Full wwPDB EM Validation Report ⓘ

Apr 3, 2025 – 02:40 pm BST

PDB ID	:	9GO6 / pdb_00009go6
EMDB ID	:	EMD-51493
Title	:	Salmonella hook-filament junction complex
Authors	:	Qin, K.; Einenkel, R.; Erhardt, E.; Bergeron, J.R.
Deposited on	:	2024-09-04
Resolution	:	2.90 Å(reported)

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

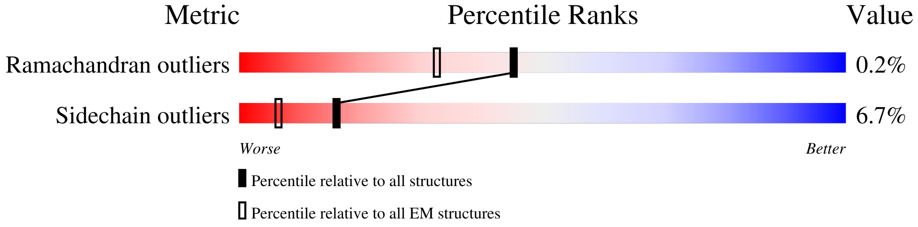
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance ⓘ

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

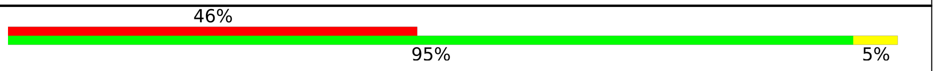
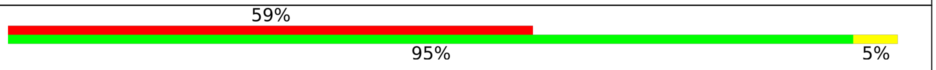
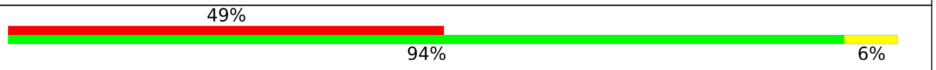
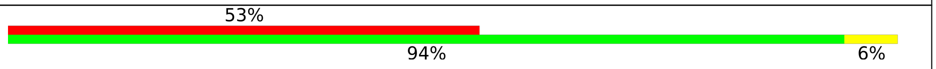
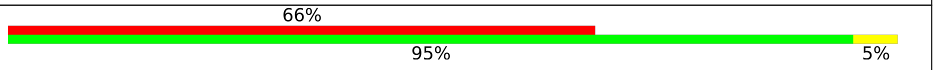
The reported resolution of this entry is 2.90 Å.

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	403	
1	2	403	
1	3	403	
1	4	403	
1	5	403	
1	6	403	
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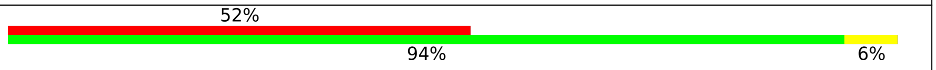
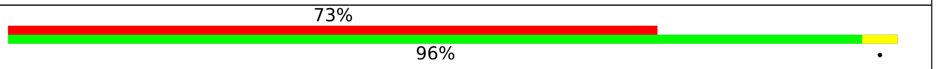
1	8	403	
1	9	403	

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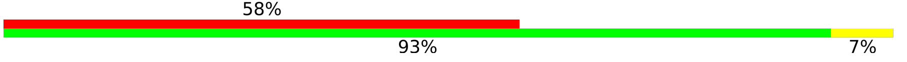
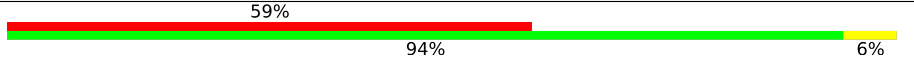
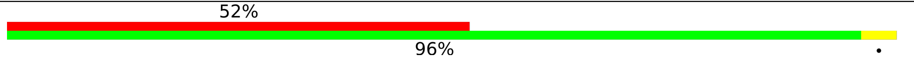
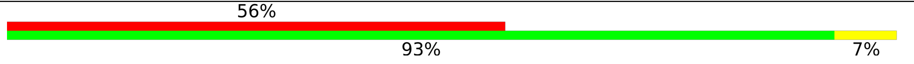
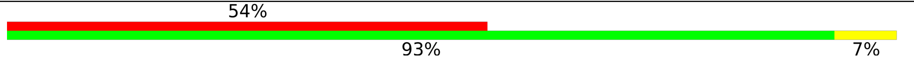
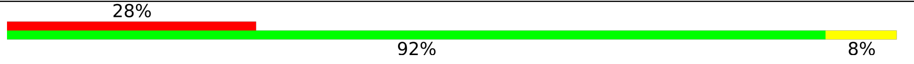
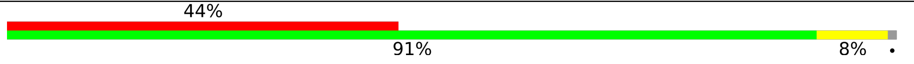
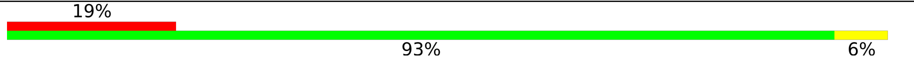
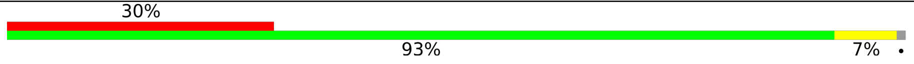
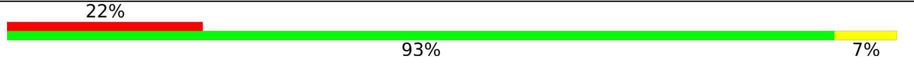
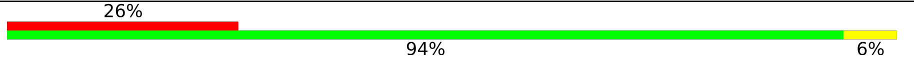
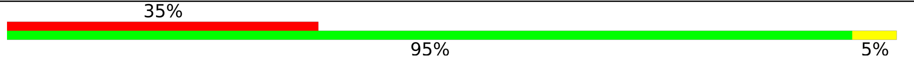
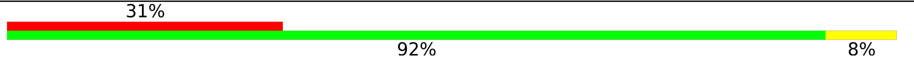
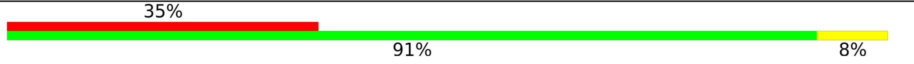
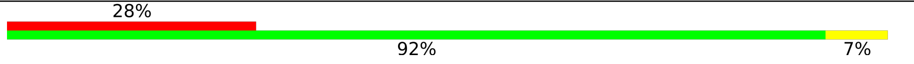
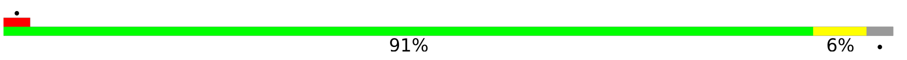
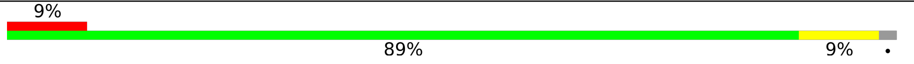
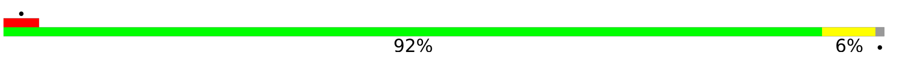
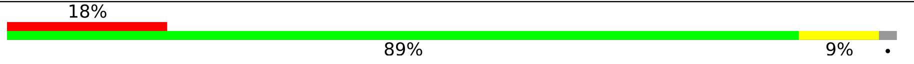
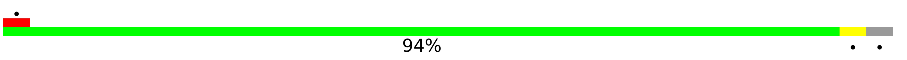
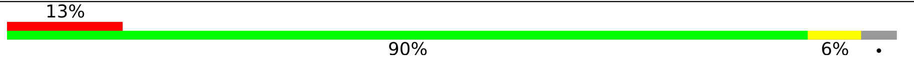
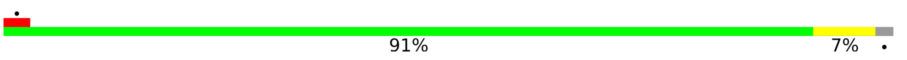
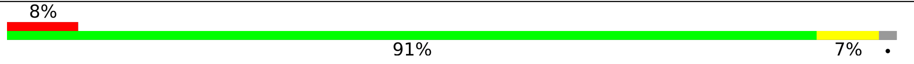
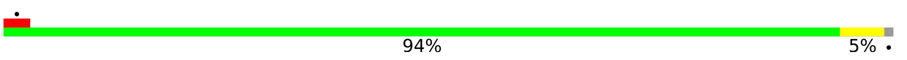
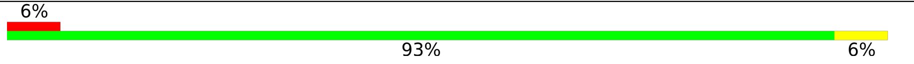
Mol	Chain	Length	Quality of chain
1	w	403	
1	x	403	
1	y	403	
1	z	403	
2	A	553	
2	B	553	
2	C	553	
2	D	553	
2	E	553	
2	F	553	
2	G	553	
2	H	553	
2	I	553	
2	J	553	
2	K	553	
3	L	317	
3	M	317	
3	N	317	
3	O	317	
3	P	317	
3	Q	317	
3	R	317	
3	S	317	
3	T	317	
3	U	317	

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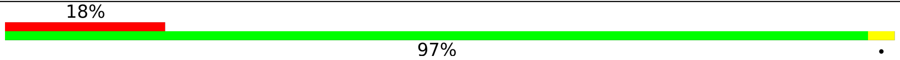
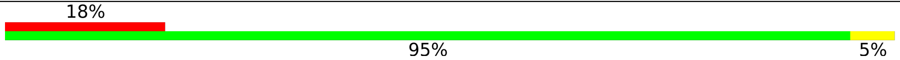
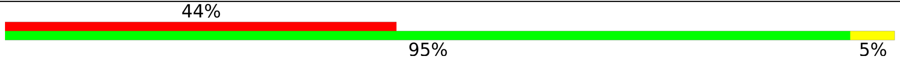
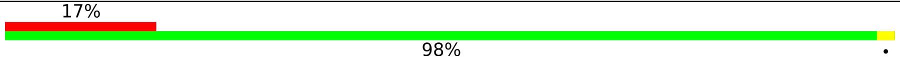
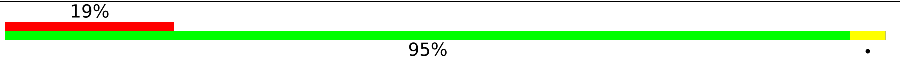
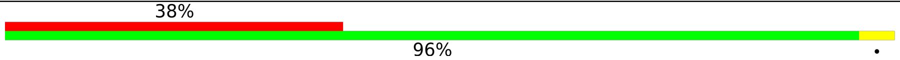
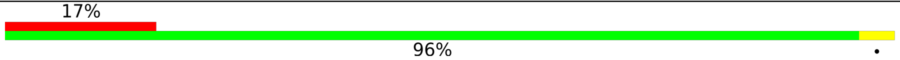
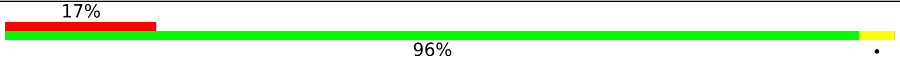
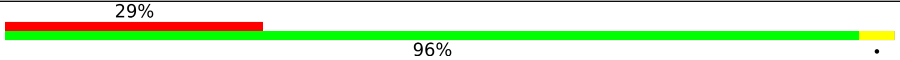
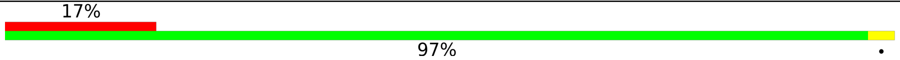
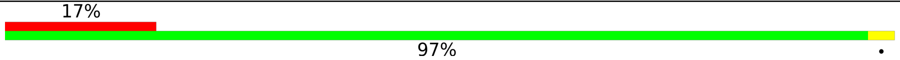
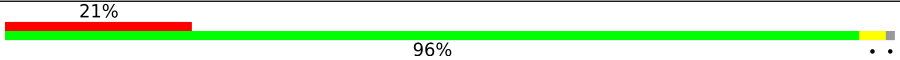
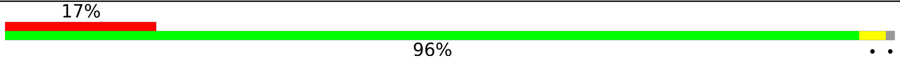
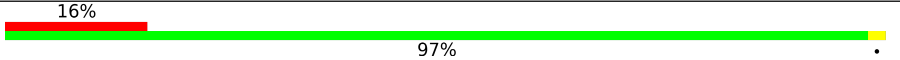
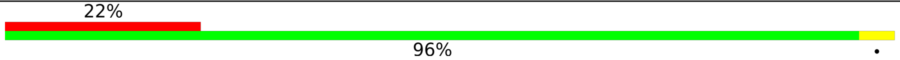
Mol	Chain	Length	Quality of chain
3	V	317	
4	a	495	
4	b	495	
4	c	495	
4	d	495	
4	e	495	
4	f	495	
4	g	495	
4	h	495	
4	i	495	
4	j	495	
4	k	495	
4	l	495	
4	m	495	
4	n	495	
4	o	495	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 324413 atoms, of which 160408 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 hook protein FlgE.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	1	403	5832	1825	2865	512	621	9	0	0
1	2	403	5832	1825	2865	512	621	9	0	0
1	3	403	5832	1825	2865	512	621	9	0	0
1	4	403	5832	1825	2865	512	621	9	0	0
1	5	403	5832	1825	2865	512	621	9	0	0
1	6	403	5832	1825	2865	512	621	9	0	0
1	7	403	5832	1825	2865	512	621	9	0	0
1	8	403	5832	1825	2865	512	621	9	0	0
1	9	403	5832	1825	2865	512	621	9	0	0
1	w	403	5832	1825	2865	512	621	9	0	0
1	x	403	5832	1825	2865	512	621	9	0	0
1	y	403	5832	1825	2865	512	621	9	0	0
1	z	403	5832	1825	2865	512	621	9	0	0

- Molecule 2 is a protein called Flagellar hook-associated protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	A	552	8201	2547	4056	722	869	7	0	0
2	B	552	8201	2547	4056	722	869	7	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	550	Total 8184	C 2542	H 4048	N 723	O 865	S 6	0	0
2	D	552	Total 8201	C 2547	H 4056	N 722	O 869	S 7	0	0
2	E	550	Total 8163	C 2536	H 4034	N 720	O 867	S 6	0	0
2	F	551	Total 8182	C 2542	H 4045	N 721	O 868	S 6	0	0
2	G	551	Total 8182	C 2542	H 4045	N 721	O 868	S 6	0	0
2	H	551	Total 8178	C 2542	H 4041	N 721	O 868	S 6	0	0
2	I	552	Total 8201	C 2547	H 4056	N 722	O 869	S 7	0	0
2	J	552	Total 8201	C 2547	H 4056	N 722	O 869	S 7	0	0
2	K	552	Total 8201	C 2547	H 4056	N 722	O 869	S 7	0	0

- Molecule 3 is a protein called Flagellar hook-associated protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	L	306	Total 4543	C 1404	H 2247	N 398	O 482	S 12	0	0
3	M	312	Total 4640	C 1436	H 2296	N 405	O 491	S 12	0	0
3	N	313	Total 4666	C 1443	H 2309	N 410	O 492	S 12	0	0
3	O	310	Total 4612	C 1428	H 2282	N 403	O 487	S 12	0	0
3	P	307	Total 4556	C 1408	H 2254	N 399	O 484	S 11	0	0
3	Q	305	Total 4529	C 1400	H 2240	N 397	O 480	S 12	0	0
3	R	310	Total 4604	C 1425	H 2277	N 402	O 488	S 12	0	0
3	S	312	Total 4653	C 1439	H 2303	N 409	O 490	S 12	0	0
3	T	314	Total 4678	C 1446	H 2315	N 411	O 494	S 12	0	0
3	U	316	Total 4681	C 1457	H 2302	N 413	O 496	S 13	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	V	315	Total 4697	C 1452	H 2326	N 412	O 495	S 12	0	0

- Molecule 4 is a protein called Flagellin.

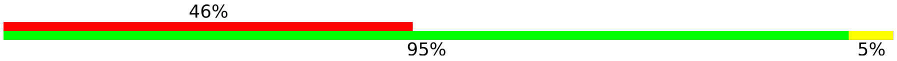
Mol	Chain	Residues	Atoms						AltConf	Trace
4	a	494	Total 7189	C 2189	H 3574	N 640	O 784	S 2	0	0
4	b	493	Total 7151	C 2186	H 3541	N 639	O 783	S 2	0	0
4	c	494	Total 7167	C 2189	H 3552	N 640	O 784	S 2	0	0
4	d	494	Total 7189	C 2189	H 3574	N 640	O 784	S 2	0	0
4	e	494	Total 7189	C 2189	H 3574	N 640	O 784	S 2	0	0
4	f	495	Total 7164	C 2194	H 3541	N 641	O 785	S 3	0	0
4	g	493	Total 7179	C 2186	H 3569	N 639	O 783	S 2	0	0
4	h	494	Total 7189	C 2189	H 3574	N 640	O 784	S 2	0	0
4	i	494	Total 7176	C 2189	H 3561	N 640	O 784	S 2	0	0
4	j	493	Total 7179	C 2186	H 3569	N 639	O 783	S 2	0	0
4	k	494	Total 7189	C 2189	H 3574	N 640	O 784	S 2	0	0
4	l	492	Total 7162	C 2181	H 3561	N 637	O 781	S 2	0	0
4	m	492	Total 7162	C 2181	H 3561	N 637	O 781	S 2	0	0
4	n	493	Total 7179	C 2186	H 3569	N 639	O 783	S 2	0	0
4	o	493	Total 7179	C 2186	H 3569	N 639	O 783	S 2	0	0

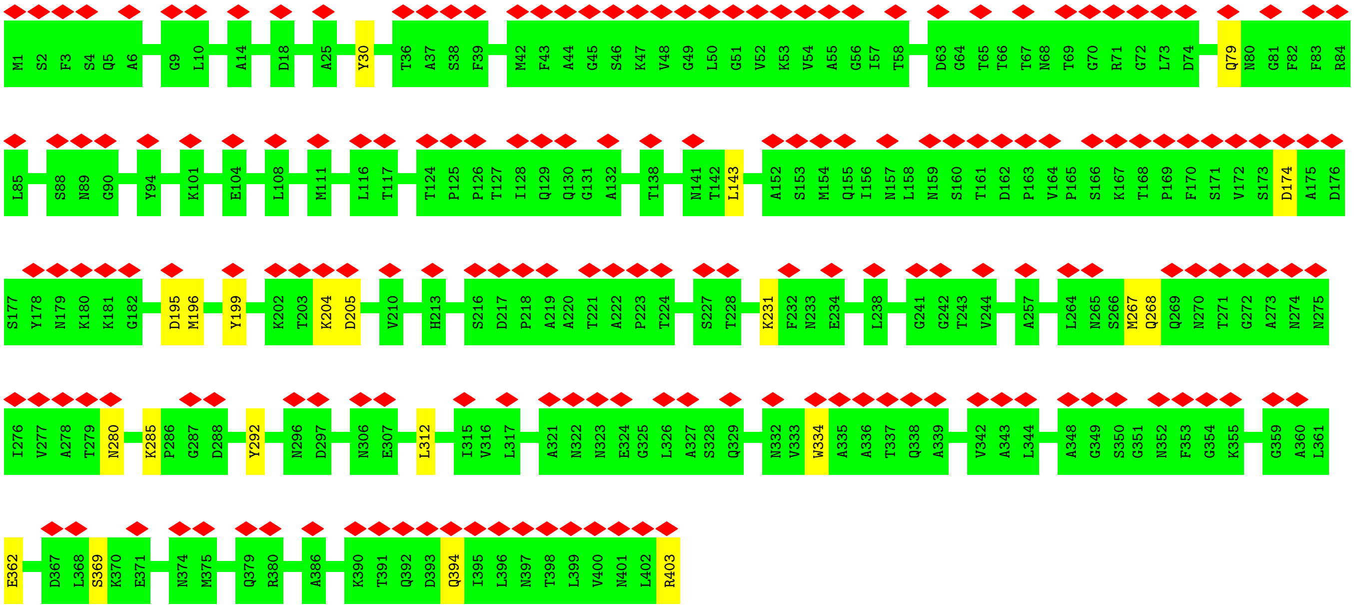
3 Residue-property plots ⓘ

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

- Molecule 1: Flagellar hook protein FlgE

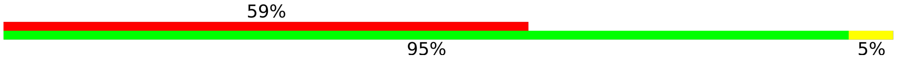
Chain 1:

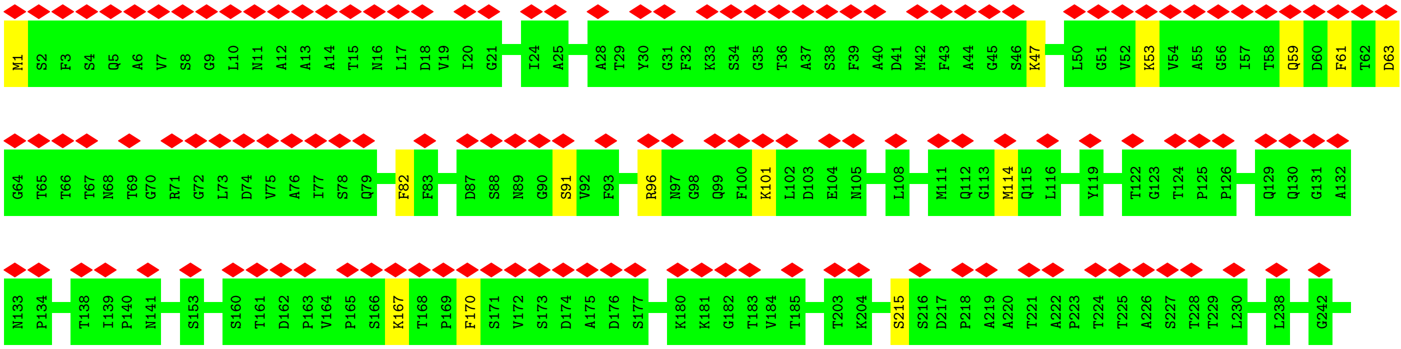


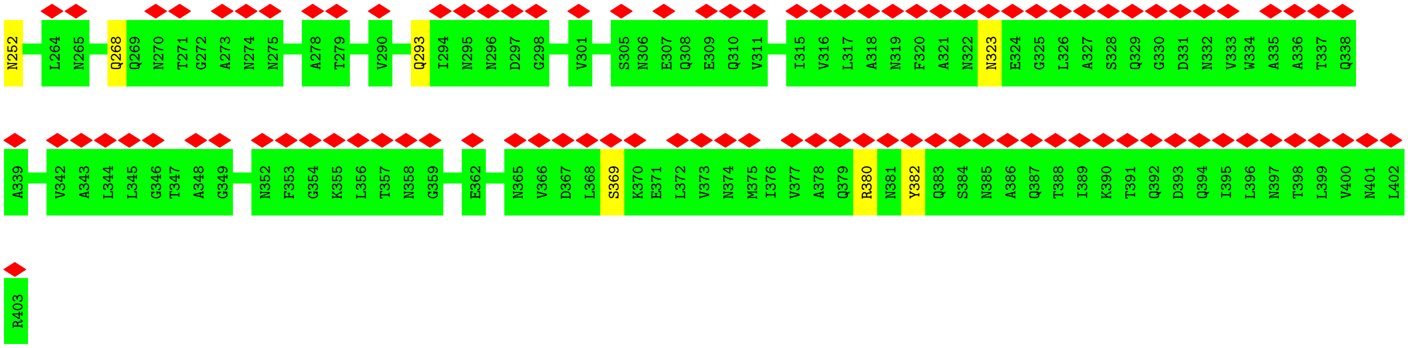


- Molecule 1: Flagellar hook protein FlgE

Chain 2:

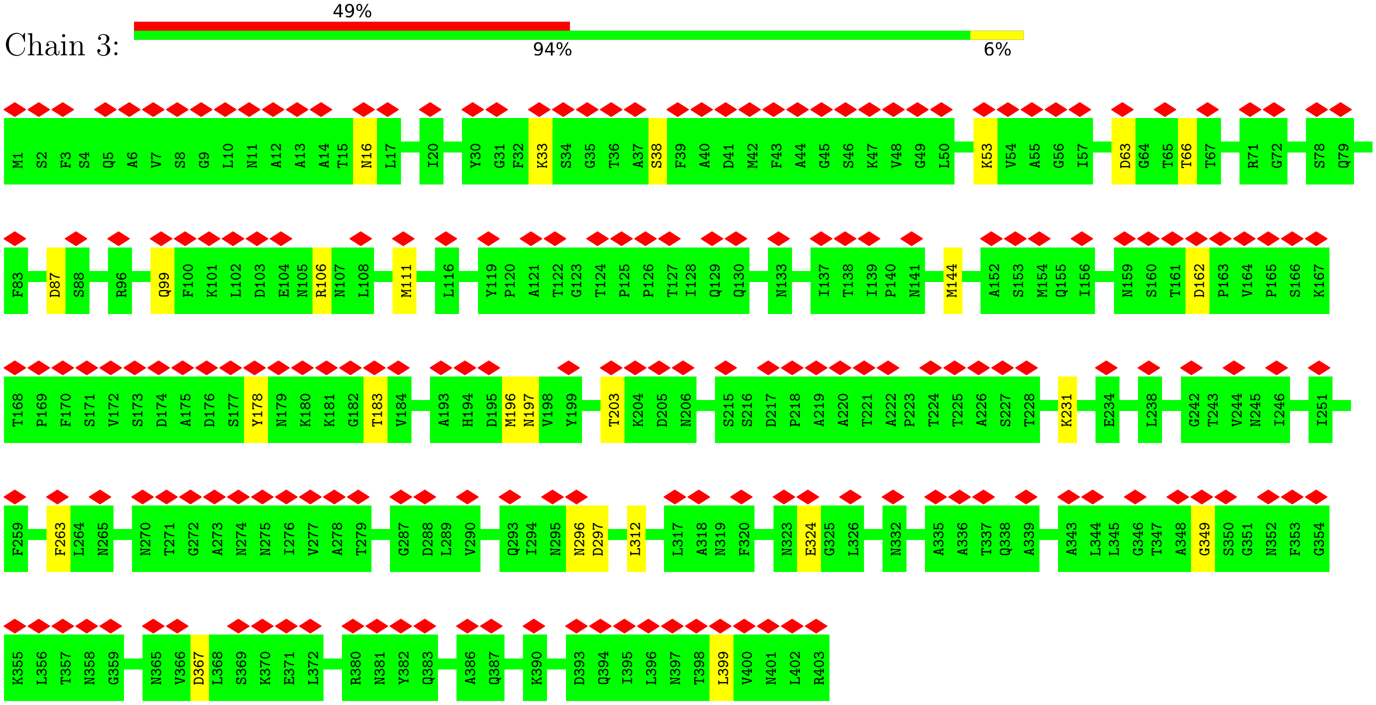






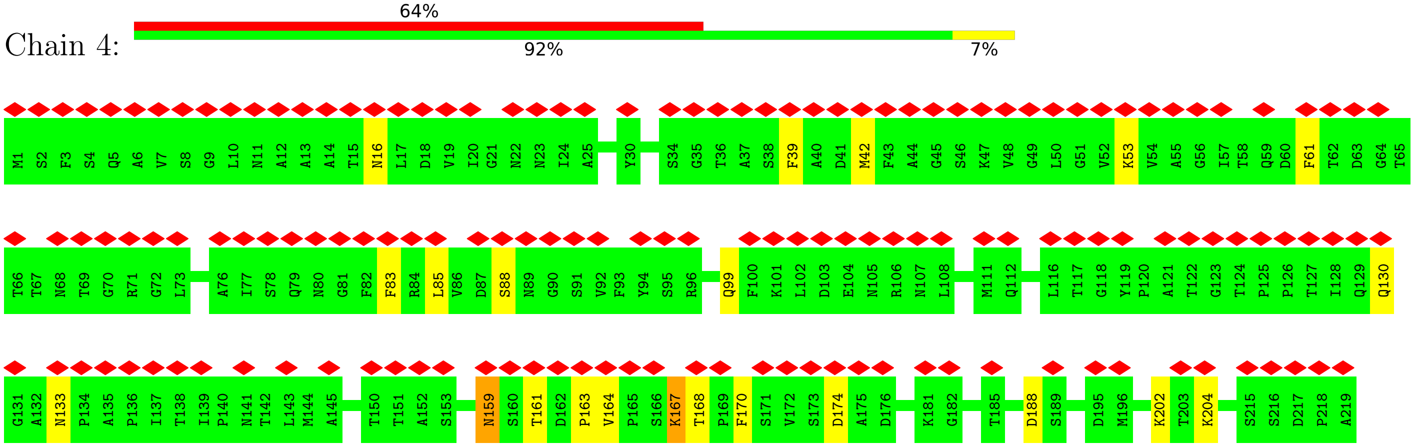
- Molecule 1: Flagellar hook protein FlgE

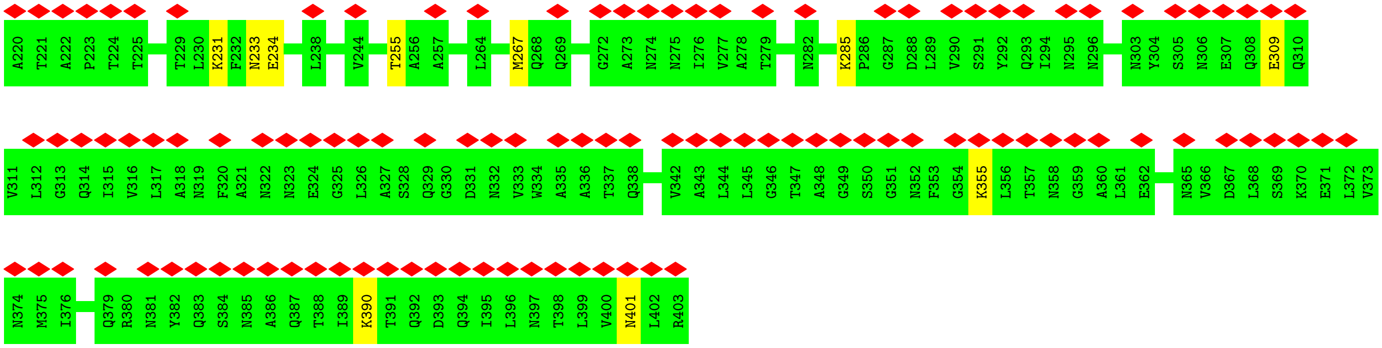
Chain 3:



- Molecule 1: Flagellar hook protein FlgE

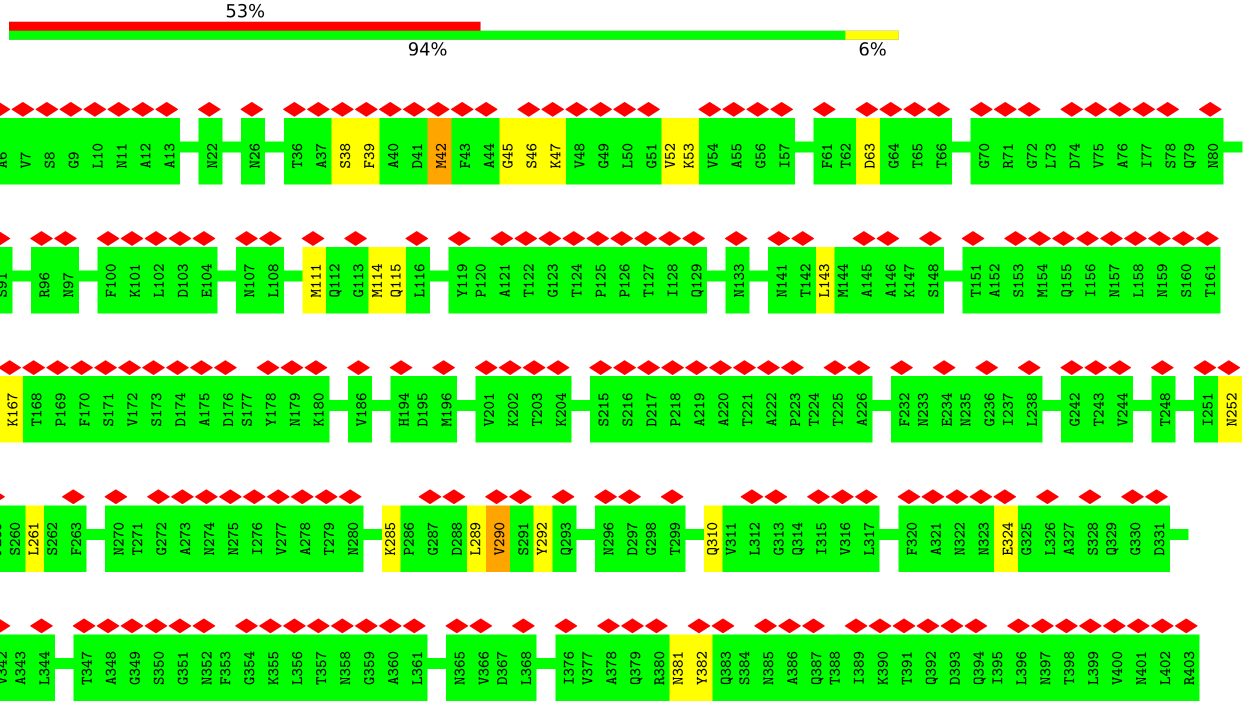
Chain 4:





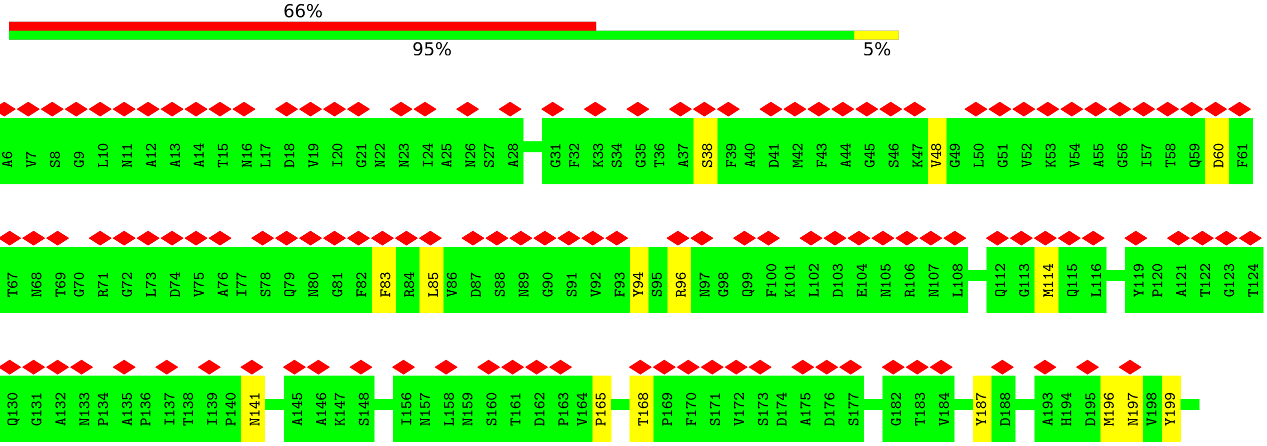
- Molecule 1: Flagellar hook protein FlgE

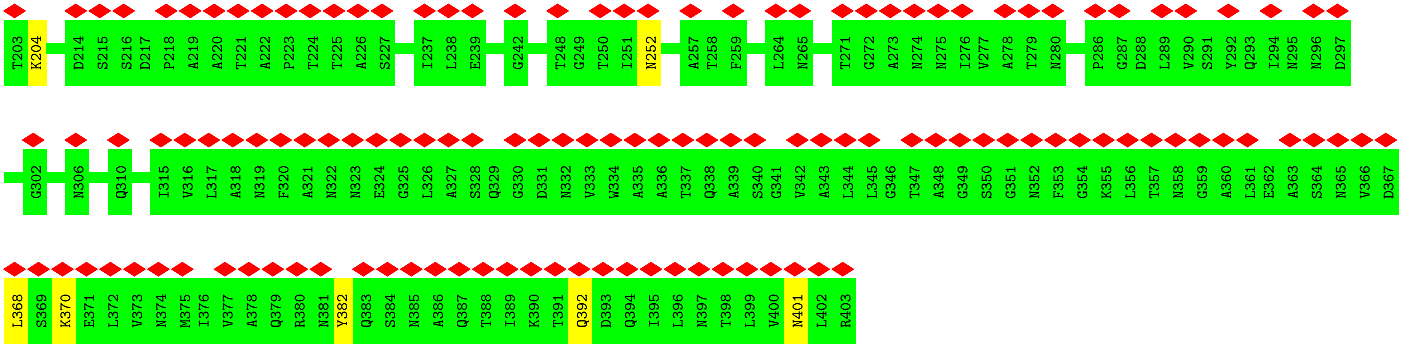
Chain 5:



- Molecule 1: Flagellar hook protein FlgE

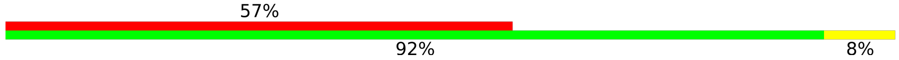
Chain 6:

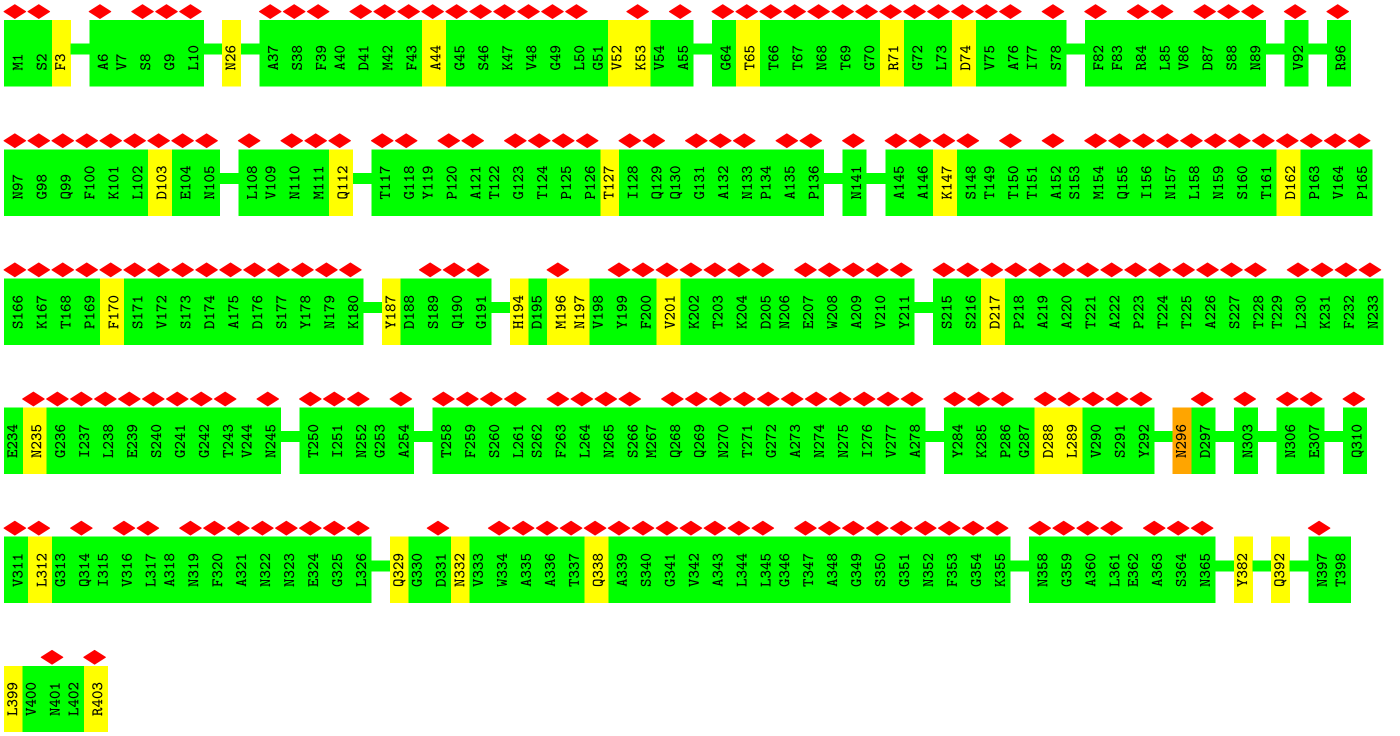




- Molecule 1: Flagellar hook protein FlgE

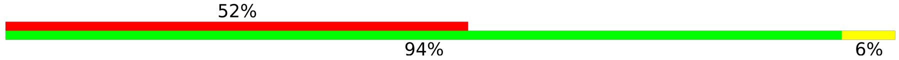
Chain 7:

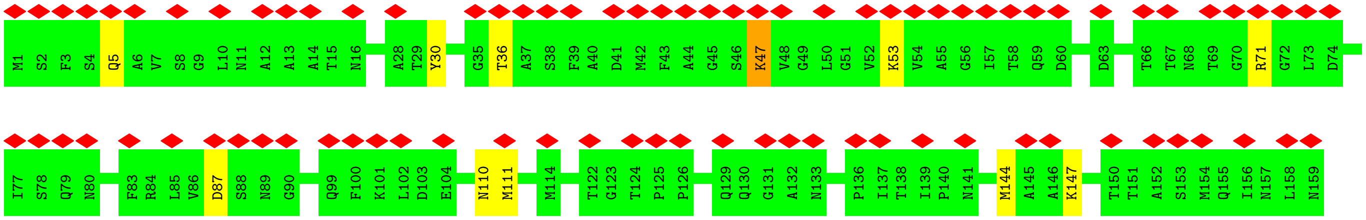


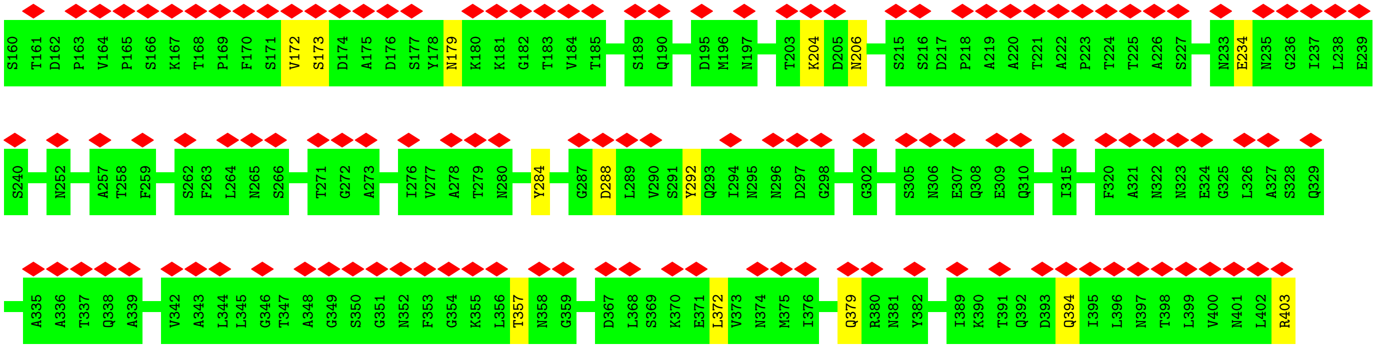


- Molecule 1: Flagellar hook protein FlgE

Chain 8:

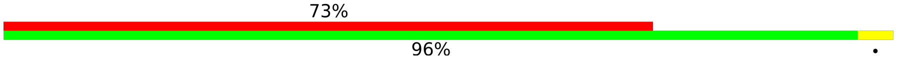


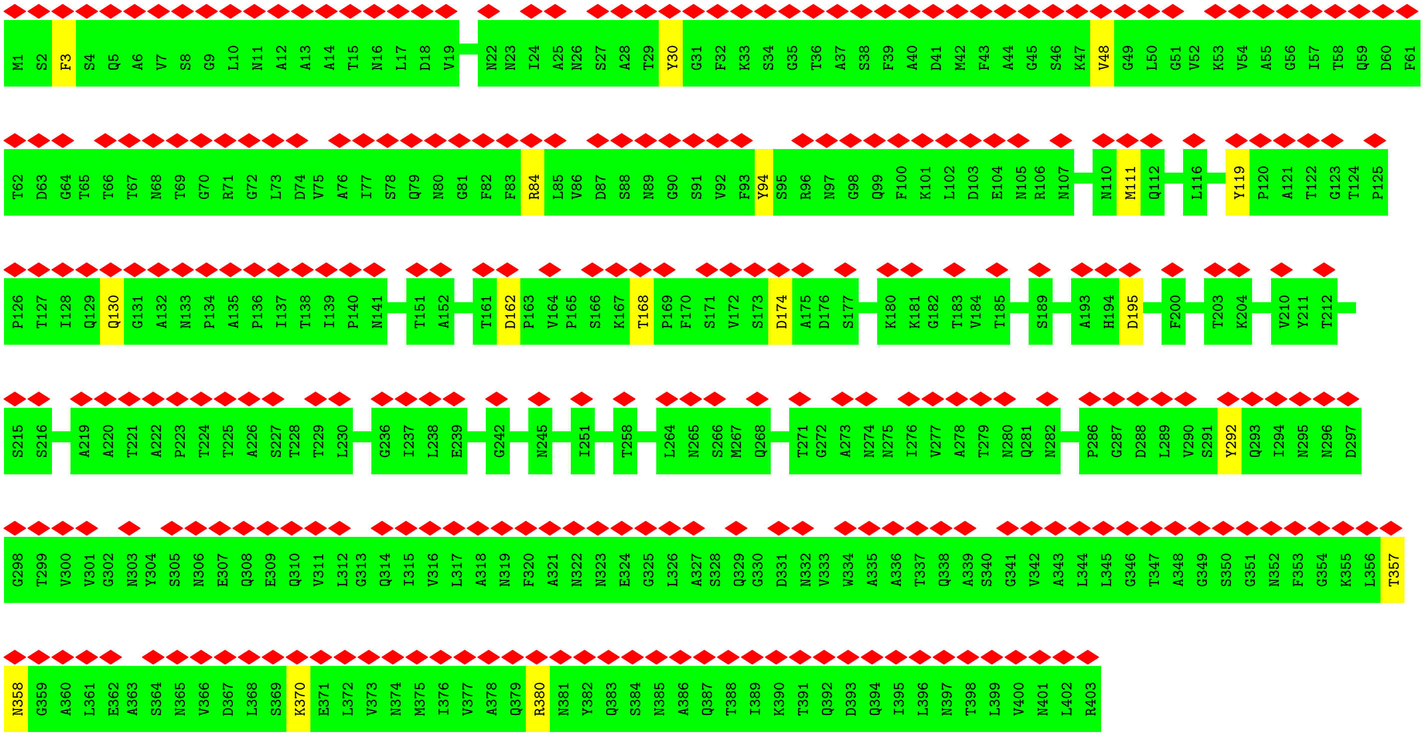




- Molecule 1: Flagellar hook protein FlgE

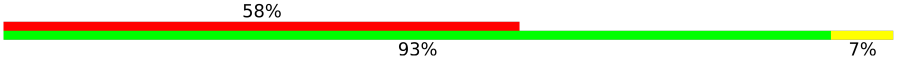
Chain 9:

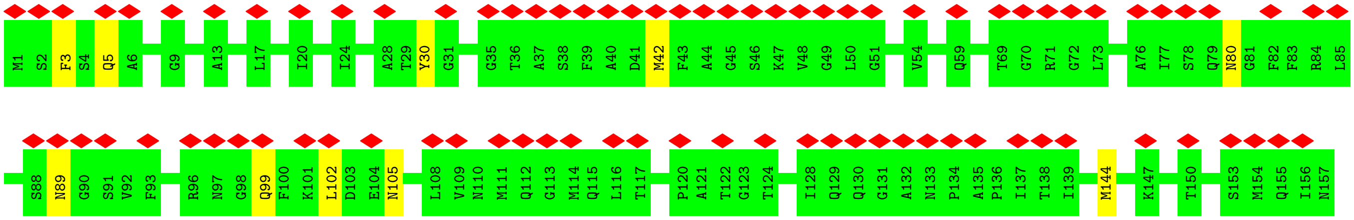


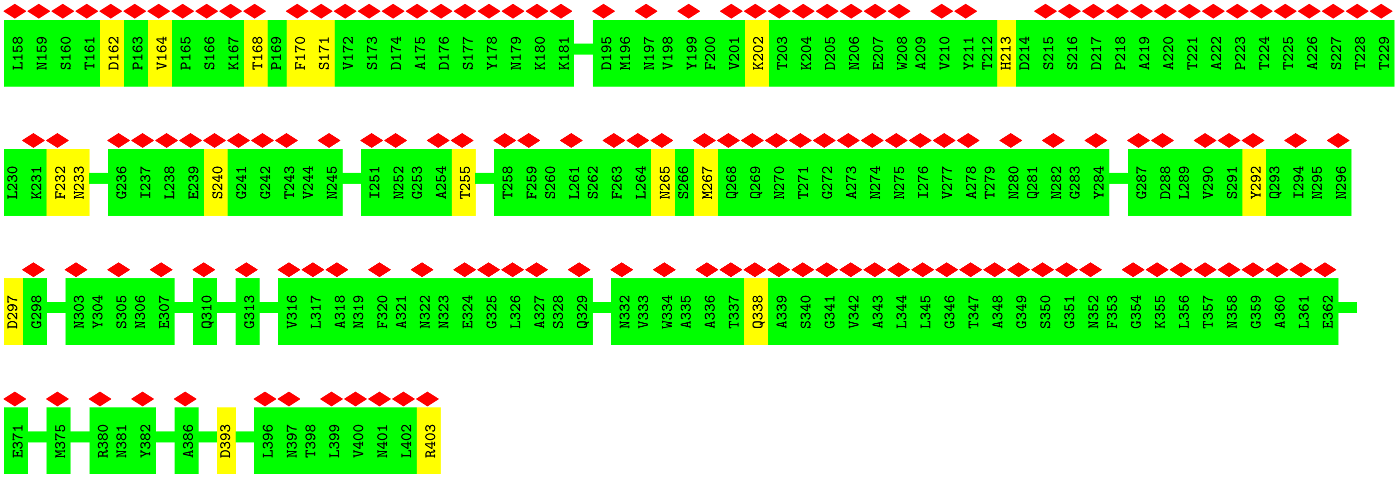


- Molecule 1: Flagellar hook protein FlgE

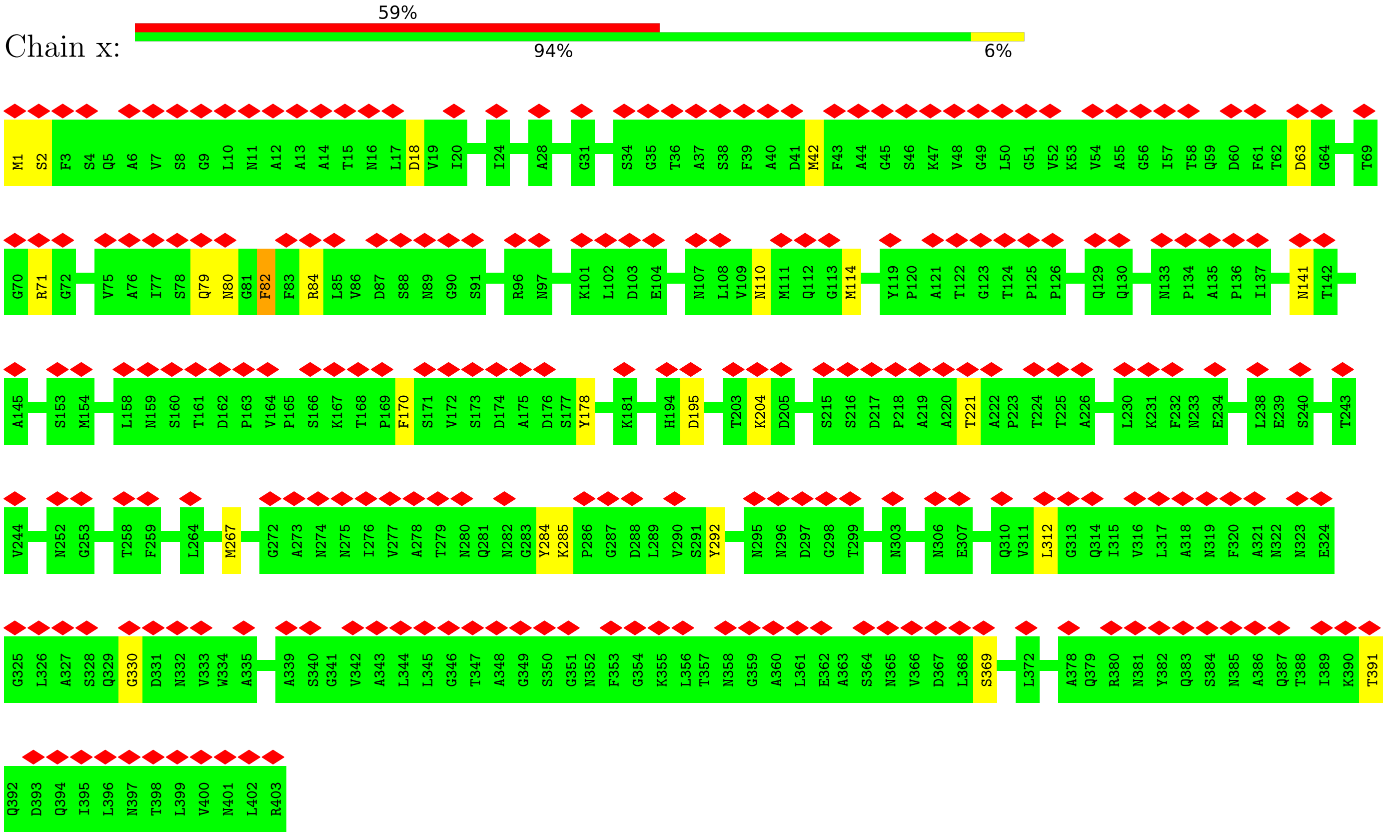
Chain w:



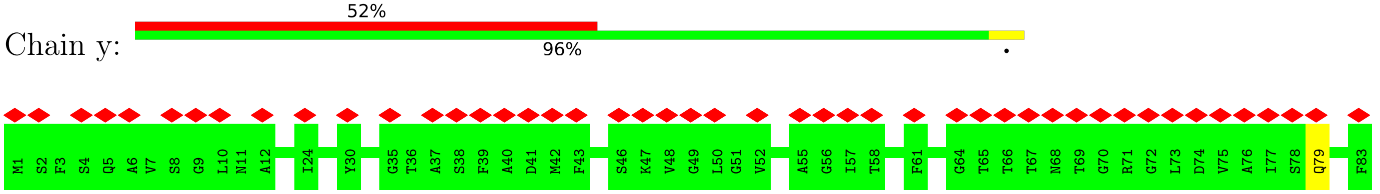


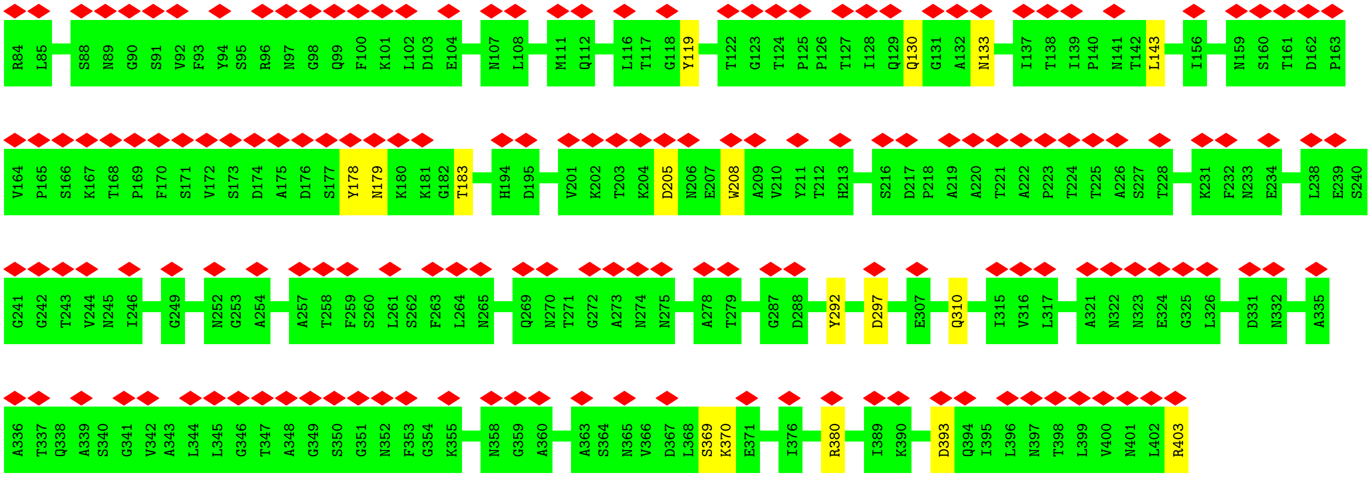


- Molecule 1: Flagellar hook protein FlgE



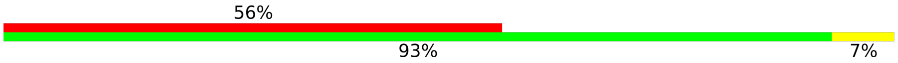
- Molecule 1: Flagellar hook protein FlgE

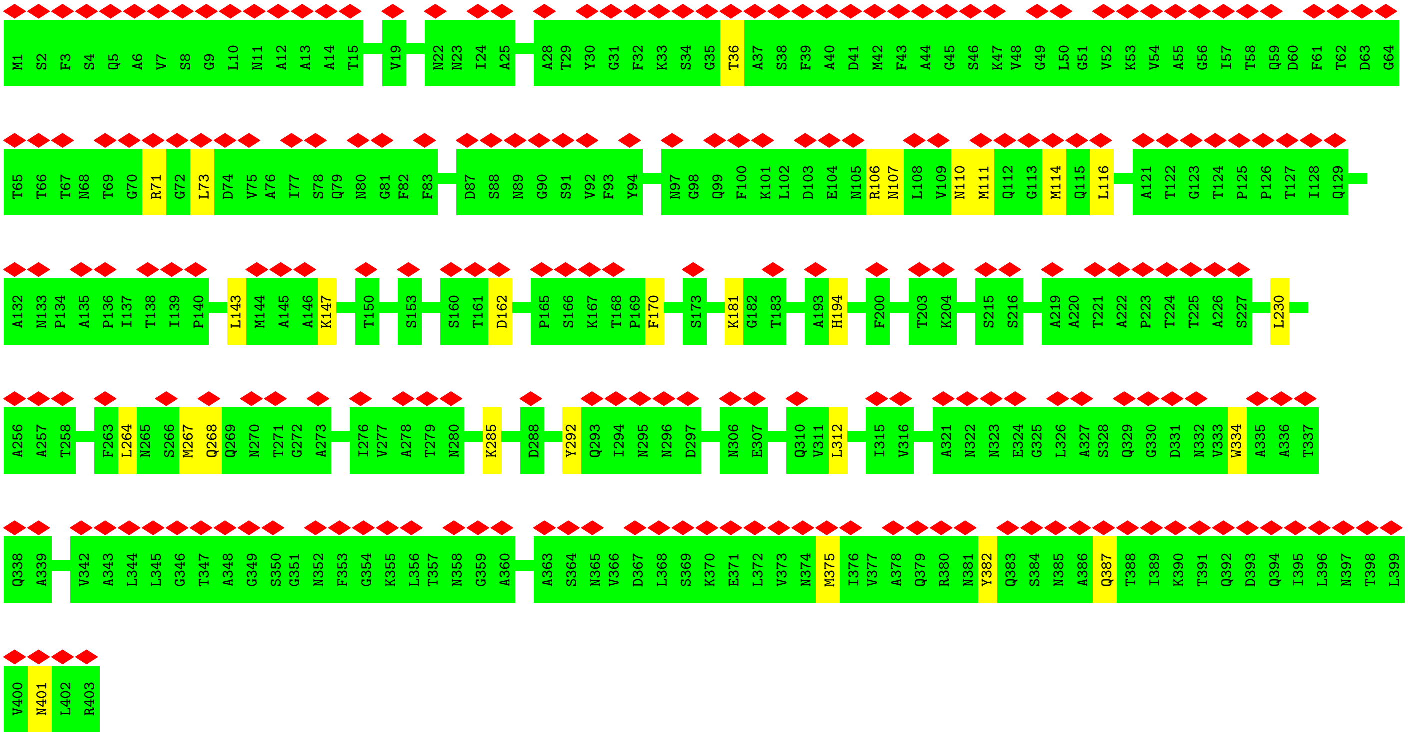




- Molecule 1: Flagellar hook protein FlgE

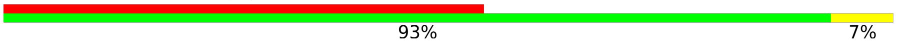
Chain z:

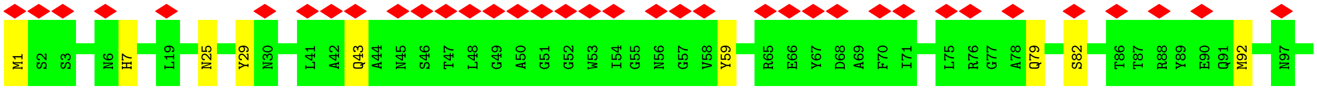


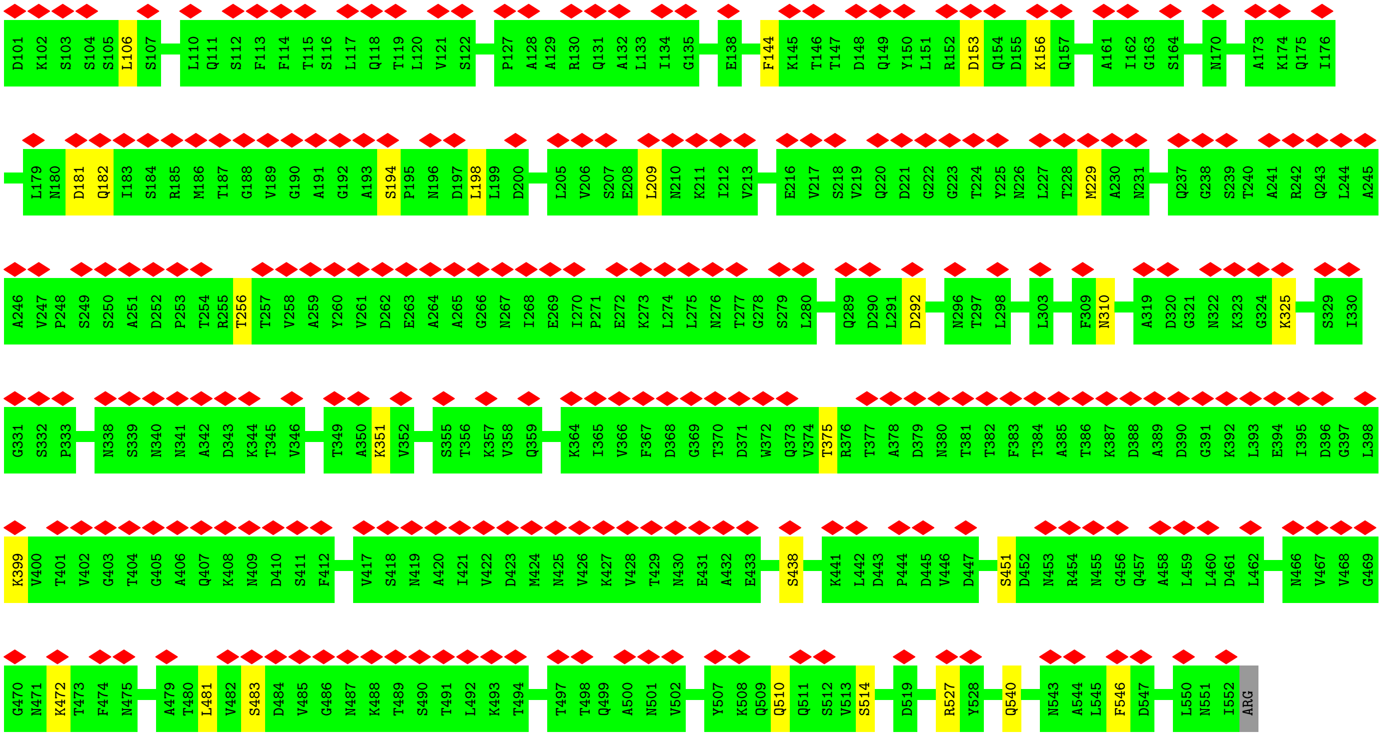


- Molecule 2: Flagellar hook-associated protein 1

Chain A:

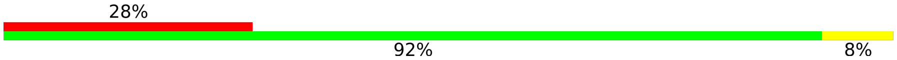


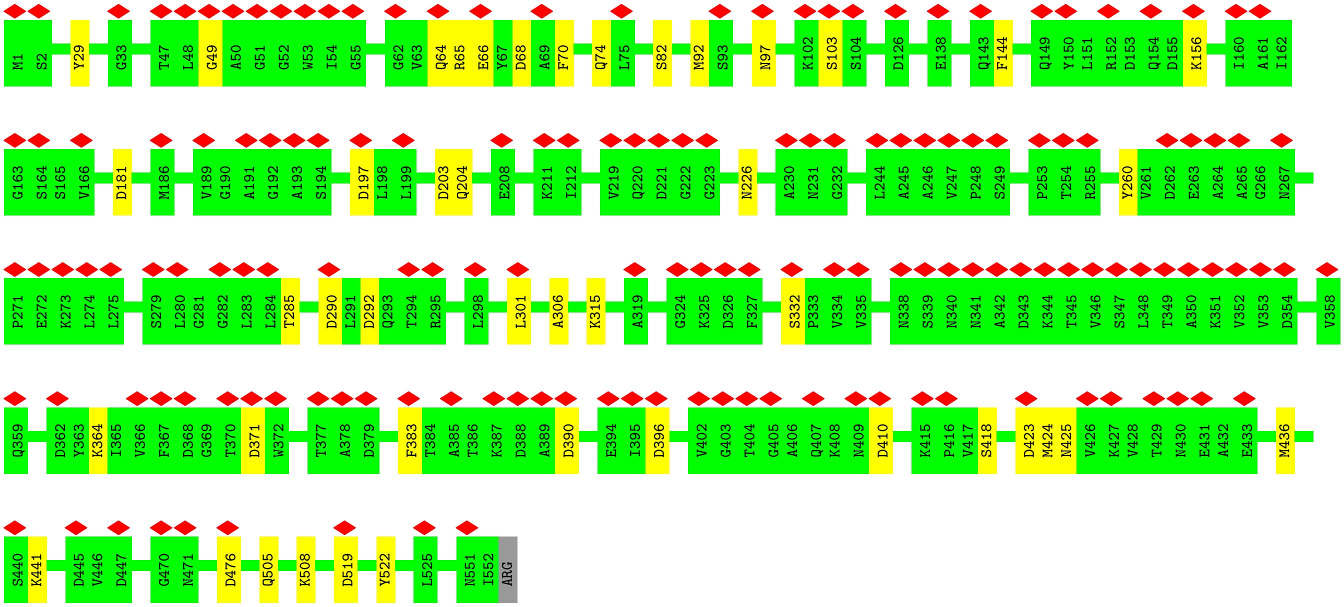




- Molecule 2: Flagellar hook-associated protein 1

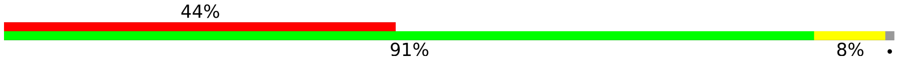
Chain B:

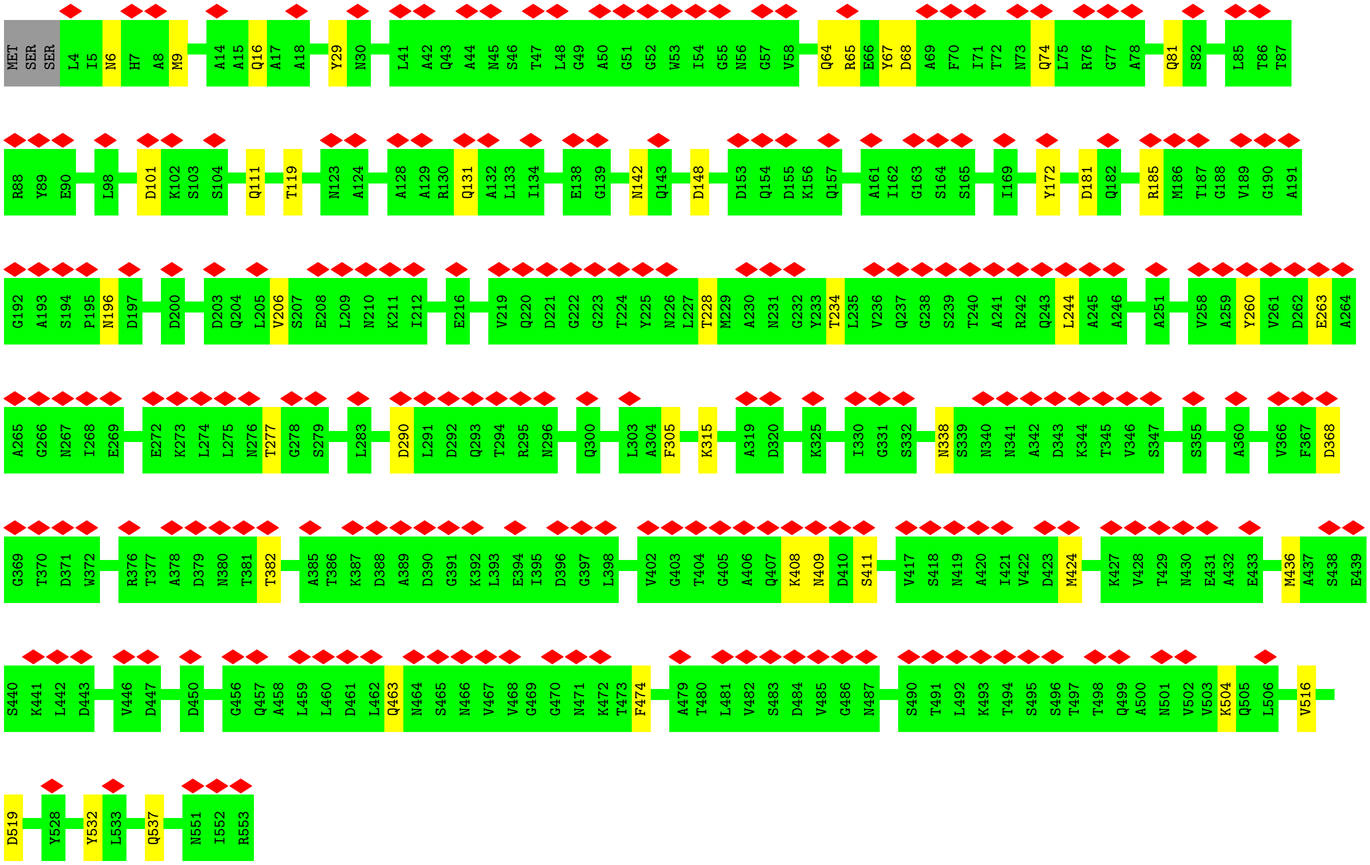




- Molecule 2: Flagellar hook-associated protein 1

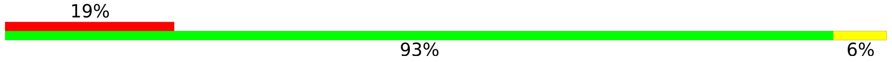
Chain C:

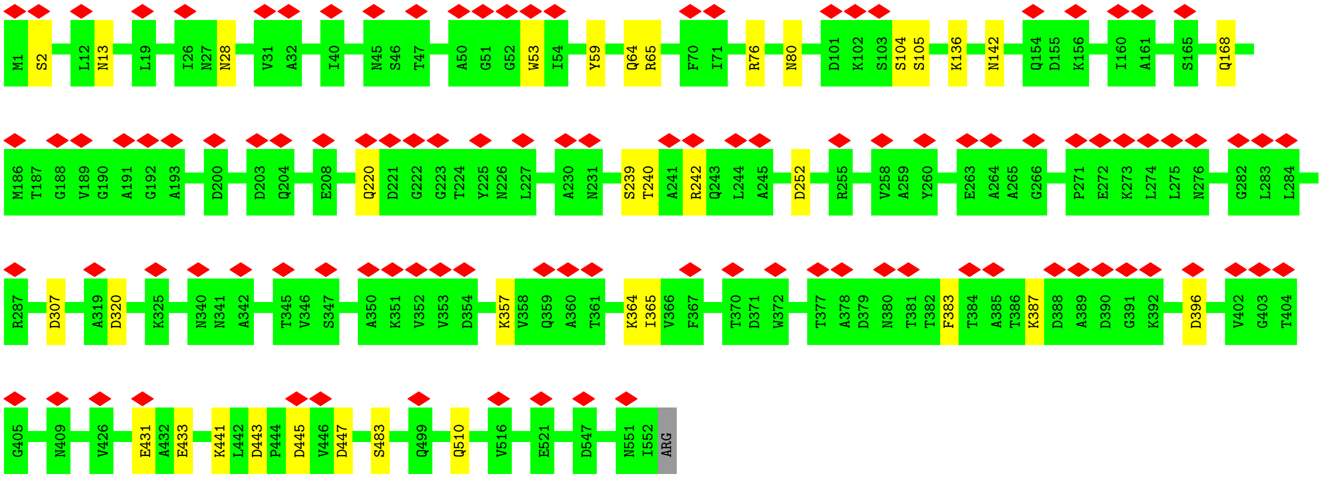




- Molecule 2: Flagellar hook-associated protein 1

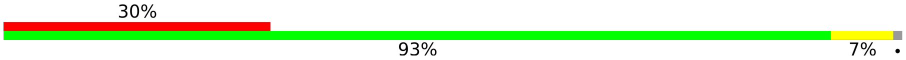
Chain D:

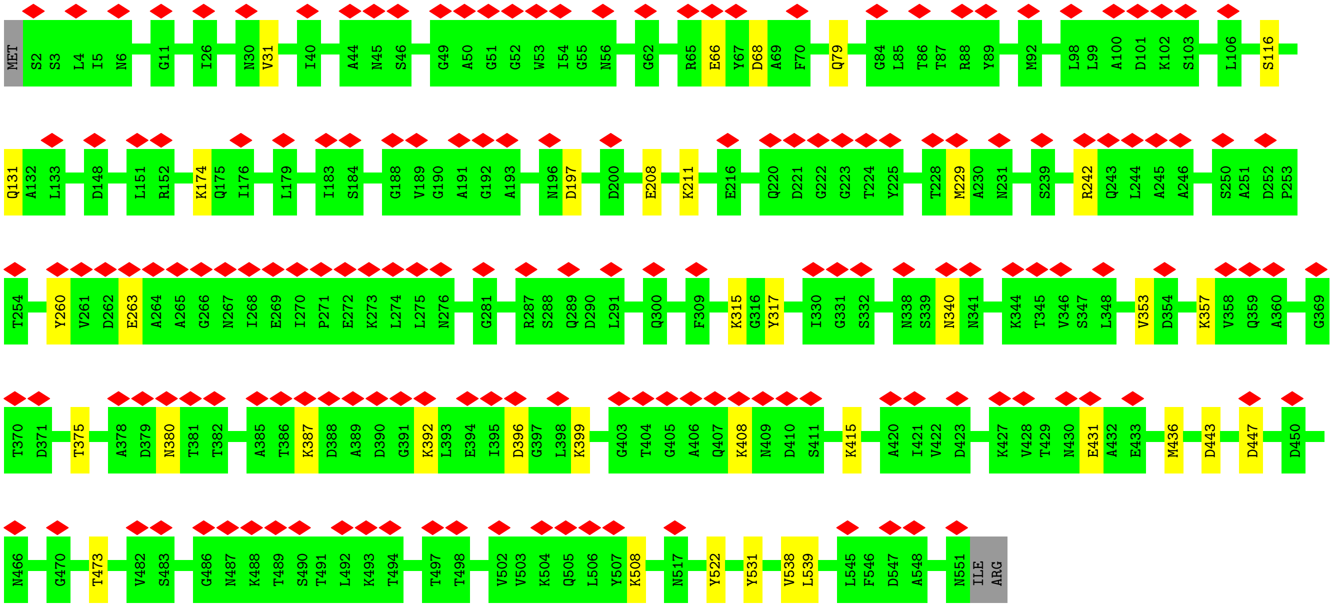




- Molecule 2: Flagellar hook-associated protein 1

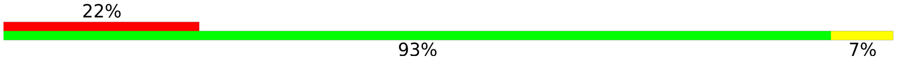
Chain E:

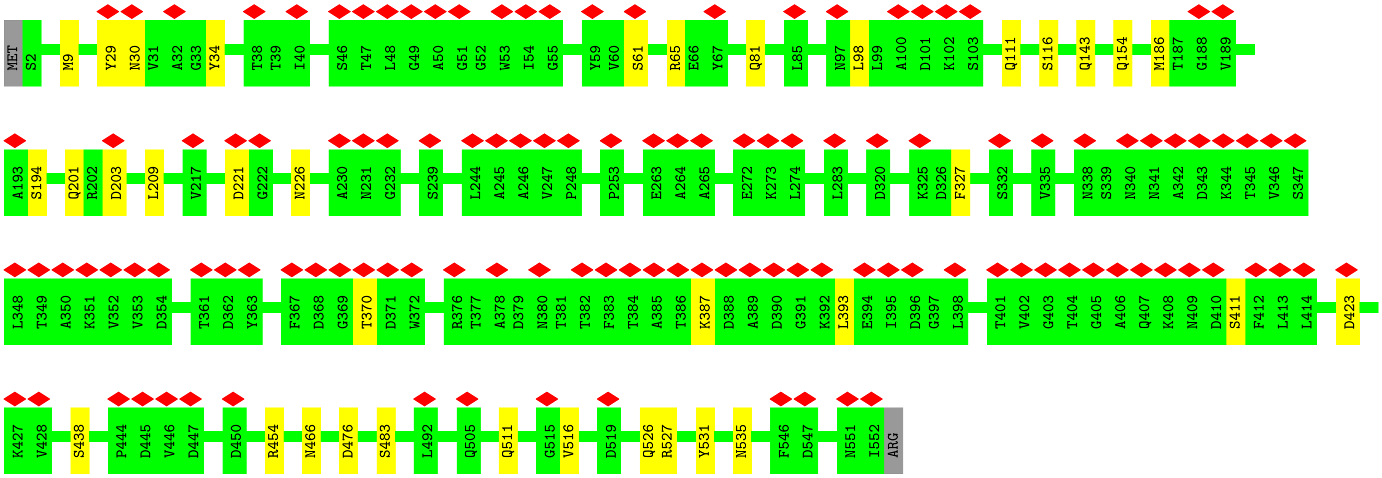




- Molecule 2: Flagellar hook-associated protein 1

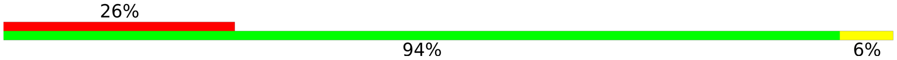
Chain F:

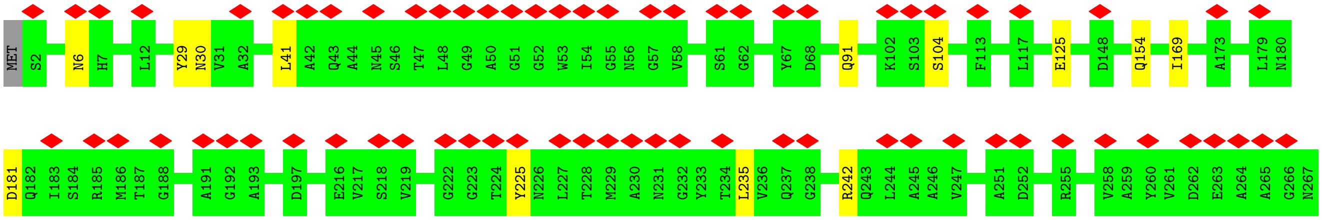


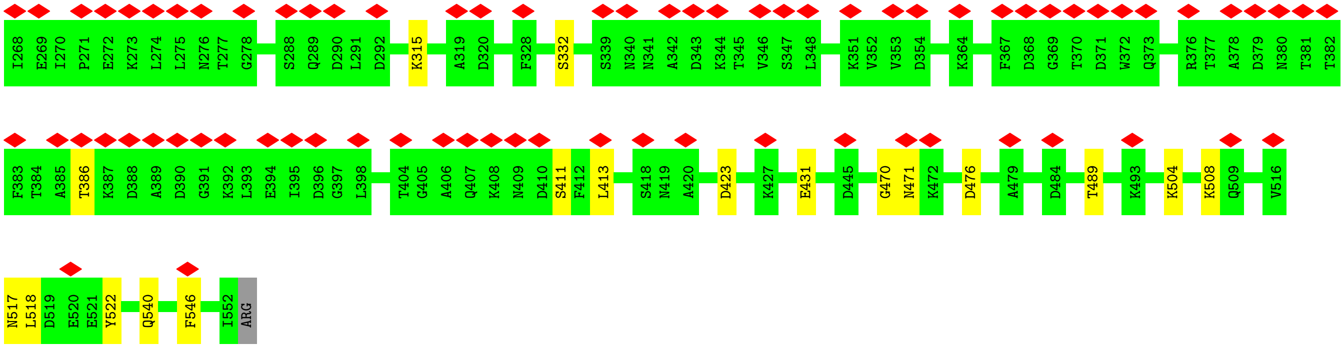


- Molecule 2: Flagellar hook-associated protein 1

Chain G:

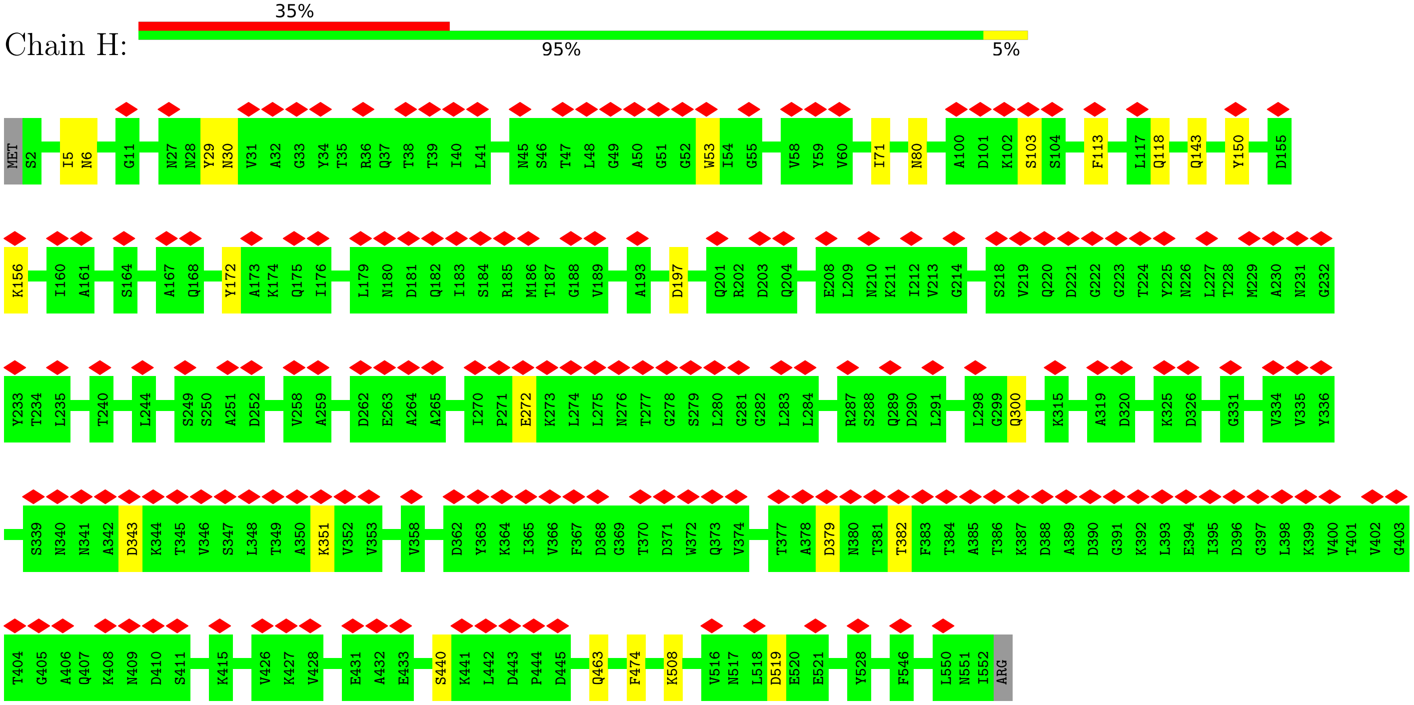






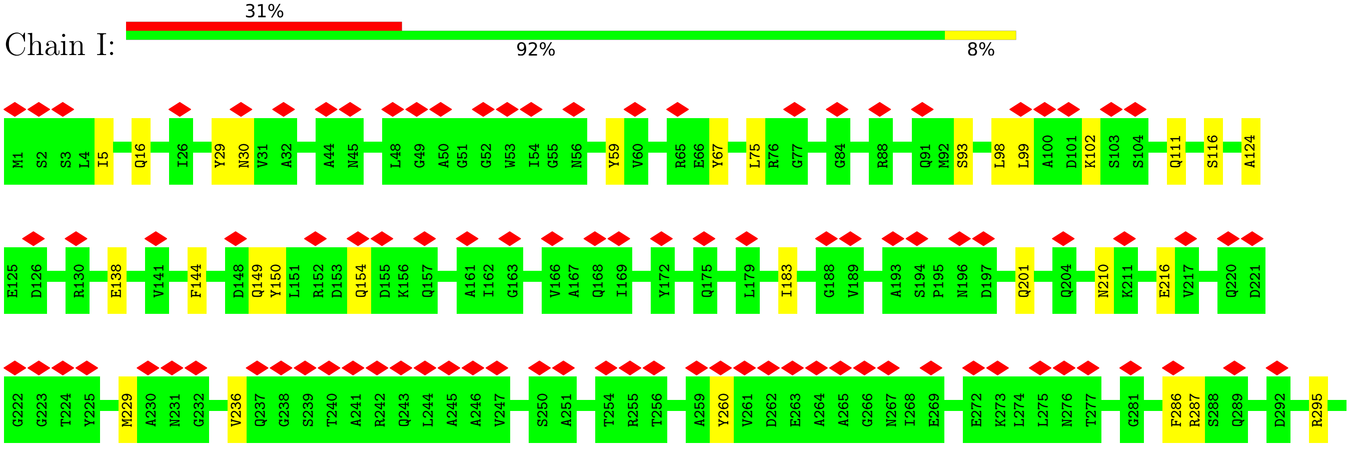
- Molecule 2: Flagellar hook-associated protein 1

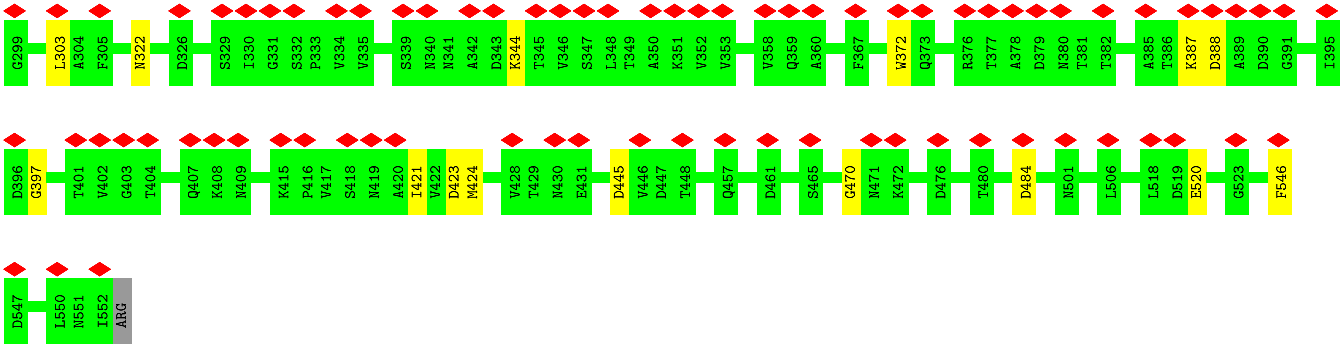
Chain H:



- Molecule 2: Flagellar hook-associated protein 1

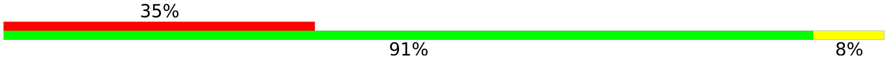
Chain I:

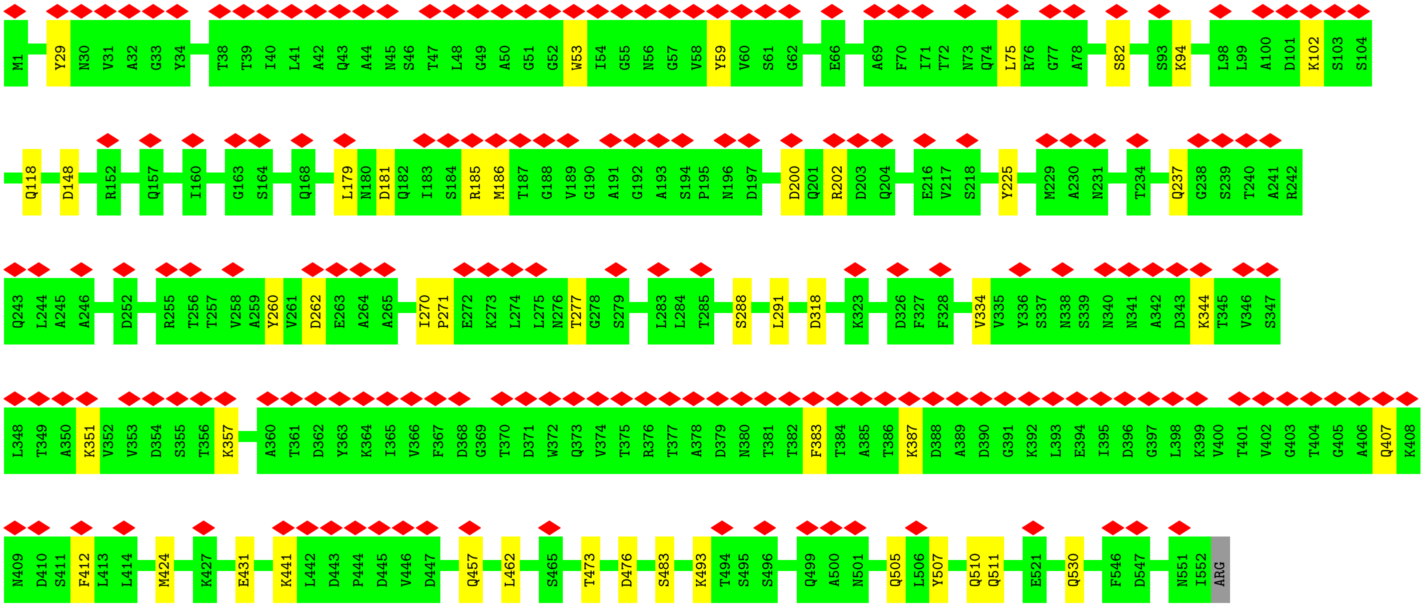




- Molecule 2: Flagellar hook-associated protein 1

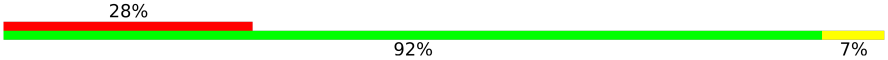
Chain J:

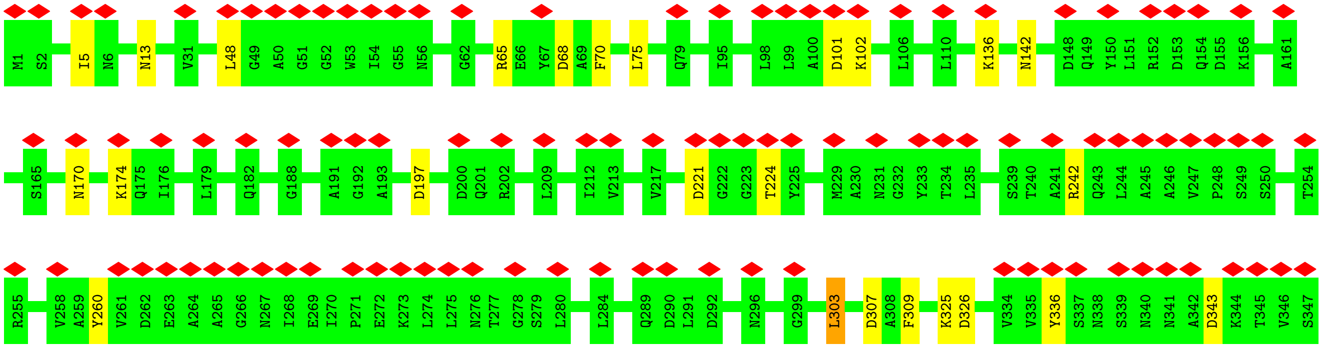


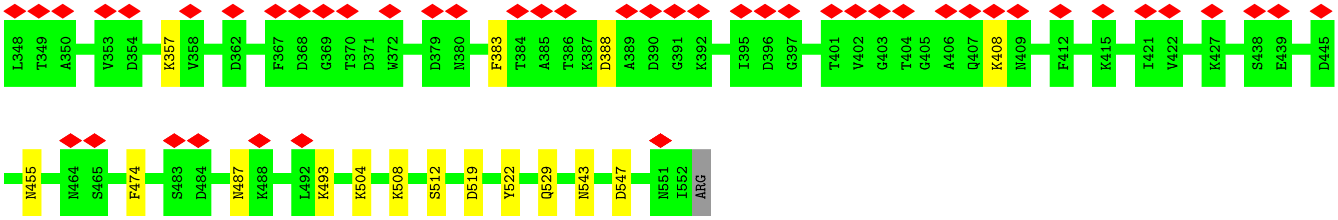


- Molecule 2: Flagellar hook-associated protein 1

Chain K:

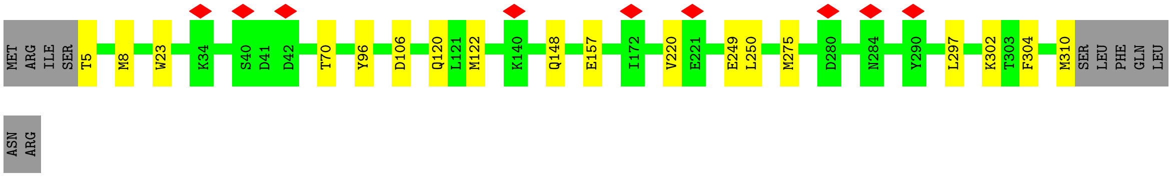






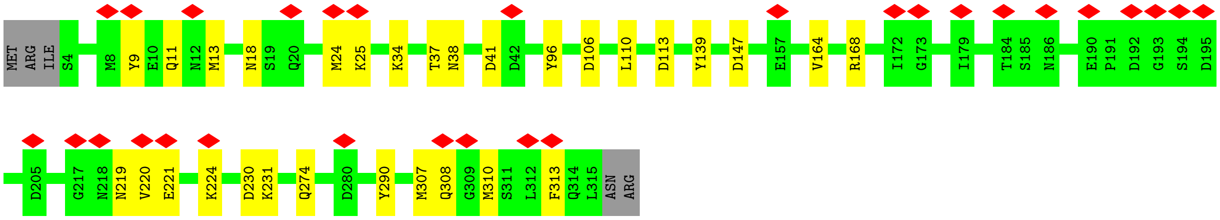
- Molecule 3: Flagellar hook-associated protein

Chain L:



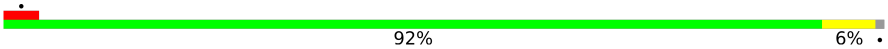
- Molecule 3: Flagellar hook-associated protein

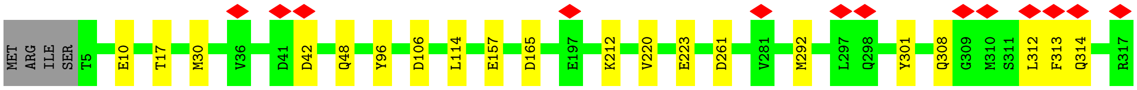
Chain M:



- Molecule 3: Flagellar hook-associated protein

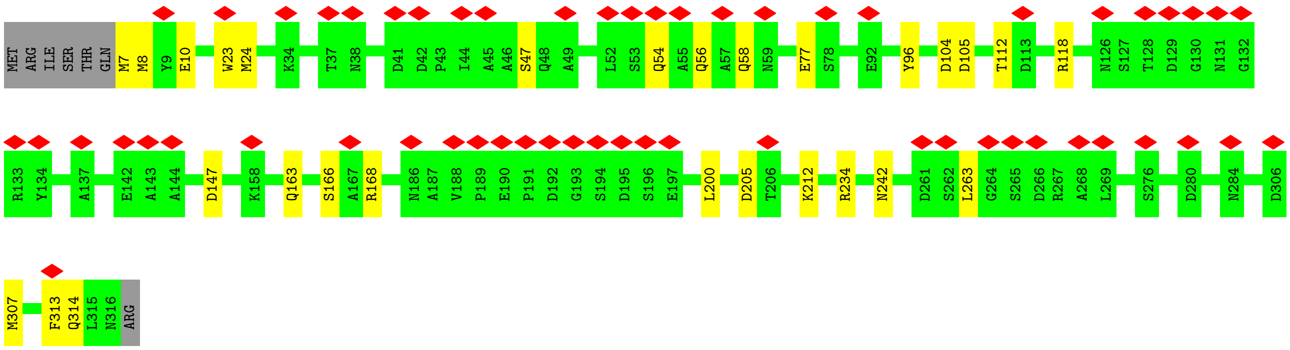
Chain N:



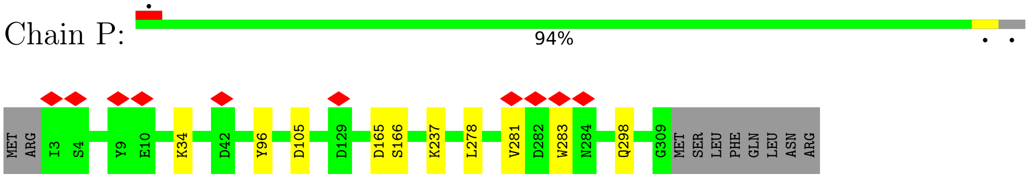


- Molecule 3: Flagellar hook-associated protein

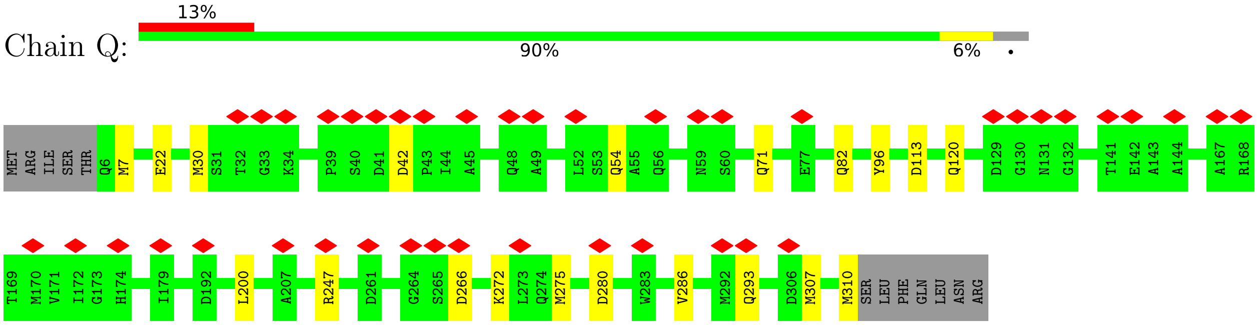
Chain O:



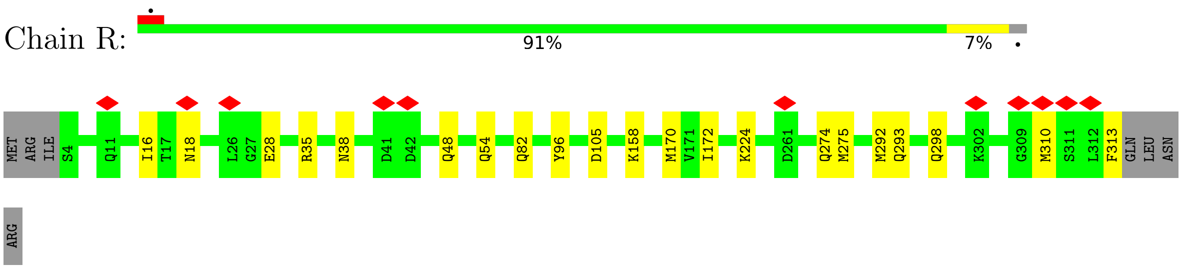
- Molecule 3: Flagellar hook-associated protein



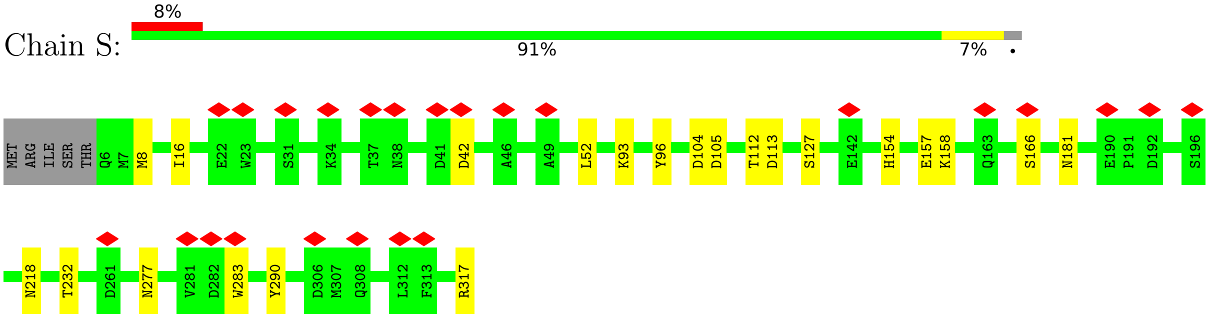
- Molecule 3: Flagellar hook-associated protein



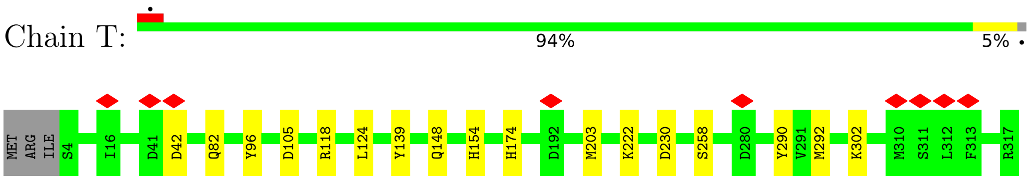
- Molecule 3: Flagellar hook-associated protein



- Molecule 3: Flagellar hook-associated protein

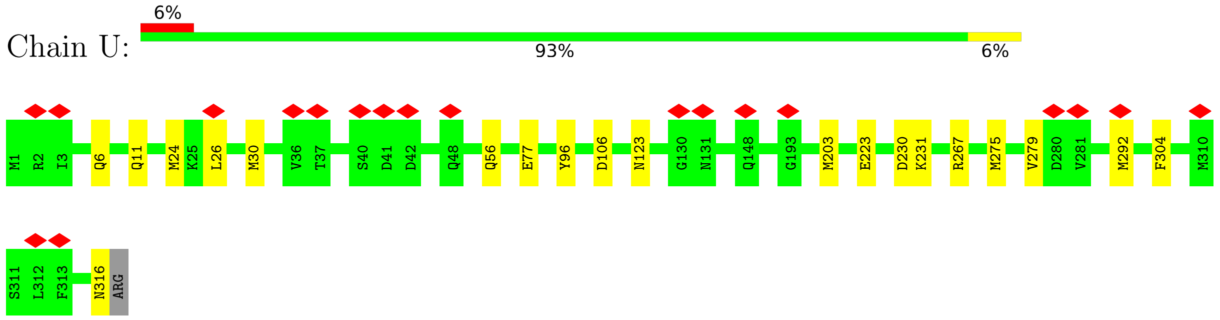


- Molecule 3: Flagellar hook-associated protein



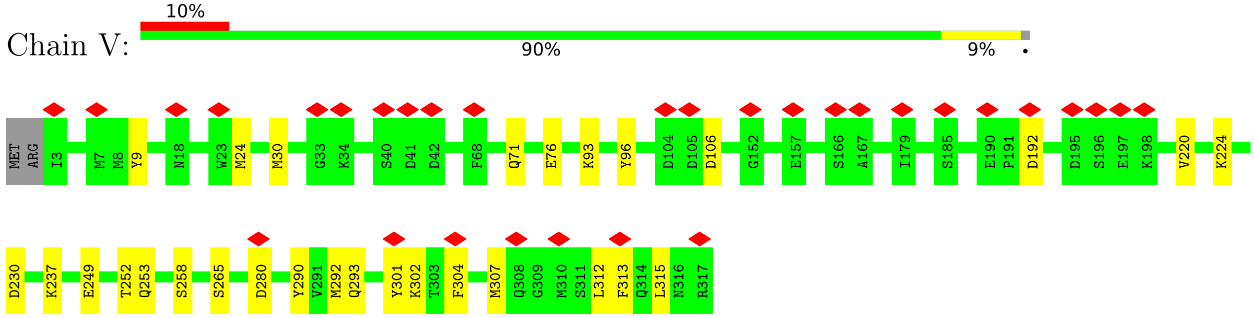
- Molecule 3: Flagellar hook-associated protein

Chain U:



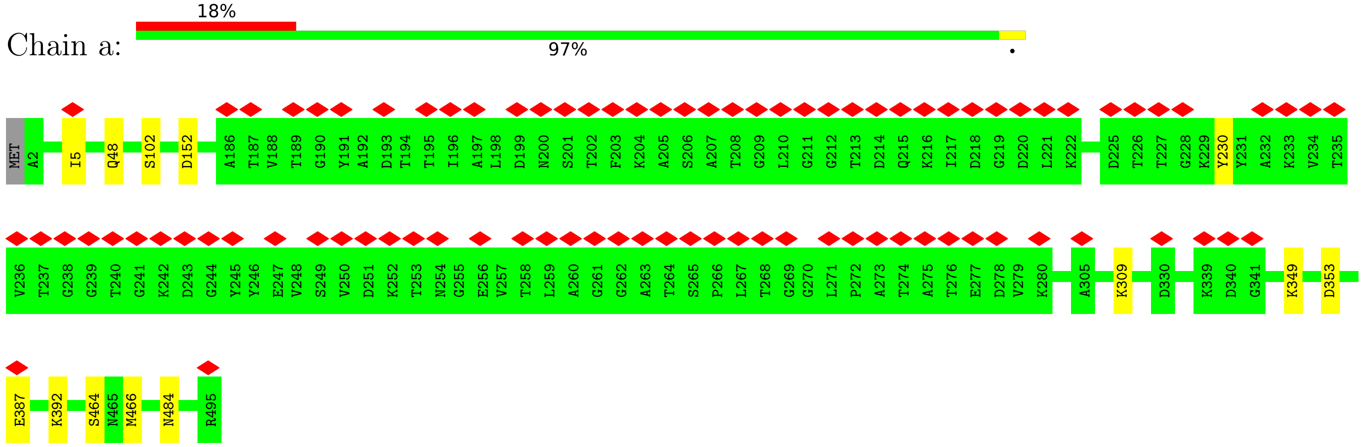
- Molecule 3: Flagellar hook-associated protein

Chain V:



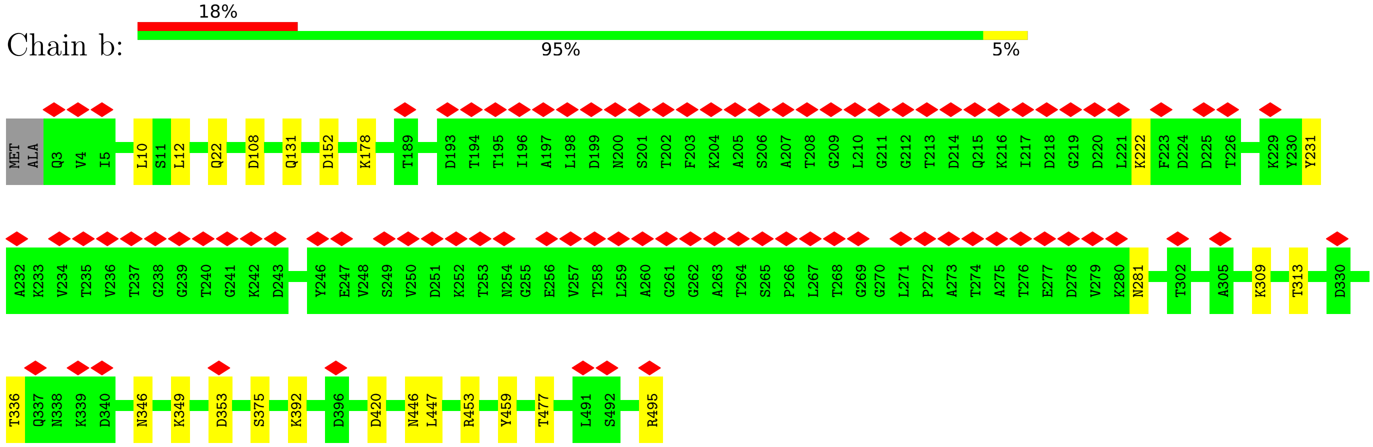
- Molecule 4: Flagellin

Chain a:



- Molecule 4: Flagellin

Chain b:

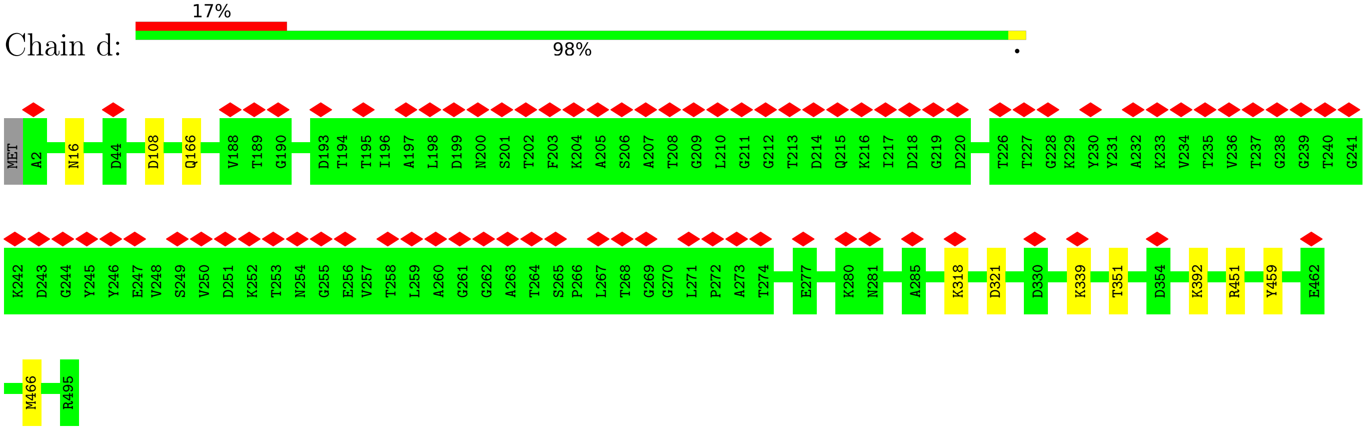


- Molecule 4: Flagellin

Chain c:

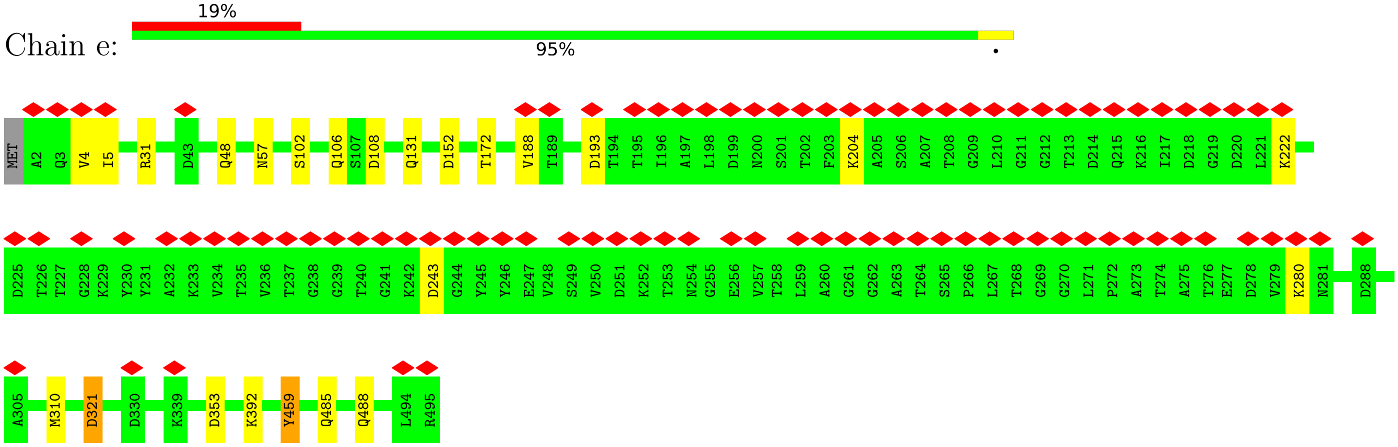
- Molecule 4: Flagellin

Chain d:



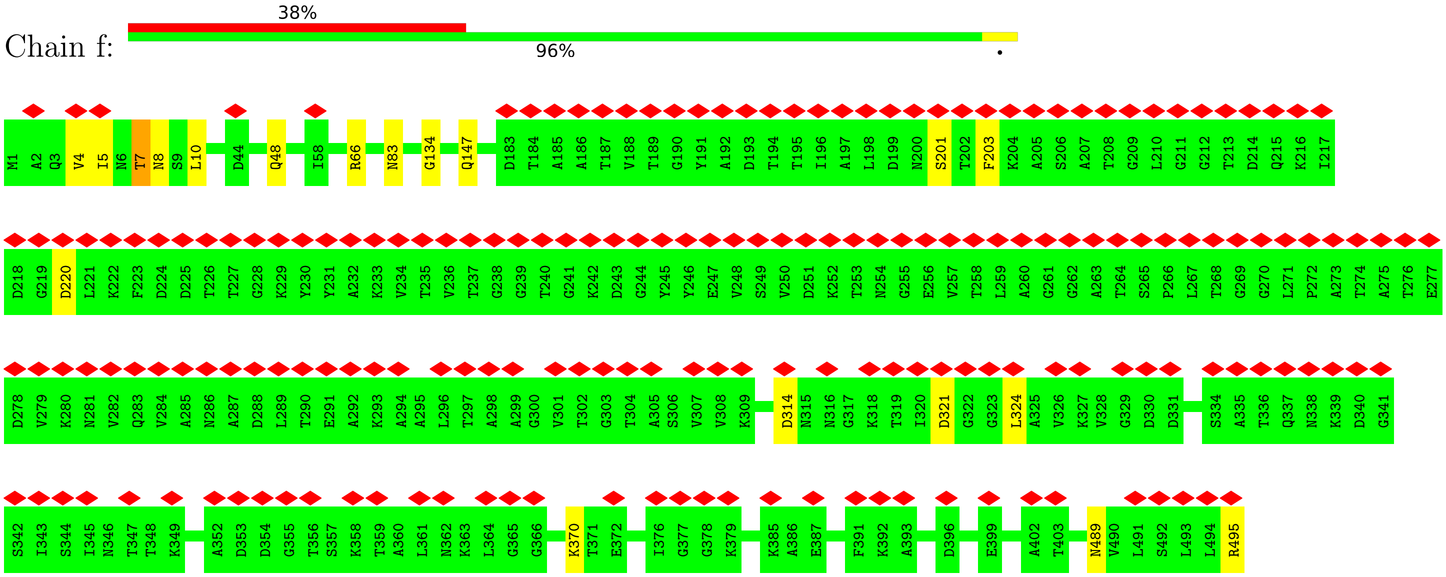
- Molecule 4: Flagellin

Chain e:



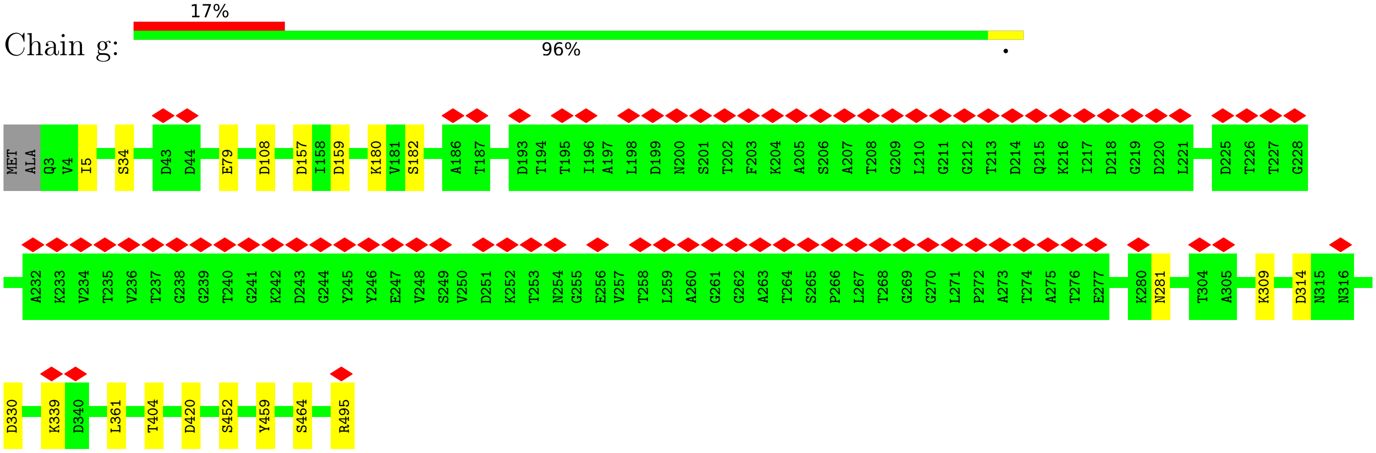
- Molecule 4: Flagellin

Chain f:



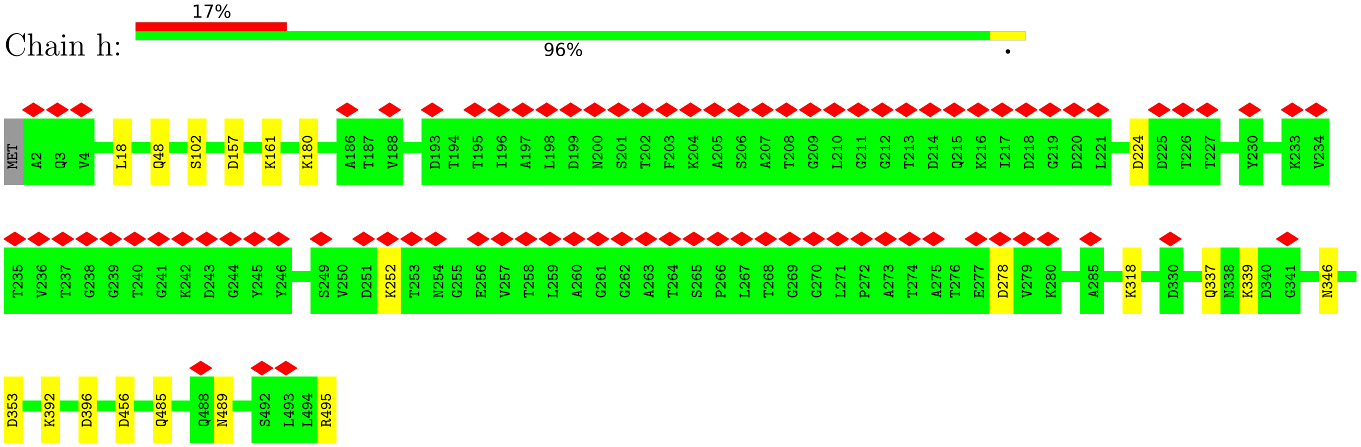
- Molecule 4: Flagellin

Chain g:

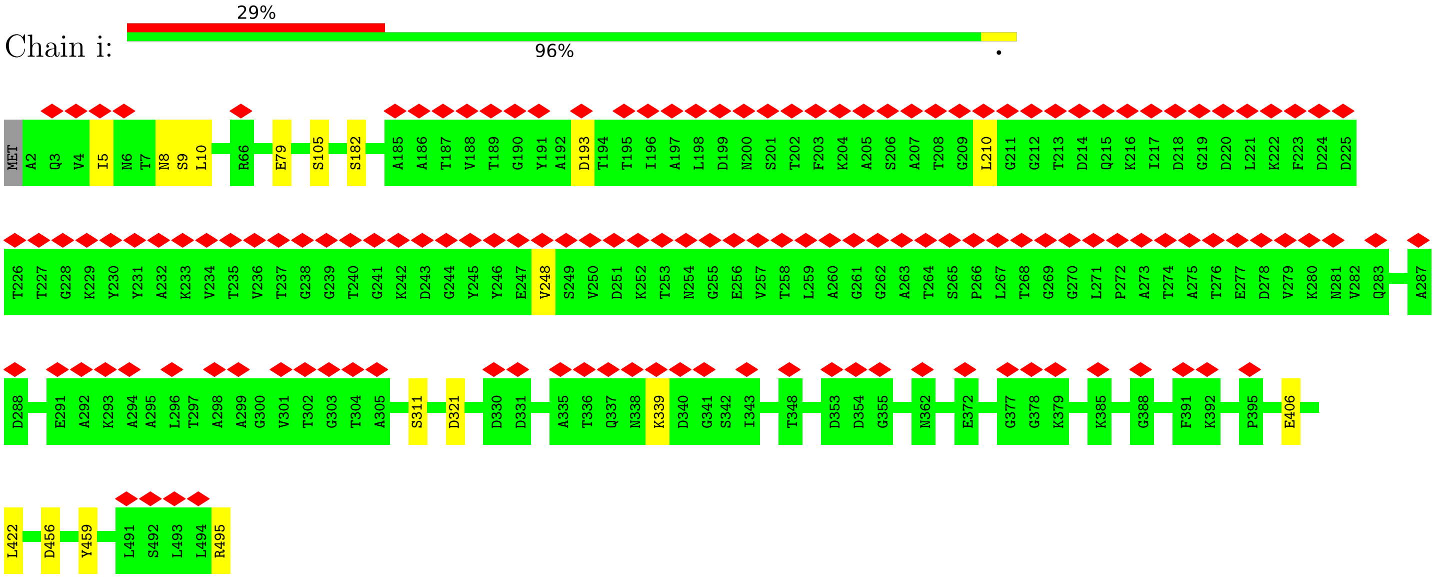


- Molecule 4: Flagellin

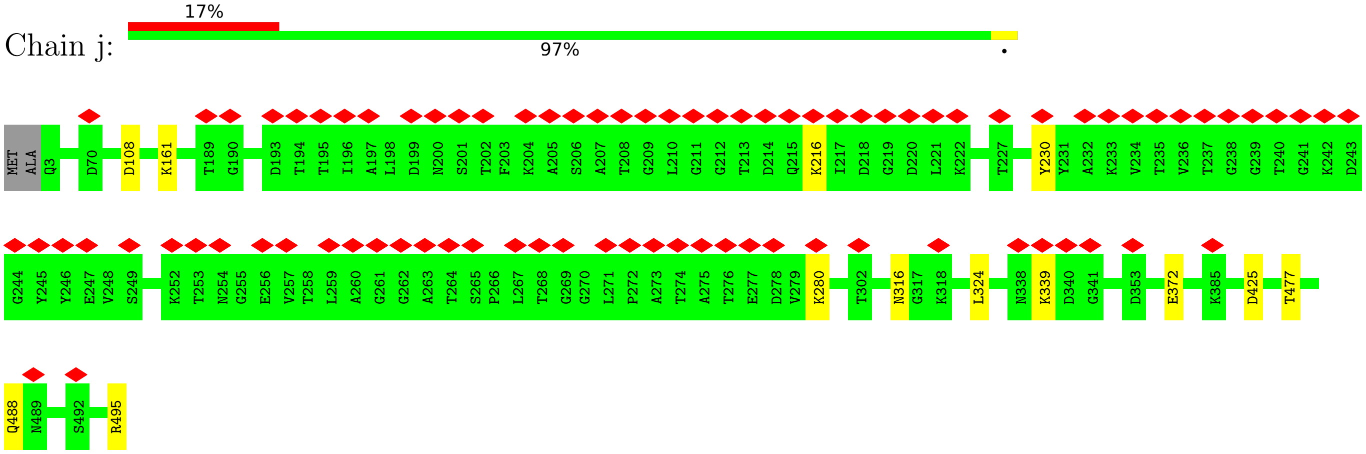
Chain h:



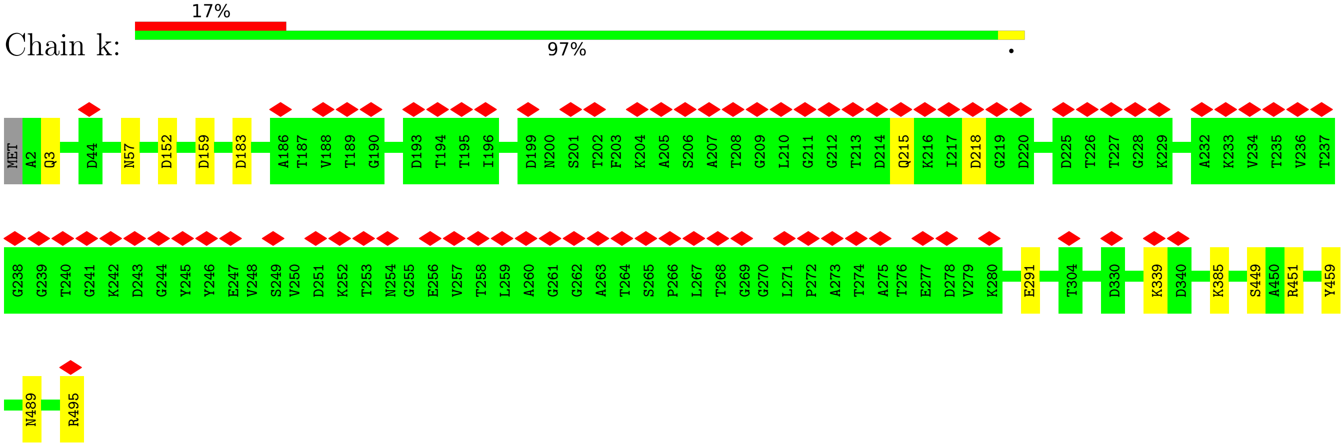
- Molecule 4: Flagellin



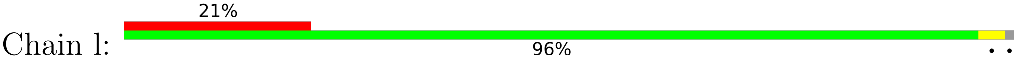
- Molecule 4: Flagellin

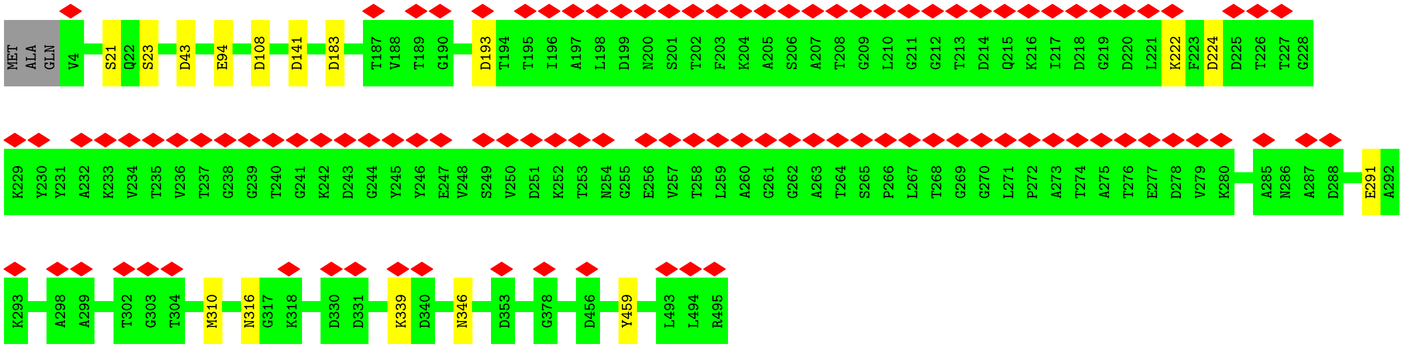


- Molecule 4: Flagellin



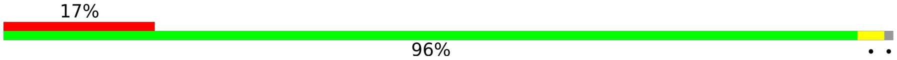
- Molecule 4: Flagellin

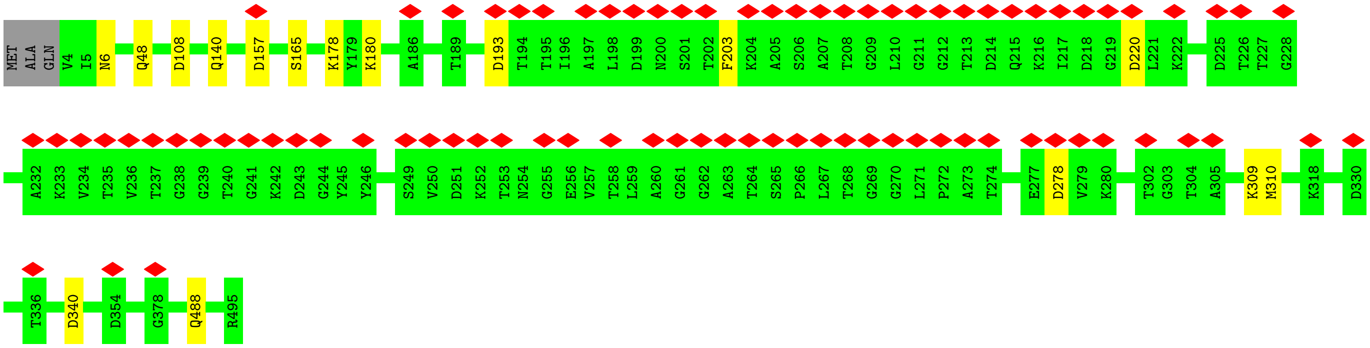




- Molecule 4: Flagellin

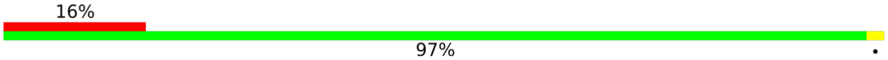
Chain m:

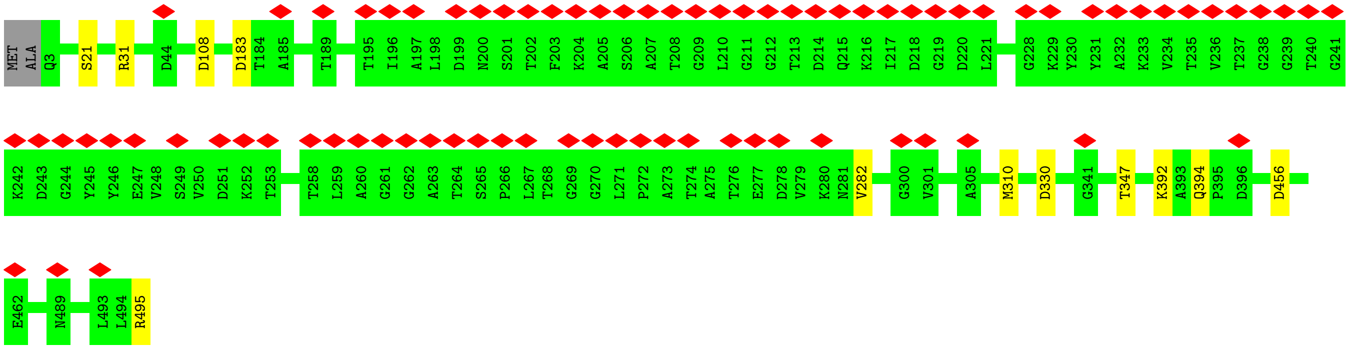




- Molecule 4: Flagellin

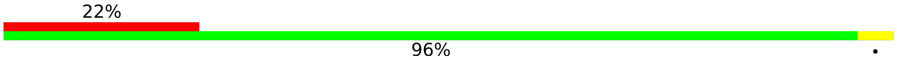
Chain n:

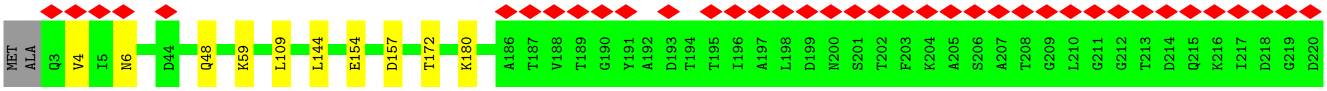


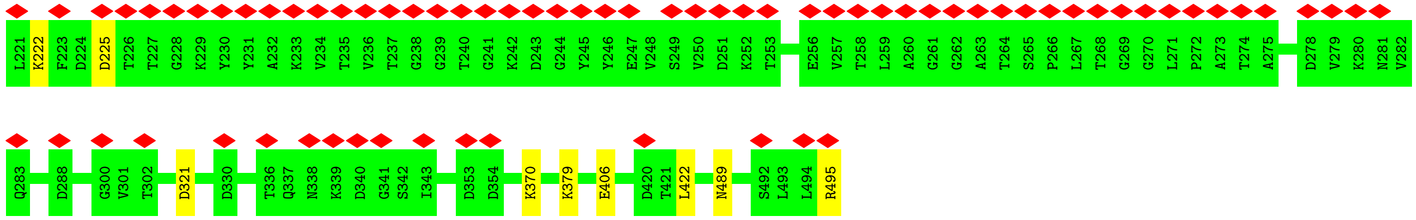


- Molecule 4: Flagellin

Chain o:






L221
K222
F223
D224
D225
T226
T227
G228
K229
Y230
Y231
A232
K233
V234
T235
V236
T237
G238
G239
T240
G241
K242
D243
G244
Y245
Y246
E247
V248
S249
V250
D251
K252
T253
E256
V257
T258
L259
A260
G261
G262
A263
T264
S265
P266
L267
T268
G269
G270
L271
P272
A273
T274
A275
D278
V279
K280
N281
V282
Q283
D288
G300
V301
T302
D321
D330
T336
Q337
N338
K339
D340
G341
S342
I343
D353
D354
K370
K379
E406
D420
T421
L422
N489
S492
L493
L494
R495

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65561	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	43	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.721	Depositor
Minimum map value	-0.376	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	539.0, 539.0, 539.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.078, 1.078, 1.078	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	1	0.30	0/3011	0.53	0/4100
1	2	0.29	0/3011	0.53	0/4100
1	3	0.29	0/3011	0.53	0/4100
1	4	0.31	0/3011	0.56	1/4100 (0.0%)
1	5	0.31	0/3011	0.56	2/4100 (0.0%)
1	6	0.30	0/3011	0.54	0/4100
1	7	0.31	0/3011	0.60	1/4100 (0.0%)
1	8	0.29	0/3011	0.55	0/4100
1	9	0.27	0/3011	0.53	0/4100
1	w	0.34	0/3011	0.60	1/4100 (0.0%)
1	x	0.30	0/3011	0.54	0/4100
1	y	0.31	0/3011	0.53	0/4100
1	z	0.33	0/3011	0.57	1/4100 (0.0%)
2	A	0.32	0/4191	0.54	0/5692
2	B	0.32	0/4191	0.54	0/5692
2	C	0.32	1/4182 (0.0%)	0.57	0/5680
2	D	0.31	0/4191	0.53	1/5692 (0.0%)
2	E	0.33	0/4175	0.54	0/5671
2	F	0.29	0/4183	0.54	0/5682
2	G	0.31	0/4183	0.55	0/5682
2	H	0.33	0/4183	0.53	0/5682
2	I	0.32	0/4191	0.56	0/5692
2	J	0.32	1/4191 (0.0%)	0.57	2/5692 (0.0%)
2	K	0.32	0/4191	0.56	0/5692
3	L	0.31	0/2321	0.53	0/3142
3	M	0.33	0/2370	0.55	1/3208 (0.0%)
3	N	0.33	0/2383	0.53	0/3225
3	O	0.33	0/2356	0.54	0/3189
3	P	0.34	0/2327	0.53	0/3151
3	Q	0.33	0/2314	0.55	0/3132
3	R	0.32	0/2353	0.51	0/3185
3	S	0.33	0/2376	0.56	0/3215
3	T	0.33	0/2389	0.53	0/3233
3	U	0.33	0/2405	0.53	0/3254

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	V	0.37	0/2397	0.58	0/3244
4	a	0.30	0/3638	0.51	0/4938
4	b	0.32	0/3633	0.53	0/4931
4	c	0.33	1/3638 (0.0%)	0.55	0/4938
4	d	0.30	0/3638	0.54	0/4938
4	e	0.30	0/3638	0.54	2/4938 (0.0%)
4	f	0.31	0/3646	0.55	2/4948 (0.0%)
4	g	0.29	0/3633	0.51	0/4931
4	h	0.30	0/3638	0.52	0/4938
4	i	0.32	0/3638	0.54	0/4938
4	j	0.29	0/3633	0.52	0/4931
4	k	0.29	0/3638	0.51	0/4938
4	l	0.30	0/3624	0.52	0/4919
4	m	0.31	0/3624	0.52	0/4919
4	n	0.31	0/3633	0.52	0/4931
4	o	0.29	0/3633	0.52	0/4931
All	All	0.31	3/165711 (0.0%)	0.54	14/225034 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	6	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	516	VAL	CB-CG2	-5.82	1.40	1.52
4	c	6	ASN	C-N	-5.48	1.21	1.34
2	J	237	GLN	CD-NE2	-5.04	1.20	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	f	4	VAL	N-CA-C	-6.20	94.27	111.00
1	5	45	GLY	N-CA-C	-6.17	97.69	113.10
2	J	271	PRO	N-CA-C	6.06	127.86	112.10
1	4	159	ASN	N-CA-C	-5.95	94.93	111.00
1	w	144	MET	CG-SD-CE	5.67	109.28	100.20
4	e	321	ASP	CB-CG-OD1	5.42	123.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	320	ASP	CB-CG-OD2	-5.32	113.51	118.30
2	J	270	ILE	N-CA-C	-5.29	96.73	111.00
4	f	7	THR	N-CA-C	-5.28	96.74	111.00
4	e	459	TYR	CA-CB-CG	5.18	123.23	113.40
1	7	296	ASN	N-CA-C	5.17	124.95	111.00
1	5	52	VAL	N-CA-C	-5.10	97.23	111.00
1	z	312	LEU	CA-CB-CG	5.07	126.96	115.30
3	M	164	VAL	CA-CB-CG2	5.05	118.48	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	6	168	THR	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1	401/403 (100%)	377 (94%)	24 (6%)	0	100	100
1	2	401/403 (100%)	360 (90%)	41 (10%)	0	100	100
1	3	401/403 (100%)	365 (91%)	35 (9%)	1 (0%)	44	73
1	4	401/403 (100%)	356 (89%)	42 (10%)	3 (1%)	19	49
1	5	401/403 (100%)	354 (88%)	45 (11%)	2 (0%)	25	56
1	6	401/403 (100%)	364 (91%)	35 (9%)	2 (0%)	25	56
1	7	401/403 (100%)	355 (88%)	44 (11%)	2 (0%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8	401/403 (100%)	372 (93%)	28 (7%)	1 (0%)	44	73
1	9	401/403 (100%)	371 (92%)	30 (8%)	0	100	100
1	w	401/403 (100%)	355 (88%)	45 (11%)	1 (0%)	44	73
1	x	401/403 (100%)	365 (91%)	32 (8%)	4 (1%)	13	40
1	y	401/403 (100%)	374 (93%)	27 (7%)	0	100	100
1	z	401/403 (100%)	361 (90%)	40 (10%)	0	100	100
2	A	550/553 (100%)	520 (94%)	30 (6%)	0	100	100
2	B	550/553 (100%)	514 (94%)	34 (6%)	2 (0%)	30	60
2	C	548/553 (99%)	512 (93%)	34 (6%)	2 (0%)	30	60
2	D	550/553 (100%)	502 (91%)	47 (8%)	1 (0%)	44	73
2	E	548/553 (99%)	500 (91%)	46 (8%)	2 (0%)	30	60
2	F	549/553 (99%)	524 (95%)	25 (5%)	0	100	100
2	G	549/553 (99%)	502 (91%)	45 (8%)	2 (0%)	30	60
2	H	549/553 (99%)	509 (93%)	40 (7%)	0	100	100
2	I	550/553 (100%)	494 (90%)	52 (10%)	4 (1%)	19	49
2	J	550/553 (100%)	506 (92%)	43 (8%)	1 (0%)	44	73
2	K	550/553 (100%)	514 (94%)	34 (6%)	2 (0%)	30	60
3	L	304/317 (96%)	286 (94%)	17 (6%)	1 (0%)	37	66
3	M	310/317 (98%)	296 (96%)	14 (4%)	0	100	100
3	N	311/317 (98%)	291 (94%)	19 (6%)	1 (0%)	37	66
3	O	308/317 (97%)	295 (96%)	13 (4%)	0	100	100
3	P	305/317 (96%)	294 (96%)	10 (3%)	1 (0%)	37	66
3	Q	303/317 (96%)	286 (94%)	17 (6%)	0	100	100
3	R	308/317 (97%)	291 (94%)	17 (6%)	0	100	100
3	S	310/317 (98%)	298 (96%)	11 (4%)	1 (0%)	37	66
3	T	312/317 (98%)	304 (97%)	8 (3%)	0	100	100
3	U	314/317 (99%)	298 (95%)	16 (5%)	0	100	100
3	V	313/317 (99%)	295 (94%)	17 (5%)	1 (0%)	37	66
4	a	492/495 (99%)	475 (96%)	17 (4%)	0	100	100
4	b	491/495 (99%)	480 (98%)	11 (2%)	0	100	100
4	c	492/495 (99%)	475 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	492/495 (99%)	473 (96%)	19 (4%)	0	100	100
4	e	492/495 (99%)	480 (98%)	10 (2%)	2 (0%)	30	60
4	f	493/495 (100%)	478 (97%)	13 (3%)	2 (0%)	30	60
4	g	491/495 (99%)	475 (97%)	16 (3%)	0	100	100
4	h	492/495 (99%)	480 (98%)	12 (2%)	0	100	100
4	i	492/495 (99%)	478 (97%)	13 (3%)	1 (0%)	44	73
4	j	491/495 (99%)	472 (96%)	19 (4%)	0	100	100
4	k	492/495 (99%)	476 (97%)	16 (3%)	0	100	100
4	l	490/495 (99%)	469 (96%)	20 (4%)	1 (0%)	44	73
4	m	490/495 (99%)	480 (98%)	10 (2%)	0	100	100
4	n	491/495 (99%)	472 (96%)	19 (4%)	0	100	100
4	o	491/495 (99%)	472 (96%)	18 (4%)	1 (0%)	44	73
All	All	22026/22234 (99%)	20695 (94%)	1287 (6%)	44 (0%)	45	73

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	7	44	ALA
2	J	29	TYR
3	N	220	VAL
3	S	127	SER
4	e	5	ILE
1	w	171	SER
1	6	48	VAL
2	G	470	GLY
2	I	344	LYS
4	f	8	ASN
1	x	330	GLY
1	4	167	LYS
1	5	42	MET
1	8	47	LYS
2	D	396	ASP
2	E	396	ASP
2	I	124	ALA
2	K	325	LYS
1	x	79	GLN
1	3	349	GLY
2	B	306	ALA

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Mol	Chain	Res	Type
4	l	43	ASP
4	o	4	VAL
1	x	2	SER
1	x	82	PHE
2	B	49	GLY
2	C	305	PHE
2	E	263	GLU
2	G	518	LEU
2	K	303	LEU
3	L	220	VAL
4	i	8	ASN
1	7	296	ASN
2	C	338	ASN
1	4	164	VAL
3	P	281	VAL
4	f	134	GLY
1	4	163	PRO
1	6	165	PRO
2	I	470	GLY
2	I	397	GLY
4	e	4	VAL
1	5	290	VAL
3	V	220	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	323/323 (100%)	302 (94%)	21 (6%)	14	40
1	2	323/323 (100%)	302 (94%)	21 (6%)	14	40
1	3	323/323 (100%)	298 (92%)	25 (8%)	10	31
1	4	323/323 (100%)	293 (91%)	30 (9%)	7	23
1	5	323/323 (100%)	299 (93%)	24 (7%)	11	34
1	6	323/323 (100%)	304 (94%)	19 (6%)	16	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7	323/323 (100%)	293 (91%)	30 (9%)	7	23
1	8	323/323 (100%)	298 (92%)	25 (8%)	10	31
1	9	323/323 (100%)	306 (95%)	17 (5%)	19	49
1	w	323/323 (100%)	297 (92%)	26 (8%)	10	30
1	x	323/323 (100%)	300 (93%)	23 (7%)	12	36
1	y	323/323 (100%)	305 (94%)	18 (6%)	17	47
1	z	323/323 (100%)	297 (92%)	26 (8%)	10	30
2	A	452/453 (100%)	416 (92%)	36 (8%)	10	30
2	B	452/453 (100%)	410 (91%)	42 (9%)	7	23
2	C	450/453 (99%)	408 (91%)	42 (9%)	7	23
2	D	452/453 (100%)	419 (93%)	33 (7%)	11	34
2	E	450/453 (99%)	415 (92%)	35 (8%)	10	31
2	F	451/453 (100%)	415 (92%)	36 (8%)	10	30
2	G	451/453 (100%)	422 (94%)	29 (6%)	14	41
2	H	451/453 (100%)	425 (94%)	26 (6%)	17	46
2	I	452/453 (100%)	412 (91%)	40 (9%)	8	26
2	J	452/453 (100%)	409 (90%)	43 (10%)	7	22
2	K	452/453 (100%)	412 (91%)	40 (9%)	8	26
3	L	250/261 (96%)	233 (93%)	17 (7%)	13	38
3	M	256/261 (98%)	227 (89%)	29 (11%)	4	15
3	N	257/261 (98%)	238 (93%)	19 (7%)	11	34
3	O	254/261 (97%)	226 (89%)	28 (11%)	5	16
3	P	251/261 (96%)	242 (96%)	9 (4%)	30	65
3	Q	249/261 (95%)	229 (92%)	20 (8%)	10	30
3	R	254/261 (97%)	233 (92%)	21 (8%)	9	28
3	S	256/261 (98%)	235 (92%)	21 (8%)	9	29
3	T	258/261 (99%)	241 (93%)	17 (7%)	14	39
3	U	260/261 (100%)	240 (92%)	20 (8%)	10	31
3	V	259/261 (99%)	231 (89%)	28 (11%)	5	17
4	a	390/391 (100%)	377 (97%)	13 (3%)	33	68
4	b	390/391 (100%)	365 (94%)	25 (6%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	c	390/391 (100%)	367 (94%)	23 (6%)	16	45
4	d	390/391 (100%)	379 (97%)	11 (3%)	38	73
4	e	390/391 (100%)	368 (94%)	22 (6%)	17	47
4	f	391/391 (100%)	375 (96%)	16 (4%)	26	60
4	g	390/391 (100%)	370 (95%)	20 (5%)	20	51
4	h	390/391 (100%)	370 (95%)	20 (5%)	20	51
4	i	390/391 (100%)	373 (96%)	17 (4%)	24	57
4	j	390/391 (100%)	377 (97%)	13 (3%)	33	68
4	k	390/391 (100%)	375 (96%)	15 (4%)	28	63
4	l	389/391 (100%)	374 (96%)	15 (4%)	27	62
4	m	389/391 (100%)	373 (96%)	16 (4%)	26	60
4	n	390/391 (100%)	378 (97%)	12 (3%)	35	70
4	o	390/391 (100%)	372 (95%)	18 (5%)	23	55
All	All	17817/17918 (99%)	16625 (93%)	1192 (7%)	16	39

All (1192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	30	TYR
1	1	79	GLN
1	1	143	LEU
1	1	174	ASP
1	1	195	ASP
1	1	196	MET
1	1	199	TYR
1	1	204	LYS
1	1	205	ASP
1	1	231	LYS
1	1	267	MET
1	1	268	GLN
1	1	280	ASN
1	1	285	LYS
1	1	292	TYR
1	1	312	LEU
1	1	334	TRP
1	1	362	GLU
1	1	369	SER

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Mol	Chain	Res	Type
1	1	394	GLN
1	1	403	ARG
1	2	1	MET
1	2	47	LYS
1	2	53	LYS
1	2	59	GLN
1	2	61	PHE
1	2	63	ASP
1	2	82	PHE
1	2	91	SER
1	2	96	ARG
1	2	101	LYS
1	2	114	MET
1	2	167	LYS
1	2	170	PHE
1	2	215	SER
1	2	252	ASN
1	2	268	GLN
1	2	293	GLN
1	2	323	ASN
1	2	369	SER
1	2	380	ARG
1	2	382	TYR
1	3	16	ASN
1	3	33	LYS
1	3	38	SER
1	3	53	LYS
1	3	63	ASP
1	3	66	THR
1	3	87	ASP
1	3	99	GLN
1	3	106	ARG
1	3	111	MET
1	3	144	MET
1	3	162	ASP
1	3	178	TYR
1	3	183	THR
1	3	196	MET
1	3	197	ASN
1	3	203	THR
1	3	231	LYS
1	3	263	PHE

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Mol	Chain	Res	Type
1	3	296	ASN
1	3	297	ASP
1	3	312	LEU
1	3	324	GLU
1	3	367	ASP
1	3	399	LEU
1	4	16	ASN
1	4	39	PHE
1	4	42	MET
1	4	53	LYS
1	4	61	PHE
1	4	83	PHE
1	4	85	LEU
1	4	88	SER
1	4	99	GLN
1	4	130	GLN
1	4	133	ASN
1	4	159	ASN
1	4	161	THR
1	4	167	LYS
1	4	168	THR
1	4	170	PHE
1	4	174	ASP
1	4	188	ASP
1	4	202	LYS
1	4	204	LYS
1	4	231	LYS
1	4	233	ASN
1	4	234	GLU
1	4	255	THR
1	4	267	MET
1	4	285	LYS
1	4	309	GLU
1	4	355	LYS
1	4	390	LYS
1	4	401	ASN
1	5	1	MET
1	5	4	SER
1	5	38	SER
1	5	39	PHE
1	5	42	MET
1	5	46	SER

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Mol	Chain	Res	Type
1	5	47	LYS
1	5	53	LYS
1	5	63	ASP
1	5	111	MET
1	5	114	MET
1	5	115	GLN
1	5	143	LEU
1	5	167	LYS
1	5	252	ASN
1	5	261	LEU
1	5	285	LYS
1	5	289	LEU
1	5	290	VAL
1	5	292	TYR
1	5	310	GLN
1	5	324	GLU
1	5	381	ASN
1	5	382	TYR
1	6	38	SER
1	6	60	ASP
1	6	83	PHE
1	6	85	LEU
1	6	94	TYR
1	6	96	ARG
1	6	114	MET
1	6	141	ASN
1	6	187	TYR
1	6	196	MET
1	6	197	ASN
1	6	199	TYR
1	6	204	LYS
1	6	252	ASN
1	6	368	LEU
1	6	370	LYS
1	6	382	TYR
1	6	392	GLN
1	6	401	ASN
1	7	3	PHE
1	7	26	ASN
1	7	52	VAL
1	7	53	LYS
1	7	65	THR

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Mol	Chain	Res	Type
1	7	71	ARG
1	7	74	ASP
1	7	103	ASP
1	7	112	GLN
1	7	127	THR
1	7	147	LYS
1	7	162	ASP
1	7	170	PHE
1	7	187	TYR
1	7	194	HIS
1	7	196	MET
1	7	197	ASN
1	7	201	VAL
1	7	217	ASP
1	7	235	ASN
1	7	288	ASP
1	7	289	LEU
1	7	312	LEU
1	7	329	GLN
1	7	332	ASN
1	7	338	GLN
1	7	382	TYR
1	7	392	GLN
1	7	399	LEU
1	7	403	ARG
1	8	5	GLN
1	8	30	TYR
1	8	36	THR
1	8	47	LYS
1	8	53	LYS
1	8	71	ARG
1	8	87	ASP
1	8	110	ASN
1	8	111	MET
1	8	144	MET
1	8	147	LYS
1	8	172	VAL
1	8	173	SER
1	8	179	ASN
1	8	204	LYS
1	8	206	ASN
1	8	234	GLU

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Mol	Chain	Res	Type
1	8	284	TYR
1	8	288	ASP
1	8	292	TYR
1	8	357	THR
1	8	372	LEU
1	8	379	GLN
1	8	394	GLN
1	8	403	ARG
1	9	3	PHE
1	9	30	TYR
1	9	48	VAL
1	9	84	ARG
1	9	94	TYR
1	9	111	MET
1	9	119	TYR
1	9	130	GLN
1	9	162	ASP
1	9	168	THR
1	9	174	ASP
1	9	195	ASP
1	9	292	TYR
1	9	357	THR
1	9	358	ASN
1	9	370	LYS
1	9	380	ARG
2	A	1	MET
2	A	7	HIS
2	A	25	ASN
2	A	29	TYR
2	A	43	GLN
2	A	59	TYR
2	A	79	GLN
2	A	82	SER
2	A	92	MET
2	A	106	LEU
2	A	144	PHE
2	A	153	ASP
2	A	156	LYS
2	A	181	ASP
2	A	182	GLN
2	A	194	SER
2	A	198	LEU

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Mol	Chain	Res	Type
2	A	209	LEU
2	A	229	MET
2	A	256	THR
2	A	292	ASP
2	A	310	ASN
2	A	325	LYS
2	A	351	LYS
2	A	375	THR
2	A	399	LYS
2	A	438	SER
2	A	451	SER
2	A	472	LYS
2	A	481	LEU
2	A	483	SER
2	A	510	GLN
2	A	514	SER
2	A	527	ARG
2	A	540	GLN
2	A	546	PHE
2	B	29	TYR
2	B	64	GLN
2	B	65	ARG
2	B	66	GLU
2	B	68	ASP
2	B	70	PHE
2	B	74	GLN
2	B	82	SER
2	B	92	MET
2	B	97	ASN
2	B	103	SER
2	B	144	PHE
2	B	156	LYS
2	B	181	ASP
2	B	197	ASP
2	B	203	ASP
2	B	204	GLN
2	B	226	ASN
2	B	260	TYR
2	B	285	THR
2	B	290	ASP
2	B	292	ASP
2	B	301	LEU

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Mol	Chain	Res	Type
2	B	315	LYS
2	B	332	SER
2	B	364	LYS
2	B	371	ASP
2	B	383	PHE
2	B	390	ASP
2	B	396	ASP
2	B	410	ASP
2	B	418	SER
2	B	423	ASP
2	B	424	MET
2	B	425	ASN
2	B	436	MET
2	B	441	LYS
2	B	476	ASP
2	B	505	GLN
2	B	508	LYS
2	B	519	ASP
2	B	522	TYR
2	C	6	ASN
2	C	9	MET
2	C	16	GLN
2	C	29	TYR
2	C	64	GLN
2	C	65	ARG
2	C	67	TYR
2	C	68	ASP
2	C	74	GLN
2	C	81	GLN
2	C	101	ASP
2	C	111	GLN
2	C	119	THR
2	C	131	GLN
2	C	142	ASN
2	C	148	ASP
2	C	172	TYR
2	C	181	ASP
2	C	185	ARG
2	C	196	ASN
2	C	206	VAL
2	C	228	THR
2	C	234	THR

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Mol	Chain	Res	Type
2	C	244	LEU
2	C	260	TYR
2	C	263	GLU
2	C	277	THR
2	C	290	ASP
2	C	315	LYS
2	C	368	ASP
2	C	382	THR
2	C	408	LYS
2	C	409	ASN
2	C	411	SER
2	C	424	MET
2	C	436	MET
2	C	463	GLN
2	C	474	PHE
2	C	504	LYS
2	C	519	ASP
2	C	532	TYR
2	C	537	GLN
2	D	2	SER
2	D	13	ASN
2	D	28	ASN
2	D	53	TRP
2	D	59	TYR
2	D	64	GLN
2	D	65	ARG
2	D	76	ARG
2	D	80	ASN
2	D	104	SER
2	D	105	SER
2	D	136	LYS
2	D	142	ASN
2	D	168	GLN
2	D	220	GLN
2	D	239	SER
2	D	240	THR
2	D	242	ARG
2	D	252	ASP
2	D	307	ASP
2	D	357	LYS
2	D	364	LYS
2	D	365	ILE

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Mol	Chain	Res	Type
2	D	383	PHE
2	D	387	LYS
2	D	431	GLU
2	D	433	GLU
2	D	441	LYS
2	D	443	ASP
2	D	445	ASP
2	D	447	ASP
2	D	483	SER
2	D	510	GLN
2	E	31	VAL
2	E	66	GLU
2	E	68	ASP
2	E	79	GLN
2	E	116	SER
2	E	131	GLN
2	E	174	LYS
2	E	197	ASP
2	E	208	GLU
2	E	211	LYS
2	E	229	MET
2	E	242	ARG
2	E	260	TYR
2	E	315	LYS
2	E	317	TYR
2	E	340	ASN
2	E	353	VAL
2	E	357	LYS
2	E	375	THR
2	E	380	ASN
2	E	387	LYS
2	E	392	LYS
2	E	399	LYS
2	E	408	LYS
2	E	415	LYS
2	E	431	GLU
2	E	436	MET
2	E	443	ASP
2	E	447	ASP
2	E	473	THR
2	E	508	LYS
2	E	522	TYR

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Mol	Chain	Res	Type
2	E	531	TYR
2	E	538	VAL
2	E	539	LEU
2	F	9	MET
2	F	29	TYR
2	F	30	ASN
2	F	34	TYR
2	F	61	SER
2	F	65	ARG
2	F	81	GLN
2	F	98	LEU
2	F	111	GLN
2	F	116	SER
2	F	143	GLN
2	F	154	GLN
2	F	186	MET
2	F	194	SER
2	F	201	GLN
2	F	203	ASP
2	F	209	LEU
2	F	221	ASP
2	F	226	ASN
2	F	327	PHE
2	F	370	THR
2	F	387	LYS
2	F	393	LEU
2	F	411	SER
2	F	423	ASP
2	F	438	SER
2	F	454	ARG
2	F	466	ASN
2	F	476	ASP
2	F	483	SER
2	F	511	GLN
2	F	516	VAL
2	F	526	GLN
2	F	527	ARG
2	F	531	TYR
2	F	535	ASN
2	G	6	ASN
2	G	29	TYR
2	G	30	ASN

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Mol	Chain	Res	Type
2	G	41	LEU
2	G	91	GLN
2	G	104	SER
2	G	125	GLU
2	G	154	GLN
2	G	169	ILE
2	G	181	ASP
2	G	225	TYR
2	G	235	LEU
2	G	242	ARG
2	G	315	LYS
2	G	332	SER
2	G	386	THR
2	G	411	SER
2	G	413	LEU
2	G	423	ASP
2	G	431	GLU
2	G	471	ASN
2	G	476	ASP
2	G	489	THR
2	G	504	LYS
2	G	508	LYS
2	G	517	ASN
2	G	522	TYR
2	G	540	GLN
2	G	546	PHE
2	H	5	ILE
2	H	6	ASN
2	H	29	TYR
2	H	30	ASN
2	H	53	TRP
2	H	71	ILE
2	H	80	ASN
2	H	103	SER
2	H	113	PHE
2	H	118	GLN
2	H	143	GLN
2	H	150	TYR
2	H	156	LYS
2	H	172	TYR
2	H	197	ASP
2	H	272	GLU

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Mol	Chain	Res	Type
2	H	300	GLN
2	H	343	ASP
2	H	351	LYS
2	H	379	ASP
2	H	382	THR
2	H	440	SER
2	H	463	GLN
2	H	474	PHE
2	H	508	LYS
2	H	519	ASP
2	I	5	ILE
2	I	16	GLN
2	I	29	TYR
2	I	30	ASN
2	I	59	TYR
2	I	67	TYR
2	I	75	LEU
2	I	93	SER
2	I	98	LEU
2	I	99	LEU
2	I	102	LYS
2	I	111	GLN
2	I	116	SER
2	I	138	GLU
2	I	144	PHE
2	I	149	GLN
2	I	150	TYR
2	I	154	GLN
2	I	183	ILE
2	I	201	GLN
2	I	210	ASN
2	I	216	GLU
2	I	229	MET
2	I	236	VAL
2	I	260	TYR
2	I	286	PHE
2	I	287	ARG
2	I	295	ARG
2	I	303	LEU
2	I	322	ASN
2	I	372	TRP
2	I	387	LYS

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Mol	Chain	Res	Type
2	I	388	ASP
2	I	421	ILE
2	I	423	ASP
2	I	424	MET
2	I	445	ASP
2	I	484	ASP
2	I	520	GLU
2	I	546	PHE
2	J	53	TRP
2	J	59	TYR
2	J	75	LEU
2	J	82	SER
2	J	94	LYS
2	J	102	LYS
2	J	118	GLN
2	J	148	ASP
2	J	179	LEU
2	J	181	ASP
2	J	185	ARG
2	J	186	MET
2	J	200	ASP
2	J	202	ARG
2	J	225	TYR
2	J	260	TYR
2	J	262	ASP
2	J	277	THR
2	J	288	SER
2	J	291	LEU
2	J	318	ASP
2	J	334	VAL
2	J	344	LYS
2	J	351	LYS
2	J	357	LYS
2	J	383	PHE
2	J	387	LYS
2	J	407	GLN
2	J	412	PHE
2	J	424	MET
2	J	431	GLU
2	J	441	LYS
2	J	457	GLN
2	J	462	LEU

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Mol	Chain	Res	Type
2	J	473	THR
2	J	476	ASP
2	J	483	SER
2	J	493	LYS
2	J	505	GLN
2	J	507	TYR
2	J	510	GLN
2	J	511	GLN
2	J	530	GLN
2	K	5	ILE
2	K	13	ASN
2	K	48	LEU
2	K	65	ARG
2	K	68	ASP
2	K	70	PHE
2	K	75	LEU
2	K	101	ASP
2	K	102	LYS
2	K	136	LYS
2	K	142	ASN
2	K	170	ASN
2	K	174	LYS
2	K	197	ASP
2	K	221	ASP
2	K	224	THR
2	K	242	ARG
2	K	260	TYR
2	K	303	LEU
2	K	307	ASP
2	K	309	PHE
2	K	326	ASP
2	K	336	TYR
2	K	343	ASP
2	K	357	LYS
2	K	383	PHE
2	K	388	ASP
2	K	408	LYS
2	K	455	ASN
2	K	474	PHE
2	K	487	ASN
2	K	493	LYS
2	K	504	LYS

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Mol	Chain	Res	Type
2	K	508	LYS
2	K	512	SER
2	K	519	ASP
2	K	522	TYR
2	K	529	GLN
2	K	543	ASN
2	K	547	ASP
3	L	5	THR
3	L	8	MET
3	L	23	TRP
3	L	70	THR
3	L	96	TYR
3	L	106	ASP
3	L	120	GLN
3	L	122	MET
3	L	148	GLN
3	L	157	GLU
3	L	249	GLU
3	L	250	LEU
3	L	275	MET
3	L	297	LEU
3	L	302	LYS
3	L	304	PHE
3	L	310	MET
3	M	9	TYR
3	M	11	GLN
3	M	13	MET
3	M	18	ASN
3	M	24	MET
3	M	25	LYS
3	M	34	LYS
3	M	37	THR
3	M	38	ASN
3	M	41	ASP
3	M	96	TYR
3	M	106	ASP
3	M	110	LEU
3	M	113	ASP
3	M	139	TYR
3	M	147	ASP
3	M	168	ARG
3	M	219	ASN

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Mol	Chain	Res	Type
3	M	220	VAL
3	M	221	GLU
3	M	224	LYS
3	M	230	ASP
3	M	231	LYS
3	M	274	GLN
3	M	290	TYR
3	M	307	MET
3	M	308	GLN
3	M	310	MET
3	M	313	PHE
3	N	10	GLU
3	N	17	THR
3	N	30	MET
3	N	42	ASP
3	N	48	GLN
3	N	96	TYR
3	N	106	ASP
3	N	114	LEU
3	N	157	GLU
3	N	165	ASP
3	N	212	LYS
3	N	223	GLU
3	N	261	ASP
3	N	292	MET
3	N	301	TYR
3	N	308	GLN
3	N	312	LEU
3	N	313	PHE
3	N	314	GLN
3	O	7	MET
3	O	8	MET
3	O	10	GLU
3	O	23	TRP
3	O	24	MET
3	O	47	SER
3	O	54	GLN
3	O	56	GLN
3	O	58	GLN
3	O	77	GLU
3	O	96	TYR
3	O	104	ASP

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Mol	Chain	Res	Type
3	O	105	ASP
3	O	112	THR
3	O	118	ARG
3	O	147	ASP
3	O	163	GLN
3	O	166	SER
3	O	168	ARG
3	O	200	LEU
3	O	205	ASP
3	O	212	LYS
3	O	234	ARG
3	O	242	ASN
3	O	263	LEU
3	O	307	MET
3	O	313	PHE
3	O	314	GLN
3	P	34	LYS
3	P	96	TYR
3	P	105	ASP
3	P	165	ASP
3	P	166	SER
3	P	237	LYS
3	P	278	LEU
3	P	283	TRP
3	P	298	GLN
3	Q	7	MET
3	Q	22	GLU
3	Q	30	MET
3	Q	42	ASP
3	Q	54	GLN
3	Q	71	GLN
3	Q	82	GLN
3	Q	96	TYR
3	Q	113	ASP
3	Q	120	GLN
3	Q	200	LEU
3	Q	247	ARG
3	Q	266	ASP
3	Q	272	LYS
3	Q	275	MET
3	Q	280	ASP
3	Q	286	VAL

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Mol	Chain	Res	Type
3	Q	293	GLN
3	Q	307	MET
3	Q	310	MET
3	R	16	ILE
3	R	18	ASN
3	R	28	GLU
3	R	35	ARG
3	R	38	ASN
3	R	48	GLN
3	R	54	GLN
3	R	82	GLN
3	R	96	TYR
3	R	105	ASP
3	R	158	LYS
3	R	170	MET
3	R	172	ILE
3	R	224	LYS
3	R	274	GLN
3	R	275	MET
3	R	292	MET
3	R	293	GLN
3	R	298	GLN
3	R	310	MET
3	R	313	PHE
3	S	8	MET
3	S	16	ILE
3	S	42	ASP
3	S	52	LEU
3	S	93	LYS
3	S	96	TYR
3	S	104	ASP
3	S	105	ASP
3	S	112	THR
3	S	113	ASP
3	S	154	HIS
3	S	157	GLU
3	S	158	LYS
3	S	166	SER
3	S	181	ASN
3	S	218	ASN
3	S	232	THR
3	S	277	ASN

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Mol	Chain	Res	Type
3	S	283	TRP
3	S	290	TYR
3	S	317	ARG
3	T	42	ASP
3	T	82	GLN
3	T	96	TYR
3	T	105	ASP
3	T	118	ARG
3	T	124	LEU
3	T	139	TYR
3	T	148	GLN
3	T	154	HIS
3	T	174	HIS
3	T	203	MET
3	T	222	LYS
3	T	230	ASP
3	T	258	SER
3	T	290	TYR
3	T	292	MET
3	T	302	LYS
3	U	6	GLN
3	U	11	GLN
3	U	24	MET
3	U	26	LEU
3	U	30	MET
3	U	56	GLN
3	U	77	GLU
3	U	96	TYR
3	U	106	ASP
3	U	123	ASN
3	U	203	MET
3	U	223	GLU
3	U	230	ASP
3	U	231	LYS
3	U	267	ARG
3	U	275	MET
3	U	279	VAL
3	U	292	MET
3	U	304	PHE
3	U	316	ASN
3	V	9	TYR
3	V	24	MET

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Mol	Chain	Res	Type
3	V	30	MET
3	V	71	GLN
3	V	76	GLU
3	V	93	LYS
3	V	96	TYR
3	V	106	ASP
3	V	192	ASP
3	V	224	LYS
3	V	230	ASP
3	V	237	LYS
3	V	249	GLU
3	V	252	THR
3	V	253	GLN
3	V	258	SER
3	V	265	SER
3	V	280	ASP
3	V	290	TYR
3	V	292	MET
3	V	293	GLN
3	V	301	TYR
3	V	302	LYS
3	V	304	PHE
3	V	307	MET
3	V	312	LEU
3	V	313	PHE
3	V	315	LEU
4	a	5	ILE
4	a	48	GLN
4	a	102	SER
4	a	152	ASP
4	a	230	TYR
4	a	309	LYS
4	a	349	LYS
4	a	353	ASP
4	a	387	GLU
4	a	392	LYS
4	a	464	SER
4	a	466	MET
4	a	484	ASN
4	b	10	LEU
4	b	12	LEU
4	b	22	GLN

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Mol	Chain	Res	Type
4	b	108	ASP
4	b	131	GLN
4	b	152	ASP
4	b	178	LYS
4	b	222	LYS
4	b	231	TYR
4	b	281	ASN
4	b	309	LYS
4	b	313	THR
4	b	336	THR
4	b	346	ASN
4	b	349	LYS
4	b	353	ASP
4	b	375	SER
4	b	392	LYS
4	b	420	ASP
4	b	446	ASN
4	b	447	LEU
4	b	453	ARG
4	b	459	TYR
4	b	477	THR
4	b	495	ARG
4	c	9	SER
4	c	12	LEU
4	c	13	LEU
4	c	32	LEU
4	c	108	ASP
4	c	157	ASP
4	c	164	ASN
4	c	171	ASP
4	c	203	PHE
4	c	213	THR
4	c	229	LYS
4	c	252	LYS
4	c	310	MET
4	c	321	ASP
4	c	339	LYS
4	c	406	GLU
4	c	424	SER
4	c	445	ASN
4	c	451	ARG
4	c	459	TYR

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Mol	Chain	Res	Type
4	c	473	GLN
4	c	484	ASN
4	c	495	ARG
4	d	16	ASN
4	d	108	ASP
4	d	166	GLN
4	d	318	LYS
4	d	321	ASP
4	d	339	LYS
4	d	351	THR
4	d	392	LYS
4	d	451	ARG
4	d	459	TYR
4	d	466	MET
4	e	31	ARG
4	e	48	GLN
4	e	57	ASN
4	e	102	SER
4	e	106	GLN
4	e	108	ASP
4	e	131	GLN
4	e	152	ASP
4	e	172	THR
4	e	188	VAL
4	e	193	ASP
4	e	204	LYS
4	e	222	LYS
4	e	243	ASP
4	e	280	LYS
4	e	310	MET
4	e	321	ASP
4	e	353	ASP
4	e	392	LYS
4	e	459	TYR
4	e	485	GLN
4	e	488	GLN
4	f	5	ILE
4	f	7	THR
4	f	10	LEU
4	f	48	GLN
4	f	66	ARG
4	f	83	ASN

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Mol	Chain	Res	Type
4	f	147	GLN
4	f	201	SER
4	f	203	PHE
4	f	220	ASP
4	f	314	ASP
4	f	321	ASP
4	f	324	LEU
4	f	370	LYS
4	f	489	ASN
4	f	495	ARG
4	g	5	ILE
4	g	34	SER
4	g	79	GLU
4	g	108	ASP
4	g	157	ASP
4	g	159	ASP
4	g	180	LYS
4	g	182	SER
4	g	281	ASN
4	g	309	LYS
4	g	314	ASP
4	g	330	ASP
4	g	339	LYS
4	g	361	LEU
4	g	404	THR
4	g	420	ASP
4	g	452	SER
4	g	459	TYR
4	g	464	SER
4	g	495	ARG
4	h	18	LEU
4	h	48	GLN
4	h	102	SER
4	h	157	ASP
4	h	161	LYS
4	h	180	LYS
4	h	224	ASP
4	h	252	LYS
4	h	278	ASP
4	h	318	LYS
4	h	337	GLN
4	h	339	LYS

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Mol	Chain	Res	Type
4	h	346	ASN
4	h	353	ASP
4	h	392	LYS
4	h	396	ASP
4	h	456	ASP
4	h	485	GLN
4	h	489	ASN
4	h	495	ARG
4	i	5	ILE
4	i	9	SER
4	i	10	LEU
4	i	79	GLU
4	i	105	SER
4	i	182	SER
4	i	193	ASP
4	i	210	LEU
4	i	248	VAL
4	i	311	SER
4	i	321	ASP
4	i	339	LYS
4	i	406	GLU
4	i	422	LEU
4	i	456	ASP
4	i	459	TYR
4	i	495	ARG
4	j	108	ASP
4	j	161	LYS
4	j	216	LYS
4	j	230	TYR
4	j	280	LYS
4	j	316	ASN
4	j	324	LEU
4	j	339	LYS
4	j	372	GLU
4	j	425	ASP
4	j	477	THR
4	j	488	GLN
4	j	495	ARG
4	k	3	GLN
4	k	57	ASN
4	k	152	ASP
4	k	159	ASP

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Mol	Chain	Res	Type
4	k	183	ASP
4	k	215	GLN
4	k	218	ASP
4	k	291	GLU
4	k	339	LYS
4	k	385	LYS
4	k	449	SER
4	k	451	ARG
4	k	459	TYR
4	k	489	ASN
4	k	495	ARG
4	l	21	SER
4	l	23	SER
4	l	94	GLU
4	l	108	ASP
4	l	141	ASP
4	l	183	ASP
4	l	193	ASP
4	l	222	LYS
4	l	224	ASP
4	l	291	GLU
4	l	310	MET
4	l	316	ASN
4	l	339	LYS
4	l	346	ASN
4	l	459	TYR
4	m	6	ASN
4	m	48	GLN
4	m	108	ASP
4	m	140	GLN
4	m	157	ASP
4	m	165	SER
4	m	178	LYS
4	m	180	LYS
4	m	193	ASP
4	m	203	PHE
4	m	220	ASP
4	m	278	ASP
4	m	309	LYS
4	m	310	MET
4	m	340	ASP
4	m	488	GLN

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Mol	Chain	Res	Type
4	n	21	SER
4	n	31	ARG
4	n	108	ASP
4	n	183	ASP
4	n	282	VAL
4	n	310	MET
4	n	330	ASP
4	n	347	THR
4	n	392	LYS
4	n	394	GLN
4	n	456	ASP
4	n	495	ARG
4	o	6	ASN
4	o	48	GLN
4	o	59	LYS
4	o	109	LEU
4	o	144	LEU
4	o	154	GLU
4	o	157	ASP
4	o	172	THR
4	o	180	LYS
4	o	222	LYS
4	o	225	ASP
4	o	321	ASP
4	o	370	LYS
4	o	379	LYS
4	o	406	GLU
4	o	422	LEU
4	o	489	ASN
4	o	495	ARG
1	w	3	PHE
1	w	5	GLN
1	w	30	TYR
1	w	42	MET
1	w	80	ASN
1	w	89	ASN
1	w	99	GLN
1	w	102	LEU
1	w	105	ASN
1	w	162	ASP
1	w	164	VAL
1	w	168	THR

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Mol	Chain	Res	Type
1	w	170	PHE
1	w	202	LYS
1	w	213	HIS
1	w	232	PHE
1	w	233	ASN
1	w	240	SER
1	w	255	THR
1	w	265	ASN
1	w	267	MET
1	w	292	TYR
1	w	297	ASP
1	w	338	GLN
1	w	393	ASP
1	w	403	ARG
1	x	1	MET
1	x	18	ASP
1	x	42	MET
1	x	63	ASP
1	x	71	ARG
1	x	80	ASN
1	x	82	PHE
1	x	84	ARG
1	x	110	ASN
1	x	114	MET
1	x	141	ASN
1	x	170	PHE
1	x	178	TYR
1	x	195	ASP
1	x	204	LYS
1	x	221	THR
1	x	267	MET
1	x	284	TYR
1	x	285	LYS
1	x	292	TYR
1	x	312	LEU
1	x	369	SER
1	x	391	THR
1	y	79	GLN
1	y	119	TYR
1	y	130	GLN
1	y	133	ASN
1	y	143	LEU

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Mol	Chain	Res	Type
1	y	178	TYR
1	y	179	ASN
1	y	183	THR
1	y	205	ASP
1	y	208	TRP
1	y	292	TYR
1	y	297	ASP
1	y	310	GLN
1	y	369	SER
1	y	370	LYS
1	y	380	ARG
1	y	393	ASP
1	y	403	ARG
1	z	36	THR
1	z	71	ARG
1	z	73	LEU
1	z	106	ARG
1	z	107	ASN
1	z	110	ASN
1	z	111	MET
1	z	114	MET
1	z	116	LEU
1	z	143	LEU
1	z	147	LYS
1	z	162	ASP
1	z	170	PHE
1	z	181	LYS
1	z	194	HIS
1	z	230	LEU
1	z	264	LEU
1	z	267	MET
1	z	268	GLN
1	z	285	LYS
1	z	292	TYR
1	z	334	TRP
1	z	375	MET
1	z	382	TYR
1	z	387	GLN
1	z	401	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	11	ASN
1	1	80	ASN
1	1	352	ASN
1	1	381	ASN
1	2	5	GLN
1	3	265	ASN
1	4	159	ASN
1	4	275	ASN
1	6	332	ASN
1	7	110	ASN
1	7	194	HIS
1	7	392	GLN
1	8	392	GLN
1	9	194	HIS
2	A	37	GLN
2	A	43	GLN
2	A	201	GLN
2	A	310	ASN
2	A	453	ASN
2	B	300	GLN
2	B	487	ASN
2	B	543	ASN
2	C	56	ASN
2	D	20	ASN
2	D	175	GLN
2	E	97	ASN
2	F	74	GLN
2	F	157	GLN
2	F	505	GLN
2	G	20	ASN
2	G	97	ASN
2	G	517	ASN
2	G	540	GLN
2	G	551	ASN
2	H	123	ASN
2	H	142	ASN
2	H	237	GLN
2	H	540	GLN
2	H	543	ASN
2	J	24	ASN
2	J	80	ASN
2	J	118	GLN
2	J	171	ASN

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Mol	Chain	Res	Type
2	K	74	GLN
2	K	168	GLN
2	K	220	GLN
2	K	226	ASN
2	K	359	GLN
3	L	20	GLN
3	L	162	GLN
3	M	274	GLN
3	M	308	GLN
3	N	277	ASN
3	N	294	GLN
3	N	308	GLN
3	N	316	ASN
3	O	162	GLN
3	O	277	ASN
3	P	253	GLN
3	P	274	GLN
3	P	277	ASN
3	Q	11	GLN
3	Q	56	GLN
3	Q	277	ASN
3	Q	293	GLN
3	S	11	GLN
3	S	12	ASN
3	S	29	GLN
3	S	48	GLN
3	T	12	ASN
3	U	6	GLN
3	U	11	GLN
3	U	12	ASN
3	U	298	GLN
3	V	11	GLN
3	V	12	ASN
3	V	20	GLN
3	V	293	GLN
4	a	3	GLN
4	b	48	GLN
4	c	3	GLN
4	c	15	GLN
4	c	16	ASN
4	c	315	ASN
4	e	3	GLN

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Mol	Chain	Res	Type
4	f	8	ASN
4	g	489	ASN
4	i	17	ASN
4	i	48	GLN
4	i	52	ASN
4	k	3	GLN
4	k	485	GLN
4	l	48	GLN
4	m	485	GLN
1	w	192	ASN
1	w	332	ASN
1	x	133	ASN
1	x	306	ASN
1	x	332	ASN
1	y	23	ASN
1	y	130	GLN
1	y	383	GLN
1	y	387	GLN
1	z	22	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

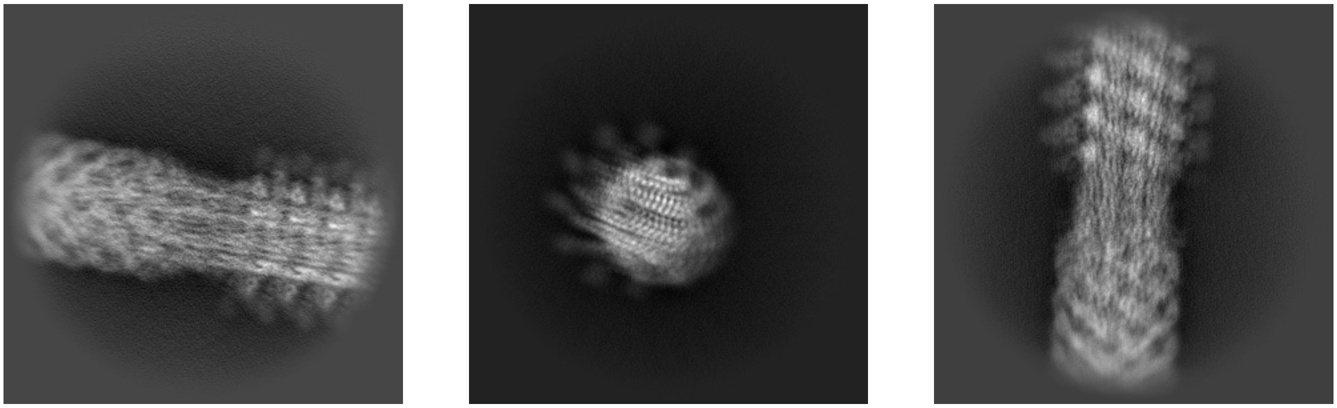
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-51493. 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.

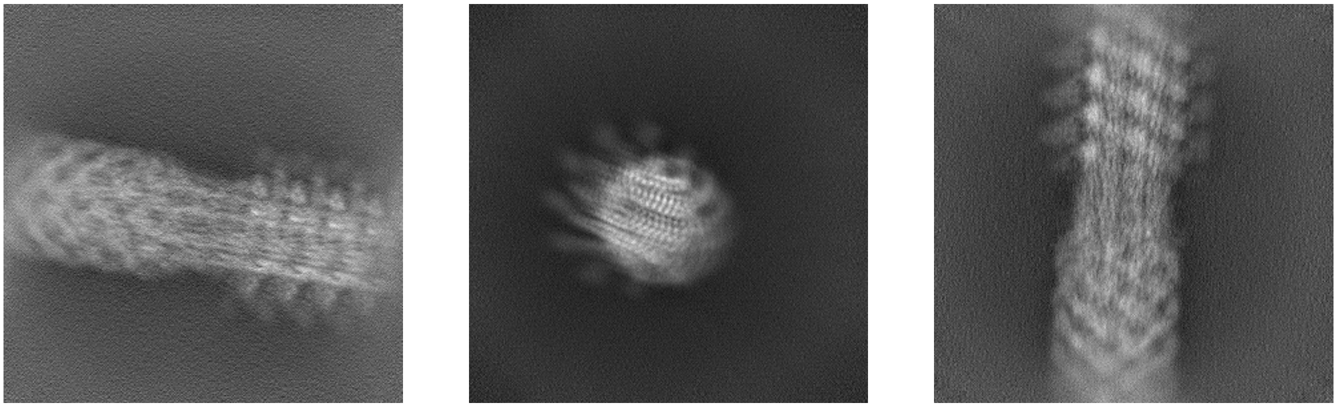
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

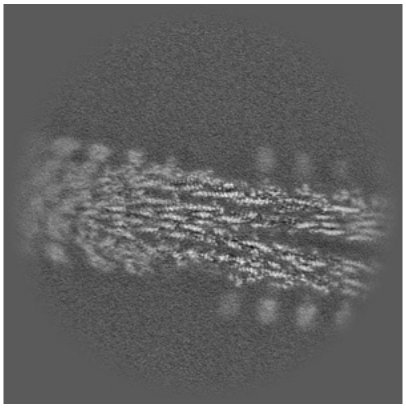


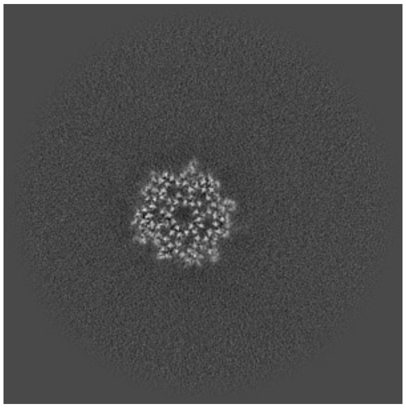
X Y Z

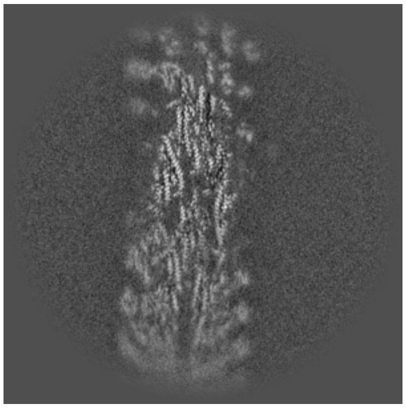
The images above show the map projected in three orthogonal directions.

6.2 Central slices

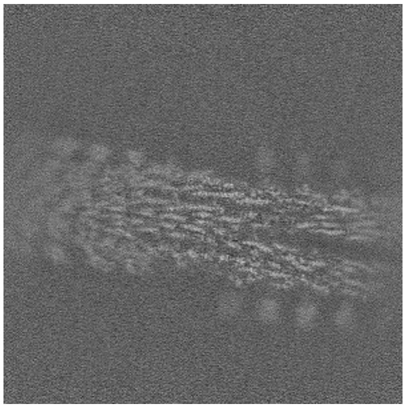
6.2.1 Primary map

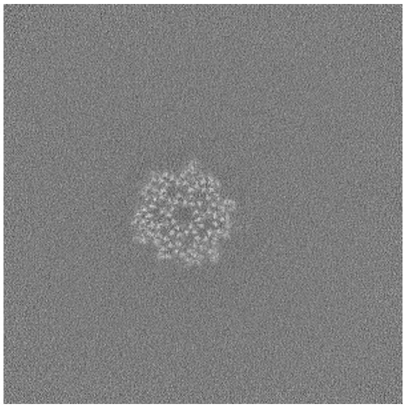

X Index: 250

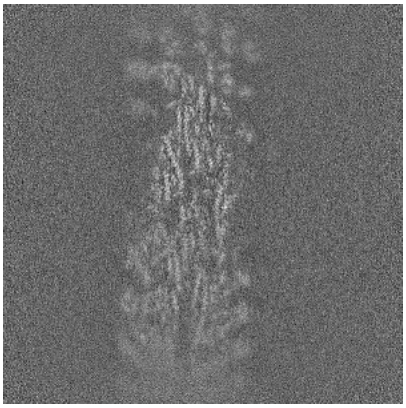

Y Index: 250


Z Index: 250

6.2.2 Raw map


X Index: 250

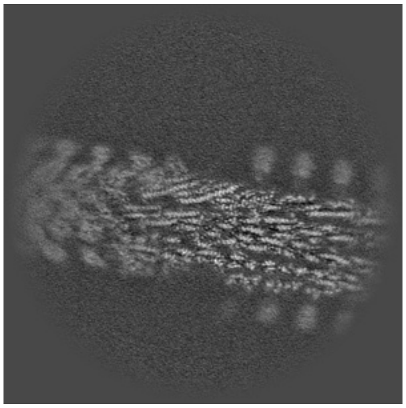

Y Index: 250


Z Index: 250

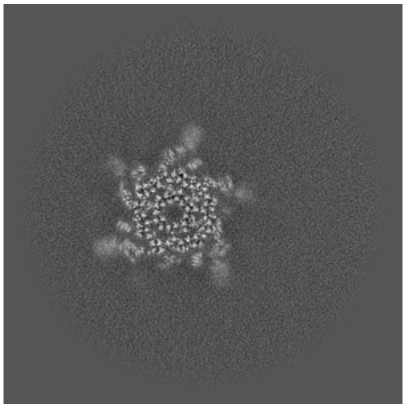
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

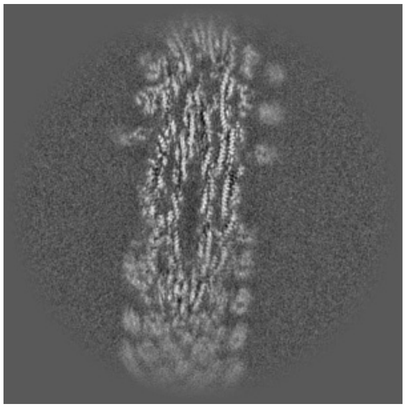
6.3.1 Primary map



X Index: 257

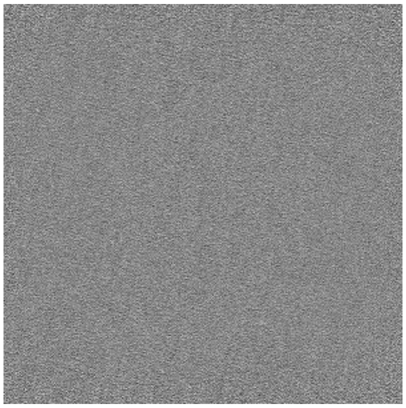


Y Index: 314

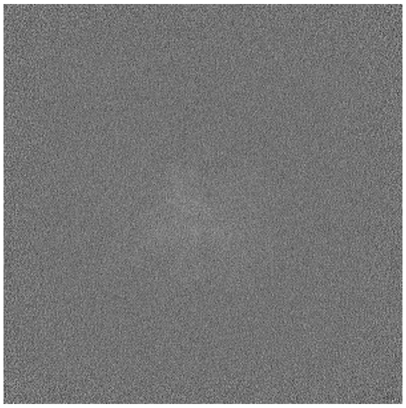


Z Index: 227

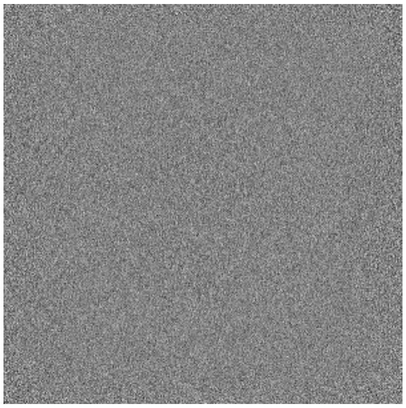
6.3.2 Raw map



X Index: 0



Y Index: 0

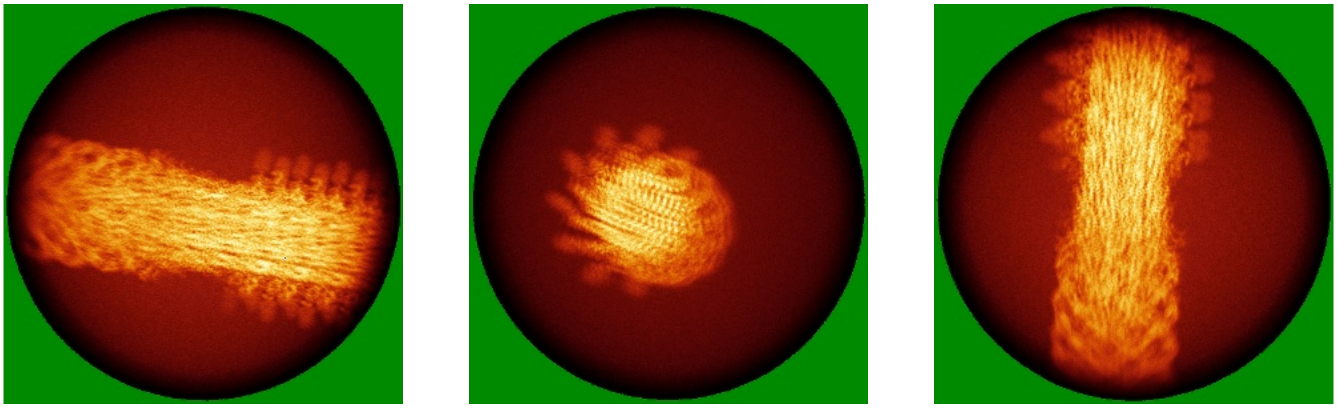


Z Index: 0

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

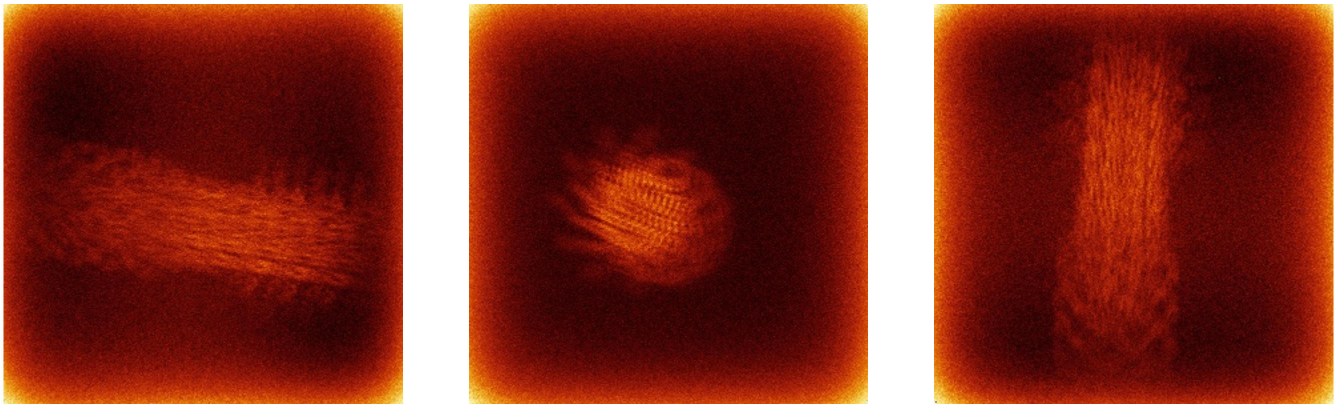
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X Y Z

6.4.2 Raw map

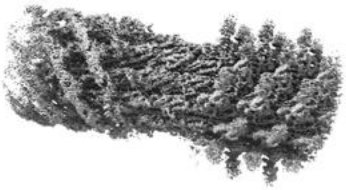


X Y Z

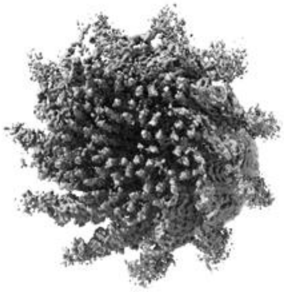
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

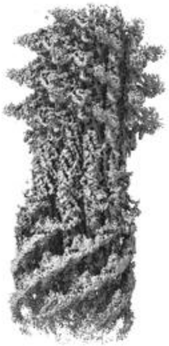
6.5.1 Primary map



X



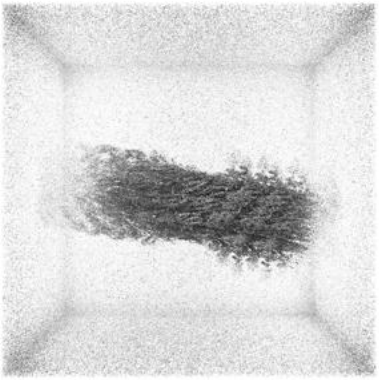
Y



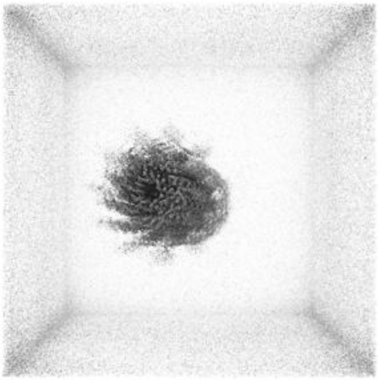
Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

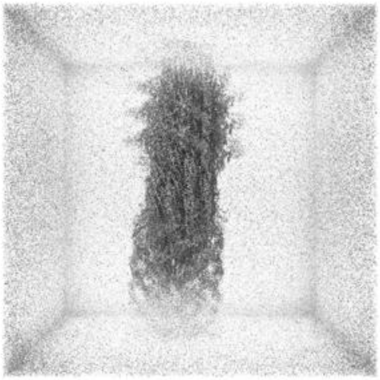
6.5.2 Raw map



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.

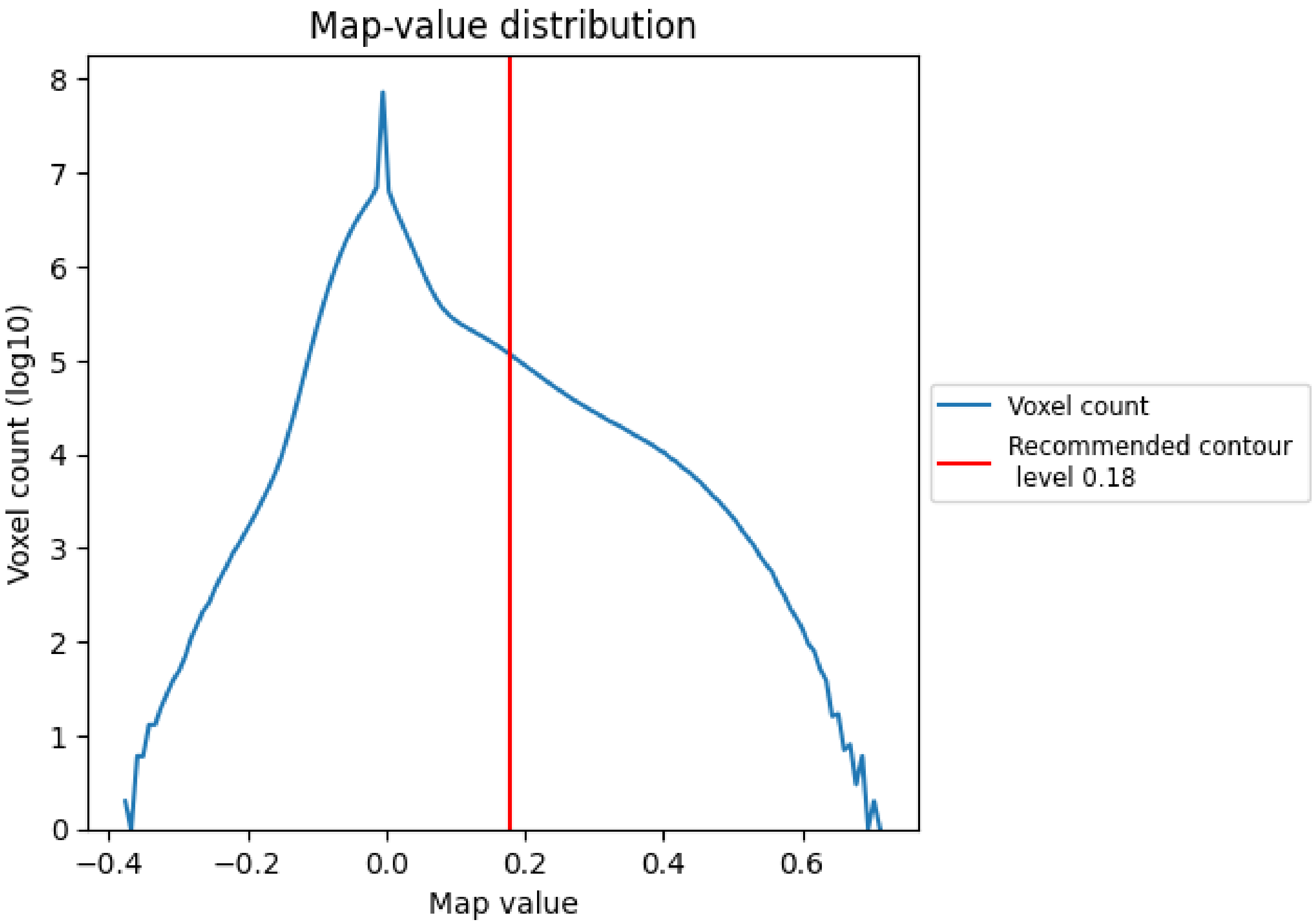
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

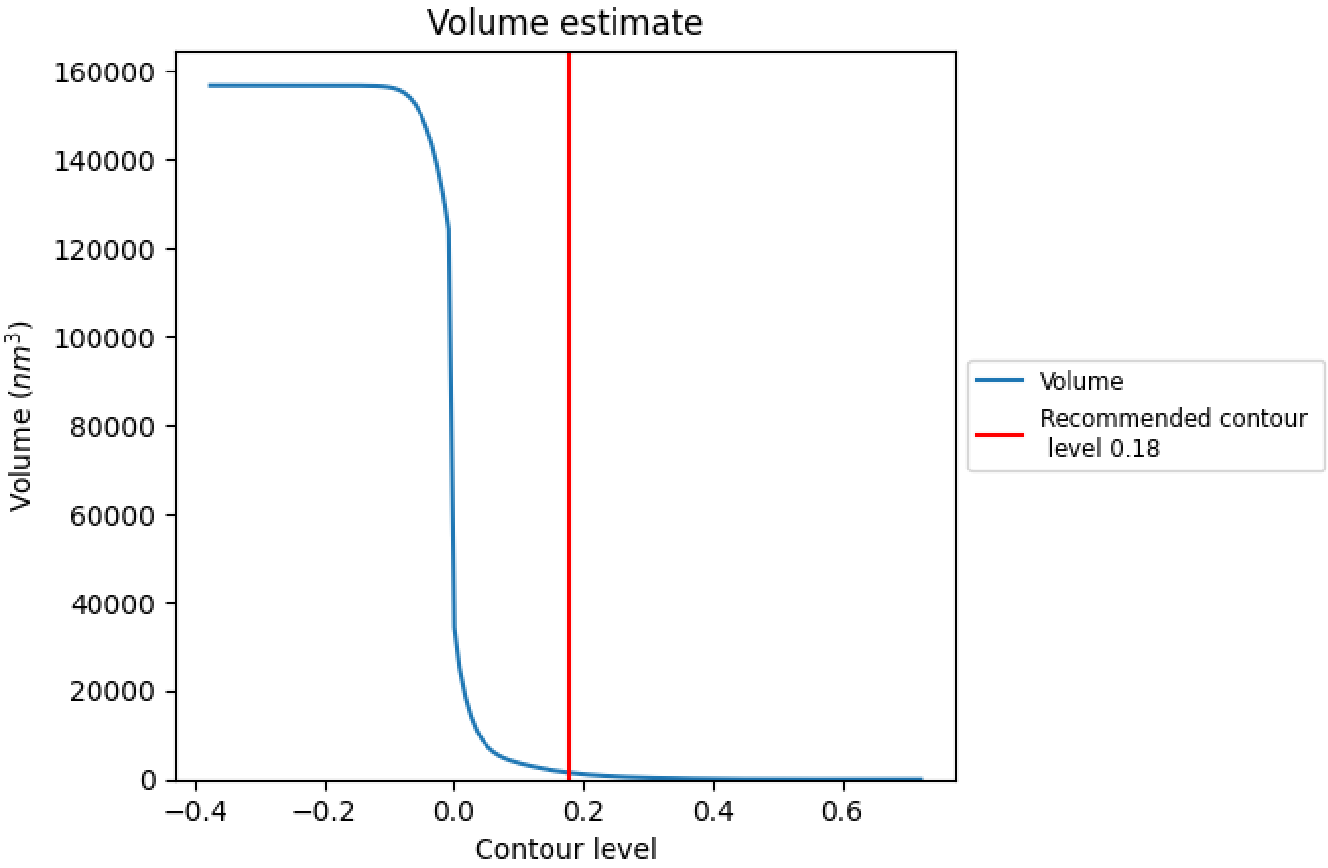
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

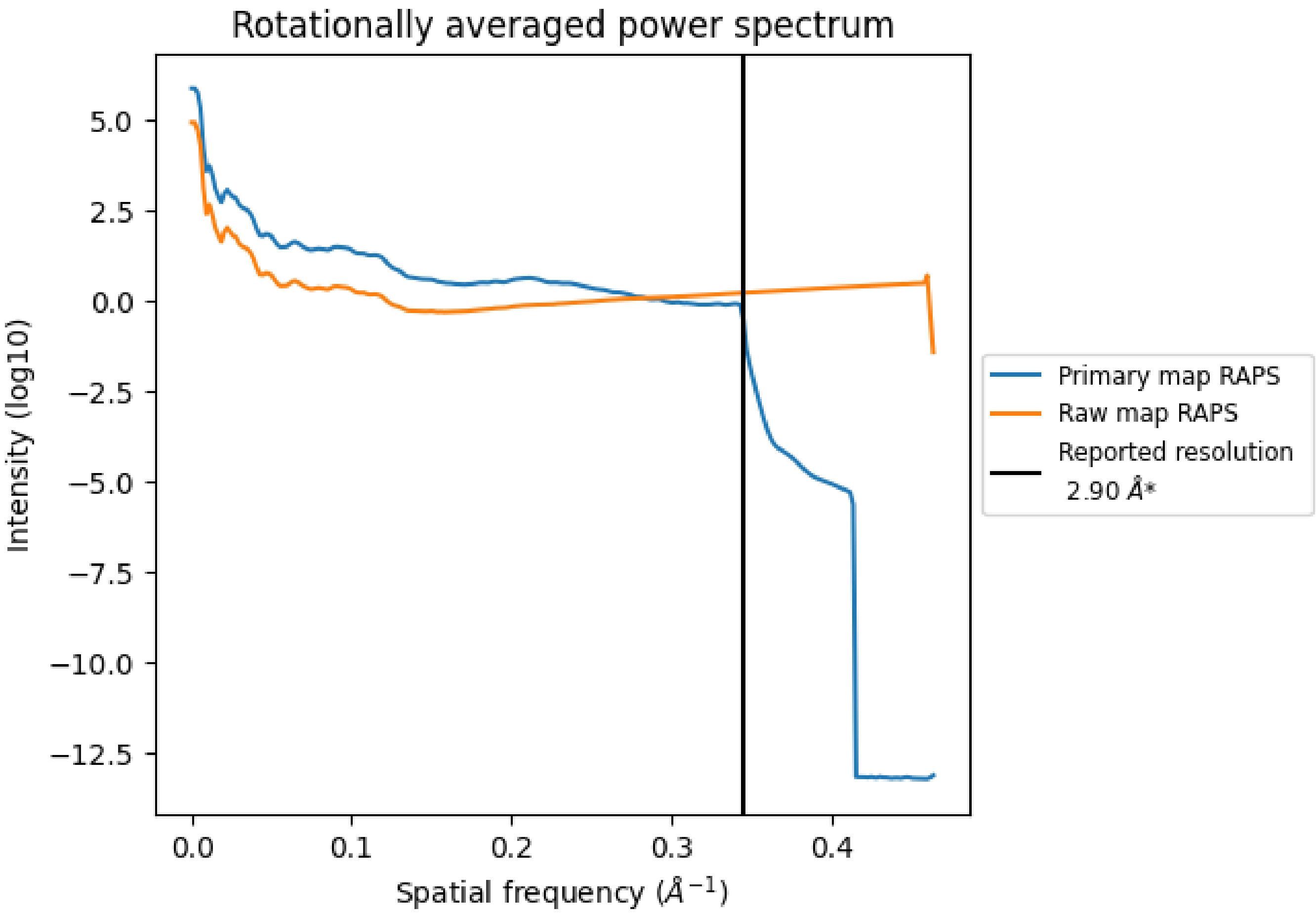
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1471 nm^3; this corresponds to an approximate mass of 1329 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

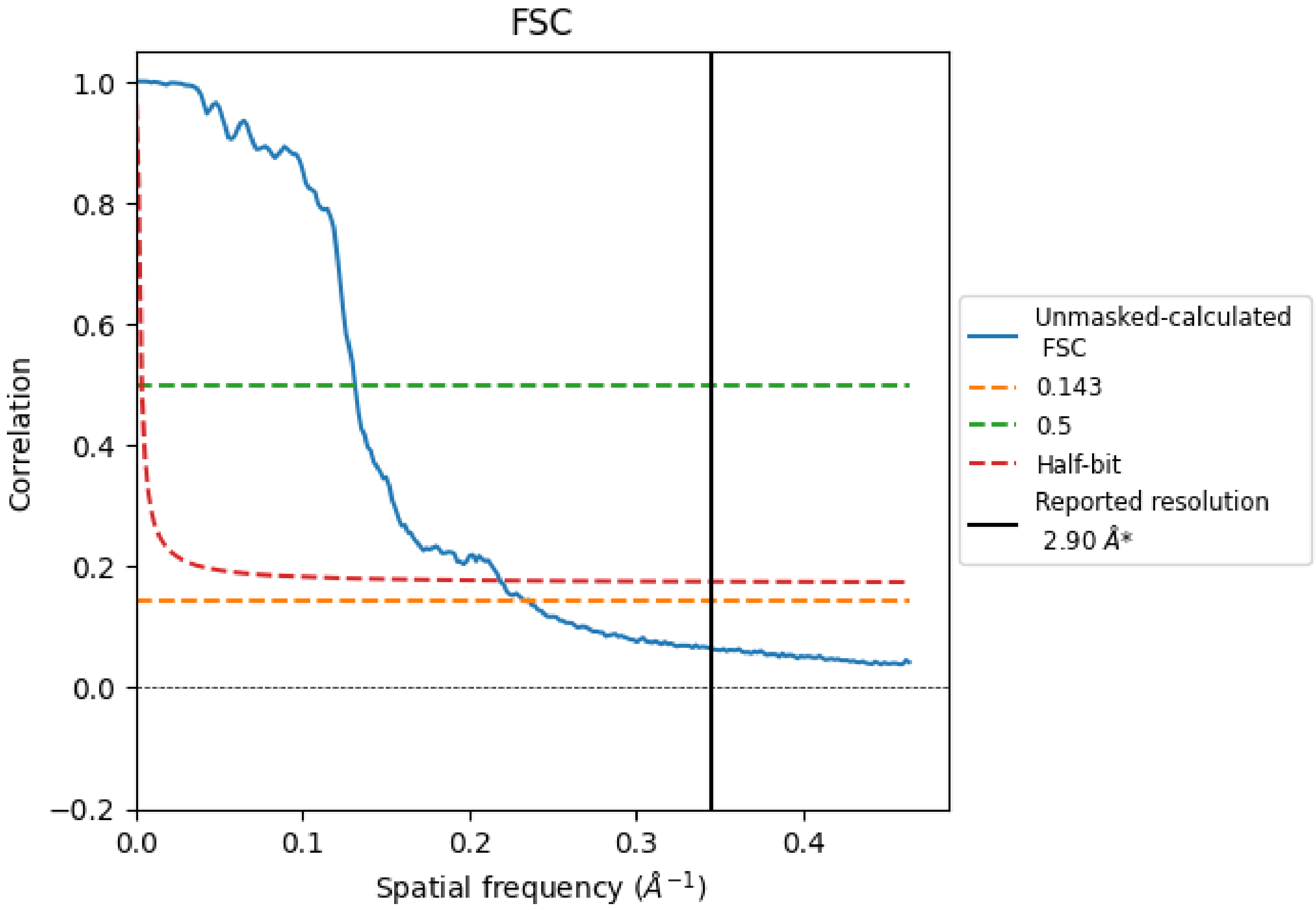


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates ⓘ

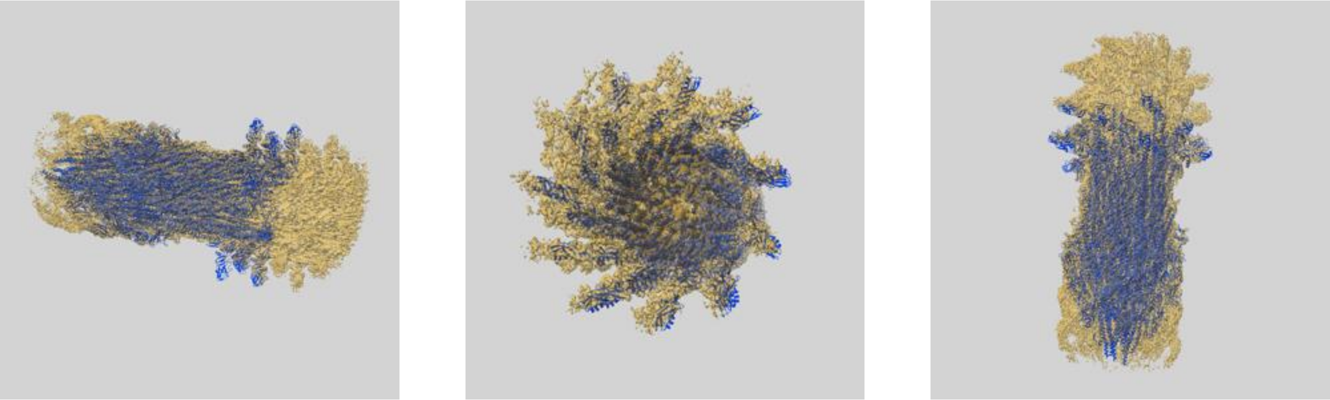
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.28	7.60	4.57

*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 4.28 differs from the reported value 2.9 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-51493 and PDB model 9GO6. Per-residue inclusion information can be found in section 3 on page 8.

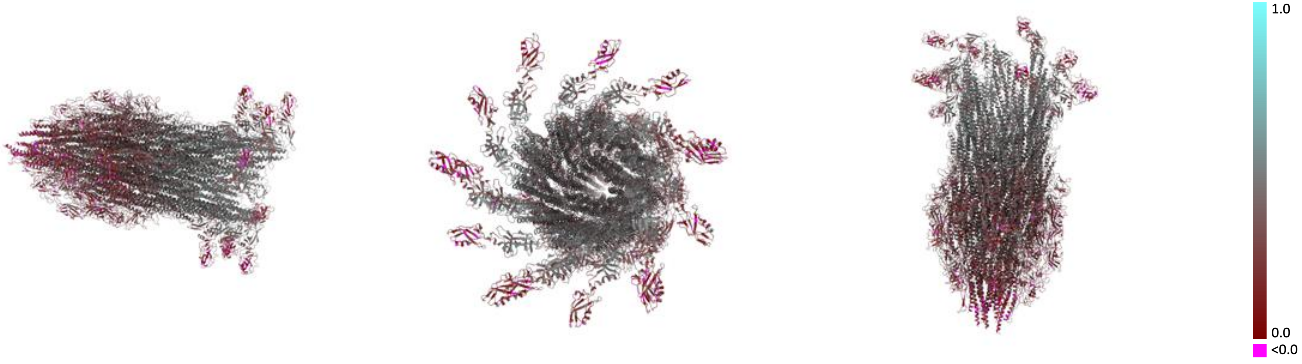
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.18 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.

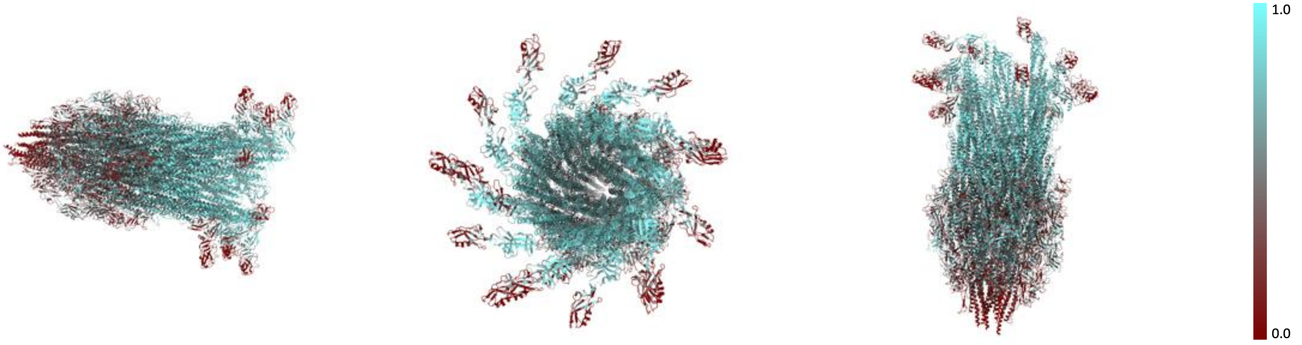
9.2 Q-score mapped to coordinate model ⓘ



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.

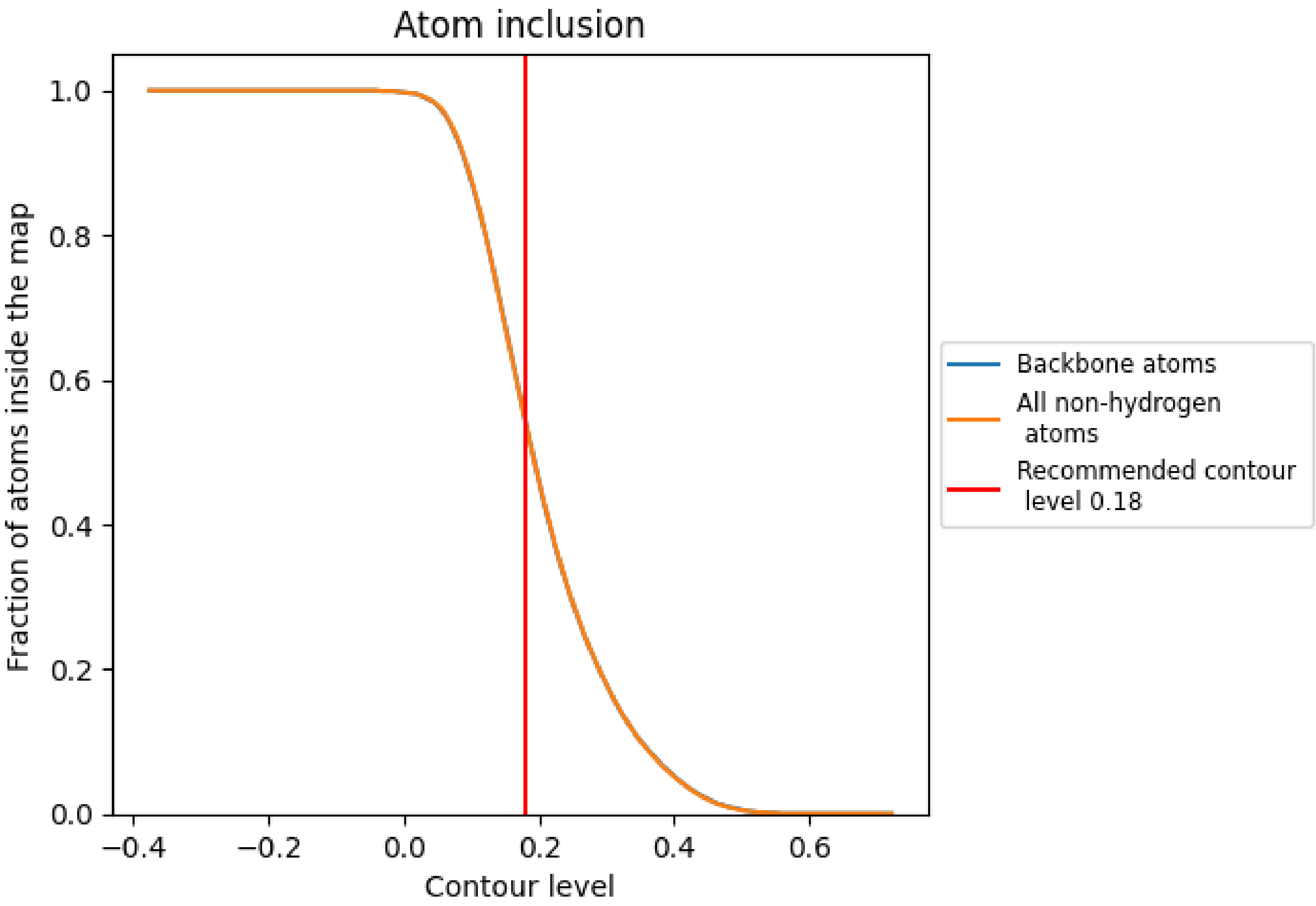
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.18).

9.4 Atom inclusion ⓘ



At the recommended contour level, 54% of all backbone atoms, 54% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5420	0.3490
1	0.4310	0.3030
2	0.3670	0.2460
3	0.4200	0.2880
4	0.3200	0.2300
5	0.3850	0.2650
6	0.3070	0.2320
7	0.3430	0.2750
8	0.3900	0.2620
9	0.2720	0.1930
A	0.3700	0.2830
B	0.5380	0.3250
C	0.4460	0.3070
D	0.5890	0.3610
E	0.5320	0.3380
F	0.5780	0.3610
G	0.5480	0.3300
H	0.5130	0.3390
I	0.5090	0.2960
J	0.5010	0.3390
K	0.5500	0.3070
L	0.7320	0.4140
M	0.6990	0.4170
N	0.7400	0.4280
O	0.6230	0.3320
P	0.7510	0.4370
Q	0.6500	0.3850
R	0.7420	0.4440
S	0.6870	0.3980
T	0.7360	0.4380
U	0.7080	0.4060
V	0.6950	0.4200
a	0.6620	0.4100
b	0.6530	0.4190
c	0.4440	0.3590

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Chain	Atom inclusion	Q-score
d	0.6640	0.4080
e	0.6630	0.4160
f	0.4980	0.3840
g	0.6610	0.4060
h	0.6550	0.4180
i	0.5580	0.3960
j	0.6710	0.4060
k	0.6730	0.4130
l	0.6180	0.3960
m	0.6680	0.4020
n	0.6710	0.4120
o	0.6350	0.4050
w	0.3450	0.2620
x	0.3550	0.2420
y	0.3890	0.3100
z	0.3660	0.2350