:j:364:VAL:HG22	1:k:315:ILE:HA	1.85	0.57
1:G:294:GLU:HA	1:G:309:VAL:HG12	1.86	0.57
1:I:287:SER:HB2	1:I:371:SER:HB3	1.85	0.57
1:b:294:GLU:HA	1:b:309:VAL:HG12	1.85	0.57
1:l:265:SER:HB2	1:l:268:ARG:HG3	1.85	0.57
1:A:501:ARG:HG2	1:A:504:ARG:HH21	1.69	0.57
1:D:409:MET:HE2	1:D:457:ARG:HE	1.69	0.57
1:H:294:GLU:HA	1:H:309:VAL:HG12	1.86	0.57
1:K:393:TRP:CE2	1:K:414:TYR:HB2	2.39	0.57
1:V:364:VAL:HG22	1:W:315:ILE:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:293:ILE:HD13	1:l:313:THR:HG21	1.85	0.56
1:A:294:GLU:HA	1:A:309:VAL:HG12	1.85	0.56
1:C:501:ARG:HG2	1:C:504:ARG:HH21	1.70	0.56
1:f:237:LEU:O	1:f:241:GLU:HG2	2.05	0.56
1:a:424:ASN:O	1:a:428:VAL:HG22	2.04	0.56
1:i:294:GLU:HA	1:i:309:VAL:HG12	1.87	0.56
1:A:315:ILE:HA	1:o:364:VAL:HG22	1.87	0.56
1:J:501:ARG:HG2	1:J:504:ARG:HH21	1.70	0.56
1:k:424:ASN:O	1:k:428:VAL:HG12	2.05	0.56
1:U:253:ARG:HG3	1:U:271:ILE:HD12	1.88	0.56
1:e:501:ARG:HG2	1:e:504:ARG:HH21	1.71	0.56
1:f:242:ARG:HH12	1:g:251:MET:HE3	1.70	0.56
1:Y:294:GLU:HA	1:Y:309:VAL:HG12	1.87	0.56
1:c:298:GLN:HE22	1:c:305:ASN:HA	1.71	0.56
1:d:356:ASN:H	1:e:323:GLU:HB3	1.71	0.56
1:j:265:SER:HB3	1:j:268:ARG:HG3	1.88	0.56
1:B:391:GLY:HA2	1:B:417:MET:HG2	1.88	0.56
1:E:291:ALA:HB3	1:E:367:ASN:HB2	1.88	0.56
1:M:501:ARG:HG2	1:M:504:ARG:HH21	1.71	0.55
1:T:430:GLN:HA	1:T:443:ILE:HD12	1.88	0.55
1:T:501:ARG:HG2	1:T:504:ARG:HH21	1.71	0.55
1:b:237:LEU:O	1:b:241:GLU:HG2	2.06	0.55
1:L:294:GLU:HA	1:L:309:VAL:HG12	1.88	0.55
1:E:293:ILE:HD13	1:E:313:THR:HG21	1.86	0.55
1:R:291:ALA:HB3	1:R:367:ASN:HB2	1.89	0.55
1:N:501:ARG:HG2	1:N:504:ARG:HH21	1.72	0.55
1:V:324:TYR:HA	1:V:355:TYR:H	1.72	0.55
1:d:273:ARG:HB2	1:e:432:SER:HB2	1.88	0.55
1:C:393:TRP:CE2	1:C:414:TYR:HB2	2.42	0.55
1:H:501:ARG:HG2	1:H:504:ARG:HH21	1.72	0.55
1:O:323:GLU:HG3	1:O:324:TYR:H	1.71	0.55
1:J:298:GLN:HE22	1:J:305:ASN:HA	1.72	0.55
1:K:287:SER:HB2	1:K:371:SER:HB3	1.88	0.55
1:o:298:GLN:HE22	1:o:305:ASN:HA	1.71	0.55
1:D:293:ILE:HD13	1:D:313:THR:HG21	1.88	0.54
1:K:501:ARG:HG2	1:K:504:ARG:HH21	1.73	0.54
1:D:319:THR:HG22	1:D:360:GLU:HG3	1.89	0.54
1:D:323:GLU:HG3	1:D:324:TYR:H	1.72	0.54
1:E:390:ASP:CG	1:E:452:ARG:HH21	2.16	0.54
1:f:393:TRP:CE2	1:f:414:TYR:HB2	2.41	0.54
1:f:501:ARG:HG2	1:f:504:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:393:TRP:CE2	1:i:414:TYR:HB2	2.42	0.54
1:E:287:SER:HB2	1:E:371:SER:HB3	1.90	0.54
1:F:390:ASP:CG	1:F:452:ARG:HH21	2.15	0.54
1:A:291:ALA:HB3	1:A:367:ASN:HB2	1.90	0.54
1:F:294:GLU:HA	1:F:309:VAL:HG12	1.89	0.54
1:Q:273:ARG:HB2	1:R:432:SER:HB2	1.89	0.54
1:c:501:ARG:HG2	1:c:504:ARG:HH21	1.71	0.54
1:h:501:ARG:HG2	1:h:504:ARG:HH21	1.72	0.54
1:G:268:ARG:HH12	1:G:417:MET:HE3	1.73	0.54
1:G:291:ALA:HB3	1:G:367:ASN:HB2	1.90	0.54
1:P:288:LYS:HB3	1:Q:368:GLU:HB2	1.89	0.54
1:N:294:GLU:HA	1:N:309:VAL:HG12	1.89	0.54
1:S:501:ARG:HG2	1:S:504:ARG:HH21	1.72	0.54
1:Q:364:VAL:HG22	1:R:315:ILE:HA	1.89	0.53
1:I:289:GLU:HB2	1:I:369:LYS:HB3	1.89	0.53
1:X:393:TRP:CE2	1:X:414:TYR:HB2	2.43	0.53
1:B:319:THR:HG22	1:B:360:GLU:HG3	1.89	0.53
1:h:324:TYR:HA	1:h:354:LYS:HA	1.90	0.53
1:k:299:ASP:HB2	1:k:302:ALA:HB2	1.90	0.53
1:M:393:TRP:CE2	1:M:414:TYR:HB2	2.44	0.53
1:O:393:TRP:CE2	1:O:414:TYR:HB2	2.44	0.53
1:Z:291:ALA:HB3	1:Z:367:ASN:HB2	1.90	0.53
1:B:271:ILE:HG23	1:B:387:ILE:HG12	1.90	0.53
1:D:390:ASP:CG	1:D:452:ARG:HH21	2.17	0.53
1:N:393:TRP:CE2	1:N:414:TYR:HB2	2.44	0.53
1:E:501:ARG:HG2	1:E:504:ARG:HH21	1.72	0.53
1:Z:390:ASP:CG	1:Z:452:ARG:HH21	2.16	0.53
1:e:291:ALA:HB3	1:e:367:ASN:HB2	1.90	0.53
1:B:294:GLU:HA	1:B:309:VAL:HG12	1.91	0.53
1:H:298:GLN:HE22	1:H:305:ASN:HA	1.73	0.53
1:N:390:ASP:HB2	1:N:450:PHE:CD1	2.43	0.53
1:i:390:ASP:HB2	1:i:450:PHE:CD1	2.44	0.53
1:N:319:THR:HG22	1:N:360:GLU:HG3	1.91	0.53
1:F:238:ALA:HB2	1:G:377:PRO:HB2	1.91	0.52
1:G:393:TRP:CE2	1:G:414:TYR:HB2	2.44	0.52
1:U:393:TRP:CE2	1:U:414:TYR:HB2	2.44	0.52
1:R:294:GLU:HA	1:R:309:VAL:HG12	1.91	0.52
1:g:393:TRP:CE2	1:g:414:TYR:HB2	2.44	0.52
1:g:501:ARG:HG2	1:g:504:ARG:HH21	1.74	0.52
1:i:237:LEU:O	1:i:241:GLU:HG2	2.09	0.52
1:J:293:ILE:HG21	1:J:313:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:393:TRP:CE2	1:J:414:TYR:HB2	2.45	0.52
1:h:355:TYR:HA	1:i:323:GLU:HB3	1.91	0.52
1:D:324:TYR:HA	1:D:354:LYS:HA	1.91	0.52
1:Q:298:GLN:HE22	1:Q:305:ASN:HA	1.74	0.52
1:d:501:ARG:HG2	1:d:504:ARG:HH21	1.75	0.52
1:H:356:ASN:HB3	1:I:323:GLU:HB3	1.91	0.52
1:O:390:ASP:CG	1:O:452:ARG:HH21	2.18	0.52
1:Q:393:TRP:CE2	1:Q:414:TYR:HB2	2.45	0.52
1:f:390:ASP:CG	1:f:452:ARG:HH21	2.18	0.52
1:D:424:ASN:O	1:D:428:VAL:HG12	2.09	0.52
1:E:409:MET:HE2	1:E:457:ARG:HE	1.73	0.52
1:J:390:ASP:CG	1:J:452:ARG:HH21	2.18	0.52
1:b:252:LEU:HD13	1:b:433:PHE:HE2	1.75	0.52
1:k:237:LEU:O	1:k:241:GLU:HG2	2.10	0.52
1:S:238:ALA:HB2	1:T:377:PRO:HB2	1.92	0.52
1:X:240:LYS:HZ2	1:X:243:LYS:HD3	1.76	0.51
1:i:268:ARG:HH12	1:i:417:MET:HE3	1.75	0.51
1:P:393:TRP:CE3	1:P:456:PHE:HE2	2.28	0.51
1:H:360:GLU:OE2	1:H:362:LYS:HD3	2.10	0.51
1:V:501:ARG:HG2	1:V:504:ARG:HH21	1.76	0.51
1:n:248:TYR:CE2	1:n:380:ILE:HD11	2.45	0.51
1:V:294:GLU:HA	1:V:309:VAL:HG12	1.92	0.51
1:l:501:ARG:HG2	1:l:504:ARG:HH21	1.75	0.51
1:m:273:ARG:HH12	1:m:275:ASN:HD22	1.58	0.51
1:D:275:ASN:O	1:D:383:VAL:HA	2.10	0.51
1:J:248:TYR:CE2	1:J:380:ILE:HD11	2.46	0.51
1:W:287:SER:HB2	1:W:371:SER:HB3	1.92	0.51
1:a:375:LYS:HG2	1:a:376:GLU:O	2.10	0.51
1:d:288:LYS:HE2	1:d:370:LYS:HE3	1.93	0.51
1:i:395:PHE:CD1	1:i:410:ARG:HD2	2.46	0.51
1:A:393:TRP:CE2	1:A:414:TYR:HB2	2.46	0.51
1:Y:253:ARG:HG3	1:Y:271:ILE:HD12	1.92	0.51
1:I:253:ARG:HG3	1:I:271:ILE:HD12	1.93	0.51
1:S:289:GLU:HB2	1:S:369:LYS:HB3	1.92	0.50
1:U:235:ILE:HG21	1:V:240:LYS:HG3	1.92	0.50
1:V:287:SER:HB2	1:V:371:SER:HB3	1.93	0.50
1:L:501:ARG:HG2	1:L:504:ARG:HH21	1.76	0.50
1:N:275:ASN:O	1:N:383:VAL:HA	2.11	0.50
1:Q:315:ILE:HD13	1:Q:365:ALA:HB2	1.93	0.50
1:T:393:TRP:CE2	1:T:414:TYR:HB2	2.46	0.50
1:a:293:ILE:HD13	1:a:313:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:268:ARG:HH12	1:K:417:MET:HE3	1.77	0.50
1:Y:393:TRP:CE2	1:Y:414:TYR:HB2	2.46	0.50
1:J:291:ALA:HB3	1:J:367:ASN:HB2	1.94	0.50
1:E:294:GLU:HA	1:E:309:VAL:HG12	1.94	0.50
1:J:287:SER:HB2	1:J:371:SER:HB3	1.94	0.50
1:K:252:LEU:HD13	1:K:433:PHE:HE1	1.77	0.50
1:L:375:LYS:HG2	1:L:376:GLU:O	2.11	0.50
1:j:388:PHE:CD2	1:k:428:VAL:HG11	2.47	0.50
1:K:390:ASP:CG	1:K:452:ARG:HH21	2.20	0.50
1:B:390:ASP:CG	1:B:452:ARG:HH21	2.20	0.50
1:H:375:LYS:HG2	1:H:376:GLU:O	2.12	0.50
1:Q:390:ASP:CG	1:Q:452:ARG:HH21	2.20	0.50
1:Z:298:GLN:HE21	1:Z:305:ASN:HA	1.77	0.50
1:a:390:ASP:CG	1:a:452:ARG:HH21	2.20	0.50
1:g:242:ARG:HH12	1:h:251:MET:HE3	1.77	0.50
1:K:290:TYR:H	1:L:367:ASN:ND2	2.10	0.50
1:N:290:TYR:H	1:O:367:ASN:ND2	2.10	0.50
1:Q:252:LEU:HD13	1:Q:433:PHE:HE1	1.77	0.50
1:e:299:ASP:HB2	1:e:302:ALA:HB2	1.93	0.50
1:j:268:ARG:HH12	1:j:417:MET:HE3	1.77	0.50
1:j:393:TRP:CE2	1:j:414:TYR:HB2	2.47	0.50
1:m:253:ARG:HG3	1:m:271:ILE:HD12	1.93	0.50
1:k:501:ARG:HG2	1:k:504:ARG:HH21	1.75	0.49
1:d:238:ALA:HB2	1:e:377:PRO:HB2	1.93	0.49
1:d:393:TRP:CE2	1:d:414:TYR:HB2	2.47	0.49
1:D:268:ARG:HH12	1:D:417:MET:HE3	1.77	0.49
1:H:390:ASP:CG	1:H:452:ARG:HH21	2.20	0.49
1:L:393:TRP:CE3	1:L:456:PHE:HE2	2.30	0.49
1:X:390:ASP:HB2	1:X:450:PHE:CD1	2.47	0.49
1:M:252:LEU:HD13	1:M:433:PHE:HE1	1.77	0.49
1:b:393:TRP:CE2	1:b:414:TYR:HB2	2.48	0.49
1:m:238:ALA:HB2	1:n:377:PRO:HB2	1.94	0.49
1:O:275:ASN:O	1:O:383:VAL:HA	2.12	0.49
1:l:253:ARG:HG3	1:l:271:ILE:HD12	1.94	0.49
1:F:275:ASN:O	1:F:383:VAL:HA	2.12	0.49
1:G:252:LEU:HD13	1:G:433:PHE:HE1	1.77	0.49
1:Q:294:GLU:HA	1:Q:309:VAL:HG12	1.94	0.49
1:k:390:ASP:CG	1:k:452:ARG:HH21	2.20	0.49
1:n:275:ASN:O	1:n:383:VAL:HA	2.13	0.49
1:f:393:TRP:CE3	1:f:456:PHE:HE2	2.30	0.49
1:m:294:GLU:HA	1:m:309:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:253:ARG:HG3	1:k:271:ILE:HD12	1.94	0.49
1:B:291:ALA:HB3	1:B:367:ASN:HB2	1.93	0.49
1:P:430:GLN:HA	1:P:443:ILE:HD12	1.95	0.49
1:S:385:LEU:HG	1:S:443:ILE:HG23	1.95	0.49
1:l:294:GLU:HA	1:l:309:VAL:HG12	1.94	0.49
1:T:385:LEU:HG	1:T:443:ILE:HG23	1.95	0.49
1:g:238:ALA:HB2	1:h:377:PRO:HB2	1.95	0.49
1:M:390:ASP:CG	1:M:452:ARG:HH21	2.21	0.48
1:N:395:PHE:CD1	1:N:410:ARG:HD2	2.48	0.48
1:O:287:SER:HB2	1:O:371:SER:HB3	1.94	0.48
1:P:393:TRP:CE2	1:P:414:TYR:HB2	2.48	0.48
1:R:390:ASP:CG	1:R:452:ARG:HH21	2.21	0.48
1:f:291:ALA:HB3	1:f:367:ASN:HB2	1.95	0.48
1:S:248:TYR:CE2	1:S:380:ILE:HD11	2.48	0.48
1:V:252:LEU:HD13	1:V:433:PHE:HE1	1.78	0.48
1:F:393:TRP:CE2	1:F:414:TYR:HB2	2.48	0.48
1:G:418:ALA:HB3	1:G:421:GLU:HG2	1.96	0.48
1:O:271:ILE:HG23	1:O:387:ILE:HG12	1.95	0.48
1:f:294:GLU:HA	1:f:309:VAL:HG12	1.96	0.48
1:A:390:ASP:CG	1:A:452:ARG:HH21	2.21	0.48
1:D:393:TRP:CE2	1:D:414:TYR:HB2	2.49	0.48
1:M:293:ILE:HD13	1:M:313:THR:HG21	1.95	0.48
1:a:238:ALA:HB2	1:b:377:PRO:HB2	1.95	0.48
1:b:360:GLU:OE2	1:b:362:LYS:HD2	2.14	0.48
1:c:393:TRP:CE2	1:c:414:TYR:HB2	2.48	0.48
1:Z:388:PHE:HD1	1:Z:448:ILE:HD12	1.78	0.48
1:o:287:SER:HB2	1:o:371:SER:HB3	1.95	0.48
1:C:390:ASP:CG	1:C:452:ARG:HH21	2.21	0.48
1:G:390:ASP:CG	1:G:452:ARG:HH21	2.21	0.48
1:I:393:TRP:CE2	1:I:414:TYR:HB2	2.49	0.48
1:K:294:GLU:HA	1:K:309:VAL:HG12	1.96	0.48
1:B:393:TRP:CE2	1:B:414:TYR:HB2	2.49	0.48
1:G:375:LYS:HG2	1:G:376:GLU:O	2.13	0.48
1:a:393:TRP:CE2	1:a:414:TYR:HB2	2.49	0.48
1:c:253:ARG:HG3	1:c:271:ILE:HD12	1.94	0.48
1:l:275:ASN:O	1:l:383:VAL:HA	2.14	0.48
1:I:501:ARG:HG2	1:I:504:ARG:HH21	1.79	0.48
1:S:252:LEU:HD13	1:S:433:PHE:HE1	1.79	0.48
1:a:375:LYS:NZ	1:a:379:ARG:HE	2.12	0.48
1:l:252:LEU:HD13	1:l:433:PHE:HE2	1.78	0.48
1:n:393:TRP:CE2	1:n:414:TYR:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:ILE:HA	1:F:317:SER:O	2.14	0.47
1:E:393:TRP:CE2	1:E:414:TYR:HB2	2.48	0.47
1:W:262:LYS:HE3	1:W:262:LYS:HB3	1.69	0.47
1:Y:288:LYS:HB3	1:Z:368:GLU:HB2	1.96	0.47
1:h:264:LEU:HD22	1:h:417:MET:HE1	1.96	0.47
1:E:268:ARG:HH12	1:E:417:MET:HE3	1.80	0.47
1:G:253:ARG:HG3	1:G:271:ILE:HD12	1.96	0.47
1:L:288:LYS:HE2	1:L:290:TYR:CE1	2.48	0.47
1:R:252:LEU:HD13	1:R:433:PHE:HE1	1.80	0.47
1:R:393:TRP:CE2	1:R:414:TYR:HB2	2.49	0.47
1:U:391:GLY:HA2	1:U:417:MET:HG2	1.95	0.47
1:b:393:TRP:CE3	1:b:456:PHE:HE2	2.32	0.47
1:d:268:ARG:HH12	1:d:417:MET:HE3	1.79	0.47
1:g:390:ASP:CG	1:g:452:ARG:HH21	2.22	0.47
1:l:248:TYR:CE2	1:l:380:ILE:HD11	2.49	0.47
1:W:275:ASN:O	1:W:383:VAL:HA	2.14	0.47
1:i:315:ILE:HD13	1:i:365:ALA:HB2	1.95	0.47
1:U:252:LEU:HD13	1:U:433:PHE:HE2	1.79	0.47
1:W:360:GLU:OE2	1:W:362:LYS:HD2	2.14	0.47
1:i:245:LYS:O	1:i:249:GLU:HG3	2.15	0.47
1:B:248:TYR:CE2	1:B:380:ILE:HD11	2.50	0.47
1:X:248:TYR:CE1	1:X:380:ILE:HD11	2.49	0.47
1:Z:248:TYR:CE2	1:Z:380:ILE:HD11	2.50	0.47
1:e:391:GLY:HA2	1:e:417:MET:HG2	1.96	0.47
1:o:391:GLY:HA2	1:o:417:MET:HG2	1.95	0.47
1:B:252:LEU:HD13	1:B:433:PHE:HE2	1.79	0.47
1:X:289:GLU:HB2	1:X:369:LYS:HB3	1.96	0.47
1:C:248:TYR:CE2	1:C:380:ILE:HD11	2.49	0.47
1:G:430:GLN:HA	1:G:443:ILE:HD12	1.96	0.47
1:K:245:LYS:O	1:K:249:GLU:HG3	2.15	0.47
1:P:275:ASN:O	1:P:383:VAL:HA	2.15	0.47
1:R:248:TYR:CE2	1:R:380:ILE:HD11	2.49	0.47
1:U:390:ASP:CG	1:U:452:ARG:HH21	2.23	0.47
1:Y:248:TYR:CE2	1:Y:380:ILE:HD11	2.50	0.47
1:e:393:TRP:CE3	1:e:456:PHE:HE2	2.33	0.47
1:i:390:ASP:CG	1:i:452:ARG:HH21	2.23	0.47
1:l:390:ASP:CG	1:l:452:ARG:HH21	2.22	0.47
1:I:275:ASN:O	1:I:383:VAL:HA	2.15	0.47
1:Q:238:ALA:HB2	1:R:377:PRO:HB2	1.97	0.47
1:X:298:GLN:NE2	1:X:305:ASN:HA	2.30	0.47
1:d:287:SER:OG	1:d:371:SER:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:252:LEU:HD13	1:g:433:PHE:HE2	1.79	0.47
1:h:393:TRP:CE2	1:h:414:TYR:HB2	2.49	0.47
1:A:245:LYS:O	1:A:249:GLU:HG3	2.15	0.47
1:A:248:TYR:CE2	1:A:380:ILE:HD11	2.50	0.47
1:C:253:ARG:HG3	1:C:271:ILE:HD12	1.97	0.47
1:H:248:TYR:CE2	1:H:380:ILE:HD11	2.50	0.47
1:i:393:TRP:CE3	1:i:456:PHE:HE2	2.32	0.47
1:m:270:MET:HE3	1:m:271:ILE:H	1.80	0.47
1:H:395:PHE:HB3	1:H:410:ARG:HD2	1.96	0.47
1:P:240:LYS:HD3	1:P:240:LYS:HA	1.66	0.47
1:S:314:ILE:H	1:S:314:ILE:HG13	1.53	0.47
1:D:282:LYS:HD3	1:E:374:GLU:OE1	2.15	0.46
1:D:298:GLN:NE2	1:D:305:ASN:HA	2.31	0.46
1:I:390:ASP:CG	1:I:452:ARG:HH21	2.23	0.46
1:J:253:ARG:HG3	1:J:271:ILE:HD12	1.97	0.46
1:O:298:GLN:NE2	1:O:305:ASN:HA	2.29	0.46
1:P:298:GLN:NE2	1:P:305:ASN:HA	2.30	0.46
1:T:238:ALA:HB2	1:U:377:PRO:HB2	1.97	0.46
1:V:238:ALA:HB2	1:W:377:PRO:HB2	1.97	0.46
1:e:375:LYS:NZ	1:e:379:ARG:HE	2.13	0.46
1:A:253:ARG:HG3	1:A:271:ILE:HD12	1.97	0.46
1:M:375:LYS:NZ	1:M:379:ARG:HE	2.12	0.46
1:O:268:ARG:HH12	1:O:417:MET:HE3	1.79	0.46
1:W:393:TRP:CE2	1:W:414:TYR:HB2	2.50	0.46
1:X:275:ASN:O	1:X:383:VAL:HA	2.15	0.46
1:j:291:ALA:HB3	1:j:367:ASN:HB2	1.97	0.46
1:D:248:TYR:CE2	1:D:380:ILE:HD11	2.50	0.46
1:T:248:TYR:CE2	1:T:380:ILE:HD11	2.51	0.46
1:c:245:LYS:O	1:c:249:GLU:HG3	2.15	0.46
1:I:234:ARG:HH21	1:J:377:PRO:HA	1.80	0.46
1:N:248:TYR:CE1	1:N:380:ILE:HD11	2.50	0.46
1:h:248:TYR:CE2	1:h:380:ILE:HD11	2.50	0.46
1:n:299:ASP:HB2	1:n:302:ALA:HB2	1.97	0.46
1:A:287:SER:O	1:A:370:LYS:HA	2.16	0.46
1:L:390:ASP:CG	1:L:452:ARG:HH21	2.24	0.46
1:Q:240:LYS:HA	1:Q:240:LYS:HD3	1.70	0.46
1:c:252:LEU:HD13	1:c:433:PHE:HE1	1.81	0.46
1:C:273:ARG:HB2	1:D:432:SER:HB2	1.98	0.46
1:I:268:ARG:HH12	1:I:417:MET:HE3	1.80	0.46
1:S:390:ASP:HB2	1:S:450:PHE:CD1	2.51	0.46
1:c:262:LYS:HE3	1:c:262:LYS:HB3	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:393:TRP:CE3	1:d:456:PHE:HE2	2.33	0.46
1:e:393:TRP:CE2	1:e:414:TYR:HB2	2.50	0.46
1:i:238:ALA:HB2	1:j:377:PRO:HB2	1.98	0.46
1:l:245:LYS:O	1:l:249:GLU:HG3	2.15	0.46
1:o:252:LEU:HD13	1:o:433:PHE:HE1	1.81	0.46
1:K:262:LYS:HE3	1:K:262:LYS:HB3	1.79	0.46
1:L:390:ASP:HB2	1:L:450:PHE:CD1	2.51	0.46
1:R:405:ILE:HG12	1:R:464:PHE:HZ	1.81	0.46
1:d:298:GLN:HE22	1:d:305:ASN:HA	1.81	0.46
1:k:287:SER:O	1:k:370:LYS:HA	2.16	0.46
1:m:288:LYS:HD3	1:m:370:LYS:HD3	1.97	0.46
1:A:298:GLN:NE2	1:A:305:ASN:HA	2.30	0.46
1:O:417:MET:H	1:O:447:ASN:ND2	2.11	0.46
1:T:287:SER:OG	1:T:371:SER:HB3	2.15	0.46
1:Y:252:LEU:HD13	1:Y:433:PHE:HE1	1.80	0.46
1:Z:393:TRP:CE2	1:Z:414:TYR:HB2	2.51	0.46
1:e:390:ASP:CG	1:e:452:ARG:HH21	2.24	0.46
1:K:248:TYR:CE2	1:K:380:ILE:HD11	2.50	0.46
1:l:240:LYS:HA	1:l:240:LYS:HD3	1.67	0.46
1:F:390:ASP:HB2	1:F:450:PHE:CD1	2.51	0.46
1:S:245:LYS:O	1:S:249:GLU:HG3	2.16	0.46
1:W:298:GLN:NE2	1:W:305:ASN:HA	2.30	0.46
1:Y:237:LEU:HB3	1:Z:377:PRO:HG2	1.98	0.46
1:Z:315:ILE:HD13	1:Z:365:ALA:HB2	1.98	0.46
1:N:293:ILE:HD13	1:N:313:THR:HG21	1.98	0.45
1:S:410:ARG:HB3	1:S:460:ASP:OD1	2.17	0.45
1:T:252:LEU:HD13	1:T:433:PHE:HE2	1.81	0.45
1:T:262:LYS:HE3	1:T:262:LYS:HB3	1.85	0.45
1:c:238:ALA:HB2	1:d:377:PRO:HB2	1.98	0.45
1:f:375:LYS:HG2	1:f:376:GLU:O	2.15	0.45
1:k:265:SER:HB3	1:k:268:ARG:HG3	1.98	0.45
1:f:296:GLN:O	1:f:307:ARG:HA	2.16	0.45
1:i:252:LEU:HD13	1:i:433:PHE:HE1	1.81	0.45
1:i:450:PHE:HE2	1:j:262:LYS:HE3	1.81	0.45
1:m:296:GLN:O	1:m:307:ARG:HA	2.16	0.45
1:n:405:ILE:HG12	1:n:464:PHE:HZ	1.81	0.45
1:o:390:ASP:CG	1:o:452:ARG:HH21	2.24	0.45
1:E:245:LYS:O	1:E:249:GLU:HG3	2.16	0.45
1:L:393:TRP:CE2	1:L:414:TYR:HB2	2.52	0.45
1:S:393:TRP:CE3	1:S:456:PHE:HE2	2.35	0.45
1:X:294:GLU:HA	1:X:309:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:298:GLN:NE2	1:c:305:ASN:HA	2.30	0.45
1:d:390:ASP:CG	1:d:452:ARG:HH21	2.25	0.45
1:m:265:SER:HB3	1:m:268:ARG:HG3	1.99	0.45
1:E:364:VAL:HG22	1:F:315:ILE:HA	1.99	0.45
1:H:315:ILE:HD13	1:H:365:ALA:HB2	1.97	0.45
1:O:375:LYS:HG2	1:O:376:GLU:O	2.16	0.45
1:P:248:TYR:CE2	1:P:380:ILE:HD11	2.52	0.45
1:R:390:ASP:HB2	1:R:450:PHE:CD1	2.51	0.45
1:U:375:LYS:HG2	1:U:376:GLU:O	2.15	0.45
1:X:268:ARG:HH12	1:X:417:MET:HE3	1.80	0.45
1:m:390:ASP:CG	1:m:452:ARG:HH21	2.24	0.45
1:D:294:GLU:HA	1:D:309:VAL:HG12	1.99	0.45
1:L:278:LEU:HD22	1:L:378:ALA:HB1	1.99	0.45
1:M:296:GLN:O	1:M:307:ARG:HA	2.17	0.45
1:O:253:ARG:HG3	1:O:271:ILE:HD12	1.98	0.45
1:U:296:GLN:O	1:U:307:ARG:HA	2.16	0.45
1:V:393:TRP:CE2	1:V:414:TYR:HB2	2.52	0.45
1:Y:390:ASP:CG	1:Y:452:ARG:HH21	2.25	0.45
1:c:294:GLU:HA	1:c:309:VAL:HG12	1.98	0.45
1:i:298:GLN:NE2	1:i:305:ASN:HA	2.31	0.45
1:n:405:ILE:HG12	1:n:464:PHE:CZ	2.52	0.45
1:o:275:ASN:O	1:o:383:VAL:HA	2.17	0.45
1:A:315:ILE:HG12	1:A:363:ASN:O	2.17	0.45
1:F:248:TYR:CE2	1:F:380:ILE:HD11	2.52	0.45
1:F:388:PHE:CD1	1:F:448:ILE:HD12	2.52	0.45
1:H:253:ARG:HG3	1:H:271:ILE:HD12	1.99	0.45
1:a:265:SER:HB3	1:a:268:ARG:HG3	1.98	0.45
1:b:264:LEU:HD22	1:b:269:PHE:HB3	1.99	0.45
1:c:275:ASN:O	1:c:383:VAL:HA	2.16	0.45
1:h:298:GLN:NE2	1:h:305:ASN:HA	2.32	0.45
1:l:262:LYS:HE3	1:l:262:LYS:HB3	1.78	0.45
1:A:406:GLU:OE1	1:A:411:LYS:HB2	2.16	0.45
1:N:252:LEU:HD13	1:N:433:PHE:HE1	1.82	0.45
1:e:296:GLN:O	1:e:307:ARG:HA	2.17	0.45
1:h:287:SER:HG	1:h:371:SER:HB3	1.82	0.45
1:k:287:SER:HB2	1:k:371:SER:HB3	1.99	0.45
1:k:293:ILE:HD13	1:k:313:THR:HG21	1.98	0.45
1:C:287:SER:O	1:C:370:LYS:HA	2.17	0.45
1:O:245:LYS:O	1:O:249:GLU:HG3	2.16	0.45
1:R:375:LYS:HG2	1:R:376:GLU:O	2.16	0.45
1:Z:501:ARG:HG2	1:Z:504:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:390:ASP:CG	1:c:452:ARG:HH21	2.25	0.45
1:C:271:ILE:HG23	1:C:387:ILE:HG12	1.99	0.45
1:V:390:ASP:CG	1:V:452:ARG:HH21	2.25	0.45
1:f:252:LEU:HD13	1:f:433:PHE:HE2	1.81	0.45
1:h:287:SER:OG	1:h:371:SER:HB3	2.17	0.45
1:E:248:TYR:CE1	1:E:380:ILE:HD11	2.52	0.45
1:G:245:LYS:O	1:G:249:GLU:HG3	2.17	0.45
1:J:275:ASN:O	1:J:383:VAL:HA	2.17	0.45
1:L:430:GLN:HA	1:L:443:ILE:HD12	1.99	0.45
1:M:245:LYS:O	1:M:249:GLU:HG3	2.17	0.45
1:R:375:LYS:NZ	1:R:379:ARG:HE	2.14	0.45
1:a:360:GLU:HB3	1:b:319:THR:HG23	1.98	0.45
1:c:293:ILE:HD13	1:c:313:THR:HG21	1.99	0.45
1:d:298:GLN:NE2	1:d:305:ASN:HA	2.32	0.45
1:j:390:ASP:CG	1:j:452:ARG:HH21	2.25	0.45
1:m:262:LYS:HE3	1:m:262:LYS:HB3	1.76	0.45
1:N:245:LYS:O	1:N:249:GLU:HG3	2.17	0.44
1:O:248:TYR:CE2	1:O:380:ILE:HD11	2.52	0.44
1:Z:298:GLN:NE2	1:Z:305:ASN:HA	2.31	0.44
1:c:391:GLY:H	1:c:414:TYR:HE1	1.64	0.44
1:k:245:LYS:O	1:k:249:GLU:HG3	2.17	0.44
1:m:298:GLN:NE2	1:m:305:ASN:HA	2.32	0.44
1:H:393:TRP:CE3	1:H:456:PHE:HE2	2.35	0.44
1:e:298:GLN:NE2	1:e:305:ASN:HA	2.31	0.44
1:g:298:GLN:NE2	1:g:305:ASN:HA	2.32	0.44
1:C:391:GLY:H	1:C:414:TYR:HE1	1.65	0.44
1:Y:389:VAL:HG23	1:Y:447:ASN:HA	1.99	0.44
1:b:288:LYS:HD3	1:b:370:LYS:HE3	2.00	0.44
1:g:296:GLN:O	1:g:307:ARG:HA	2.18	0.44
1:j:253:ARG:HG3	1:j:271:ILE:HD12	1.99	0.44
1:C:245:LYS:O	1:C:249:GLU:HG3	2.16	0.44
1:C:275:ASN:O	1:C:383:VAL:HA	2.17	0.44
1:F:360:GLU:CD	1:F:362:LYS:HZ2	2.26	0.44
1:F:501:ARG:HG2	1:F:504:ARG:HH21	1.83	0.44
1:R:296:GLN:O	1:R:307:ARG:HA	2.17	0.44
1:R:314:ILE:HG23	1:R:362:LYS:HD2	1.99	0.44
1:g:289:GLU:HB2	1:g:369:LYS:HB3	1.99	0.44
1:h:268:ARG:HH12	1:h:417:MET:HE3	1.83	0.44
1:h:294:GLU:HA	1:h:309:VAL:HG12	1.99	0.44
1:n:292:PRO:HB2	1:n:309:VAL:HB	2.00	0.44
1:A:298:GLN:HE21	1:A:305:ASN:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:290:TYR:H	1:L:367:ASN:HD21	1.66	0.44
1:O:240:LYS:HA	1:O:240:LYS:HD2	1.68	0.44
1:Q:298:GLN:NE2	1:Q:305:ASN:HA	2.32	0.44
1:T:273:ARG:HH12	1:T:275:ASN:HD22	1.66	0.44
1:Y:375:LYS:NZ	1:Y:379:ARG:HE	2.16	0.44
1:a:355:TYR:HA	1:b:323:GLU:HB3	2.00	0.44
1:l:390:ASP:HB2	1:l:450:PHE:CD1	2.53	0.44
1:o:393:TRP:CE3	1:o:456:PHE:HE2	2.35	0.44
1:F:263:VAL:HB	1:F:264:LEU:HD12	2.00	0.44
1:J:240:LYS:HA	1:J:240:LYS:HD3	1.69	0.44
1:N:268:ARG:HH12	1:N:417:MET:HE3	1.82	0.44
1:U:298:GLN:NE2	1:U:305:ASN:HA	2.33	0.44
1:W:287:SER:O	1:W:370:LYS:HA	2.16	0.44
1:X:501:ARG:HG2	1:X:504:ARG:HH21	1.83	0.44
1:Z:391:GLY:HA2	1:Z:417:MET:HG2	2.00	0.44
1:a:287:SER:HB2	1:a:371:SER:HB3	1.99	0.44
1:c:393:TRP:CE3	1:c:456:PHE:HE2	2.36	0.44
1:e:248:TYR:CE2	1:e:380:ILE:HD11	2.52	0.44
1:e:275:ASN:O	1:e:383:VAL:HA	2.17	0.44
1:i:501:ARG:HG2	1:i:504:ARG:HH21	1.82	0.44
1:j:270:MET:HB3	1:j:388:PHE:HD1	1.83	0.44
1:j:388:PHE:HB3	1:j:448:ILE:HD12	1.99	0.44
1:l:393:TRP:CE3	1:l:456:PHE:HE2	2.35	0.44
1:n:391:GLY:H	1:n:414:TYR:HE1	1.66	0.44
1:C:448:ILE:HD13	1:D:425:ILE:HG12	1.99	0.44
1:H:314:ILE:HG23	1:H:362:LYS:HB3	2.00	0.44
1:I:299:ASP:HB2	1:I:302:ALA:HB2	1.99	0.44
1:Q:265:SER:HB2	1:Q:268:ARG:HG3	2.00	0.44
1:T:324:TYR:HA	1:T:354:LYS:HA	2.00	0.44
1:X:296:GLN:O	1:X:307:ARG:HA	2.18	0.44
1:A:360:GLU:O	1:B:318:GLN:HA	2.18	0.44
1:D:245:LYS:O	1:D:249:GLU:HG3	2.18	0.44
1:E:375:LYS:HG2	1:E:376:GLU:O	2.18	0.44
1:K:271:ILE:HG23	1:K:387:ILE:HG12	1.99	0.44
1:P:390:ASP:CG	1:P:452:ARG:HH21	2.26	0.44
1:P:501:ARG:HG2	1:P:504:ARG:HH21	1.83	0.44
1:Y:240:LYS:HD2	1:Y:240:LYS:HA	1.72	0.44
1:h:252:LEU:HD13	1:h:433:PHE:HE1	1.83	0.44
1:k:264:LEU:HD23	1:k:268:ARG:NH2	2.33	0.44
1:o:315:ILE:HD13	1:o:365:ALA:HB2	2.00	0.44
1:A:315:ILE:HD13	1:A:365:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:GLU:HB2	1:E:369:LYS:HB3	2.00	0.44
1:Z:296:GLN:O	1:Z:307:ARG:HA	2.17	0.44
1:f:242:ARG:NH1	1:g:251:MET:HG3	2.33	0.44
1:i:364:VAL:HG22	1:j:315:ILE:HA	1.99	0.44
1:I:262:LYS:HE3	1:I:262:LYS:HB3	1.85	0.43
1:S:240:LYS:HA	1:S:240:LYS:HD3	1.66	0.43
1:Z:245:LYS:O	1:Z:249:GLU:HG3	2.17	0.43
1:h:238:ALA:HB2	1:i:377:PRO:HB2	1.99	0.43
1:o:375:LYS:HG2	1:o:376:GLU:O	2.17	0.43
1:F:268:ARG:HH12	1:F:417:MET:HE3	1.82	0.43
1:N:390:ASP:CG	1:N:452:ARG:HH21	2.26	0.43
1:l:252:LEU:O	1:l:256:ILE:HG12	2.18	0.43
1:B:245:LYS:O	1:B:249:GLU:HG3	2.18	0.43
1:M:393:TRP:CE3	1:M:456:PHE:HE2	2.36	0.43
1:O:287:SER:O	1:O:370:LYS:HA	2.18	0.43
1:W:298:GLN:HE21	1:W:305:ASN:HA	1.83	0.43
1:f:238:ALA:HB2	1:g:377:PRO:HB2	1.99	0.43
1:h:288:LYS:HE2	1:h:370:LYS:HE3	2.00	0.43
1:l:287:SER:O	1:l:370:LYS:HA	2.18	0.43
1:o:298:GLN:NE2	1:o:305:ASN:HA	2.31	0.43
1:E:253:ARG:HG3	1:E:271:ILE:HD12	2.00	0.43
1:W:264:LEU:HD22	1:W:417:MET:HE1	2.01	0.43
1:X:375:LYS:HG2	1:X:376:GLU:O	2.18	0.43
1:c:246:LEU:HD23	1:c:246:LEU:HA	1.88	0.43
1:h:391:GLY:H	1:h:414:TYR:HE1	1.65	0.43
1:D:355:TYR:HA	1:E:323:GLU:HB3	2.00	0.43
1:M:274:VAL:HG22	1:M:385:LEU:HB3	2.01	0.43
1:X:390:ASP:CG	1:X:452:ARG:HH21	2.26	0.43
1:C:252:LEU:HD13	1:C:433:PHE:HE1	1.83	0.43
1:H:293:ILE:HD13	1:H:313:THR:HG21	2.00	0.43
1:I:238:ALA:HB2	1:J:377:PRO:HB2	2.00	0.43
1:M:248:TYR:CE2	1:M:380:ILE:HD11	2.53	0.43
1:T:315:ILE:HD13	1:T:365:ALA:HB2	2.00	0.43
1:X:238:ALA:HB2	1:Y:377:PRO:HB2	2.00	0.43
1:Z:287:SER:HB2	1:Z:371:SER:OG	2.18	0.43
1:j:385:LEU:HD23	1:j:443:ILE:HG12	2.00	0.43
1:k:278:LEU:HD23	1:k:278:LEU:HA	1.80	0.43
1:l:393:TRP:CE2	1:l:414:TYR:HB2	2.53	0.43
1:m:248:TYR:CE2	1:m:380:ILE:HD11	2.53	0.43
1:m:268:ARG:HH12	1:m:417:MET:HE3	1.84	0.43
1:m:390:ASP:HB2	1:m:450:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:287:SER:O	1:i:370:LYS:HA	2.19	0.43
1:H:393:TRP:CE2	1:H:414:TYR:HB2	2.53	0.43
1:O:390:ASP:HB2	1:O:450:PHE:CD1	2.54	0.43
1:Z:390:ASP:HB2	1:Z:450:PHE:CD1	2.54	0.43
1:b:298:GLN:NE2	1:b:305:ASN:HA	2.28	0.43
1:C:247:LYS:HD2	1:C:247:LYS:HA	1.90	0.43
1:Z:253:ARG:HG3	1:Z:271:ILE:HD12	2.00	0.43
1:i:237:LEU:HD22	1:j:377:PRO:HG2	2.00	0.43
1:l:237:LEU:HB3	1:m:377:PRO:HG2	2.01	0.43
1:n:390:ASP:CG	1:n:452:ARG:HH21	2.27	0.43
1:Q:262:LYS:HE3	1:Q:262:LYS:HB3	1.86	0.43
1:Q:289:GLU:HB2	1:Q:369:LYS:HB3	2.00	0.43
1:Q:292:PRO:HD3	1:R:294:GLU:O	2.19	0.43
1:V:430:GLN:HA	1:V:443:ILE:HD12	2.00	0.43
1:Y:274:VAL:HG22	1:Y:385:LEU:HB3	2.01	0.43
1:j:245:LYS:O	1:j:249:GLU:HG3	2.18	0.43
1:k:268:ARG:HH12	1:k:417:MET:HE3	1.84	0.43
1:A:262:LYS:HB3	1:A:262:LYS:HE3	1.84	0.42
1:P:375:LYS:HG2	1:P:376:GLU:O	2.18	0.42
1:Z:235:ILE:HG21	1:a:240:LYS:HG3	2.01	0.42
1:a:391:GLY:H	1:a:414:TYR:HE1	1.66	0.42
1:h:247:LYS:HD2	1:h:247:LYS:HA	1.91	0.42
1:l:292:PRO:HD3	1:m:294:GLU:O	2.19	0.42
1:m:288:LYS:HE3	1:m:288:LYS:HB2	1.95	0.42
1:n:393:TRP:CE3	1:n:456:PHE:HE2	2.37	0.42
1:J:317:SER:OG	1:J:319:THR:HG23	2.18	0.42
1:P:245:LYS:O	1:P:249:GLU:HG3	2.19	0.42
1:Q:296:GLN:O	1:Q:307:ARG:HA	2.19	0.42
1:X:288:LYS:HD3	1:X:370:LYS:HD3	2.00	0.42
1:X:315:ILE:HD13	1:X:365:ALA:HB2	2.01	0.42
1:j:278:LEU:HD23	1:j:278:LEU:HA	1.88	0.42
1:C:288:LYS:HD3	1:C:370:LYS:HD3	2.00	0.42
1:M:375:LYS:HG2	1:M:376:GLU:O	2.19	0.42
1:O:247:LYS:HD2	1:O:247:LYS:HA	1.81	0.42
1:P:298:GLN:HE21	1:P:305:ASN:HA	1.84	0.42
1:X:247:LYS:HD2	1:X:247:LYS:HA	1.88	0.42
1:b:390:ASP:CG	1:b:452:ARG:HH21	2.28	0.42
1:e:252:LEU:HD13	1:e:433:PHE:HE2	1.85	0.42
1:k:360:GLU:OE2	1:k:362:LYS:HD3	2.19	0.42
1:A:252:LEU:HD13	1:A:433:PHE:HE1	1.84	0.42
1:C:278:LEU:HD23	1:C:278:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:283:GLU:HA	1:M:372:THR:O	2.20	0.42
1:M:360:GLU:O	1:N:318:GLN:HA	2.20	0.42
1:N:376:GLU:CD	1:N:376:GLU:H	2.26	0.42
1:T:268:ARG:HH12	1:T:417:MET:HE3	1.85	0.42
1:T:294:GLU:HA	1:T:309:VAL:HG12	2.02	0.42
1:W:296:GLN:O	1:W:307:ARG:HA	2.19	0.42
1:Y:288:LYS:HE2	1:Y:290:TYR:CE1	2.54	0.42
1:f:262:LYS:HE3	1:f:262:LYS:HB3	1.85	0.42
1:i:281:SER:HB3	1:j:376:GLU:OE1	2.19	0.42
1:C:264:LEU:HD22	1:C:417:MET:HE1	2.02	0.42
1:I:388:PHE:CD1	1:I:448:ILE:HD12	2.55	0.42
1:Y:245:LYS:O	1:Y:249:GLU:HG3	2.20	0.42
1:g:275:ASN:O	1:g:383:VAL:HA	2.20	0.42
1:j:448:ILE:HD13	1:k:425:ILE:HG12	2.01	0.42
1:m:393:TRP:CE3	1:m:456:PHE:HE2	2.37	0.42
1:F:262:LYS:HB3	1:F:262:LYS:HE3	1.82	0.42
1:F:389:VAL:HG23	1:F:447:ASN:HA	2.01	0.42
1:G:393:TRP:CE3	1:G:456:PHE:HE2	2.38	0.42
1:N:253:ARG:HG3	1:N:271:ILE:HD12	2.02	0.42
1:R:262:LYS:HE3	1:R:262:LYS:HB3	1.83	0.42
1:X:412:ARG:HH21	1:X:460:ASP:CG	2.28	0.42
1:a:296:GLN:O	1:a:307:ARG:HA	2.19	0.42
1:a:501:ARG:HG2	1:a:504:ARG:HH21	1.85	0.42
1:d:360:GLU:OE2	1:d:362:LYS:HD3	2.20	0.42
1:e:391:GLY:H	1:e:414:TYR:HE1	1.68	0.42
1:g:245:LYS:O	1:g:249:GLU:HG3	2.18	0.42
1:j:248:TYR:CE2	1:j:380:ILE:HD11	2.54	0.42
1:E:315:ILE:HD13	1:E:365:ALA:HB2	2.00	0.42
1:F:247:LYS:HD3	1:F:247:LYS:HA	1.84	0.42
1:G:292:PRO:HD3	1:H:294:GLU:O	2.20	0.42
1:Q:245:LYS:O	1:Q:249:GLU:HG3	2.18	0.42
1:Q:248:TYR:CE2	1:Q:380:ILE:HD11	2.54	0.42
1:a:262:LYS:HE3	1:a:262:LYS:HB3	1.79	0.42
1:k:393:TRP:CE2	1:k:414:TYR:HB2	2.55	0.42
1:o:245:LYS:O	1:o:249:GLU:HG3	2.20	0.42
1:C:385:LEU:HD23	1:C:443:ILE:HG12	2.02	0.42
1:D:247:LYS:HD2	1:D:247:LYS:HA	1.91	0.42
1:D:289:GLU:HB2	1:D:369:LYS:HB3	2.02	0.42
1:K:410:ARG:HB3	1:K:460:ASP:OD1	2.19	0.42
1:L:262:LYS:HE3	1:L:262:LYS:HB3	1.80	0.42
1:S:253:ARG:HG3	1:S:271:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:298:GLN:NE2	1:T:305:ASN:HA	2.35	0.42
1:W:240:LYS:HD3	1:W:240:LYS:HA	1.73	0.42
1:X:240:LYS:HA	1:X:240:LYS:HD3	1.80	0.42
1:Y:296:GLN:O	1:Y:307:ARG:HA	2.20	0.42
1:b:247:LYS:HD2	1:b:247:LYS:HA	1.91	0.42
1:b:275:ASN:O	1:b:383:VAL:HA	2.20	0.42
1:g:248:TYR:CE1	1:g:380:ILE:HD11	2.55	0.42
1:l:291:ALA:HB3	1:l:367:ASN:HB2	2.01	0.42
1:D:393:TRP:CE3	1:D:456:PHE:HE2	2.38	0.42
1:S:390:ASP:CG	1:S:452:ARG:HH21	2.27	0.42
1:b:287:SER:O	1:b:370:LYS:HA	2.20	0.42
1:b:296:GLN:O	1:b:307:ARG:HA	2.19	0.42
1:i:319:THR:HG22	1:i:360:GLU:HG3	2.02	0.42
1:k:390:ASP:HB2	1:k:450:PHE:CD1	2.55	0.42
1:G:296:GLN:O	1:G:307:ARG:HA	2.20	0.42
1:M:315:ILE:HD13	1:M:365:ALA:HB2	2.02	0.42
1:W:362:LYS:HG2	1:X:317:SER:HB3	2.01	0.42
1:Z:275:ASN:O	1:Z:383:VAL:HA	2.19	0.42
1:Z:293:ILE:HD13	1:Z:313:THR:HG21	2.01	0.42
1:a:253:ARG:HG3	1:a:271:ILE:HD12	2.02	0.42
1:i:412:ARG:HH21	1:i:460:ASP:CG	2.28	0.42
1:n:406:GLU:OE1	1:n:411:LYS:HB2	2.19	0.42
1:C:293:ILE:HD13	1:C:313:THR:HG21	2.02	0.41
1:T:393:TRP:CE3	1:T:456:PHE:HE2	2.38	0.41
1:V:315:ILE:HD13	1:V:365:ALA:HB2	2.02	0.41
1:c:265:SER:OG	1:c:268:ARG:HG3	2.20	0.41
1:c:281:SER:HB3	1:d:376:GLU:OE1	2.20	0.41
1:B:260:LEU:HD11	1:B:387:ILE:HD13	2.01	0.41
1:D:238:ALA:HB2	1:E:377:PRO:HB2	2.02	0.41
1:G:293:ILE:HD13	1:G:313:THR:HG21	2.01	0.41
1:I:256:ILE:HD12	1:I:429:LEU:HD22	2.01	0.41
1:Q:232:ILE:HD13	1:Q:232:ILE:HA	1.94	0.41
1:c:296:GLN:O	1:c:307:ARG:HA	2.20	0.41
1:e:390:ASP:HB2	1:e:450:PHE:CD1	2.55	0.41
1:f:359:GLN:HA	1:g:319:THR:O	2.20	0.41
1:m:252:LEU:HD13	1:m:433:PHE:HE1	1.85	0.41
1:J:375:LYS:NZ	1:J:379:ARG:HE	2.17	0.41
1:N:288:LYS:HD3	1:N:370:LYS:HD3	2.01	0.41
1:Q:270:MET:HE3	1:Q:271:ILE:H	1.84	0.41
1:R:245:LYS:O	1:R:249:GLU:HG3	2.20	0.41
1:R:360:GLU:OE2	1:R:362:LYS:HD3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:238:ALA:HB2	1:V:377:PRO:HB2	2.01	0.41
1:X:245:LYS:O	1:X:249:GLU:HG3	2.20	0.41
1:c:386:GLY:HA2	1:c:444:THR:O	2.21	0.41
1:c:459:ILE:HD13	1:c:459:ILE:HA	1.91	0.41
1:d:262:LYS:HE3	1:d:262:LYS:HB3	1.83	0.41
1:i:247:LYS:HD3	1:i:247:LYS:HA	1.76	0.41
1:k:274:VAL:HG22	1:k:385:LEU:HB3	2.02	0.41
1:B:357:GLU:HA	1:C:321:LYS:O	2.20	0.41
1:C:270:MET:HB3	1:C:388:PHE:HD1	1.86	0.41
1:I:315:ILE:HD13	1:I:365:ALA:HB2	2.03	0.41
1:W:237:LEU:HD22	1:X:377:PRO:HG2	2.02	0.41
1:B:262:LYS:HB3	1:B:262:LYS:HE3	1.81	0.41
1:B:388:PHE:CD1	1:B:448:ILE:HD12	2.55	0.41
1:O:314:ILE:HG23	1:O:362:LYS:HD2	2.01	0.41
1:R:298:GLN:NE2	1:R:305:ASN:HA	2.33	0.41
1:k:248:TYR:CE2	1:k:380:ILE:HD11	2.55	0.41
1:m:281:SER:HB3	1:n:376:GLU:OE1	2.20	0.41
1:D:262:LYS:HE3	1:D:262:LYS:HB3	1.78	0.41
1:I:393:TRP:CE3	1:I:456:PHE:HE2	2.37	0.41
1:Q:390:ASP:HB2	1:Q:450:PHE:CD1	2.55	0.41
1:S:391:GLY:H	1:S:414:TYR:HE1	1.68	0.41
1:W:391:GLY:H	1:W:414:TYR:HE1	1.68	0.41
1:i:278:LEU:HD23	1:i:278:LEU:HA	1.82	0.41
1:m:275:ASN:O	1:m:383:VAL:HA	2.20	0.41
1:m:375:LYS:HG2	1:m:376:GLU:O	2.20	0.41
1:E:238:ALA:HB2	1:F:377:PRO:HB2	2.03	0.41
1:E:296:GLN:O	1:E:307:ARG:HA	2.21	0.41
1:F:314:ILE:HG21	1:F:317:SER:HB2	2.03	0.41
1:V:240:LYS:HD3	1:V:240:LYS:HA	1.77	0.41
1:W:252:LEU:HD13	1:W:433:PHE:HE2	1.86	0.41
1:X:262:LYS:HE3	1:X:262:LYS:HB3	1.90	0.41
1:a:248:TYR:CE2	1:a:380:ILE:HD11	2.55	0.41
1:b:265:SER:HB2	1:b:268:ARG:HG3	2.02	0.41
1:b:270:MET:HE3	1:b:271:ILE:H	1.85	0.41
1:c:247:LYS:HD2	1:c:247:LYS:HA	1.94	0.41
1:f:245:LYS:O	1:f:249:GLU:HG3	2.21	0.41
1:n:237:LEU:HD22	1:o:377:PRO:HG2	2.02	0.41
1:K:278:LEU:HA	1:K:278:LEU:HD23	1.80	0.41
1:R:409:MET:SD	1:R:457:ARG:HG2	2.61	0.41
1:Z:238:ALA:HB2	1:a:377:PRO:HB2	2.02	0.41
1:b:415:LYS:HA	1:b:416:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:238:ALA:HB2	1:k:377:PRO:HB2	2.02	0.41
1:j:288:LYS:HE2	1:j:290:TYR:CE1	2.55	0.41
1:C:393:TRP:CE3	1:C:456:PHE:HE2	2.39	0.41
1:H:314:ILE:H	1:H:314:ILE:HG13	1.68	0.41
1:N:393:TRP:CE3	1:N:456:PHE:HE2	2.39	0.41
1:N:403:PHE:HB3	1:N:410:ARG:HG3	2.03	0.41
1:P:385:LEU:HD23	1:P:443:ILE:HG12	2.02	0.41
1:R:388:PHE:CD2	1:S:263:VAL:HG21	2.56	0.41
1:a:240:LYS:HD3	1:a:240:LYS:HA	1.73	0.41
1:a:390:ASP:HB2	1:a:450:PHE:CD1	2.56	0.41
1:h:389:VAL:HG23	1:h:447:ASN:HA	2.02	0.41
1:l:268:ARG:HH12	1:l:417:MET:HE3	1.86	0.41
1:n:278:LEU:HD23	1:n:278:LEU:HA	1.92	0.41
1:n:415:LYS:HA	1:n:416:PRO:HD3	1.97	0.41
1:I:245:LYS:O	1:I:249:GLU:HG3	2.20	0.41
1:b:410:ARG:HB2	1:b:460:ASP:OD1	2.21	0.41
1:f:360:GLU:OE2	1:f:362:LYS:HD3	2.21	0.41
1:g:271:ILE:HG23	1:g:387:ILE:HG12	2.02	0.41
1:j:391:GLY:H	1:j:414:TYR:HE1	1.69	0.41
1:C:262:LYS:HE3	1:C:262:LYS:HB3	1.92	0.40
1:P:235:ILE:HG21	1:Q:240:LYS:HB3	2.03	0.40
1:Q:375:LYS:HG2	1:Q:376:GLU:O	2.20	0.40
1:R:405:ILE:HG12	1:R:464:PHE:CZ	2.57	0.40
1:U:315:ILE:HD13	1:U:365:ALA:HB2	2.03	0.40
1:g:391:GLY:H	1:g:414:TYR:HE1	1.68	0.40
1:h:278:LEU:HD23	1:h:278:LEU:HA	1.89	0.40
1:j:296:GLN:O	1:j:307:ARG:HA	2.21	0.40
1:k:356:ASN:HB3	1:l:323:GLU:HB3	2.01	0.40
1:F:355:TYR:HA	1:G:323:GLU:HB3	2.03	0.40
1:N:286:GLU:HA	1:N:371:SER:O	2.21	0.40
1:Q:375:LYS:NZ	1:Q:379:ARG:HE	2.19	0.40
1:R:238:ALA:HB2	1:S:377:PRO:HB2	2.04	0.40
1:R:393:TRP:CE3	1:R:456:PHE:HE2	2.39	0.40
1:M:405:ILE:HG12	1:M:464:PHE:HZ	1.86	0.40
1:M:406:GLU:OE1	1:M:411:LYS:HB2	2.21	0.40
1:S:278:LEU:HD23	1:S:278:LEU:HA	1.91	0.40
1:e:410:ARG:HB3	1:e:460:ASP:OD1	2.22	0.40
1:h:275:ASN:O	1:h:383:VAL:HA	2.22	0.40
1:A:393:TRP:CE3	1:A:456:PHE:HE2	2.39	0.40
1:K:286:GLU:O	1:L:369:LYS:HA	2.21	0.40
1:d:248:TYR:O	1:d:251:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:313:THR:O	1:n:364:VAL:HA	2.21	0.40
1:A:391:GLY:H	1:A:414:TYR:HE1	1.68	0.40
1:C:415:LYS:HA	1:C:416:PRO:HD3	1.98	0.40
1:F:356:ASN:H	1:G:323:GLU:HB3	1.86	0.40
1:H:245:LYS:O	1:H:249:GLU:HG3	2.22	0.40
1:J:315:ILE:HD13	1:J:365:ALA:HB2	2.04	0.40
1:K:235:ILE:HD13	1:K:235:ILE:HA	1.89	0.40
1:N:319:THR:HA	1:N:359:GLN:O	2.22	0.40
1:T:296:GLN:O	1:T:307:ARG:HA	2.21	0.40
1:b:292:PRO:HD3	1:c:294:GLU:O	2.21	0.40
1:n:262:LYS:HE3	1:n:262:LYS:HB3	1.86	0.40
1:o:240:LYS:HD2	1:o:240:LYS:HA	1.92	0.40
1:o:315:ILE:HG12	1:o:363:ASN:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/569 (45%)	245 (95%)	13 (5%)	0	100	100
1	B	258/569 (45%)	247 (96%)	11 (4%)	0	100	100
1	C	258/569 (45%)	243 (94%)	15 (6%)	0	100	100
1	D	258/569 (45%)	243 (94%)	15 (6%)	0	100	100
1	E	258/569 (45%)	243 (94%)	15 (6%)	0	100	100
1	F	258/569 (45%)	243 (94%)	15 (6%)	0	100	100
1	G	258/569 (45%)	242 (94%)	16 (6%)	0	100	100
1	H	258/569 (45%)	247 (96%)	11 (4%)	0	100	100
1	I	258/569 (45%)	251 (97%)	7 (3%)	0	100	100
1	J	258/569 (45%)	245 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	258/569 (45%)	249 (96%)	9 (4%)	0	100	100
1	L	258/569 (45%)	250 (97%)	8 (3%)	0	100	100
1	M	258/569 (45%)	245 (95%)	13 (5%)	0	100	100
1	N	258/569 (45%)	243 (94%)	15 (6%)	0	100	100
1	O	258/569 (45%)	246 (95%)	12 (5%)	0	100	100
1	P	258/569 (45%)	247 (96%)	11 (4%)	0	100	100
1	Q	258/569 (45%)	247 (96%)	11 (4%)	0	100	100
1	R	258/569 (45%)	242 (94%)	16 (6%)	0	100	100
1	S	258/569 (45%)	246 (95%)	12 (5%)	0	100	100
1	T	258/569 (45%)	245 (95%)	13 (5%)	0	100	100
1	U	258/569 (45%)	252 (98%)	6 (2%)	0	100	100
1	V	258/569 (45%)	244 (95%)	14 (5%)	0	100	100
1	W	258/569 (45%)	246 (95%)	12 (5%)	0	100	100
1	X	258/569 (45%)	245 (95%)	13 (5%)	0	100	100
1	Y	258/569 (45%)	244 (95%)	14 (5%)	0	100	100
1	Z	258/569 (45%)	246 (95%)	12 (5%)	0	100	100
1	a	258/569 (45%)	245 (95%)	13 (5%)	0	100	100
1	b	258/569 (45%)	245 (95%)	13 (5%)	0	100	100
1	c	258/569 (45%)	247 (96%)	11 (4%)	0	100	100
1	d	258/569 (45%)	248 (96%)	10 (4%)	0	100	100
1	e	258/569 (45%)	251 (97%)	7 (3%)	0	100	100
1	f	258/569 (45%)	245 (95%)	13 (5%)	0	100	100
1	g	258/569 (45%)	246 (95%)	12 (5%)	0	100	100
1	h	258/569 (45%)	242 (94%)	16 (6%)	0	100	100
1	i	258/569 (45%)	242 (94%)	16 (6%)	0	100	100
1	j	258/569 (45%)	244 (95%)	14 (5%)	0	100	100
1	k	258/569 (45%)	248 (96%)	10 (4%)	0	100	100
1	l	258/569 (45%)	245 (95%)	13 (5%)	0	100	100
1	m	258/569 (45%)	247 (96%)	11 (4%)	0	100	100
1	n	258/569 (45%)	251 (97%)	7 (3%)	0	100	100
1	o	258/569 (45%)	246 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	10578/23329 (45%)	10078 (95%)	500 (5%)	0	100 100

There are no Ramachandran outliers to report.

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	A	226/506 (45%)	219 (97%)	7 (3%)	35 59
1	B	226/506 (45%)	217 (96%)	9 (4%)	28 53
1	C	226/506 (45%)	214 (95%)	12 (5%)	20 47
1	D	226/506 (45%)	217 (96%)	9 (4%)	28 53
1	E	226/506 (45%)	221 (98%)	5 (2%)	45 63
1	F	226/506 (45%)	216 (96%)	10 (4%)	25 51
1	G	226/506 (45%)	220 (97%)	6 (3%)	39 61
1	H	226/506 (45%)	221 (98%)	5 (2%)	45 63
1	I	226/506 (45%)	223 (99%)	3 (1%)	61 71
1	J	226/506 (45%)	219 (97%)	7 (3%)	35 59
1	K	226/506 (45%)	220 (97%)	6 (3%)	39 61
1	L	226/506 (45%)	218 (96%)	8 (4%)	32 56
1	M	226/506 (45%)	218 (96%)	8 (4%)	32 56
1	N	226/506 (45%)	218 (96%)	8 (4%)	32 56
1	O	226/506 (45%)	218 (96%)	8 (4%)	32 56
1	P	226/506 (45%)	218 (96%)	8 (4%)	32 56
1	Q	226/506 (45%)	218 (96%)	8 (4%)	32 56
1	R	226/506 (45%)	220 (97%)	6 (3%)	39 61
1	S	226/506 (45%)	220 (97%)	6 (3%)	39 61
1	T	226/506 (45%)	222 (98%)	4 (2%)	51 67
1	U	226/506 (45%)	220 (97%)	6 (3%)	39 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	226/506 (45%)	218 (96%)	8 (4%)	32	56
1	W	226/506 (45%)	220 (97%)	6 (3%)	39	61
1	X	226/506 (45%)	221 (98%)	5 (2%)	45	63
1	Y	226/506 (45%)	217 (96%)	9 (4%)	28	53
1	Z	226/506 (45%)	220 (97%)	6 (3%)	39	61
1	a	226/506 (45%)	219 (97%)	7 (3%)	35	59
1	b	226/506 (45%)	220 (97%)	6 (3%)	39	61
1	c	226/506 (45%)	220 (97%)	6 (3%)	39	61
1	d	226/506 (45%)	220 (97%)	6 (3%)	39	61
1	e	226/506 (45%)	216 (96%)	10 (4%)	25	51
1	f	226/506 (45%)	219 (97%)	7 (3%)	35	59
1	g	226/506 (45%)	216 (96%)	10 (4%)	25	51
1	h	226/506 (45%)	218 (96%)	8 (4%)	32	56
1	i	226/506 (45%)	222 (98%)	4 (2%)	51	67
1	j	226/506 (45%)	218 (96%)	8 (4%)	32	56
1	k	226/506 (45%)	221 (98%)	5 (2%)	45	63
1	l	226/506 (45%)	219 (97%)	7 (3%)	35	59
1	m	226/506 (45%)	219 (97%)	7 (3%)	35	59
1	n	226/506 (45%)	221 (98%)	5 (2%)	45	63
1	o	226/506 (45%)	219 (97%)	7 (3%)	35	59
All	All	9266/20746 (45%)	8980 (97%)	286 (3%)	36	59

All (286) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	LEU
1	A	271	ILE
1	A	299	ASP
1	A	306	THR
1	A	314	ILE
1	A	374	GLU
1	A	384	SER
1	B	271	ILE
1	B	299	ASP
1	B	306	THR

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Mol	Chain	Res	Type
1	B	314	ILE
1	B	364	VAL
1	B	417	MET
1	B	432	SER
1	B	435	TYR
1	B	460	ASP
1	C	234	ARG
1	C	264	LEU
1	C	271	ILE
1	C	288	LYS
1	C	306	THR
1	C	314	ILE
1	C	319	THR
1	C	323	GLU
1	C	364	VAL
1	C	383	VAL
1	C	384	SER
1	C	388	PHE
1	D	271	ILE
1	D	288	LYS
1	D	306	THR
1	D	314	ILE
1	D	364	VAL
1	D	383	VAL
1	D	384	SER
1	D	448	ILE
1	D	460	ASP
1	E	234	ARG
1	E	271	ILE
1	E	306	THR
1	E	314	ILE
1	E	364	VAL
1	F	234	ARG
1	F	263	VAL
1	F	299	ASP
1	F	306	THR
1	F	315	ILE
1	F	364	VAL
1	F	373	SER
1	F	383	VAL
1	F	384	SER
1	F	460	ASP

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Mol	Chain	Res	Type
1	G	271	ILE
1	G	306	THR
1	G	314	ILE
1	G	319	THR
1	G	364	VAL
1	G	373	SER
1	H	299	ASP
1	H	306	THR
1	H	314	ILE
1	H	364	VAL
1	H	460	ASP
1	I	247	LYS
1	I	314	ILE
1	I	364	VAL
1	J	246	LEU
1	J	247	LYS
1	J	271	ILE
1	J	306	THR
1	J	314	ILE
1	J	364	VAL
1	J	432	SER
1	K	234	ARG
1	K	271	ILE
1	K	306	THR
1	K	314	ILE
1	K	364	VAL
1	K	448	ILE
1	L	234	ARG
1	L	271	ILE
1	L	306	THR
1	L	314	ILE
1	L	364	VAL
1	L	374	GLU
1	L	384	SER
1	L	460	ASP
1	M	264	LEU
1	M	271	ILE
1	M	299	ASP
1	M	306	THR
1	M	314	ILE
1	M	364	VAL
1	M	384	SER

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Mol	Chain	Res	Type
1	M	460	ASP
1	N	247	LYS
1	N	299	ASP
1	N	306	THR
1	N	314	ILE
1	N	364	VAL
1	N	373	SER
1	N	383	VAL
1	N	384	SER
1	O	271	ILE
1	O	299	ASP
1	O	314	ILE
1	O	364	VAL
1	O	383	VAL
1	O	384	SER
1	O	432	SER
1	O	448	ILE
1	P	234	ARG
1	P	271	ILE
1	P	288	LYS
1	P	306	THR
1	P	314	ILE
1	P	319	THR
1	P	364	VAL
1	P	383	VAL
1	Q	233	ASP
1	Q	234	ARG
1	Q	271	ILE
1	Q	288	LYS
1	Q	306	THR
1	Q	314	ILE
1	Q	319	THR
1	Q	364	VAL
1	R	271	ILE
1	R	306	THR
1	R	314	ILE
1	R	359	GLN
1	R	364	VAL
1	R	384	SER
1	S	288	LYS
1	S	306	THR
1	S	314	ILE

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Mol	Chain	Res	Type
1	S	364	VAL
1	S	373	SER
1	S	384	SER
1	T	306	THR
1	T	314	ILE
1	T	364	VAL
1	T	384	SER
1	U	271	ILE
1	U	306	THR
1	U	314	ILE
1	U	364	VAL
1	U	373	SER
1	U	384	SER
1	V	288	LYS
1	V	306	THR
1	V	314	ILE
1	V	323	GLU
1	V	364	VAL
1	V	373	SER
1	V	384	SER
1	V	432	SER
1	W	299	ASP
1	W	306	THR
1	W	314	ILE
1	W	315	ILE
1	W	384	SER
1	W	460	ASP
1	X	306	THR
1	X	314	ILE
1	X	364	VAL
1	X	383	VAL
1	X	384	SER
1	Y	237	LEU
1	Y	271	ILE
1	Y	306	THR
1	Y	314	ILE
1	Y	315	ILE
1	Y	319	THR
1	Y	364	VAL
1	Y	384	SER
1	Y	385	LEU
1	Z	234	ARG

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Mol	Chain	Res	Type
1	Z	306	THR
1	Z	314	ILE
1	Z	319	THR
1	Z	364	VAL
1	Z	384	SER
1	a	234	ARG
1	a	271	ILE
1	a	306	THR
1	a	314	ILE
1	a	319	THR
1	a	364	VAL
1	a	373	SER
1	b	271	ILE
1	b	306	THR
1	b	314	ILE
1	b	319	THR
1	b	364	VAL
1	b	410	ARG
1	c	271	ILE
1	c	306	THR
1	c	314	ILE
1	c	364	VAL
1	c	383	VAL
1	c	384	SER
1	d	271	ILE
1	d	306	THR
1	d	314	ILE
1	d	364	VAL
1	d	373	SER
1	d	432	SER
1	e	234	ARG
1	e	271	ILE
1	e	288	LYS
1	e	306	THR
1	e	314	ILE
1	e	364	VAL
1	e	370	LYS
1	e	373	SER
1	e	384	SER
1	e	448	ILE
1	f	234	ARG
1	f	299	ASP

Continued on next page...

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Mol	Chain	Res	Type
1	f	306	THR
1	f	314	ILE
1	f	319	THR
1	f	364	VAL
1	f	384	SER
1	g	234	ARG
1	g	242	ARG
1	g	271	ILE
1	g	306	THR
1	g	314	ILE
1	g	364	VAL
1	g	370	LYS
1	g	373	SER
1	g	384	SER
1	g	432	SER
1	h	234	ARG
1	h	264	LEU
1	h	299	ASP
1	h	306	THR
1	h	314	ILE
1	h	364	VAL
1	h	370	LYS
1	h	384	SER
1	i	245	LYS
1	i	306	THR
1	i	314	ILE
1	i	384	SER
1	j	263	VAL
1	j	299	ASP
1	j	306	THR
1	j	314	ILE
1	j	315	ILE
1	j	364	VAL
1	j	373	SER
1	j	388	PHE
1	k	314	ILE
1	k	319	THR
1	k	362	LYS
1	k	364	VAL
1	k	448	ILE
1	l	237	LEU
1	l	271	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	l	306	THR
1	l	314	ILE
1	l	364	VAL
1	l	383	VAL
1	l	384	SER
1	m	271	ILE
1	m	306	THR
1	m	314	ILE
1	m	315	ILE
1	m	319	THR
1	m	364	VAL
1	m	384	SER
1	n	271	ILE
1	n	314	ILE
1	n	364	VAL
1	n	373	SER
1	n	384	SER
1	o	234	ARG
1	o	237	LEU
1	o	306	THR
1	o	314	ILE
1	o	364	VAL
1	o	383	VAL
1	o	448	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	513	HIS
1	B	513	HIS
1	C	356	ASN
1	D	447	ASN
1	D	513	HIS
1	E	513	HIS
1	F	513	HIS
1	G	298	GLN
1	H	298	GLN
1	I	462	ASN
1	I	513	HIS
1	J	298	GLN
1	K	462	ASN
1	L	367	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	298	GLN
1	N	298	GLN
1	N	513	HIS
1	O	356	ASN
1	O	367	ASN
1	O	447	ASN
1	P	275	ASN
1	P	513	HIS
1	Q	298	GLN
1	Q	394	ASN
1	R	298	GLN
1	R	359	GLN
1	S	359	GLN
1	S	513	HIS
1	T	275	ASN
1	T	513	HIS
1	V	298	GLN
1	V	407	ASN
1	W	363	ASN
1	X	356	ASN
1	X	367	ASN
1	Y	298	GLN
1	a	462	ASN
1	b	298	GLN
1	b	394	ASN
1	c	298	GLN
1	c	462	ASN
1	d	298	GLN
1	e	275	ASN
1	g	298	GLN
1	h	513	HIS
1	i	356	ASN
1	i	394	ASN
1	j	298	GLN
1	l	513	HIS
1	m	275	ASN
1	n	298	GLN
1	o	275	ASN
1	o	298	GLN
1	o	513	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76344. These allow visual inspection of the internal detail of the map and identification of artifacts.

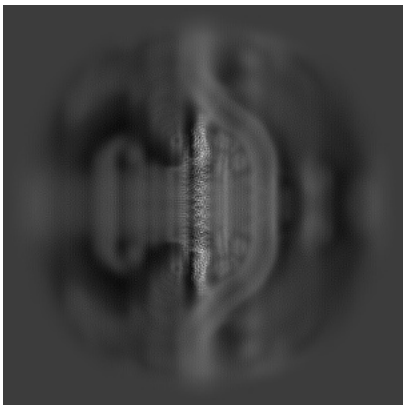
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X



Y

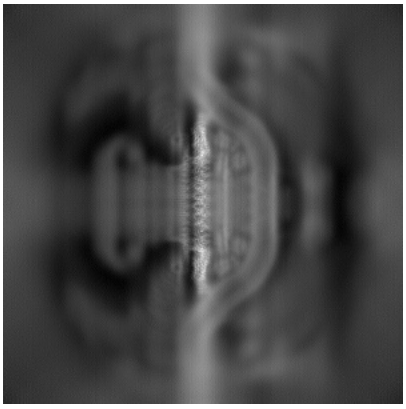


Z

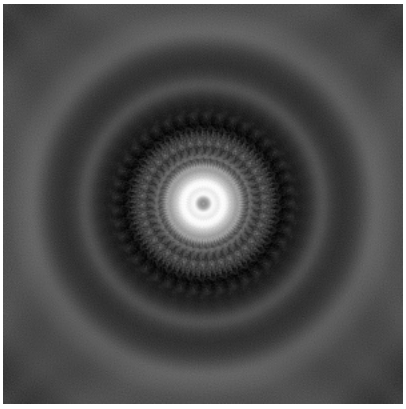
6.1.2 Raw map



X



Y

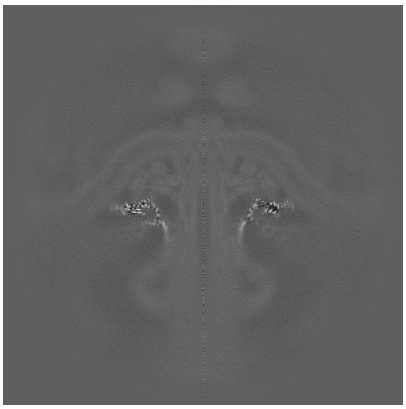


Z

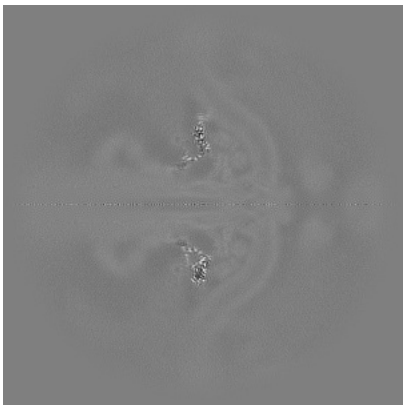
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

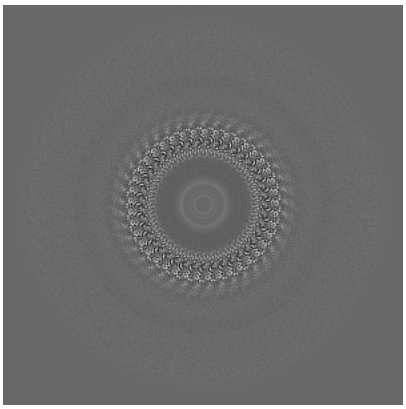
6.2.1 Primary map



X Index: 224

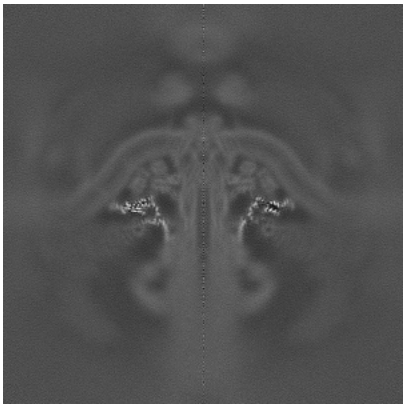


Y Index: 224

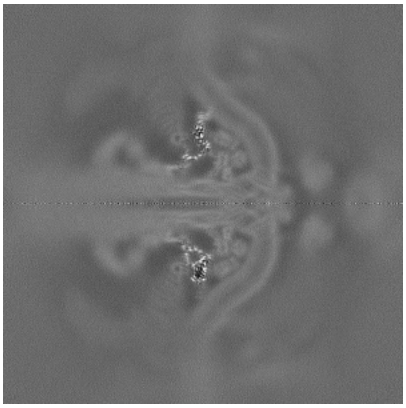


Z Index: 224

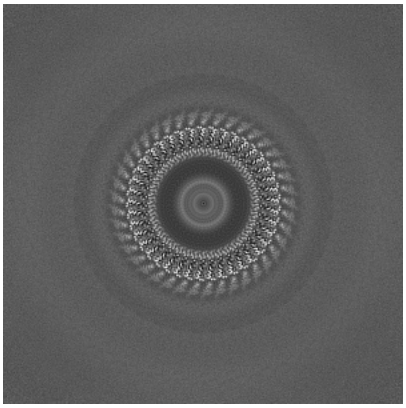
6.2.2 Raw map



X Index: 224



Y Index: 224



Z Index: 224

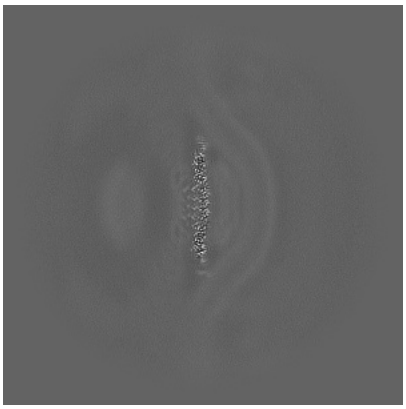
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

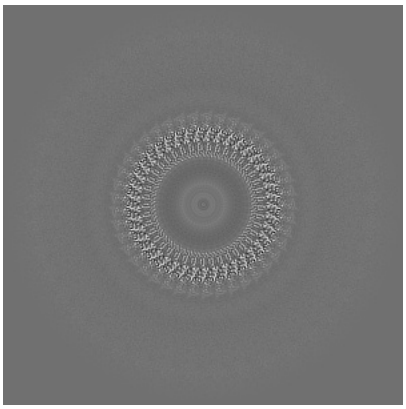
6.3.1 Primary map



X Index: 158

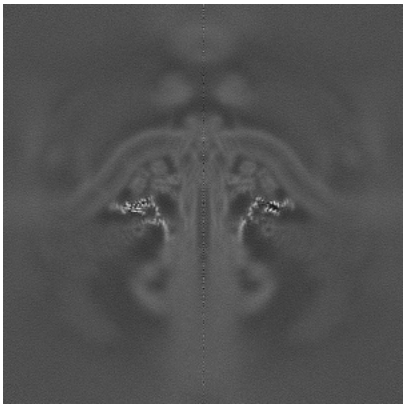


Y Index: 290

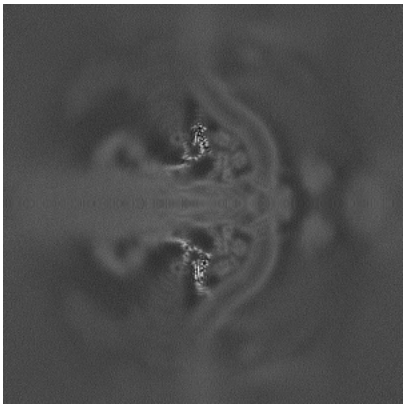


Z Index: 222

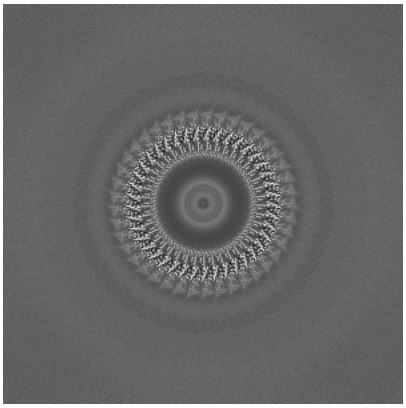
6.3.2 Raw map



X Index: 224



Y Index: 232

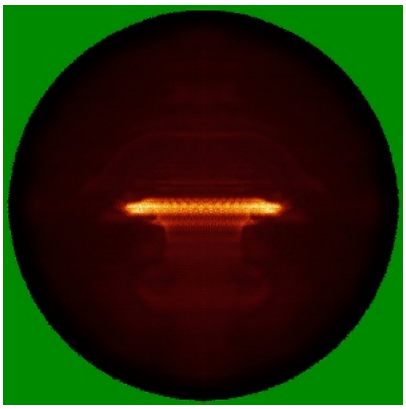


Z Index: 222

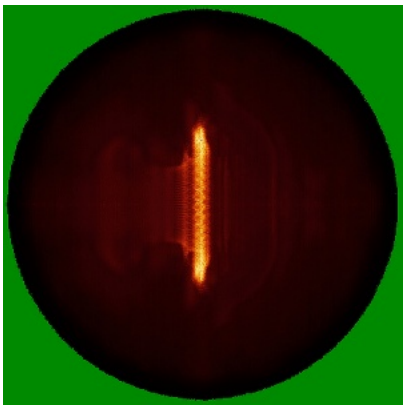
The images above show the largest variance slices of the map in three orthogonal directions.

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

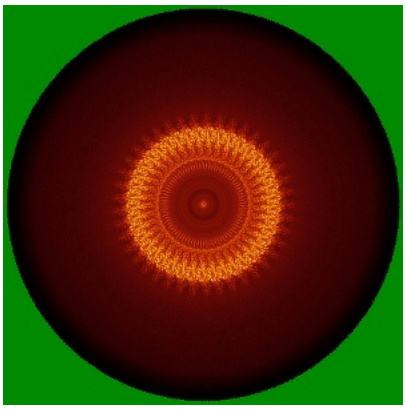
6.4.1 Primary map



X

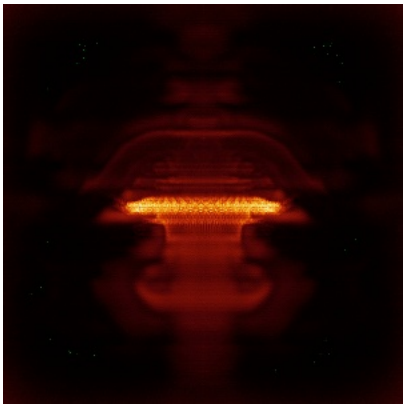


Y

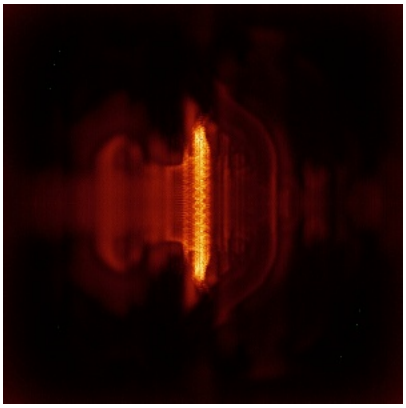


Z

6.4.2 Raw map



X



Y

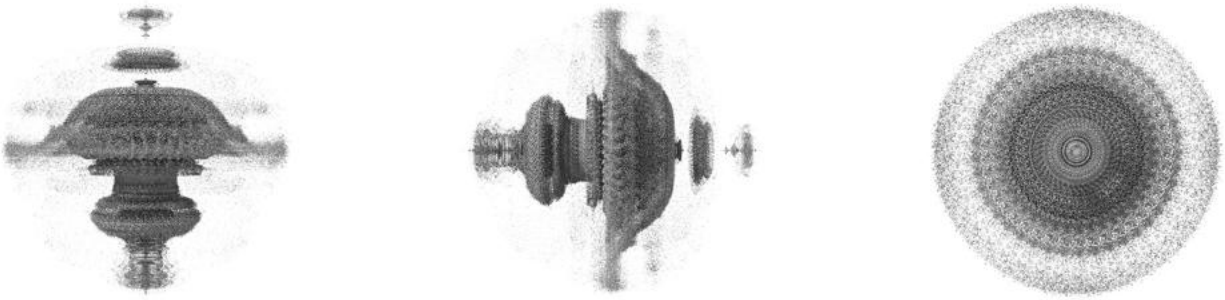


Z

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)

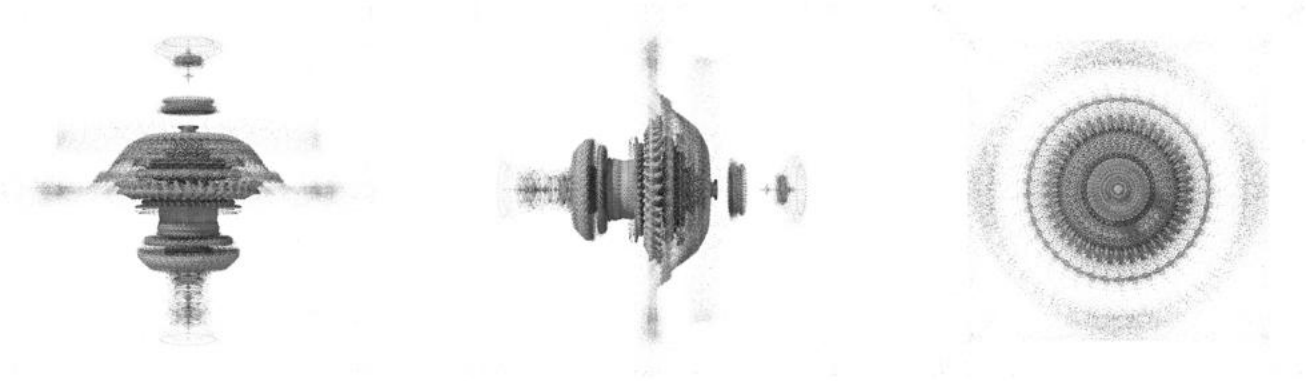
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

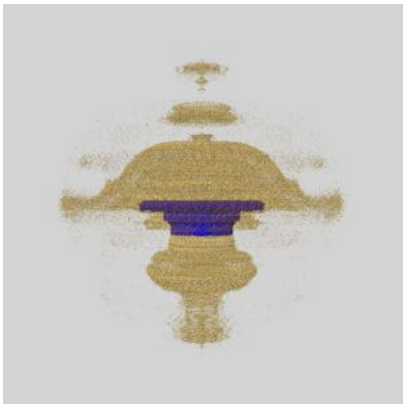
6.6 Mask visualisation (i)

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

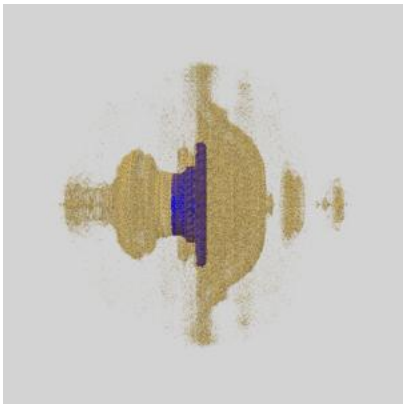
A mask typically either:

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

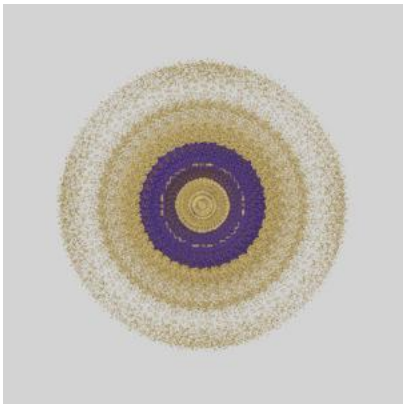
6.6.1 emd_76344_msk_1.map (i)



X



Y

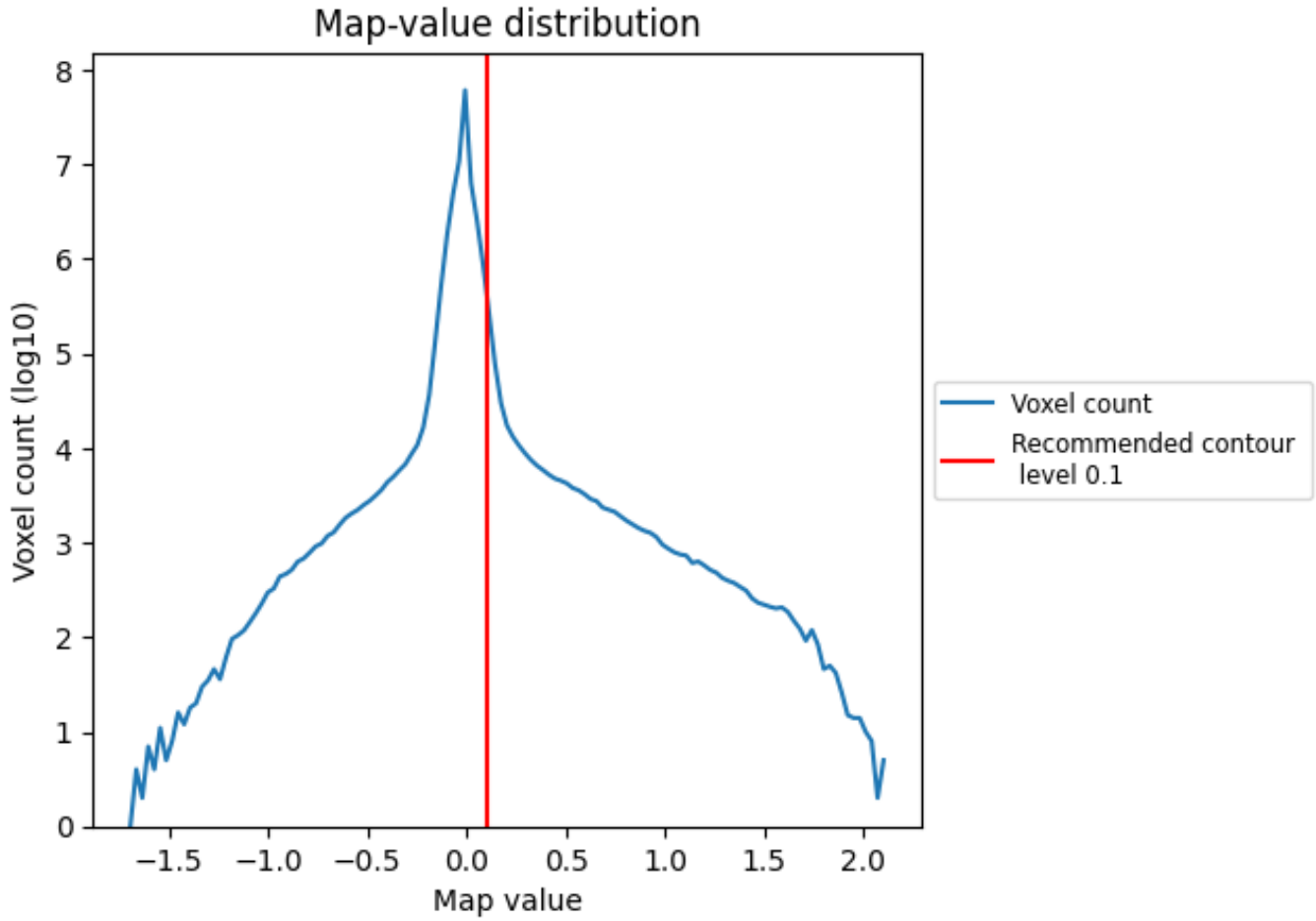


Z

7 Map analysis

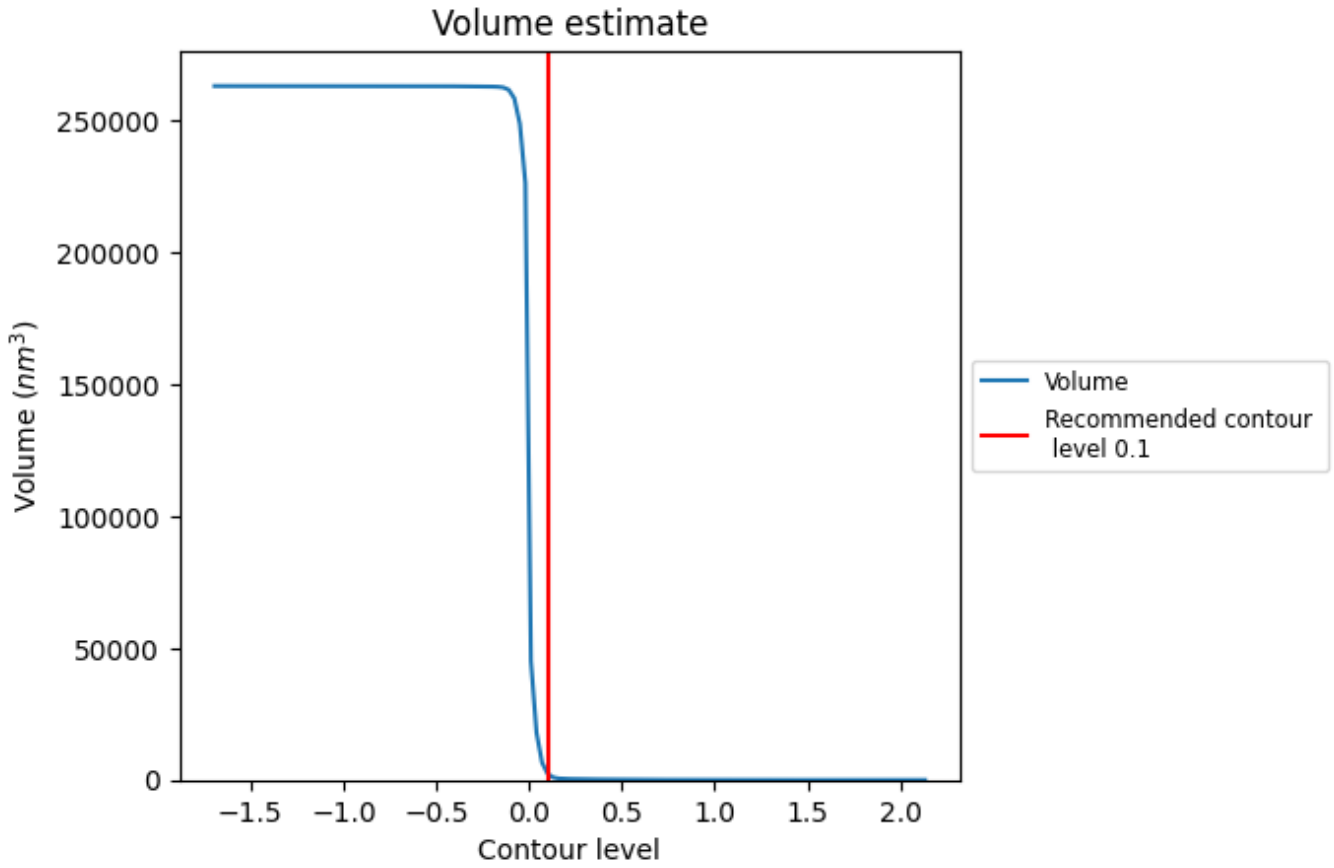
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

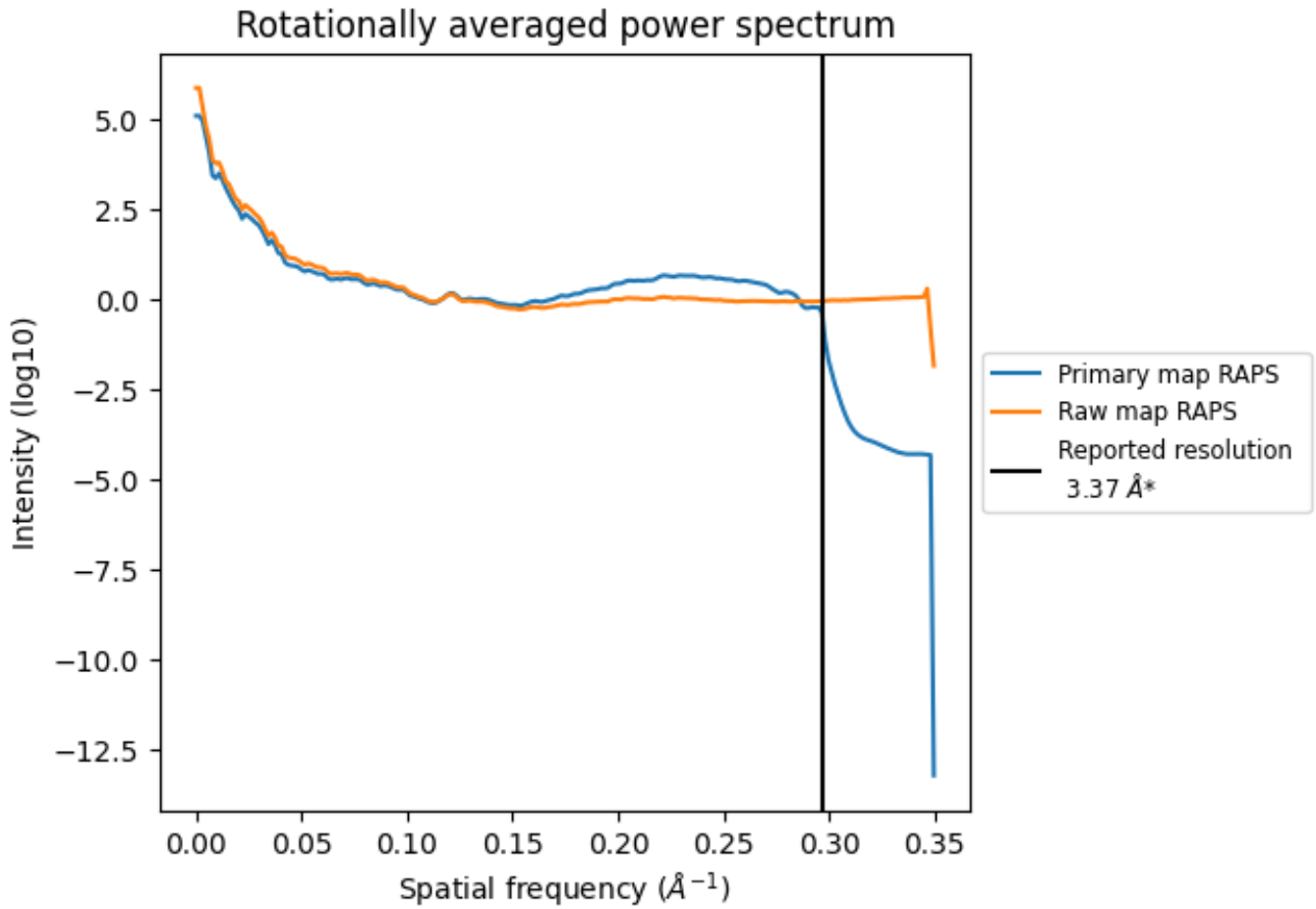
7.2 Volume estimate



The volume at the recommended contour level is 2394 nm^3; this corresponds to an approximate mass of 2163 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)

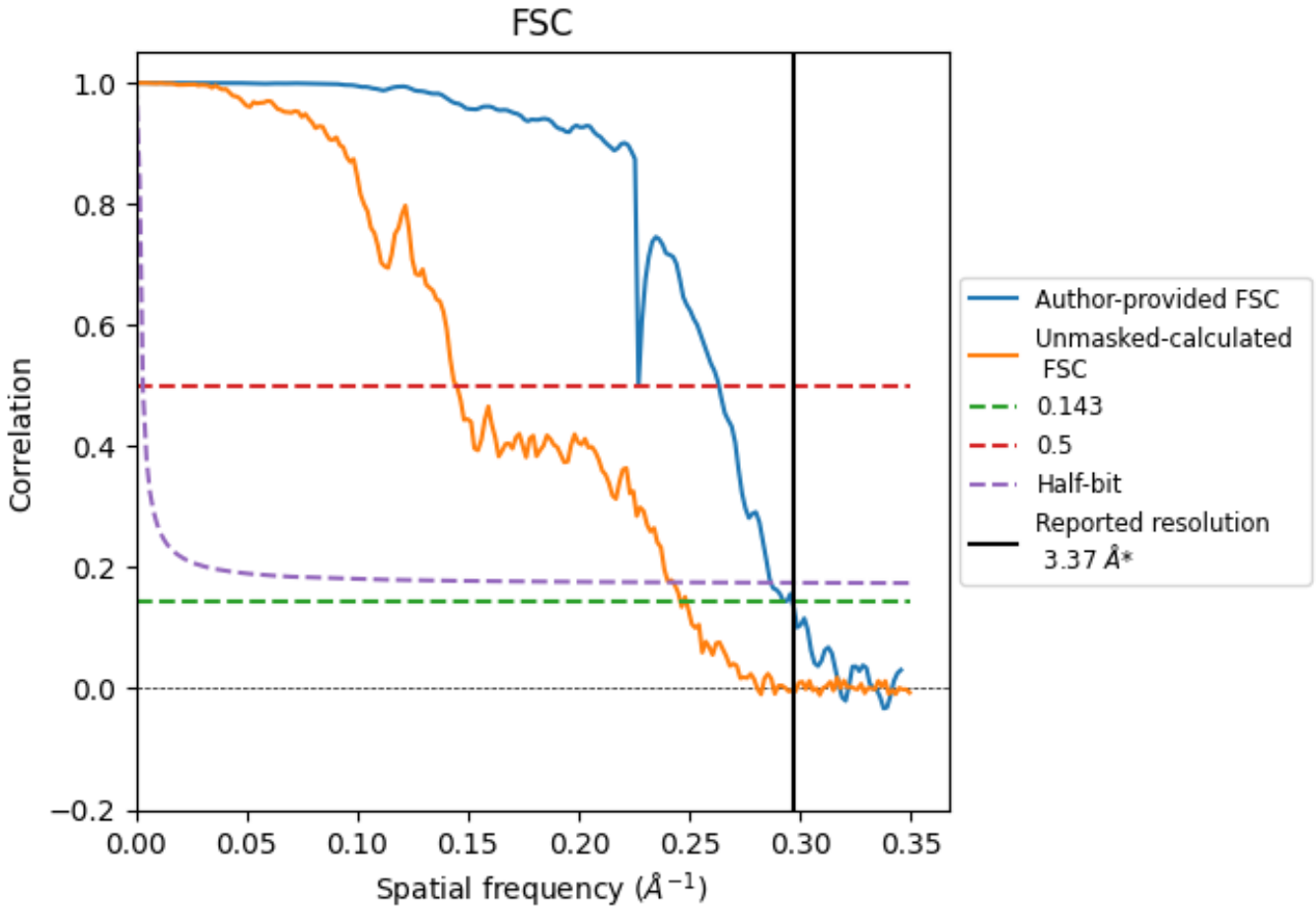


*Reported resolution corresponds to spatial frequency of 0.297 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.297 Å^{-1}

8.2 Resolution estimates (i)

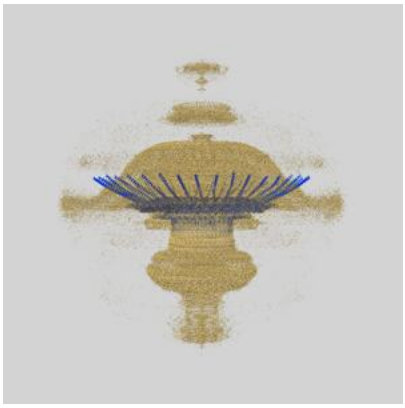
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	3.37	3.80	3.49
Unmasked-calculated*	4.07	6.90	4.12

*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 4.07 differs from the reported value 3.37 by more than 10 %

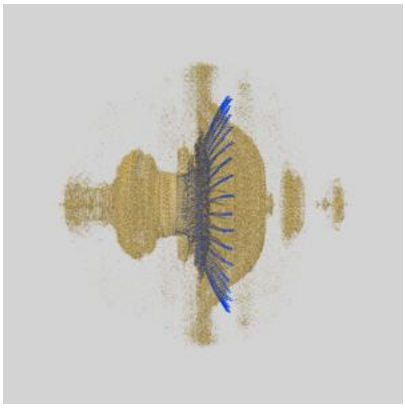
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76344 and PDB model 12DR. Per-residue inclusion information can be found in section 3 on page 8.

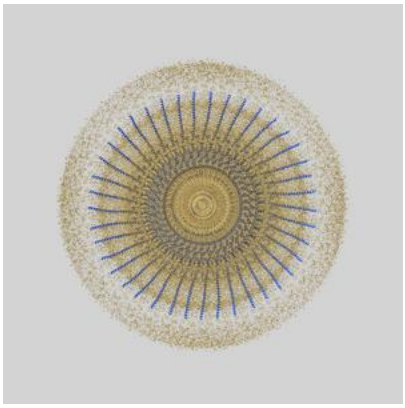
9.1 Map-model overlay



X



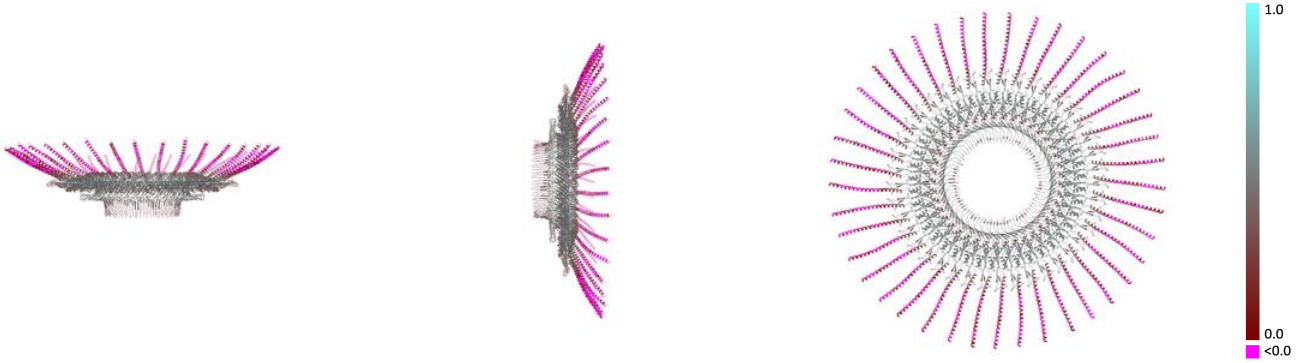
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

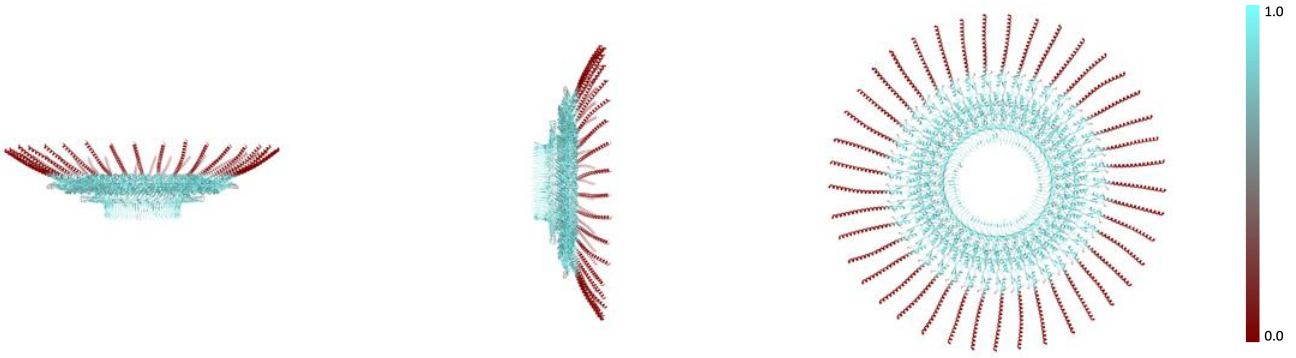
9.2 Q-score mapped to coordinate model (i)



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.

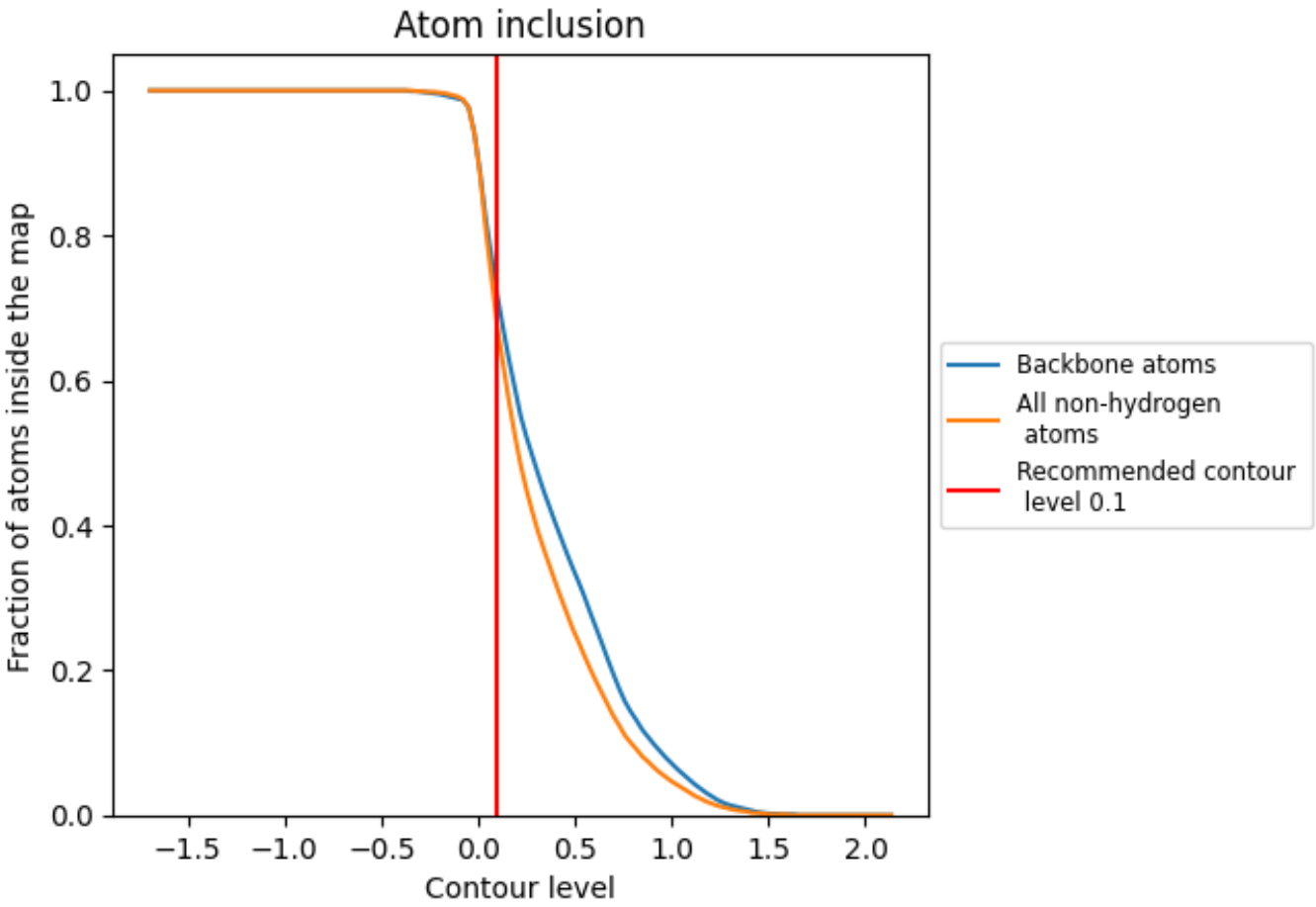
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6730	0.3500
A	0.6750	0.3540
B	0.6740	0.3430
C	0.6760	0.3510
D	0.6740	0.3610
E	0.6740	0.3490
F	0.6750	0.3590
G	0.6720	0.3490
H	0.6650	0.3410
I	0.6700	0.3450
J	0.6740	0.3600
K	0.6710	0.3460
L	0.6780	0.3510
M	0.6780	0.3500
N	0.6710	0.3450
O	0.6680	0.3500
P	0.6790	0.3570
Q	0.6710	0.3520
R	0.6760	0.3580
S	0.6610	0.3510
T	0.6760	0.3530
U	0.6690	0.3510
V	0.6690	0.3510
W	0.6740	0.3440
X	0.6760	0.3510
Y	0.6650	0.3470
Z	0.6690	0.3520
a	0.6690	0.3500
b	0.6760	0.3450
c	0.6780	0.3500
d	0.6750	0.3470
e	0.6720	0.3350
f	0.6680	0.3500
g	0.6800	0.3570
h	0.6720	0.3440



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.6740	0.3420
j	0.6750	0.3550
k	0.6680	0.3480
l	0.6650	0.3480
m	0.6710	0.3520
n	0.6750	0.3550
o	0.6710	0.3510