wwPDB EM Validation Summary Report (i)

Nov 14, 2022 – 10:47 PM EST

PDB ID	:	7KJK
EMDB ID	:	EMD-22896
Title	:	The Neck region of Phage XM1 (6-fold symmetry)
Authors	:	Wang, Z.; Klose, T.; Jiang, W.; Kuhn, R.J.
Deposited on	:	2020-10-26
Resolution	:	3.60 Å(reported)

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

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

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

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

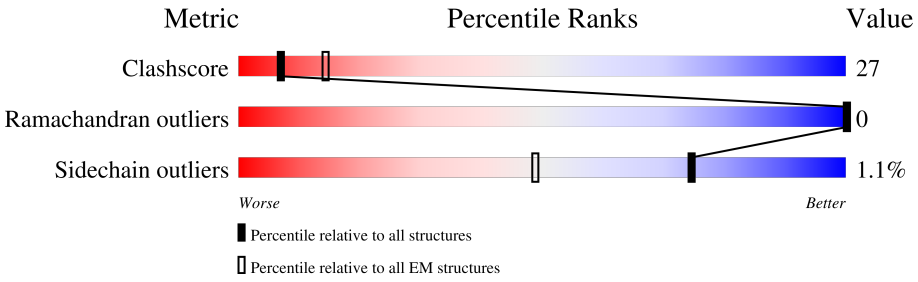
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A5	161	47% 51%
1	B5	161	44% 53%
1	C5	161	46% 52%
1	D5	161	48% 50%
1	E5	161	50% 48%
1	F5	161	45% 52%
2	A3	839	8% 7% 85%
2	B3	839	8% 7% 85%

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Mol	Chain	Length	Quality of chain
2	C3	839	9% 6% 85%
2	D3	839	7% 8% 85%
2	E3	839	9% 6% 85%
2	F3	839	9% 6% 85%
2	G3	839	8% 7% 85%
2	H3	839	9% 6% 85%
2	I3	839	9% 6% 85%
2	J3	839	8% 7% 85%
2	K3	839	8% 7% 85%
2	L3	839	9% 6% 85%
2	M3	839	8% 7% 85%
2	N3	839	9% 6% 85%
2	O3	839	8% 7% 85%
2	P3	839	8% 7% 85%
2	Q3	839	9% 6% 85%
2	R3	839	9% 6% 85%
3	A4	114	6% 47% 51%
3	B4	114	6% 44% 54%
3	C4	114	46% 52%
3	D4	114	44% 54%
3	E4	114	44% 54%
3	F4	114	5% 41% 57%
4	A7	143	5% 52% 47%
4	B7	143	5% 52% 48%
4	C7	143	5% 52% 47%

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Mol	Chain	Length	Quality of chain
4	D7	143	5% 57% 42%
4	E7	143	59% 40%
4	F7	143	5% 56% 43%
5	A6	497	6% 54% 45%
5	B6	497	5% 54% 46%
5	C6	497	10% 54% 45%
5	D6	497	6% 53% 46%
5	E6	497	6% 55% 45%
5	F6	497	6% 56% 43%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 59088 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 Tail terminator protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A5	159	Total	C	N	O	S	0	0
			1267	793	210	262	2		
1	B5	159	Total	C	N	O	S	0	0
			1267	793	210	262	2		
1	C5	159	Total	C	N	O	S	0	0
			1267	793	210	262	2		
1	D5	159	Total	C	N	O	S	0	0
			1267	793	210	262	2		
1	E5	159	Total	C	N	O	S	0	0
			1267	793	210	262	2		
1	F5	159	Total	C	N	O	S	0	0
			1267	793	210	262	2		

- Molecule 2 is a protein called Collar spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A3	126	Total	C	N	O	S	0	0
			951	594	157	199	1		
2	B3	126	Total	C	N	O	S	0	0
			951	594	157	199	1		
2	C3	126	Total	C	N	O	S	0	0
			949	593	157	198	1		
2	D3	126	Total	C	N	O	S	0	0
			951	594	157	199	1		
2	E3	126	Total	C	N	O	S	0	0
			951	594	157	199	1		
2	F3	126	Total	C	N	O	S	0	0
			949	593	157	198	1		
2	G3	126	Total	C	N	O	S	0	0
			951	594	157	199	1		
2	H3	126	Total	C	N	O	S	0	0
			951	594	157	199	1		
2	I3	126	Total	C	N	O	S	0	0
			949	593	157	198	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	J3	126	Total	C	N	O	S	0	0
			951	594	157	199	1		
2	K3	126	Total	C	N	O	S	0	0
			951	594	157	199	1		
2	L3	126	Total	C	N	O	S	0	0
			949	593	157	198	1		
2	M3	126	Total	C	N	O	S	0	0
			951	594	157	199	1		
2	N3	126	Total	C	N	O	S	0	0
			951	594	157	199	1		
2	O3	126	Total	C	N	O	S	0	0
			949	593	157	198	1		
2	P3	126	Total	C	N	O	S	0	0
			951	594	157	199	1		
2	Q3	126	Total	C	N	O	S	0	0
			951	594	157	199	1		
2	R3	126	Total	C	N	O	S	0	0
			949	593	157	198	1		

- Molecule 3 is a protein called Head completion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A4	114	Total	C	N	O	S	0	0
			918	594	148	172	4		
3	B4	114	Total	C	N	O	S	0	0
			918	594	148	172	4		
3	C4	114	Total	C	N	O	S	0	0
			918	594	148	172	4		
3	D4	114	Total	C	N	O	S	0	0
			918	594	148	172	4		
3	E4	114	Total	C	N	O	S	0	0
			918	594	148	172	4		
3	F4	114	Total	C	N	O	S	0	0
			918	594	148	172	4		

- Molecule 4 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A7	142	Total	C	N	O	S	0	0
			1091	673	192	224	2		
4	B7	142	Total	C	N	O	S	0	0
			1091	673	192	224	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	C7	142	Total	C	N	O	S	0	0
			1091	673	192	224	2		
4	D7	142	Total	C	N	O	S	0	0
			1091	673	192	224	2		
4	E7	142	Total	C	N	O	S	0	0
			1091	673	192	224	2		
4	F7	142	Total	C	N	O	S	0	0
			1091	673	192	224	2		

- Molecule 5 is a protein called Tail sheath protein.

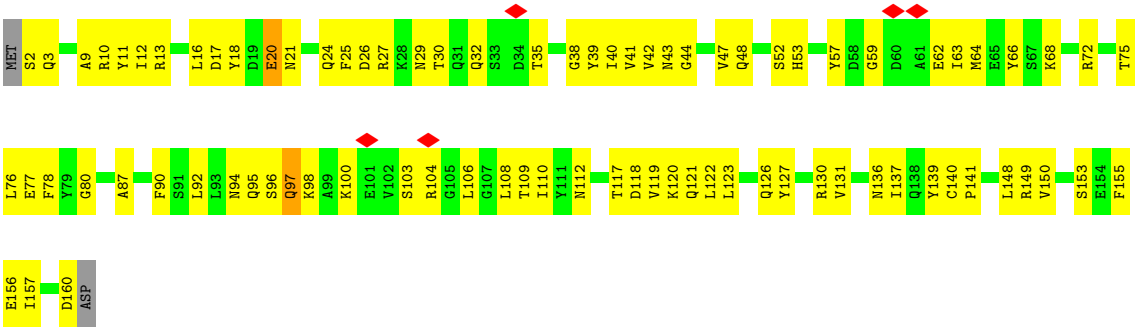
Mol	Chain	Residues	Atoms					AltConf	Trace
5	A6	497	Total	C	N	O	S	0	0
			3721	2321	616	772	12		
5	B6	497	Total	C	N	O	S	0	0
			3721	2321	616	772	12		
5	C6	497	Total	C	N	O	S	0	0
			3721	2321	616	772	12		
5	D6	497	Total	C	N	O	S	0	0
			3721	2321	616	772	12		
5	E6	497	Total	C	N	O	S	0	0
			3721	2321	616	772	12		
5	F6	497	Total	C	N	O	S	0	0
			3721	2321	616	772	12		

3 Residue-property plots (i)

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

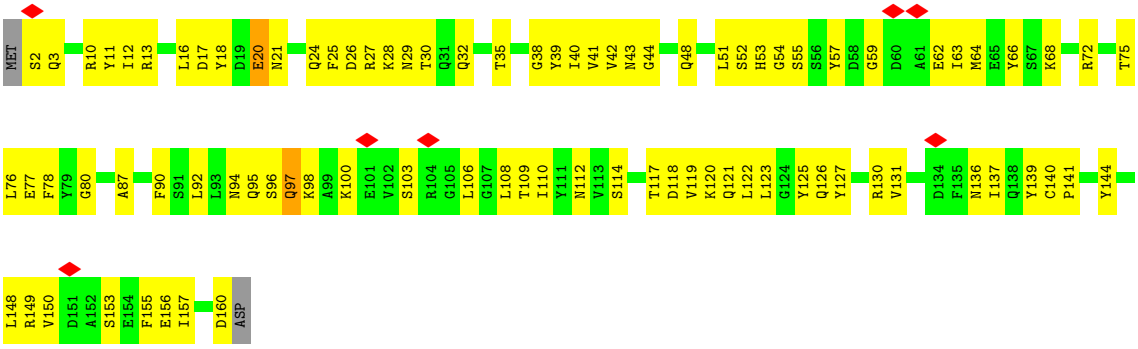
• Molecule 1: Tail terminator protein

Chain A5:



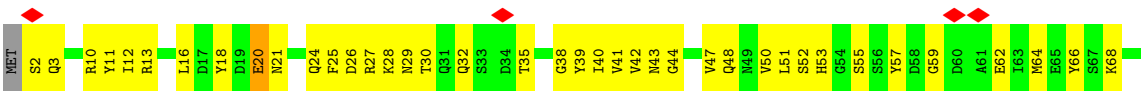
• Molecule 1: Tail terminator protein

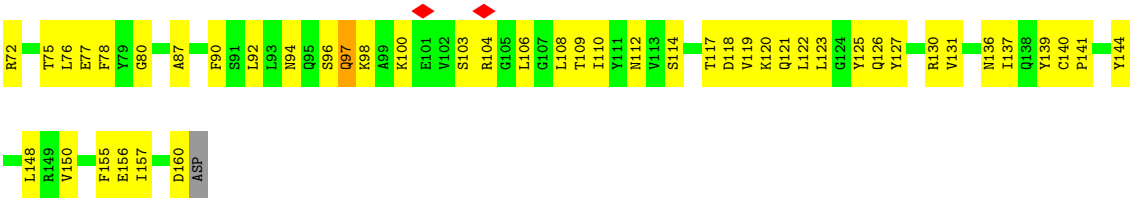
Chain B5:



• Molecule 1: Tail terminator protein

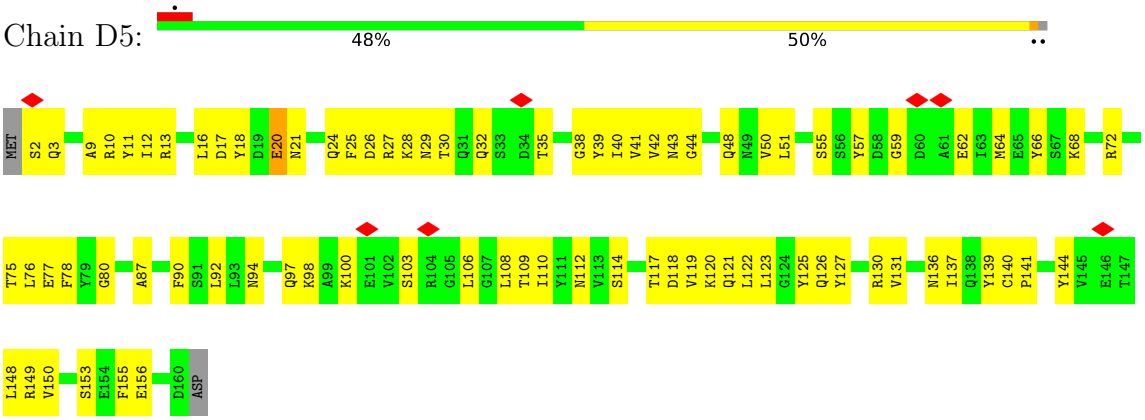
Chain C5:





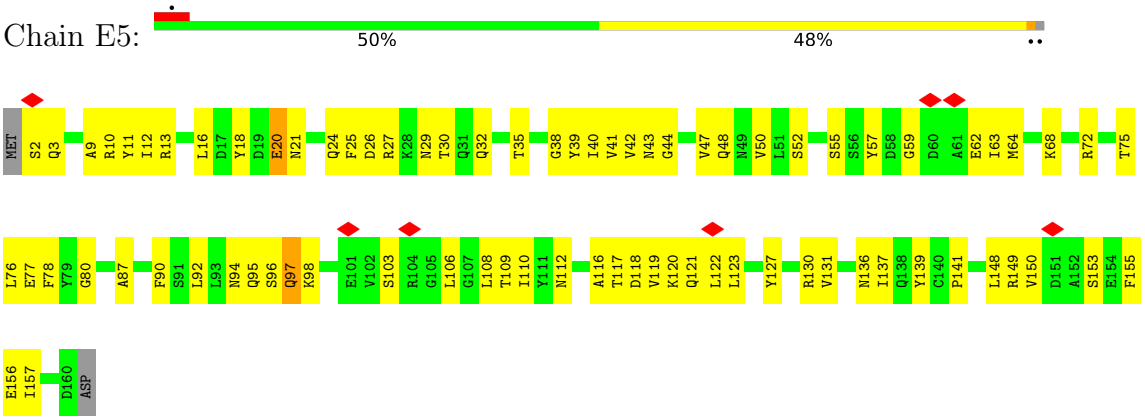
• Molecule 1: Tail terminator protein

Chain D5:



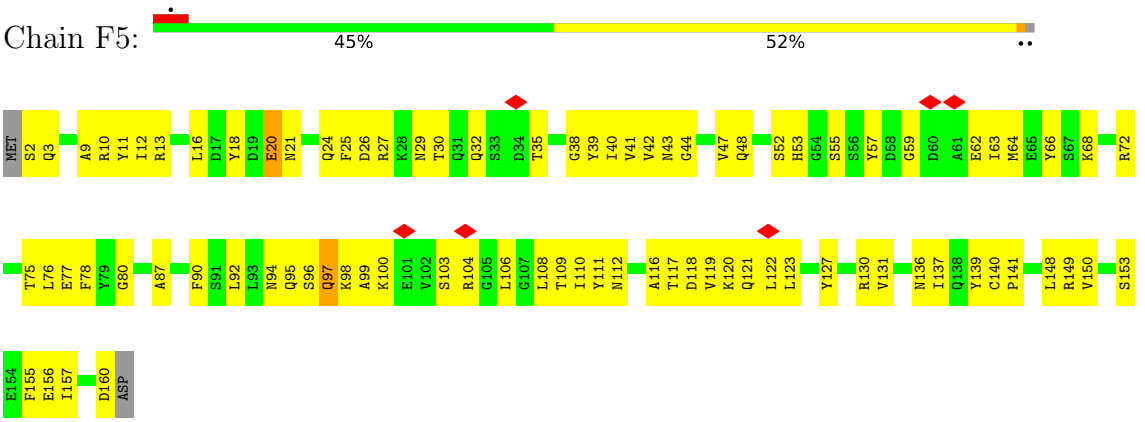
• Molecule 1: Tail terminator protein

Chain E5:



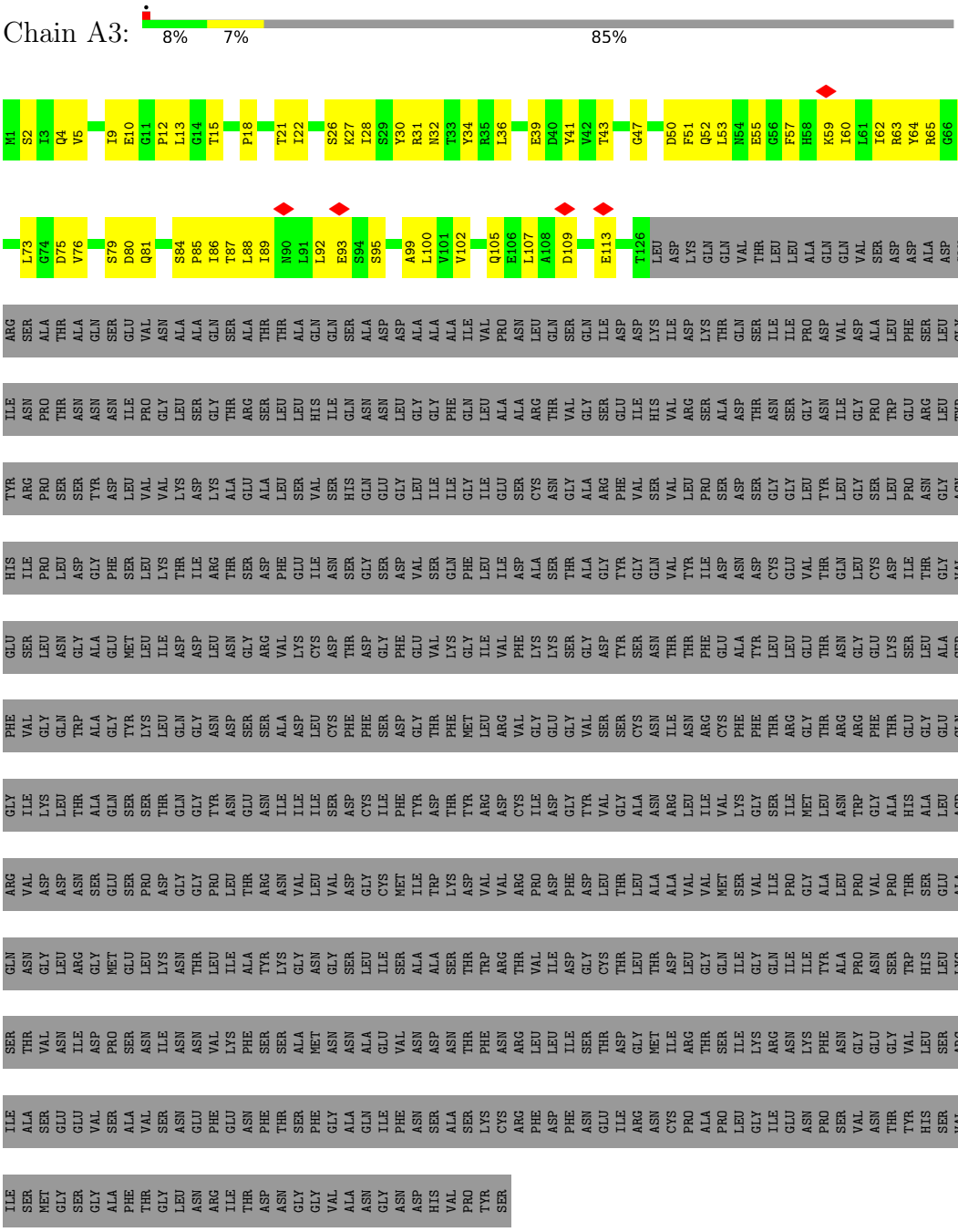
• Molecule 1: Tail terminator protein

Chain F5:



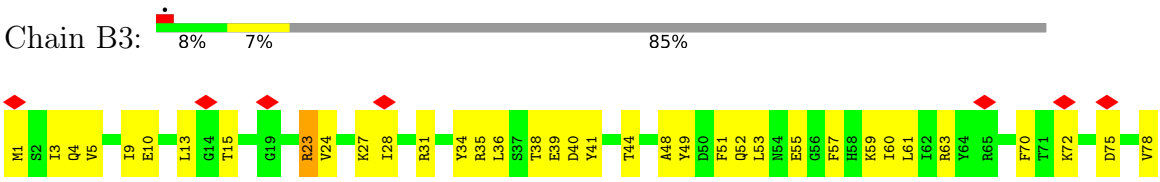
• Molecule 2: Collar spike protein

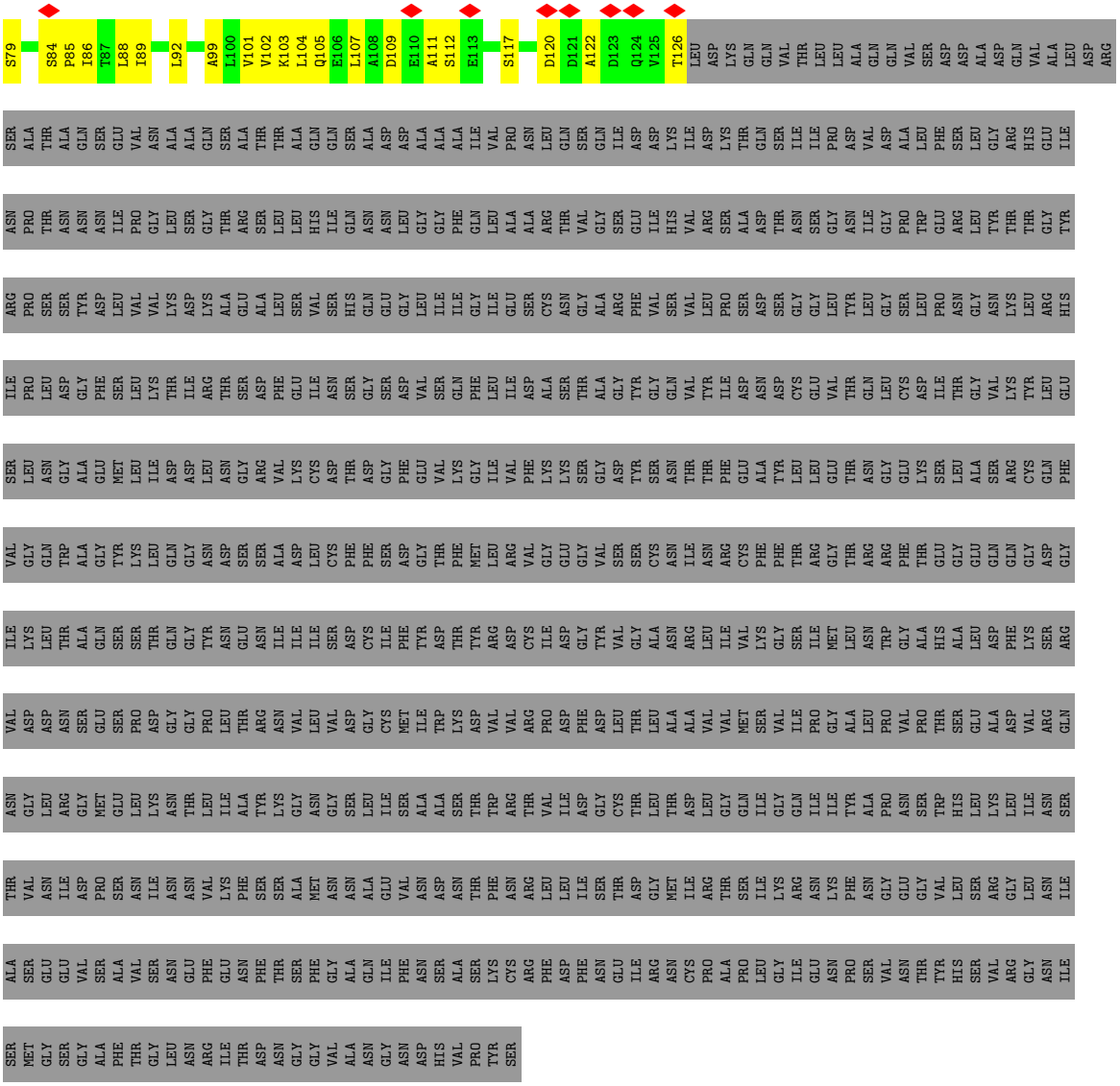
Chain A3:



• Molecule 2: Collar spike protein

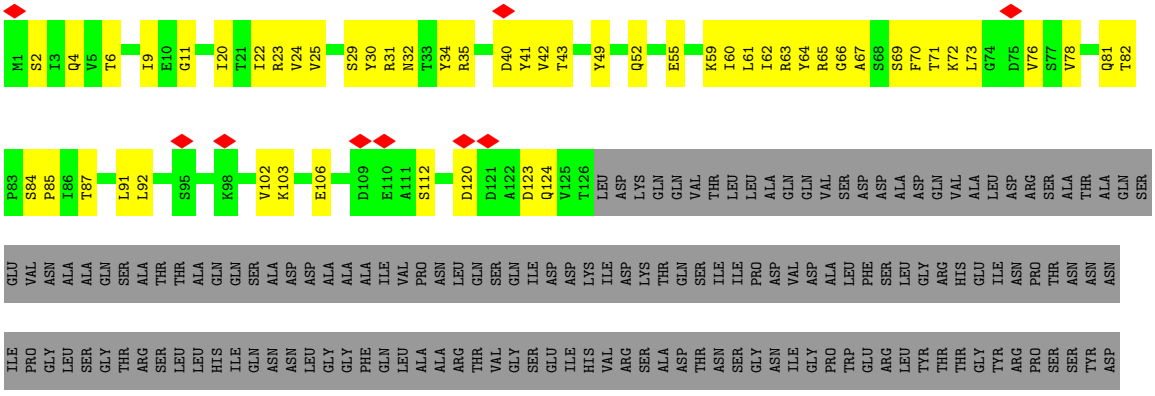
Chain B3:

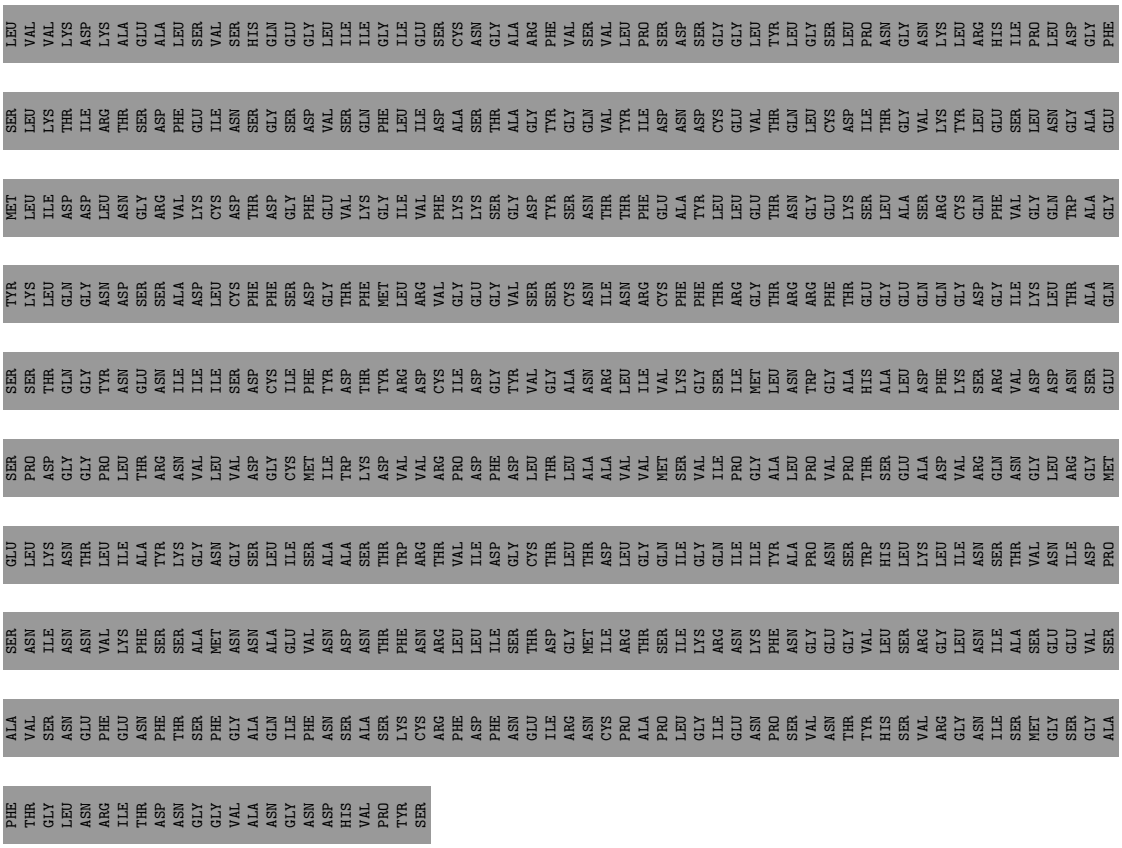




• Molecule 2: Collar spike protein

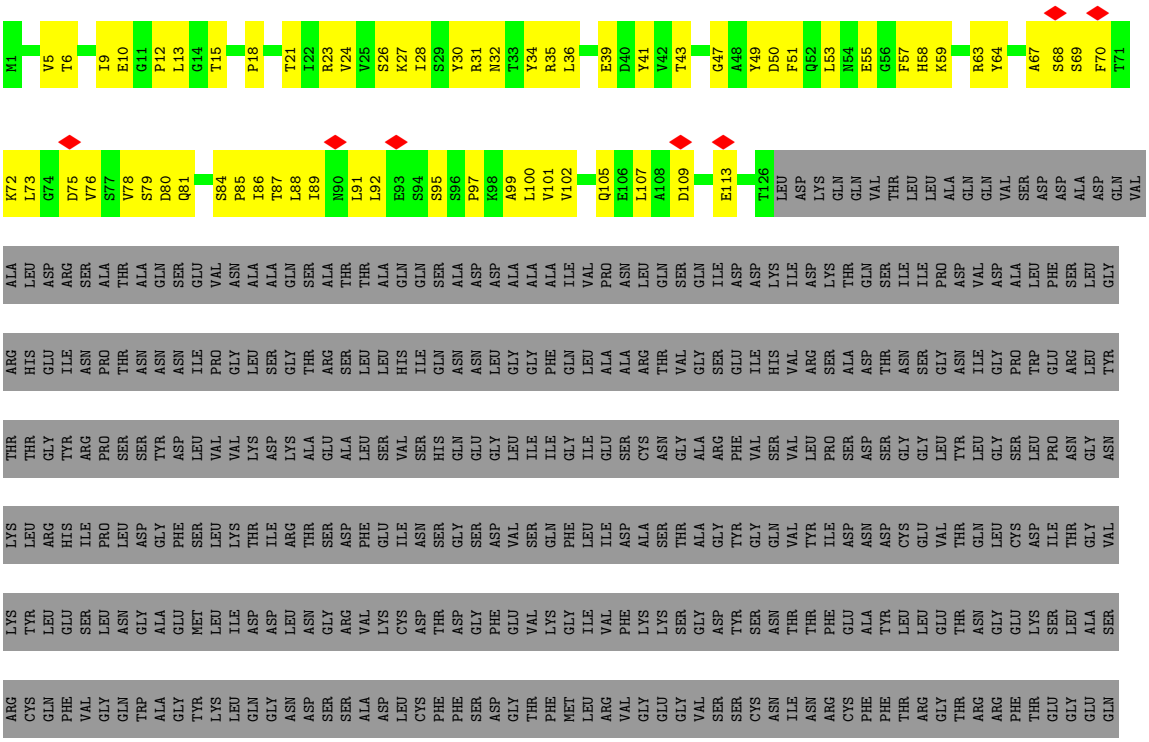
Chain C3:

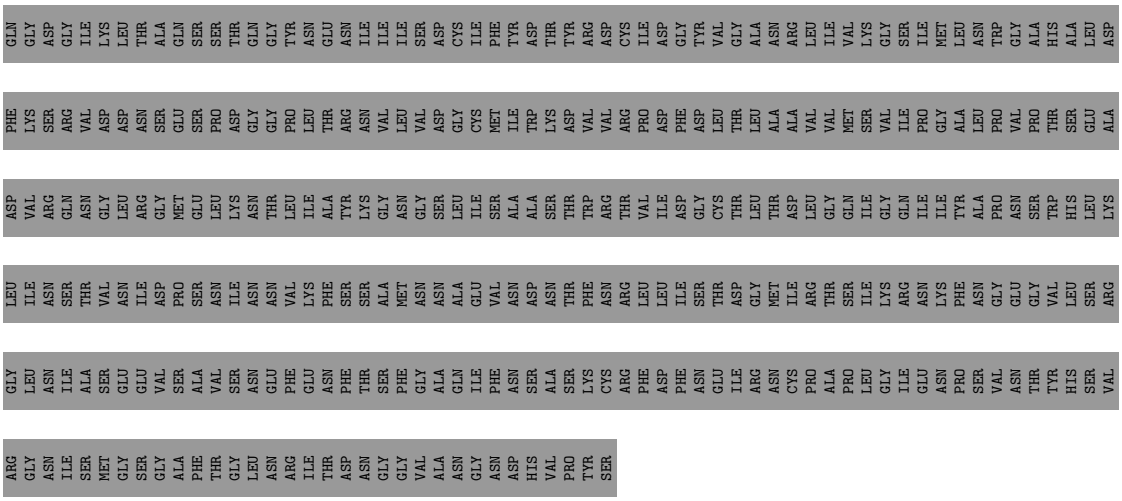




• Molecule 2: Collar spike protein

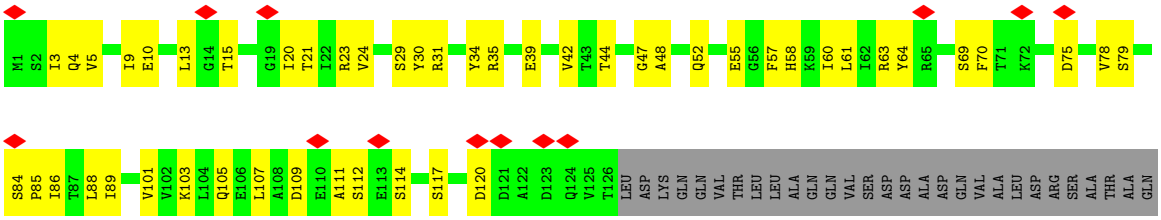
Chain D3:

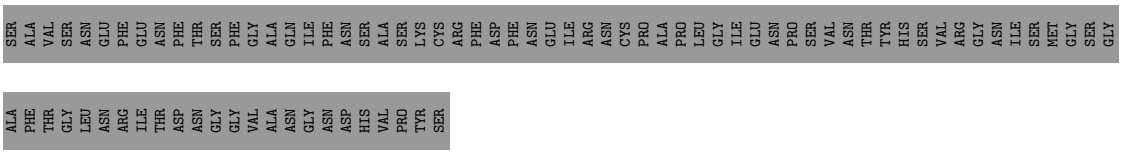




• Molecule 2: Collar spike protein

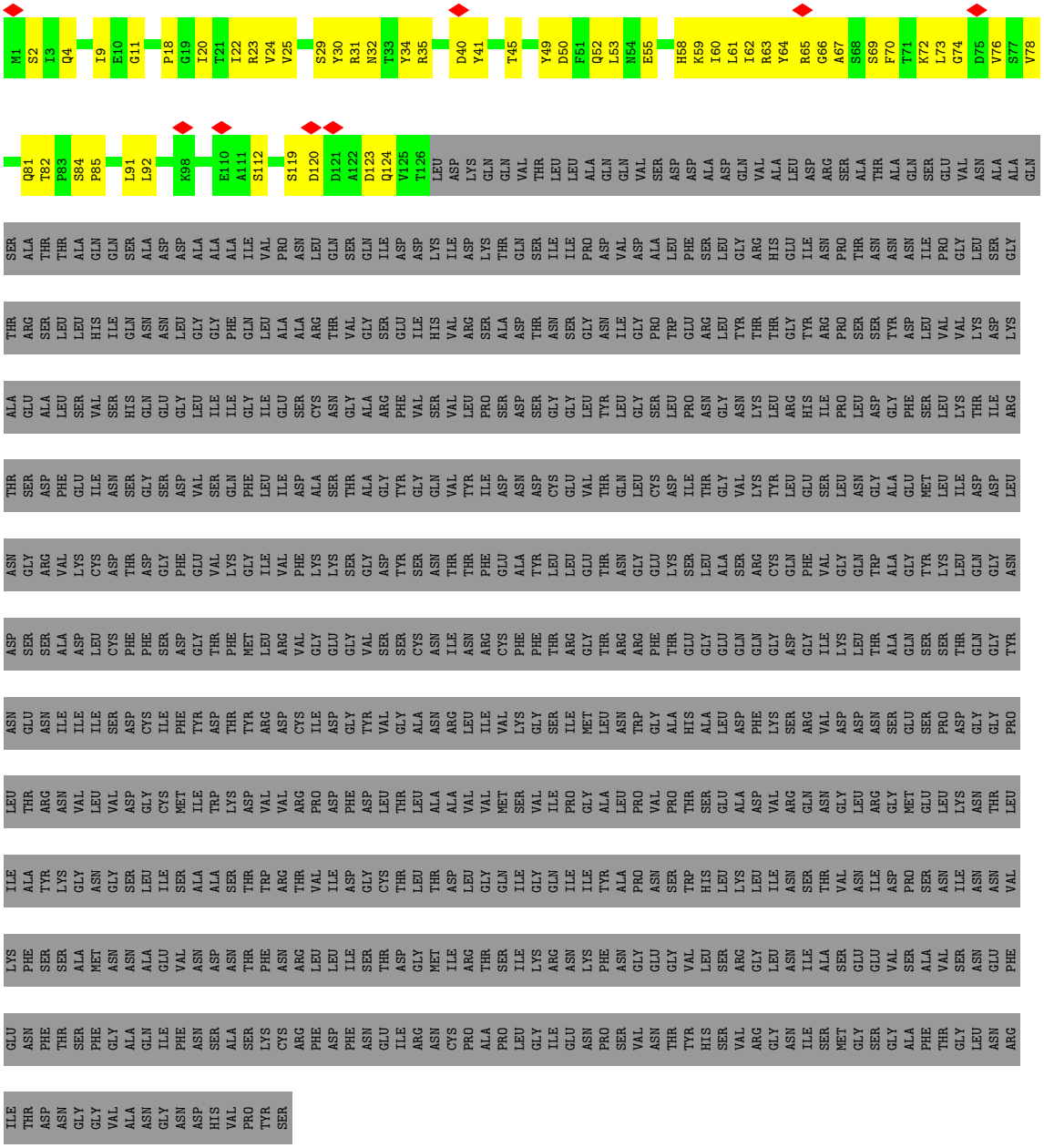
Chain E3:





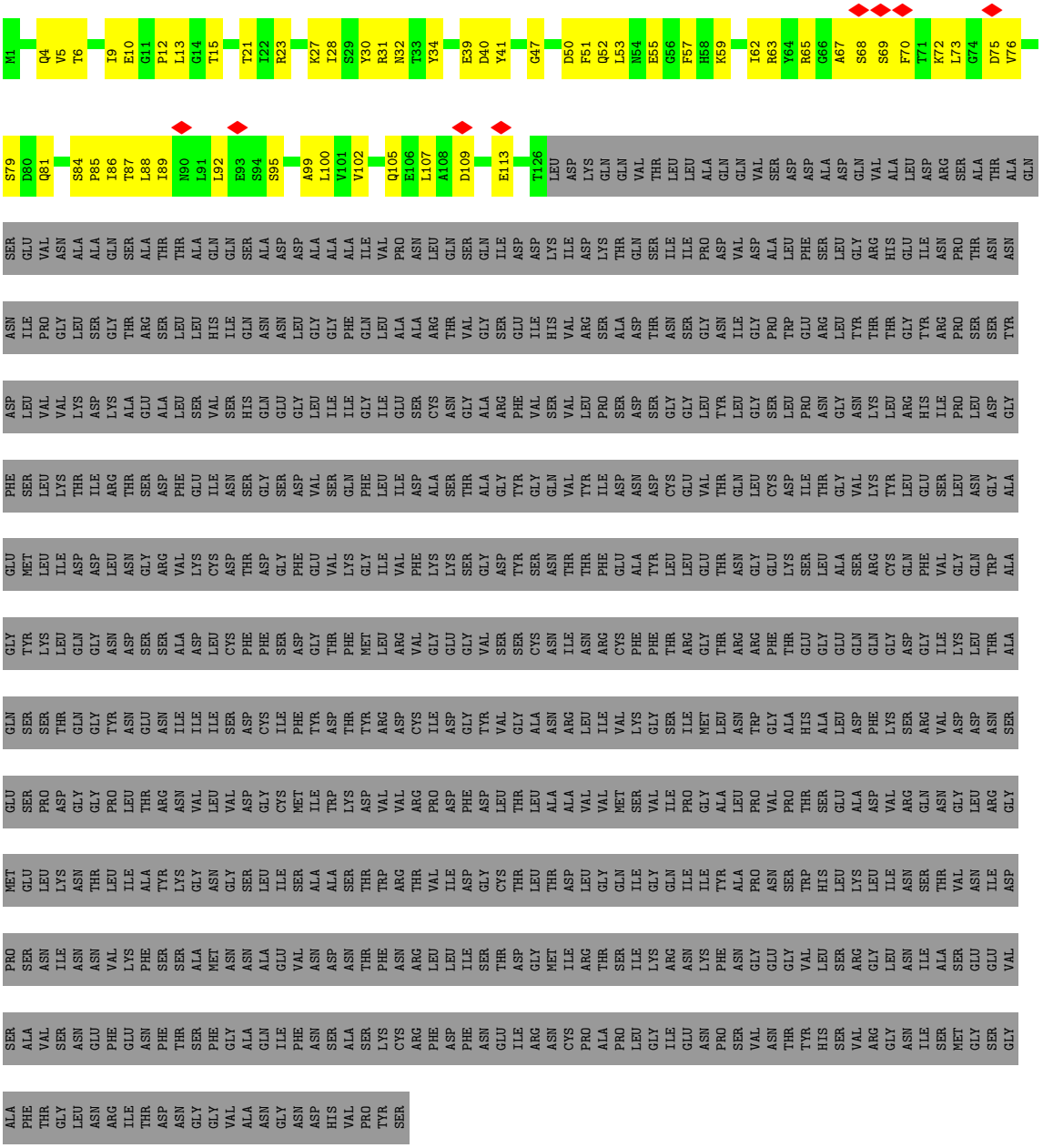
• Molecule 2: Collar spike protein

Chain F3:



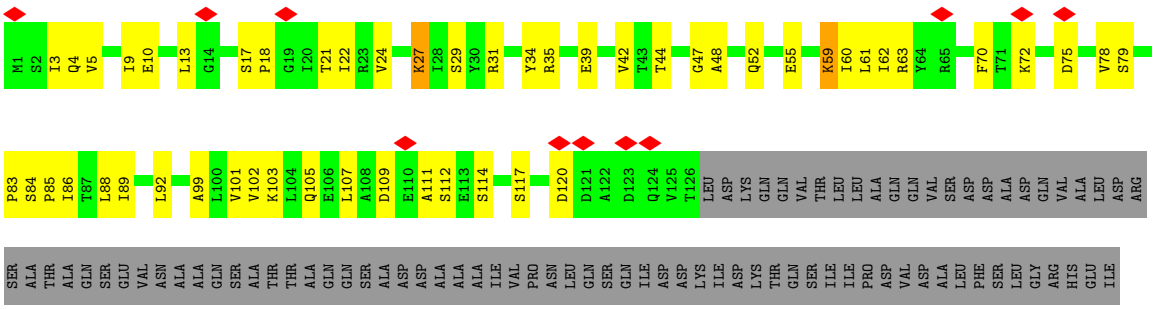
• Molecule 2: Collar spike protein

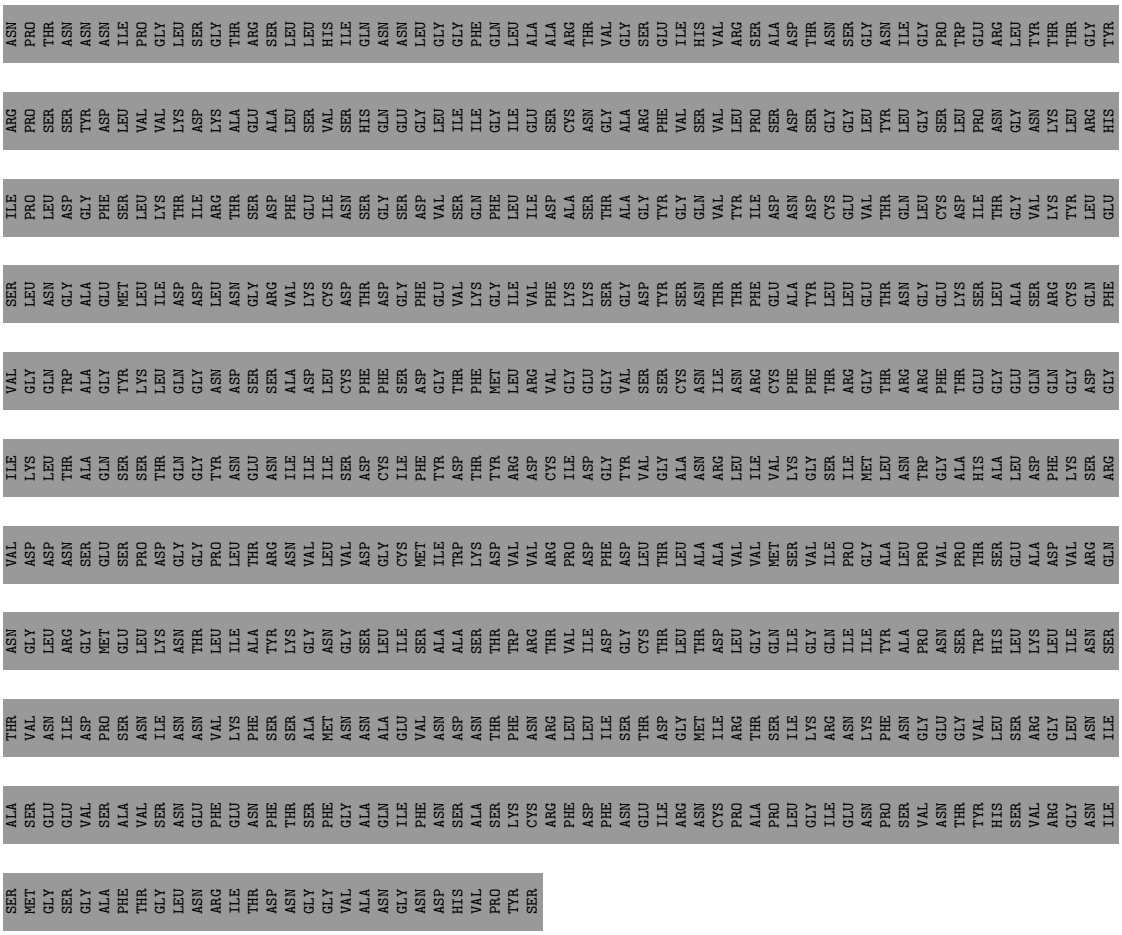
Chain G3:



• Molecule 2: Collar spike protein

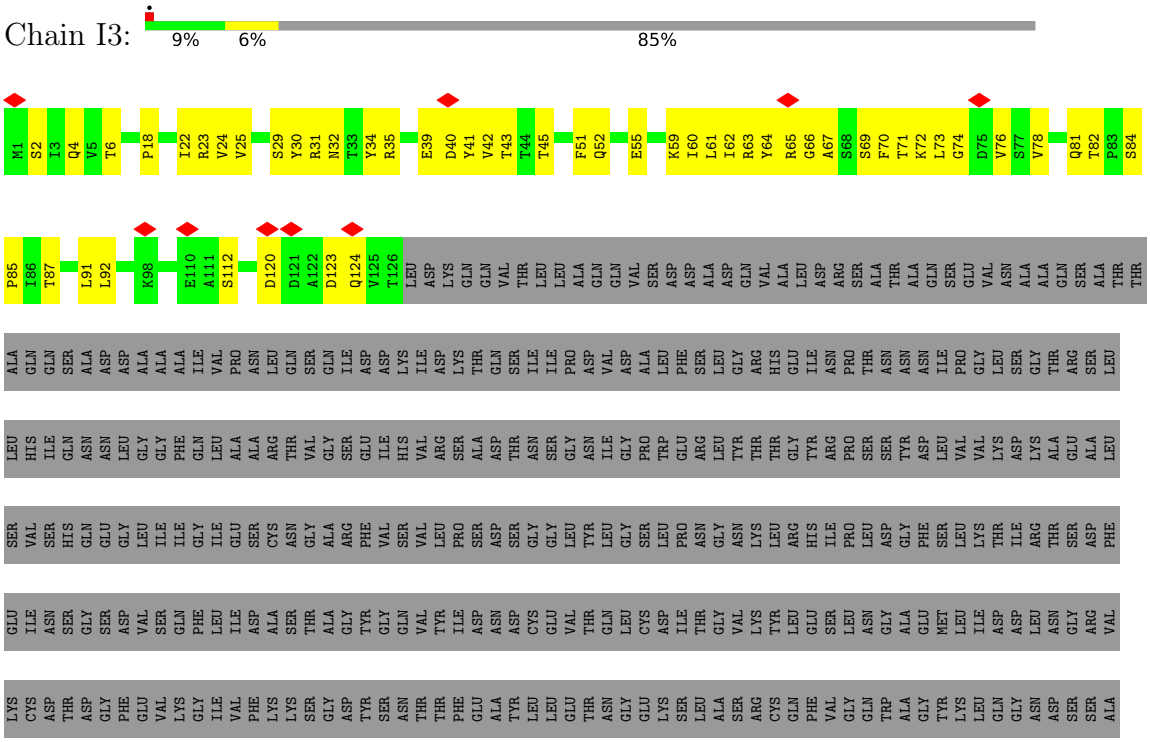
Chain H3:

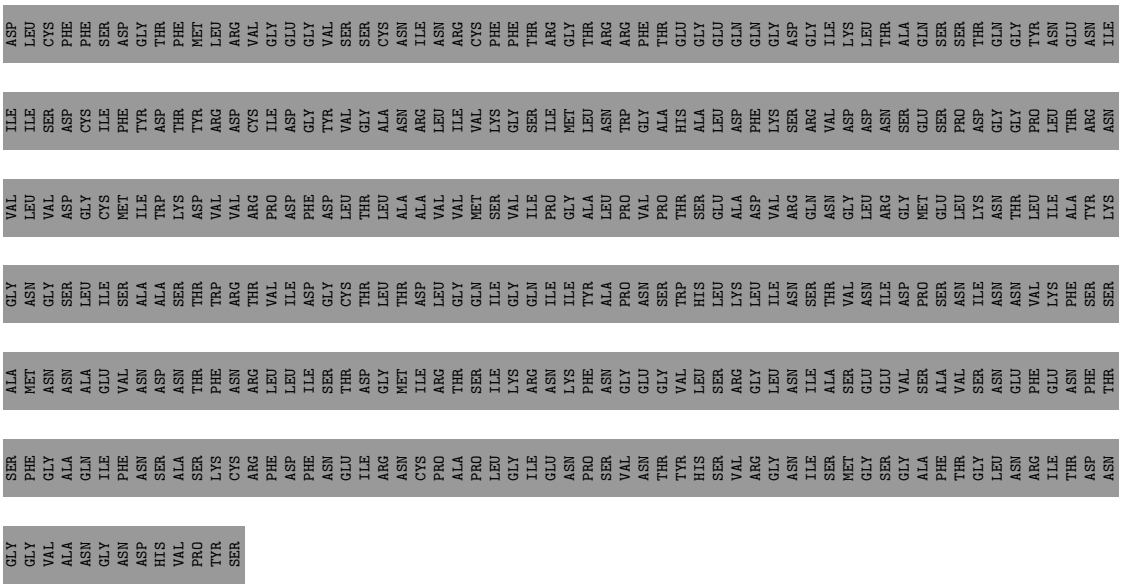




• Molecule 2: Collar spike protein

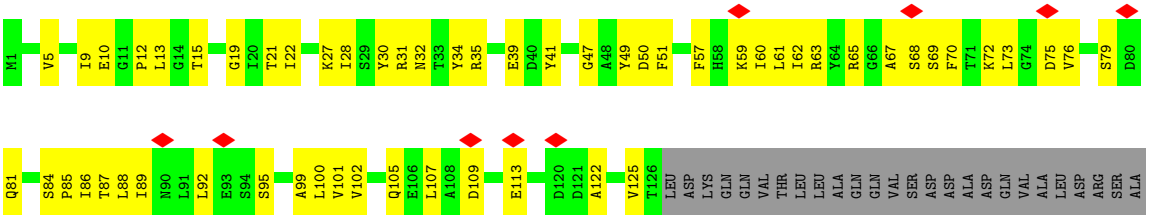
Chain I3:

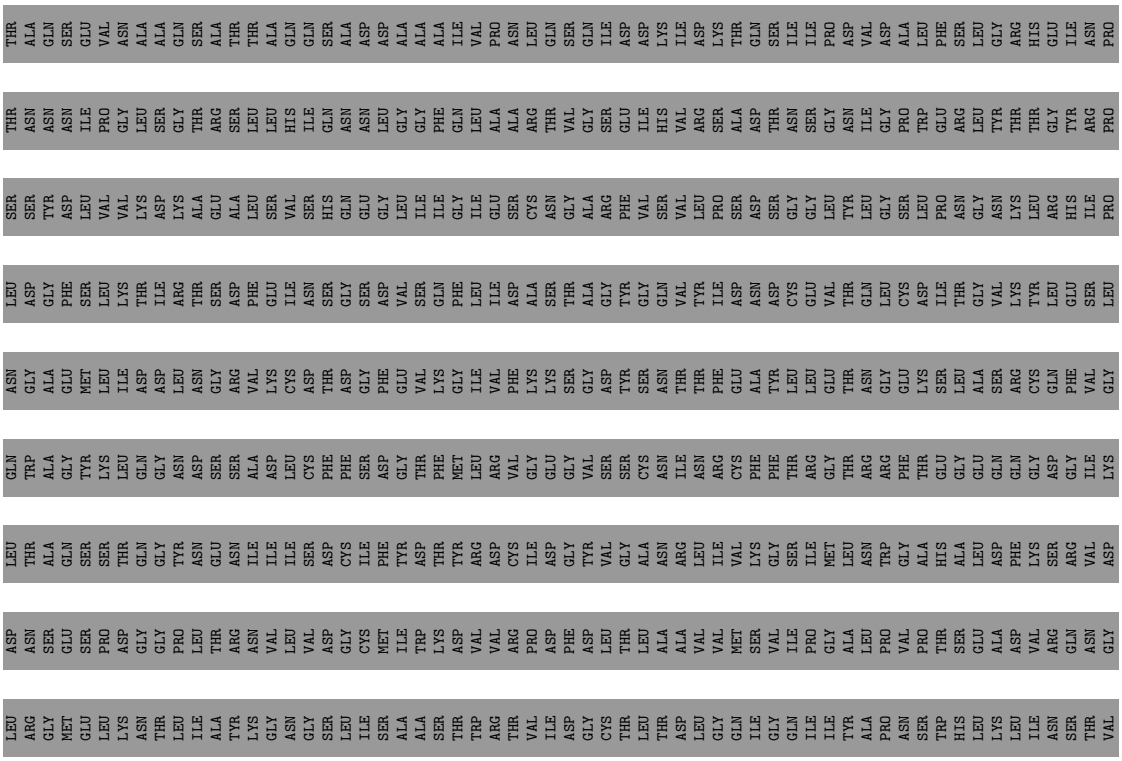


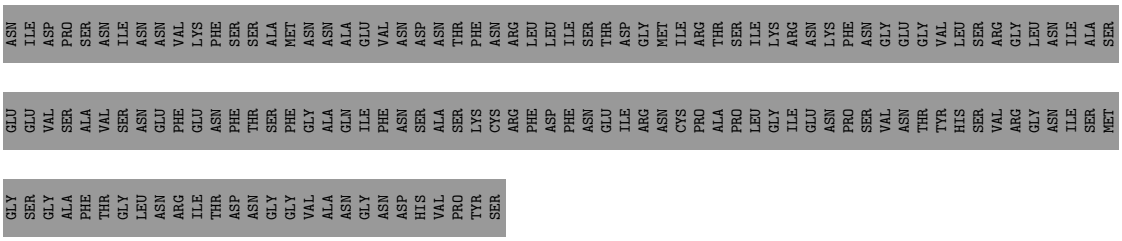


• Molecule 2: Collar spike protein

Chain J3:

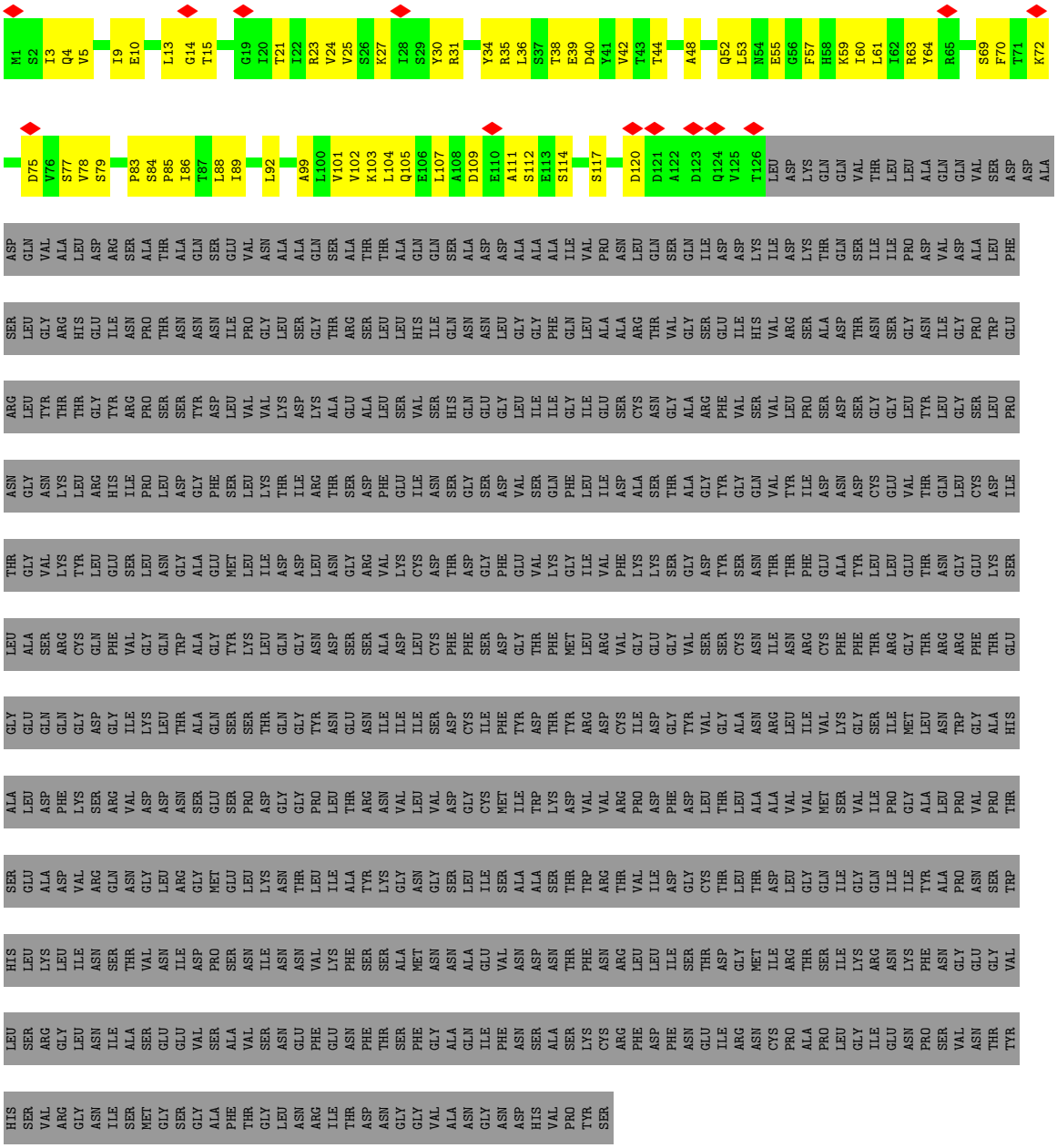






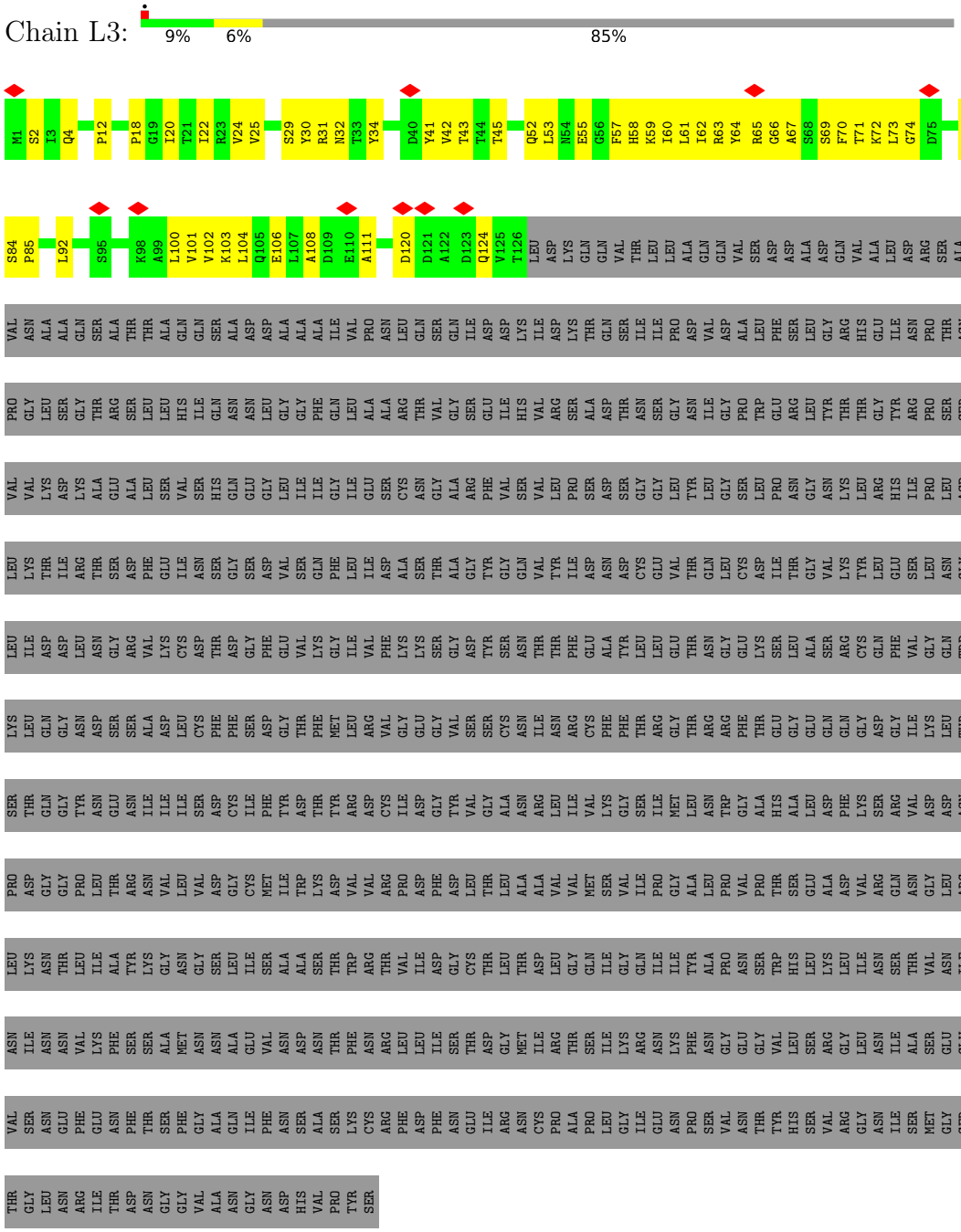
• Molecule 2: Collar spike protein

Chain K3:



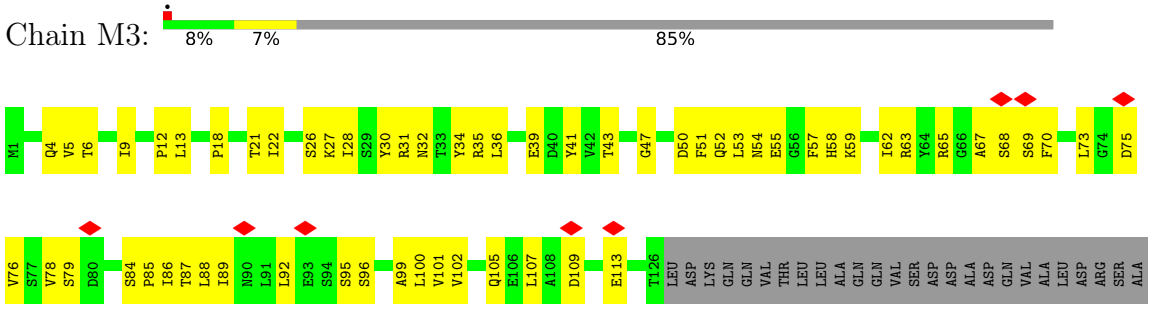
• Molecule 2: Collar spike protein

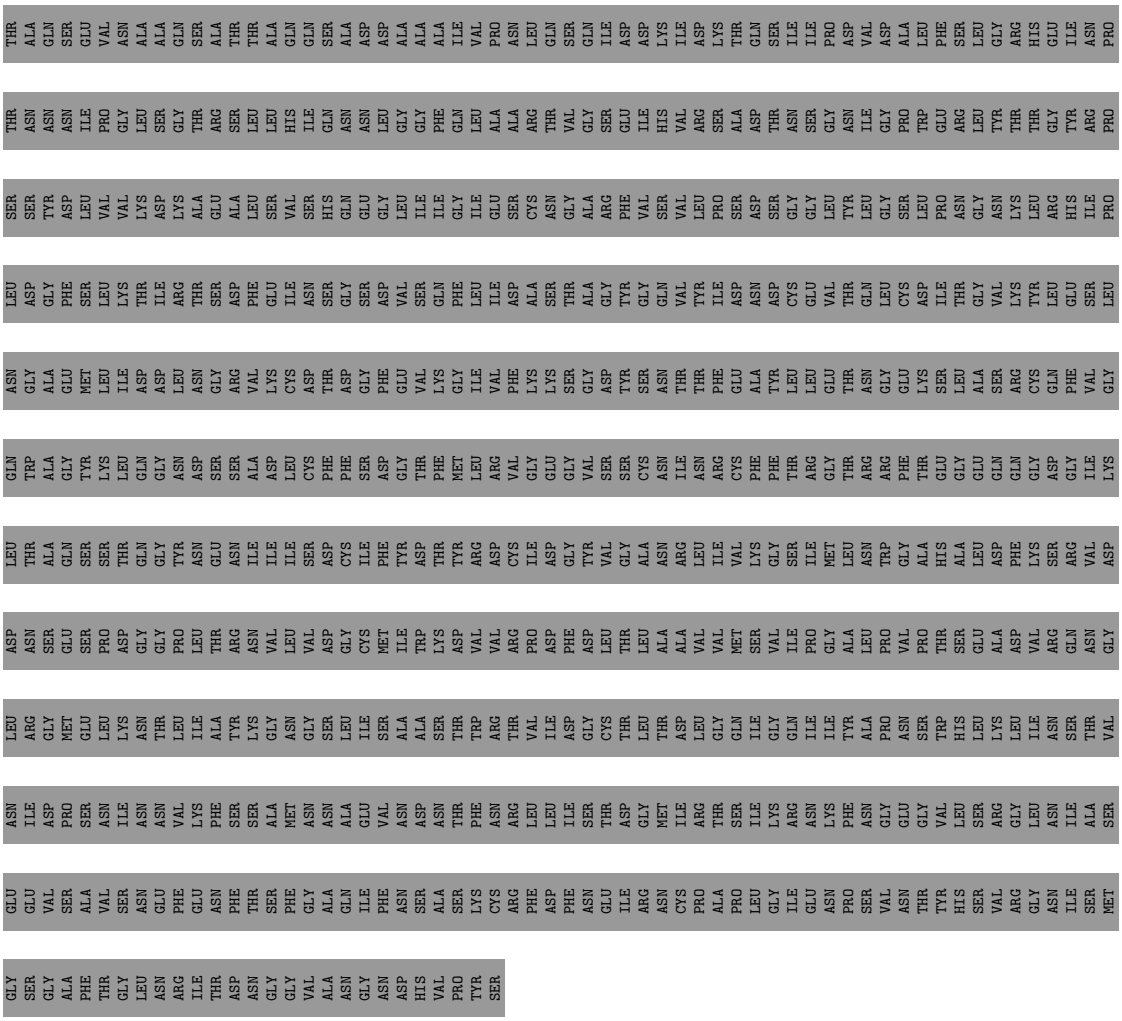
Chain L3:



• Molecule 2: Collar spike protein

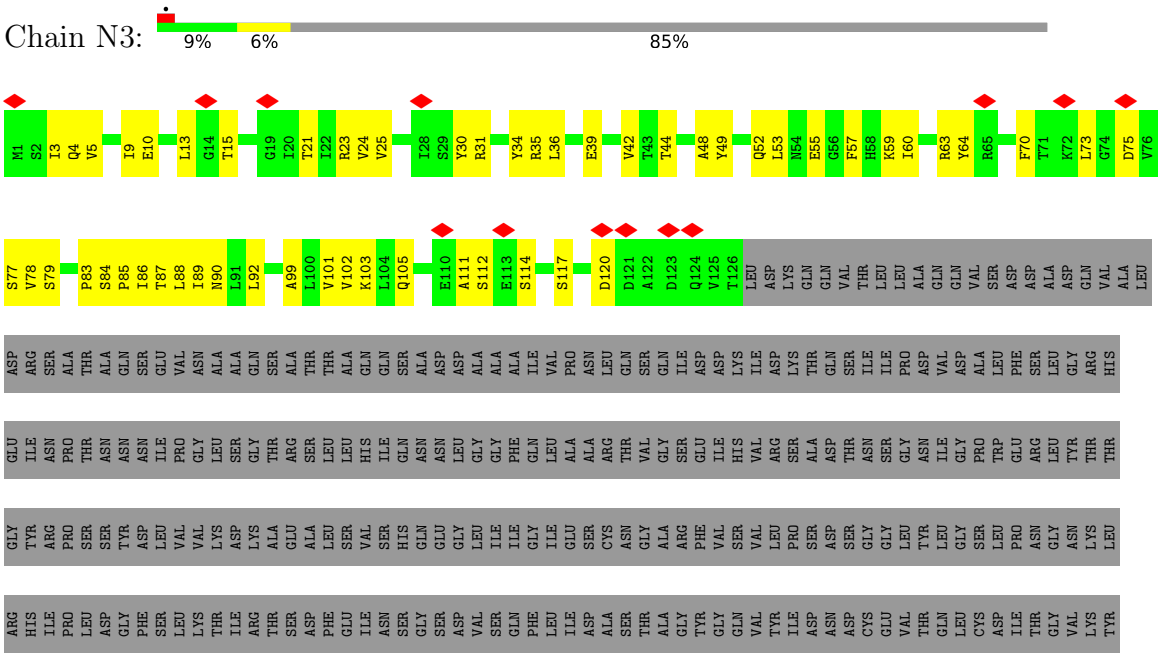
Chain M3:





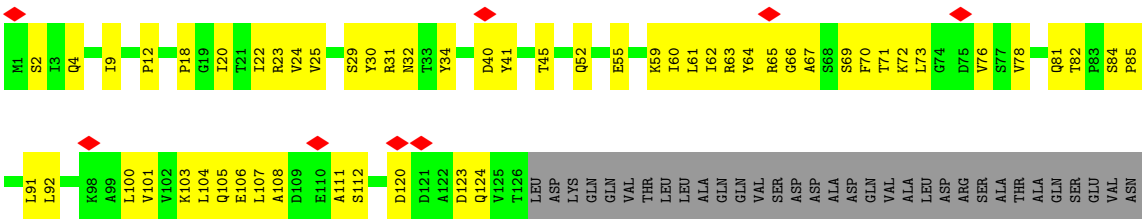
• Molecule 2: Collar spike protein

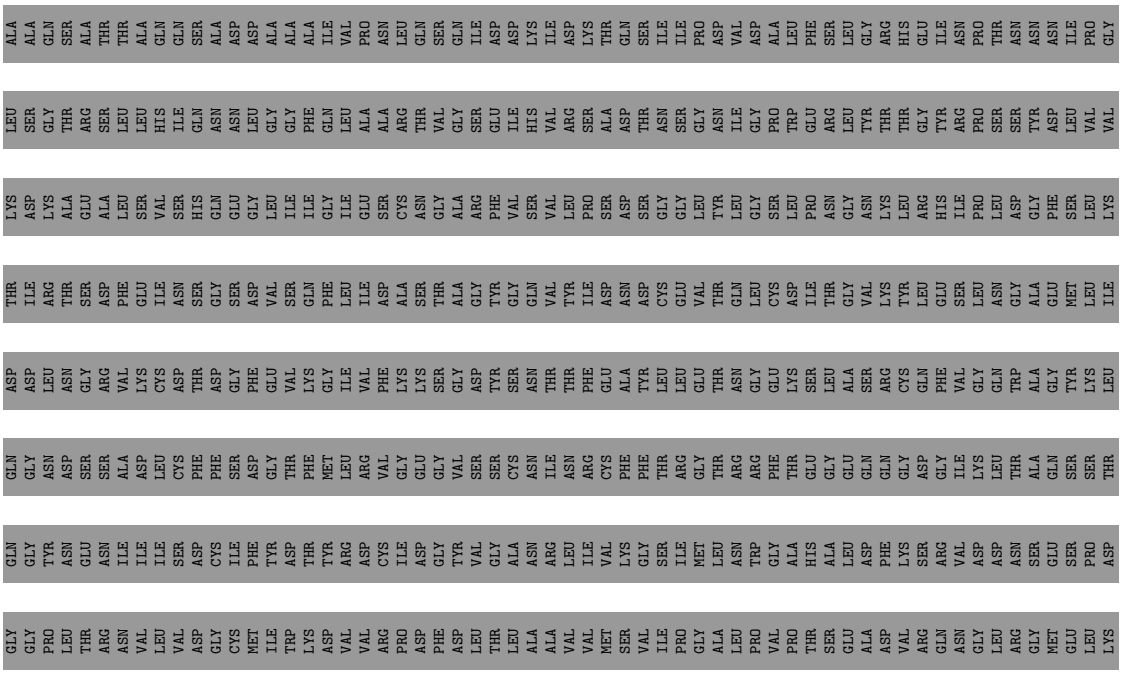
Chain N3:

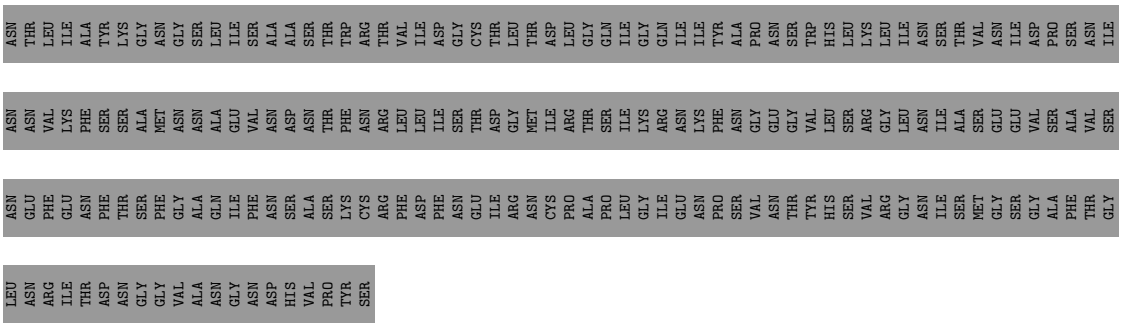


• Molecule 2: Collar spike protein

Chain O3:

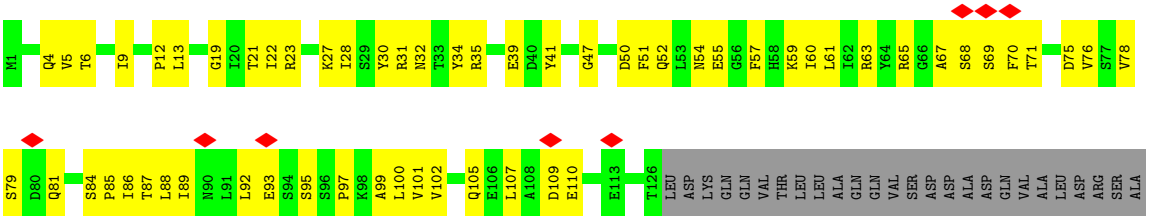


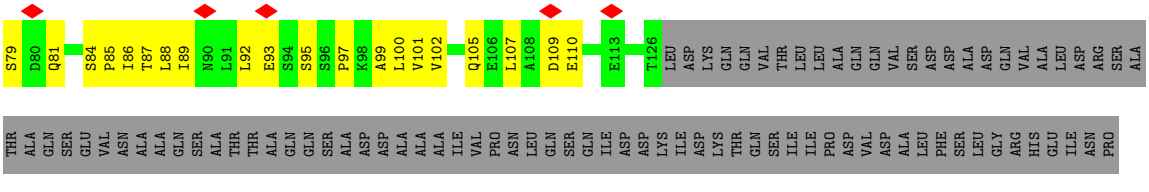


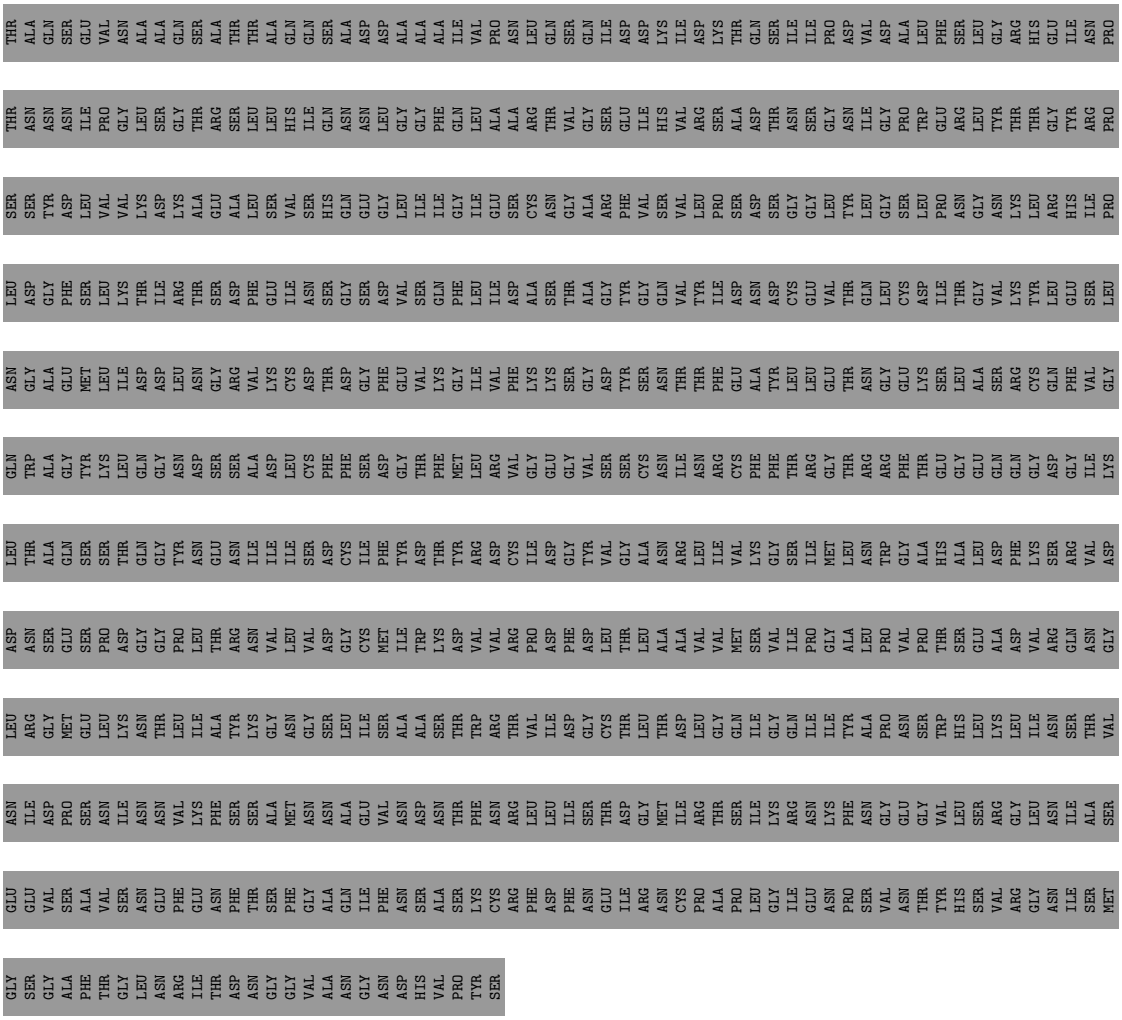


• Molecule 2: Collar spike protein

Chain P3:

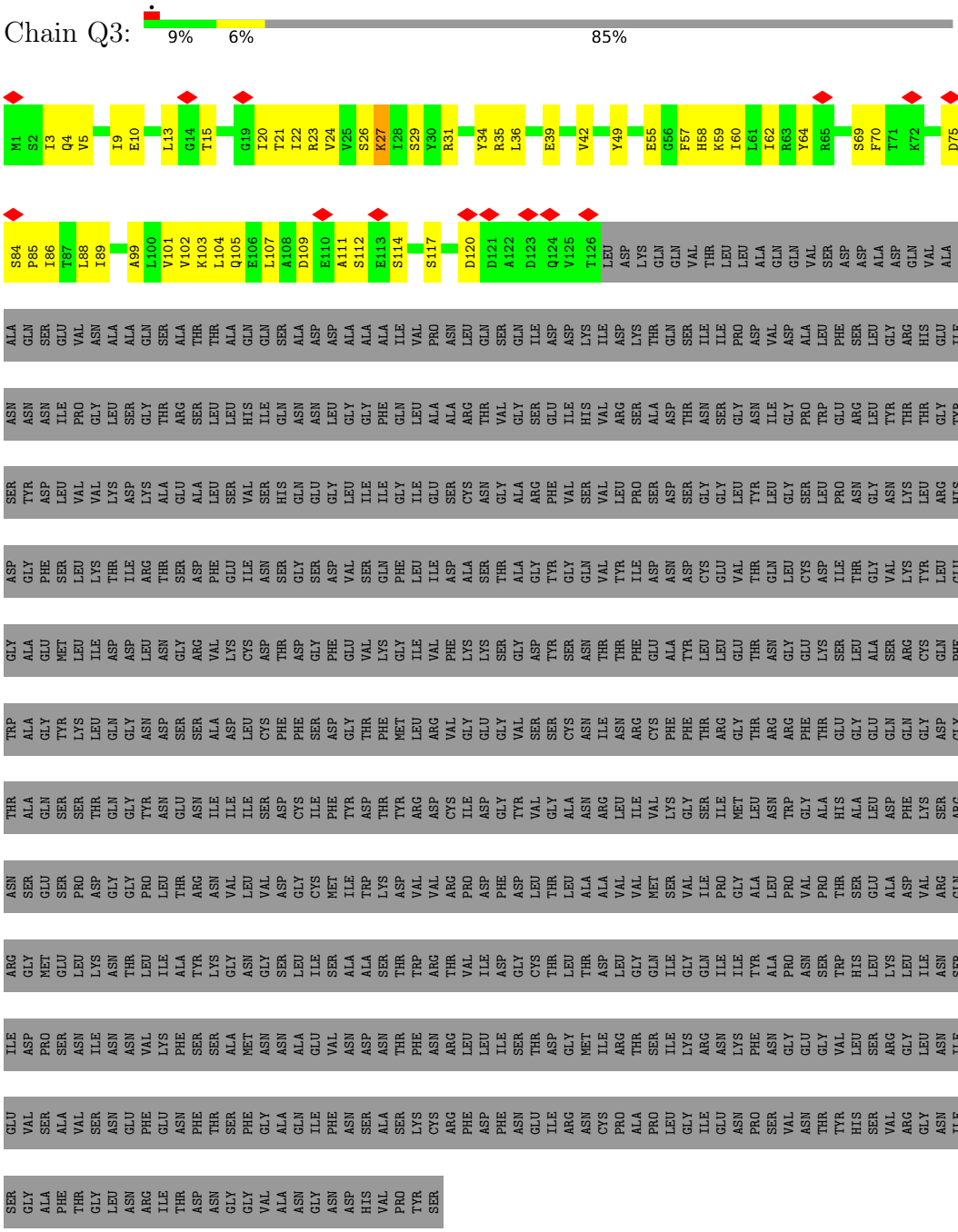






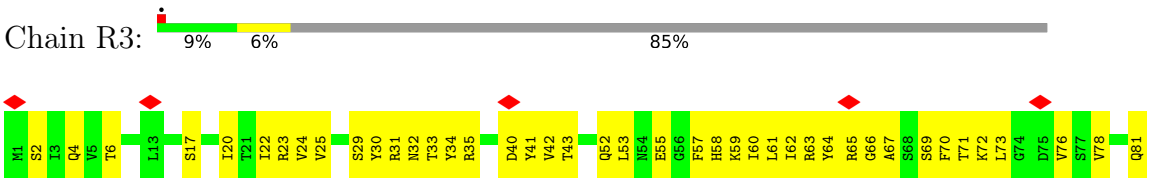
• Molecule 2: Collar spike protein

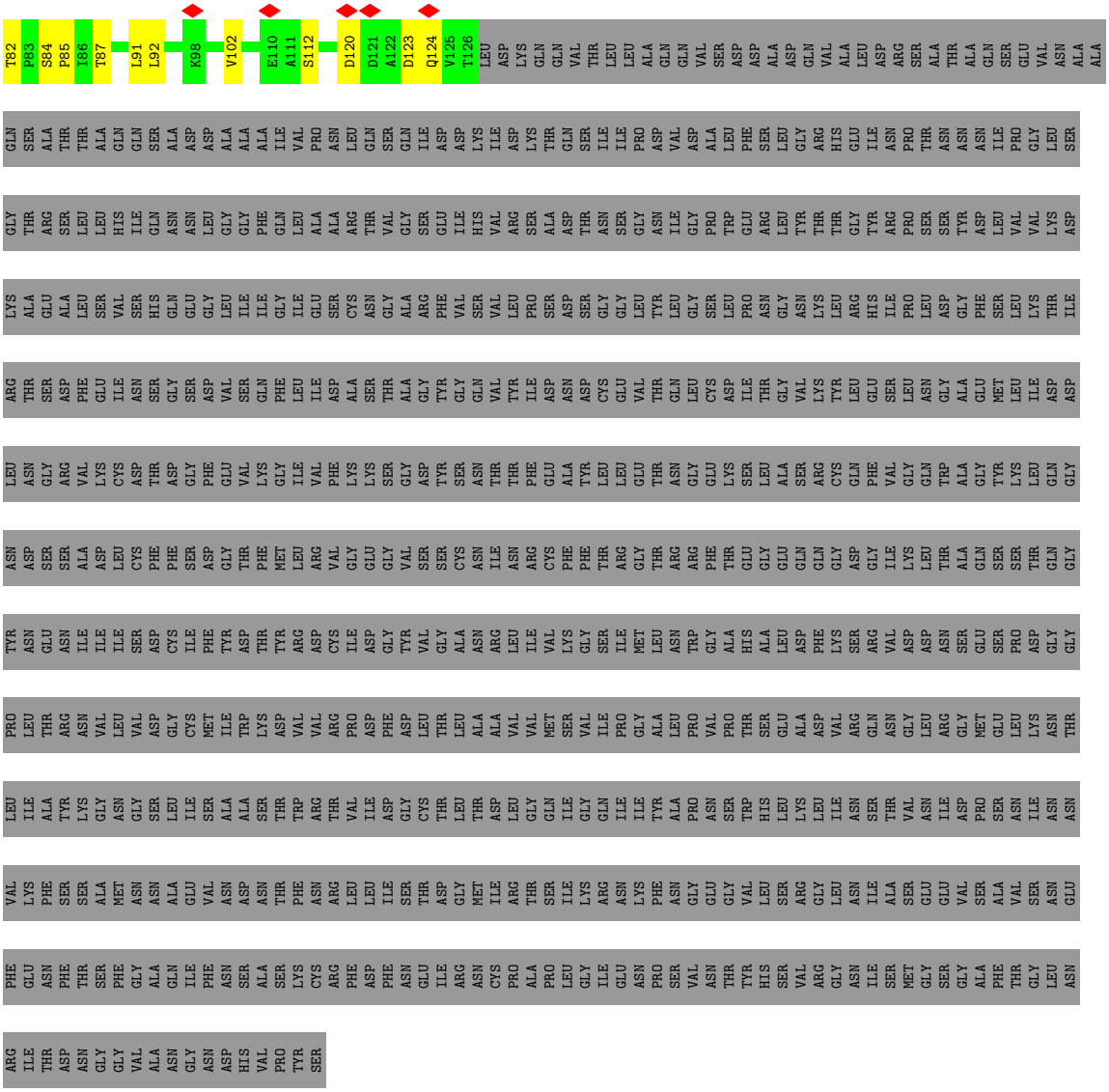
Chain Q3:



• Molecule 2: Collar spike protein

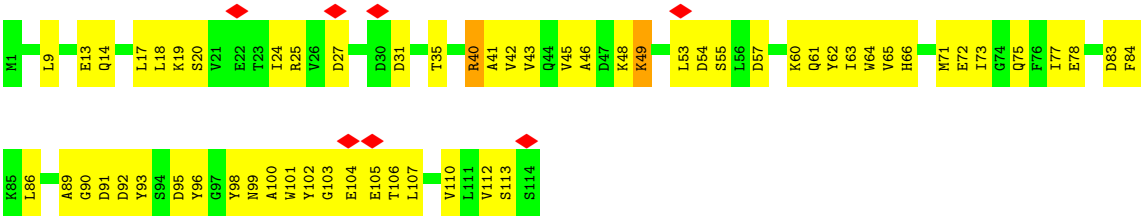
Chain R3:





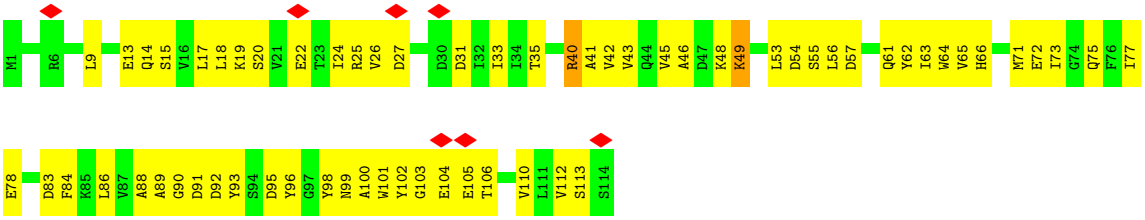
• Molecule 3: Head completion protein

Chain A4:



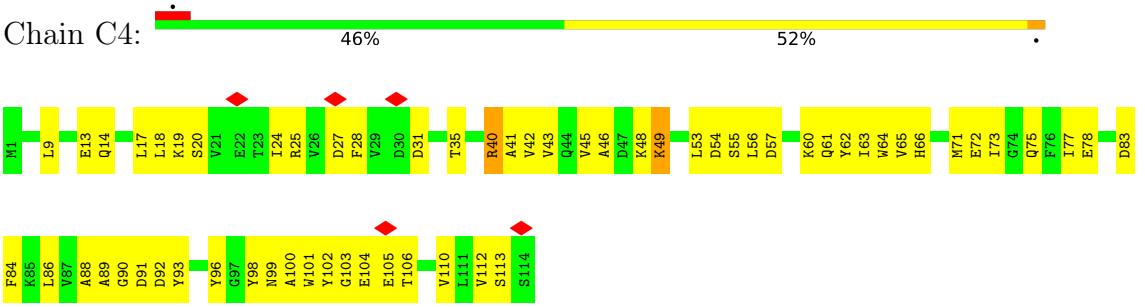
• Molecule 3: Head completion protein

Chain B4:



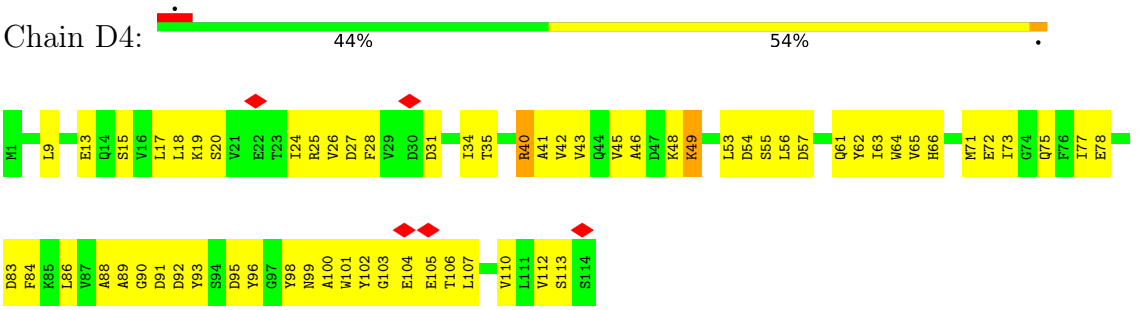
• Molecule 3: Head completion protein

Chain C4:



• Molecule 3: Head completion protein

Chain D4:

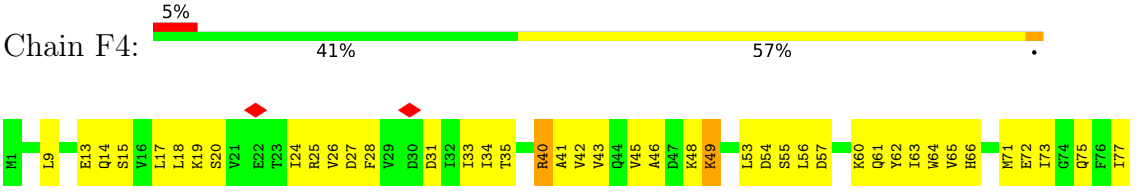


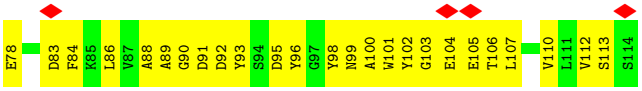
• Molecule 3: Head completion protein

Chain E4:

• Molecule 3: Head completion protein

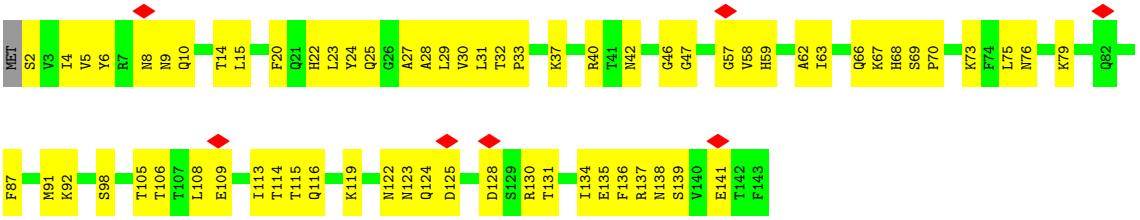
Chain F4:





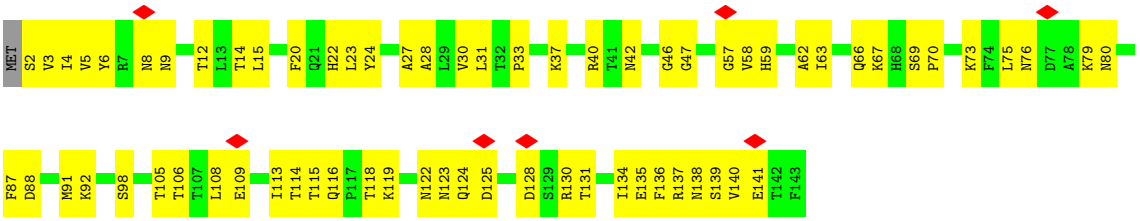
• Molecule 4: Tail tube protein

Chain A7:



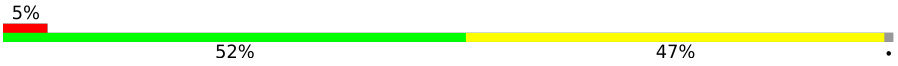
• Molecule 4: Tail tube protein

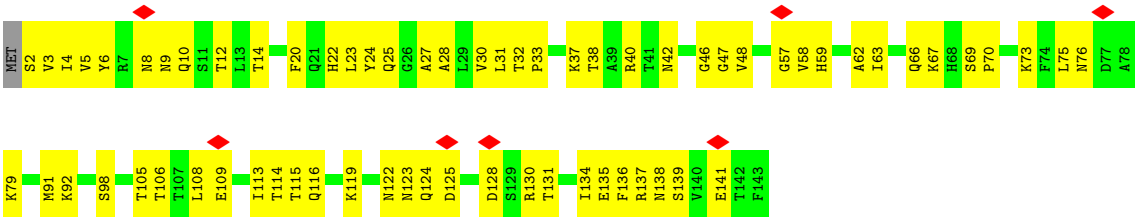
Chain B7:



• Molecule 4: Tail tube protein

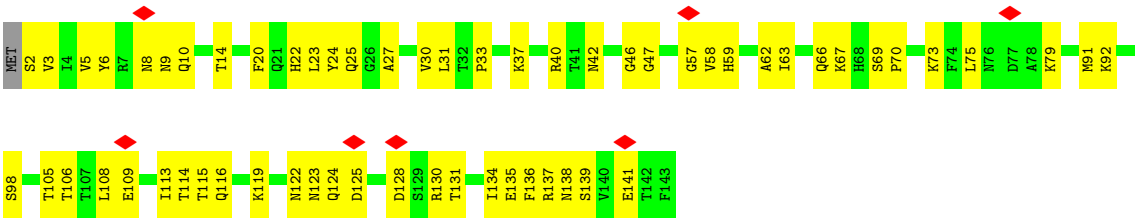
Chain C7:





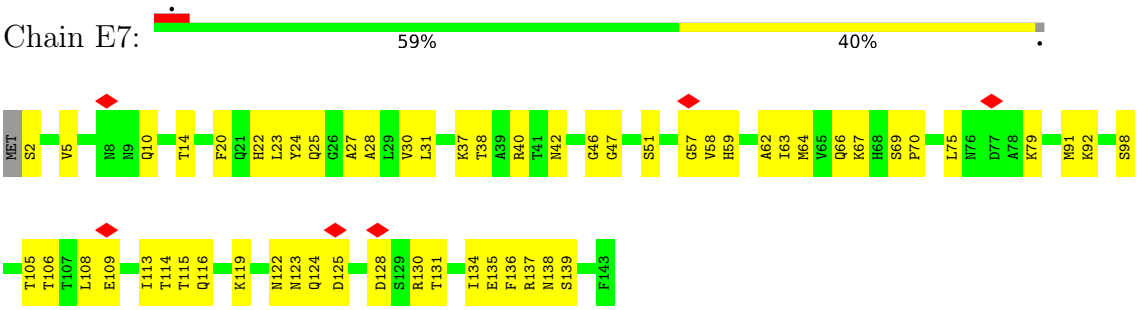
• Molecule 4: Tail tube protein

Chain D7:



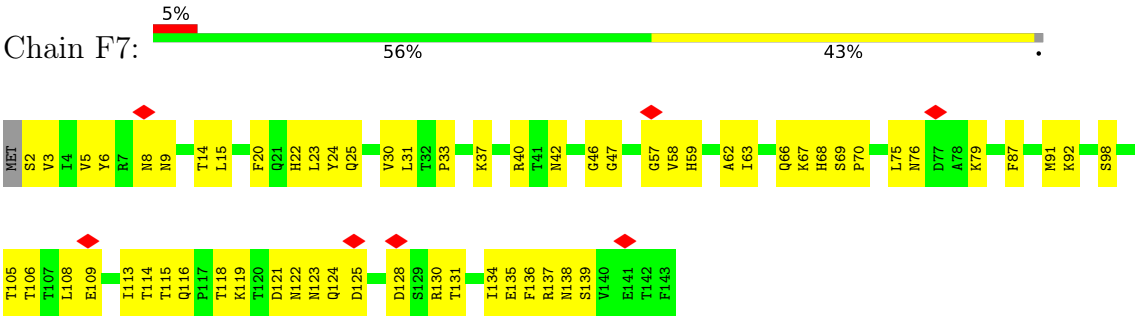
• Molecule 4: Tail tube protein

Chain E7:



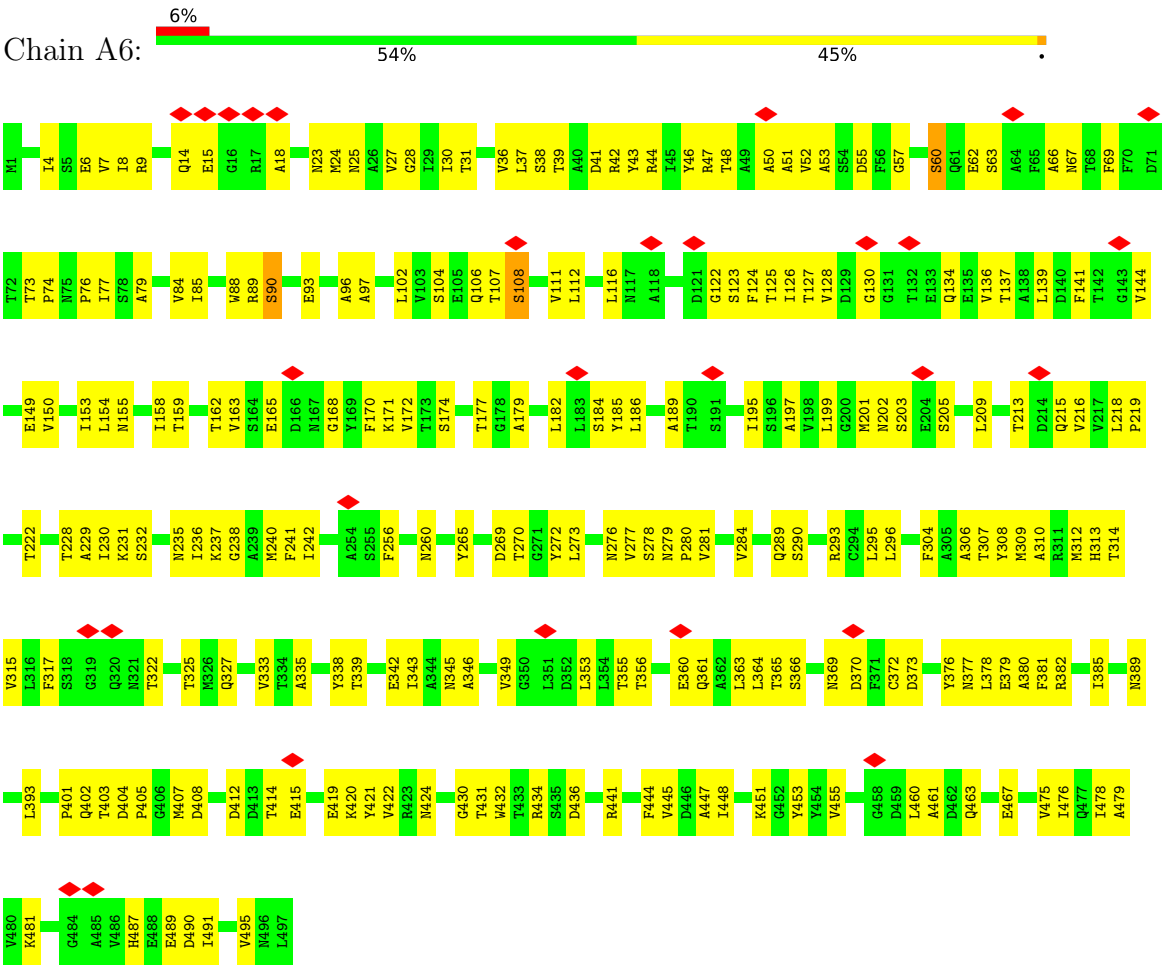
• Molecule 4: Tail tube protein

Chain F7:



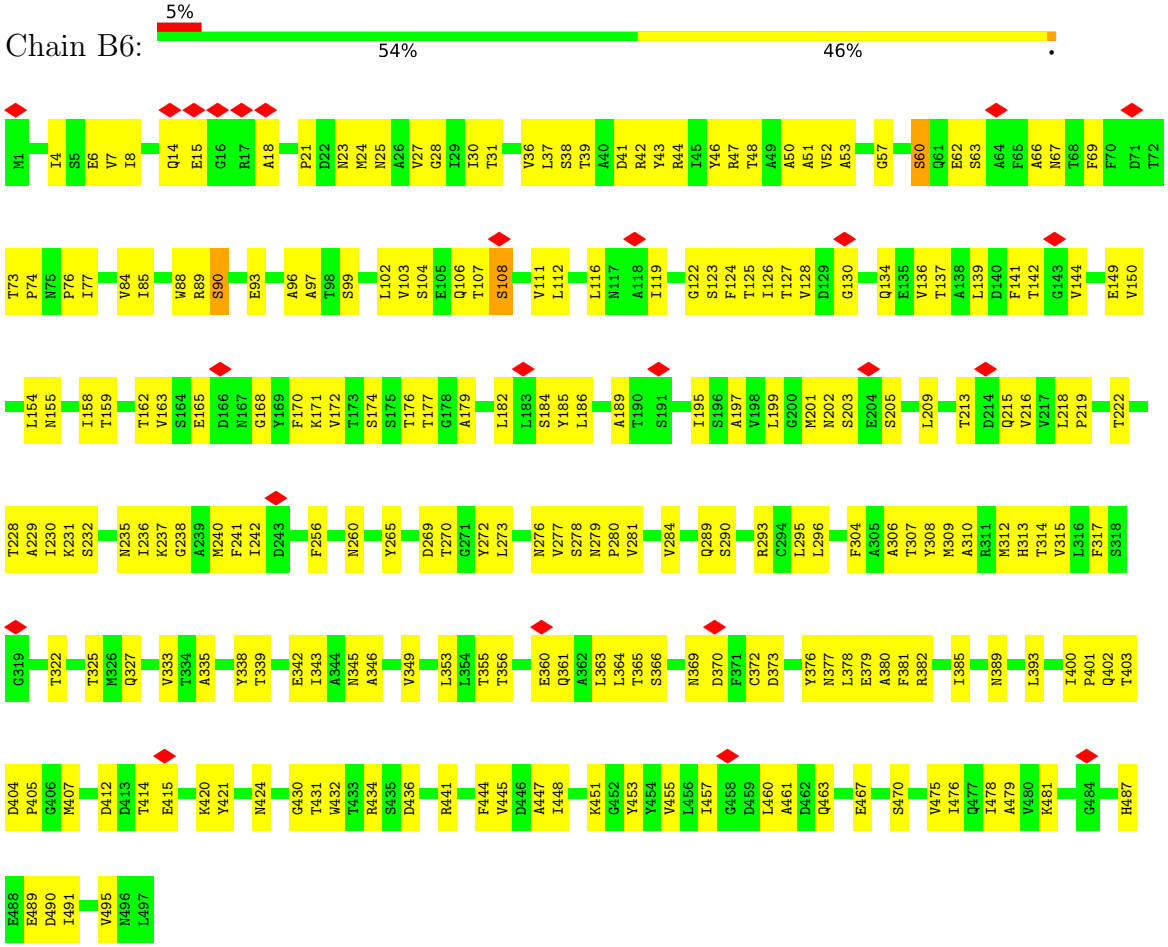
• Molecule 5: Tail sheath protein

Chain A6:



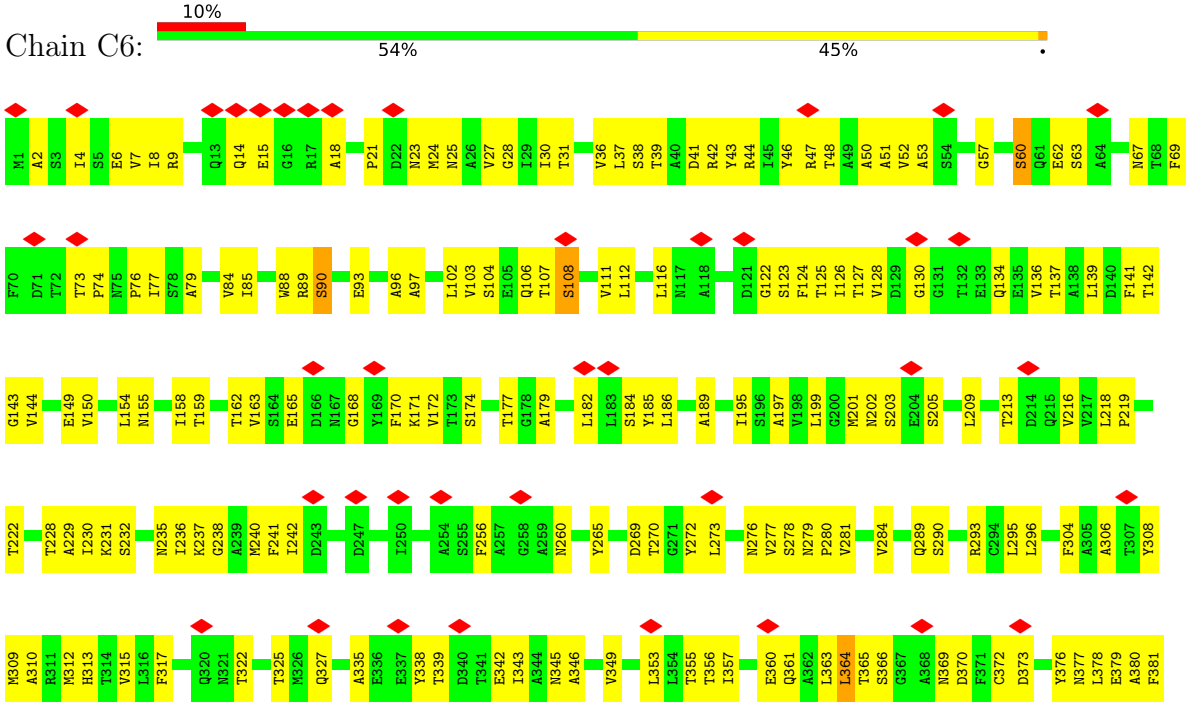
• Molecule 5: Tail sheath protein

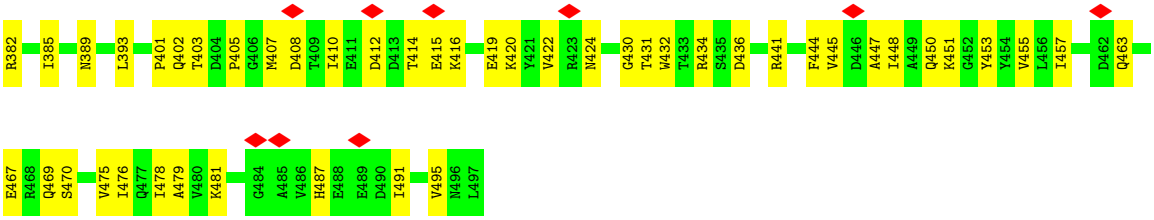
Chain B6:



• Molecule 5: Tail sheath protein

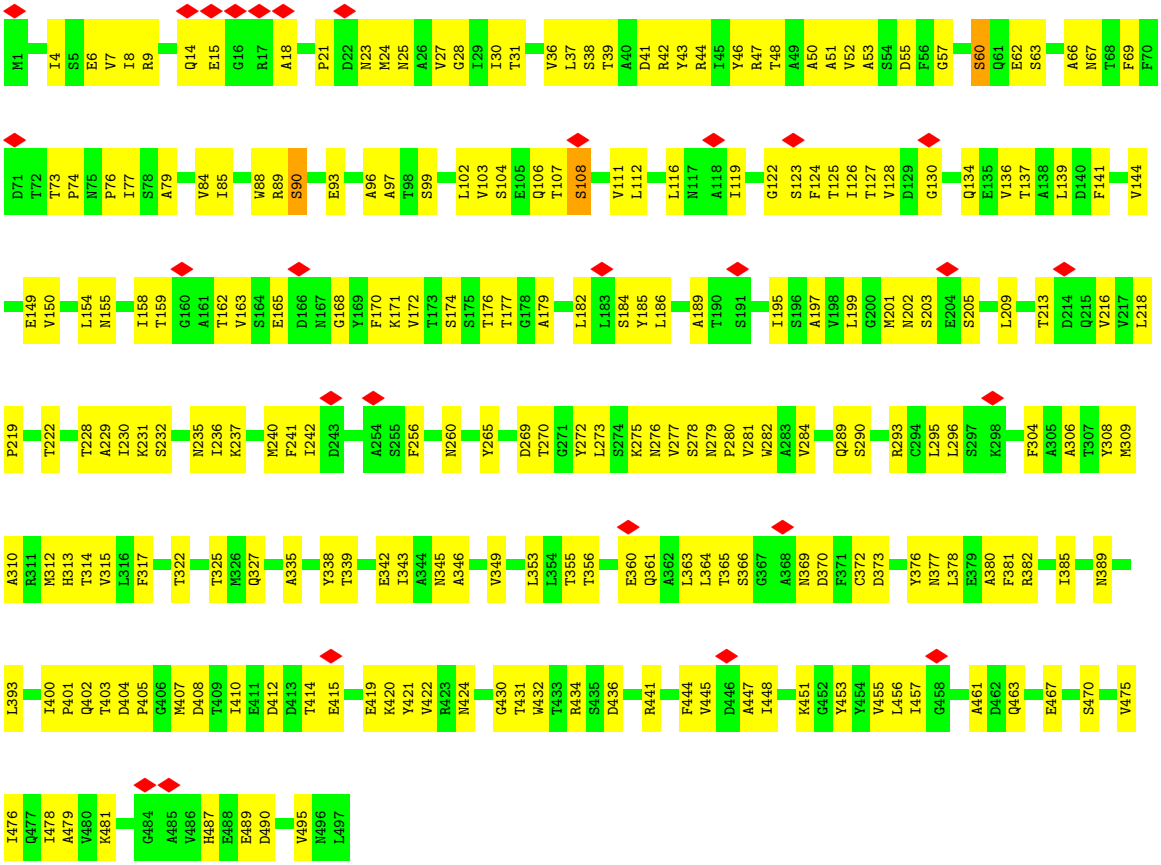
Chain C6:





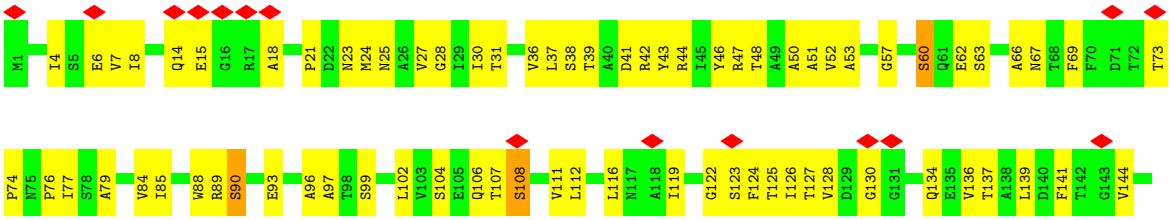
• Molecule 5: Tail sheath protein

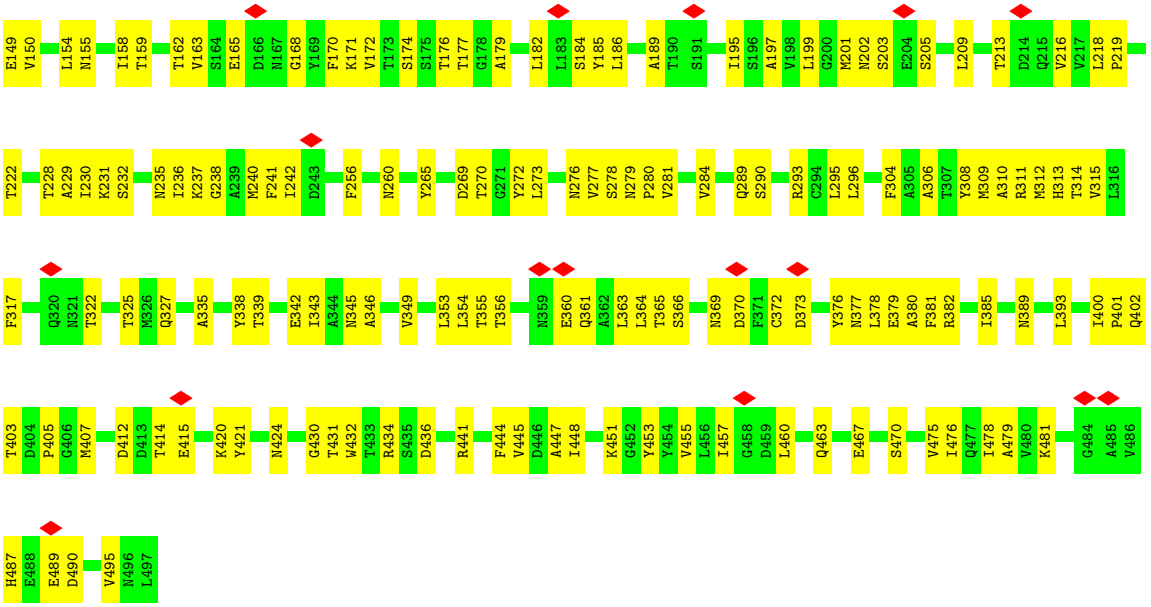
Chain D6:



• Molecule 5: Tail sheath protein

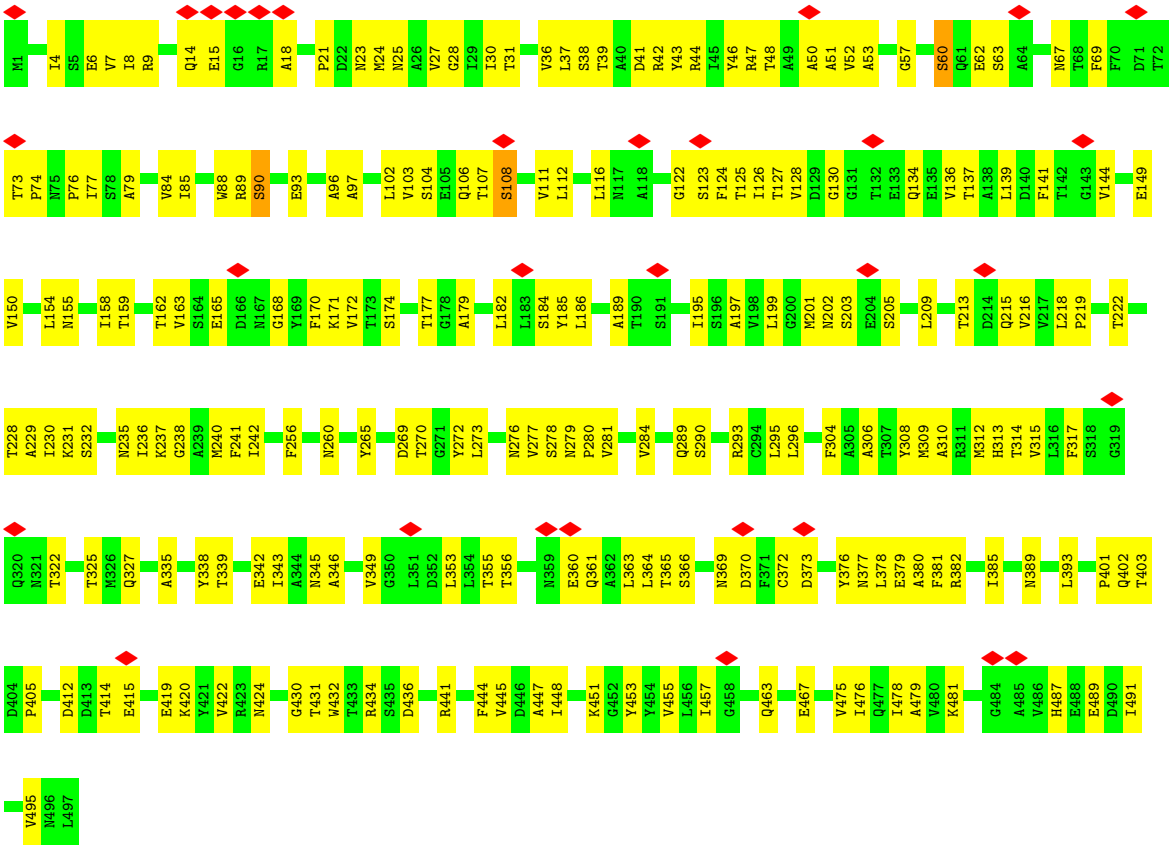
Chain E6:





• Molecule 5: Tail sheath protein

Chain F6:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10615	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-16 (4k x 4k)	Depositor
Maximum map value	12.435	Depositor
Minimum map value	-9.353	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.596	Depositor
Recommended contour level	2.63	Depositor
Map size (Å)	414.72, 414.72, 414.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	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	A5	0.55	0/1286	0.65	0/1742
1	B5	0.55	0/1286	0.65	0/1742
1	C5	0.55	0/1286	0.65	0/1742
1	D5	0.55	0/1286	0.65	0/1742
1	E5	0.55	0/1286	0.65	0/1742
1	F5	0.55	0/1286	0.65	0/1742
2	A3	0.43	0/965	0.55	0/1312
2	B3	0.51	0/965	0.67	2/1312 (0.2%)
2	C3	0.42	0/963	0.55	0/1309
2	D3	0.47	0/965	0.56	0/1312
2	E3	0.44	0/965	0.59	0/1312
2	F3	0.41	0/963	0.56	0/1309
2	G3	0.45	0/965	0.57	0/1312
2	H3	0.46	0/965	0.64	2/1312 (0.2%)
2	I3	0.43	0/963	0.54	0/1309
2	J3	0.44	0/965	0.56	0/1312
2	K3	0.46	0/965	0.60	0/1312
2	L3	0.42	0/963	0.56	0/1309
2	M3	0.45	0/965	0.57	0/1312
2	N3	0.45	0/965	0.58	0/1312
2	O3	0.42	0/963	0.55	0/1309
2	P3	0.45	0/965	0.57	0/1312
2	Q3	0.45	0/965	0.65	1/1312 (0.1%)
2	R3	0.42	0/963	0.55	0/1309
3	A4	0.53	0/939	0.65	0/1271
3	B4	0.53	0/939	0.65	0/1271
3	C4	0.53	0/939	0.65	0/1271
3	D4	0.53	0/939	0.65	0/1271
3	E4	0.53	0/939	0.65	0/1271
3	F4	0.53	0/939	0.65	0/1271
4	A7	0.50	0/1108	0.61	0/1505
4	B7	0.50	0/1108	0.61	0/1505
4	C7	0.50	0/1108	0.61	0/1505
4	D7	0.50	0/1108	0.61	0/1505

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	E7	0.50	0/1108	0.61	0/1505
4	F7	0.50	0/1108	0.61	0/1505
5	A6	0.42	0/3772	0.54	0/5134
5	B6	0.42	0/3772	0.54	0/5134
5	C6	0.42	0/3772	0.54	0/5134
5	D6	0.42	0/3772	0.54	0/5134
5	E6	0.42	0/3772	0.54	0/5134
5	F6	0.42	0/3772	0.54	0/5134
All	All	0.47	0/59988	0.59	5/81510 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B3	23	ARG	NE-CZ-NH1	-9.90	115.35	120.30
2	H3	59	LYS	CD-CE-NZ	6.10	125.73	111.70
2	Q3	27	LYS	CD-CE-NZ	-5.83	98.30	111.70
2	B3	23	ARG	NE-CZ-NH2	5.77	123.19	120.30
2	H3	27	LYS	CD-CE-NZ	-5.13	99.89	111.70

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	A5	1267	0	1214	112	0
1	B5	1267	0	1214	111	0
1	C5	1267	0	1214	110	0
1	D5	1267	0	1214	100	0
1	E5	1267	0	1214	97	0
1	F5	1267	0	1214	116	0
2	A3	951	0	950	66	0
2	B3	951	0	950	70	0
2	C3	949	0	945	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D3	951	0	950	71	0
2	E3	951	0	950	56	0
2	F3	949	0	945	42	0
2	G3	951	0	950	58	0
2	H3	951	0	950	58	0
2	I3	949	0	945	40	0
2	J3	951	0	950	72	0
2	K3	951	0	950	73	0
2	L3	949	0	945	42	0
2	M3	951	0	950	65	0
2	N3	951	0	950	61	0
2	O3	949	0	945	44	0
2	P3	951	0	950	71	0
2	Q3	951	0	950	58	0
2	R3	949	0	945	44	0
3	A4	918	0	917	62	0
3	B4	918	0	917	64	0
3	C4	918	0	917	61	0
3	D4	918	0	917	69	0
3	E4	918	0	917	75	0
3	F4	918	0	917	70	0
4	A7	1091	0	1069	96	0
4	B7	1091	0	1069	112	0
4	C7	1091	0	1069	113	0
4	D7	1091	0	1069	95	0
4	E7	1091	0	1069	82	0
4	F7	1091	0	1069	91	0
5	A6	3721	0	3660	206	0
5	B6	3721	0	3660	210	0
5	C6	3721	0	3660	207	0
5	D6	3721	0	3660	213	0
5	E6	3721	0	3660	201	0
5	F6	3721	0	3660	197	0
All	All	59088	0	58230	3179	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 27.

The worst 5 of 3179 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)
5:C6:9:ARG:NH2	5:D6:490:ASP:OD2	1.92	1.01
4:D7:137:ARG:HH12	4:E7:47:GLY:H	1.11	0.95
2:D3:34:TYR:HE1	2:E3:89:ILE:HD11	1.30	0.94
1:D5:13:ARG:HD3	2:L3:69:SER:HB2	1.50	0.93
4:B7:137:ARG:HH12	4:C7:47:GLY:H	1.09	0.93

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	A5	157/161 (98%)	129 (82%)	28 (18%)	0	100	100
1	B5	157/161 (98%)	129 (82%)	28 (18%)	0	100	100
1	C5	157/161 (98%)	129 (82%)	28 (18%)	0	100	100
1	D5	157/161 (98%)	129 (82%)	28 (18%)	0	100	100
1	E5	157/161 (98%)	129 (82%)	28 (18%)	0	100	100
1	F5	157/161 (98%)	129 (82%)	28 (18%)	0	100	100
2	A3	124/839 (15%)	114 (92%)	10 (8%)	0	100	100
2	B3	124/839 (15%)	114 (92%)	10 (8%)	0	100	100
2	C3	124/839 (15%)	110 (89%)	14 (11%)	0	100	100
2	D3	124/839 (15%)	115 (93%)	9 (7%)	0	100	100
2	E3	124/839 (15%)	117 (94%)	7 (6%)	0	100	100
2	F3	124/839 (15%)	109 (88%)	15 (12%)	0	100	100
2	G3	124/839 (15%)	113 (91%)	11 (9%)	0	100	100
2	H3	124/839 (15%)	114 (92%)	10 (8%)	0	100	100
2	I3	124/839 (15%)	110 (89%)	14 (11%)	0	100	100
2	J3	124/839 (15%)	114 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K3	124/839 (15%)	116 (94%)	8 (6%)	0	100	100
2	L3	124/839 (15%)	107 (86%)	17 (14%)	0	100	100
2	M3	124/839 (15%)	117 (94%)	7 (6%)	0	100	100
2	N3	124/839 (15%)	117 (94%)	7 (6%)	0	100	100
2	O3	124/839 (15%)	108 (87%)	16 (13%)	0	100	100
2	P3	124/839 (15%)	114 (92%)	10 (8%)	0	100	100
2	Q3	124/839 (15%)	115 (93%)	9 (7%)	0	100	100
2	R3	124/839 (15%)	111 (90%)	13 (10%)	0	100	100
3	A4	112/114 (98%)	98 (88%)	14 (12%)	0	100	100
3	B4	112/114 (98%)	98 (88%)	14 (12%)	0	100	100
3	C4	112/114 (98%)	98 (88%)	14 (12%)	0	100	100
3	D4	112/114 (98%)	98 (88%)	14 (12%)	0	100	100
3	E4	112/114 (98%)	98 (88%)	14 (12%)	0	100	100
3	F4	112/114 (98%)	98 (88%)	14 (12%)	0	100	100
4	A7	140/143 (98%)	124 (89%)	16 (11%)	0	100	100
4	B7	140/143 (98%)	124 (89%)	16 (11%)	0	100	100
4	C7	140/143 (98%)	124 (89%)	16 (11%)	0	100	100
4	D7	140/143 (98%)	124 (89%)	16 (11%)	0	100	100
4	E7	140/143 (98%)	124 (89%)	16 (11%)	0	100	100
4	F7	140/143 (98%)	124 (89%)	16 (11%)	0	100	100
5	A6	495/497 (100%)	449 (91%)	46 (9%)	0	100	100
5	B6	495/497 (100%)	448 (90%)	47 (10%)	0	100	100
5	C6	495/497 (100%)	448 (90%)	47 (10%)	0	100	100
5	D6	495/497 (100%)	450 (91%)	45 (9%)	0	100	100
5	E6	495/497 (100%)	449 (91%)	46 (9%)	0	100	100
5	F6	495/497 (100%)	449 (91%)	46 (9%)	0	100	100
All	All	7656/20592 (37%)	6834 (89%)	822 (11%)	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	A5	142/144 (99%)	138 (97%)	4 (3%)	43	72
1	B5	142/144 (99%)	139 (98%)	3 (2%)	53	78
1	C5	142/144 (99%)	139 (98%)	3 (2%)	53	78
1	D5	142/144 (99%)	139 (98%)	3 (2%)	53	78
1	E5	142/144 (99%)	139 (98%)	3 (2%)	53	78
1	F5	142/144 (99%)	138 (97%)	4 (3%)	43	72
2	A3	109/708 (15%)	109 (100%)	0	100	100
2	B3	109/708 (15%)	109 (100%)	0	100	100
2	C3	108/708 (15%)	108 (100%)	0	100	100
2	D3	109/708 (15%)	109 (100%)	0	100	100
2	E3	109/708 (15%)	109 (100%)	0	100	100
2	F3	108/708 (15%)	108 (100%)	0	100	100
2	G3	109/708 (15%)	109 (100%)	0	100	100
2	H3	109/708 (15%)	109 (100%)	0	100	100
2	I3	108/708 (15%)	108 (100%)	0	100	100
2	J3	109/708 (15%)	109 (100%)	0	100	100
2	K3	109/708 (15%)	109 (100%)	0	100	100
2	L3	108/708 (15%)	108 (100%)	0	100	100
2	M3	109/708 (15%)	109 (100%)	0	100	100
2	N3	109/708 (15%)	109 (100%)	0	100	100
2	O3	108/708 (15%)	108 (100%)	0	100	100
2	P3	109/708 (15%)	109 (100%)	0	100	100
2	Q3	109/708 (15%)	109 (100%)	0	100	100
2	R3	108/708 (15%)	108 (100%)	0	100	100
3	A4	101/101 (100%)	99 (98%)	2 (2%)	55	79
3	B4	101/101 (100%)	99 (98%)	2 (2%)	55	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C4	101/101 (100%)	99 (98%)	2 (2%)	55 79
3	D4	101/101 (100%)	99 (98%)	2 (2%)	55 79
3	E4	101/101 (100%)	99 (98%)	2 (2%)	55 79
3	F4	101/101 (100%)	99 (98%)	2 (2%)	55 79
4	A7	124/125 (99%)	124 (100%)	0	100 100
4	B7	124/125 (99%)	124 (100%)	0	100 100
4	C7	124/125 (99%)	124 (100%)	0	100 100
4	D7	124/125 (99%)	124 (100%)	0	100 100
4	E7	124/125 (99%)	124 (100%)	0	100 100
4	F7	124/125 (99%)	124 (100%)	0	100 100
5	A6	407/407 (100%)	400 (98%)	7 (2%)	60 82
5	B6	407/407 (100%)	400 (98%)	7 (2%)	60 82
5	C6	407/407 (100%)	399 (98%)	8 (2%)	55 79
5	D6	407/407 (100%)	400 (98%)	7 (2%)	60 82
5	E6	407/407 (100%)	400 (98%)	7 (2%)	60 82
5	F6	407/407 (100%)	400 (98%)	7 (2%)	60 82
All	All	6600/17406 (38%)	6525 (99%)	75 (1%)	74 88

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D6	281	VAL
5	F6	281	VAL
5	D6	364	LEU
5	E6	360	GLU
3	C4	40	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
3	F4	99	ASN
5	C6	134	GLN
5	A6	134	GLN
5	B6	134	GLN
5	C6	424	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 monosaccharides 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.

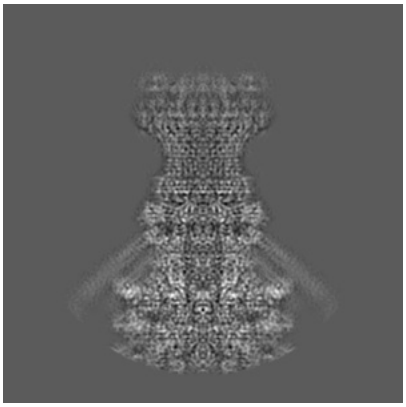
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22896. These allow visual inspection of the internal detail of the map and identification of artifacts.

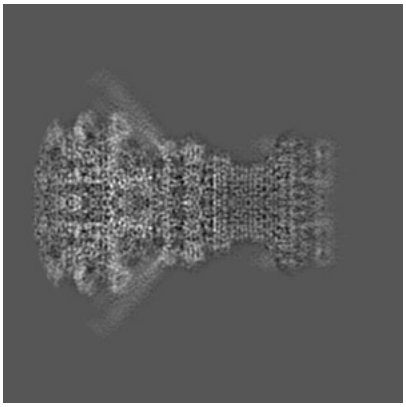
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

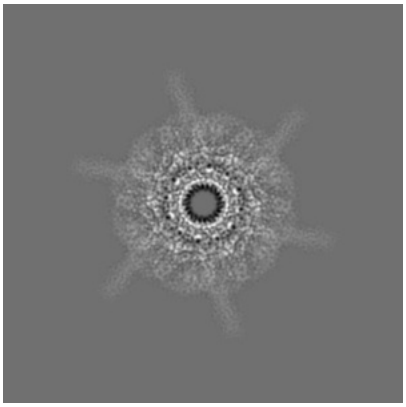
6.1.1 Primary map



X



Y

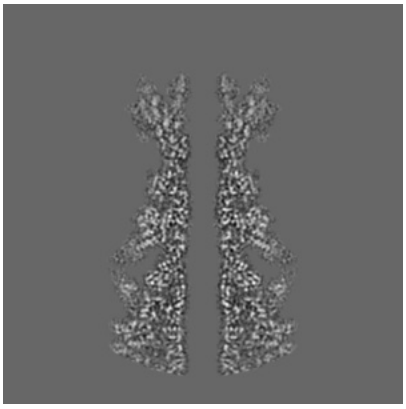


Z

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

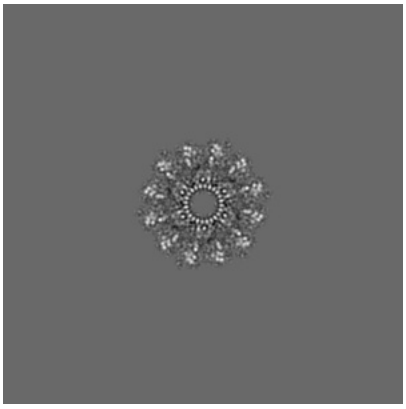
6.2 Central slices

6.2.1 Primary map



X Index: 256

Y Index: 256

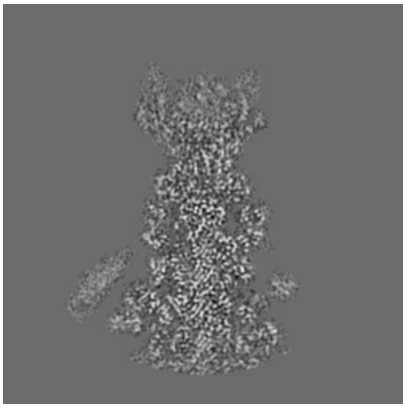


Z Index: 256

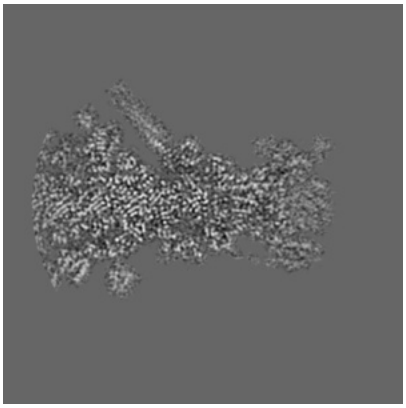
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

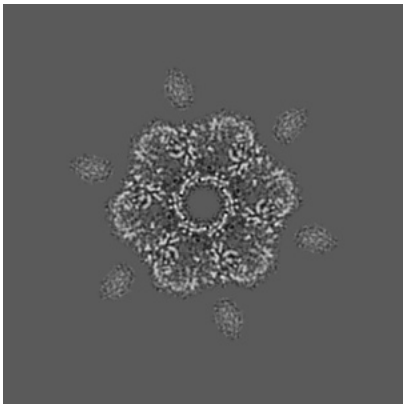
6.3.1 Primary map



X Index: 286



Y Index: 226

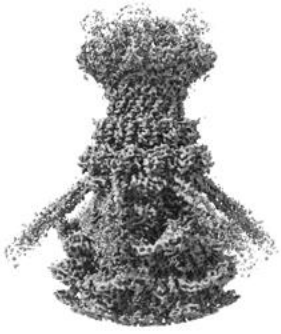


Z Index: 141

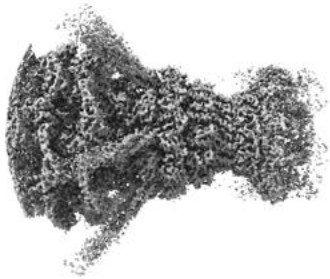
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 2.63. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

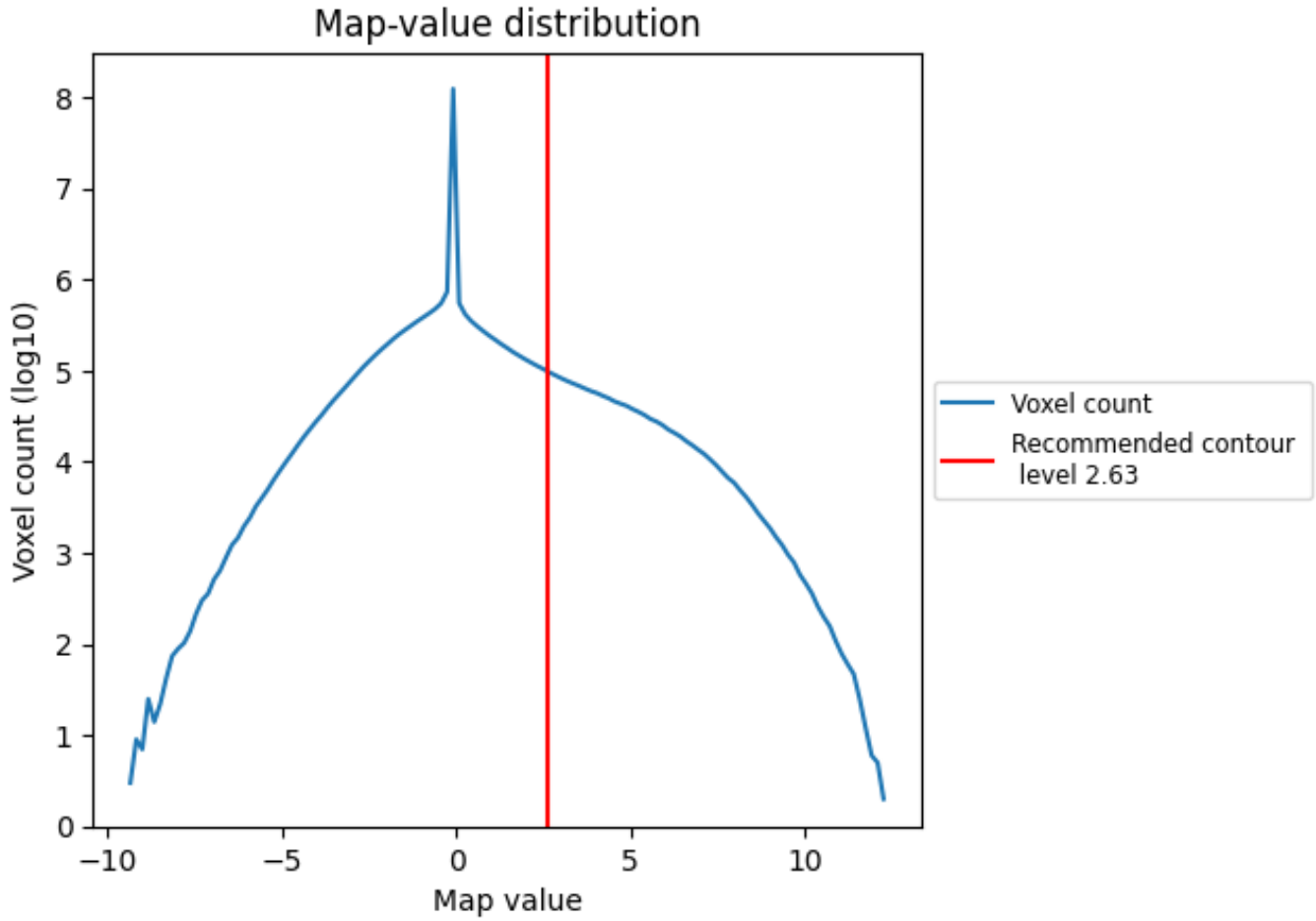
6.5 Mask visualisation (i)

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

7 Map analysis

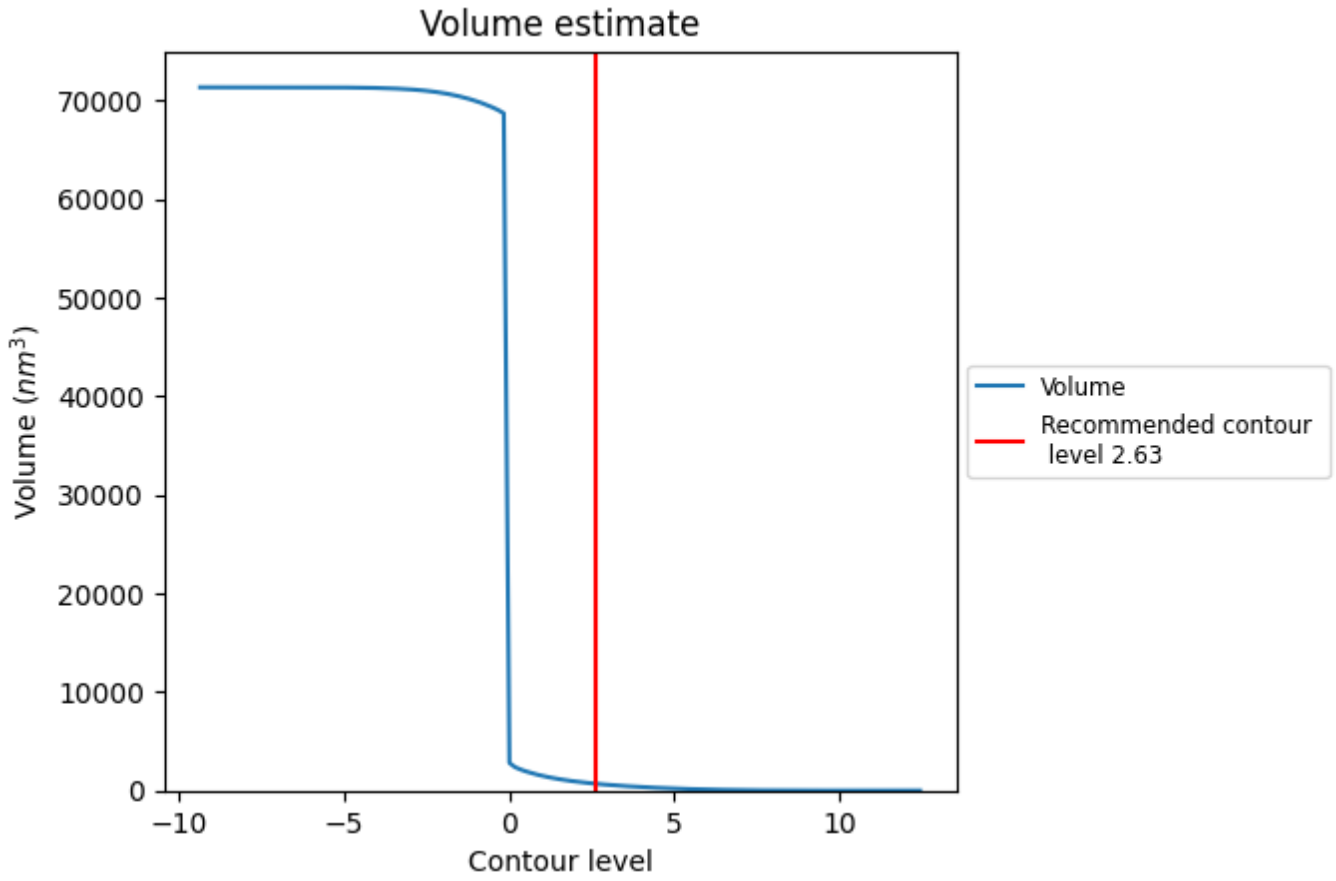
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

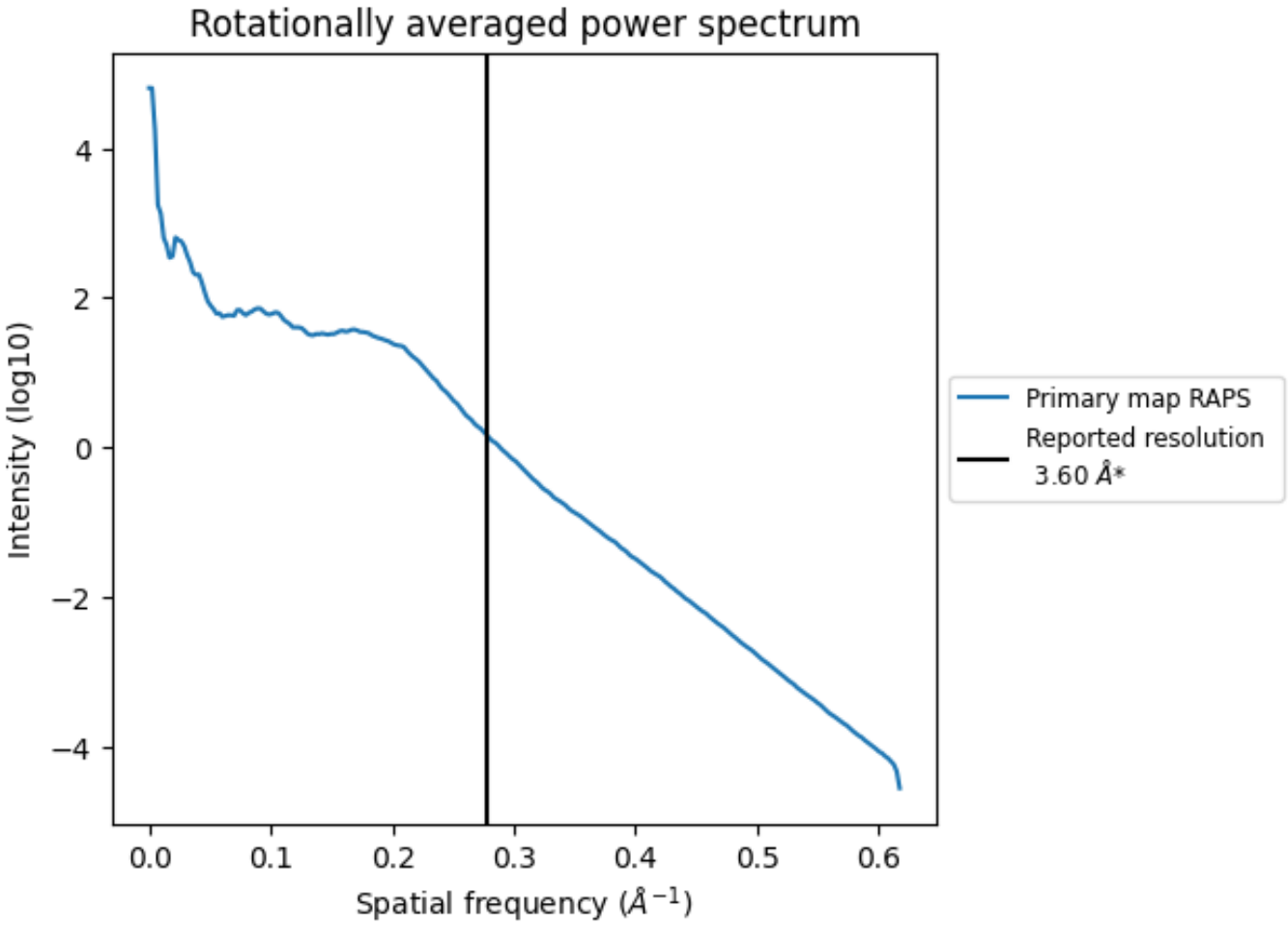
7.2 Volume estimate (i)



The volume at the recommended contour level is 688 nm^3; this corresponds to an approximate mass of 622 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)

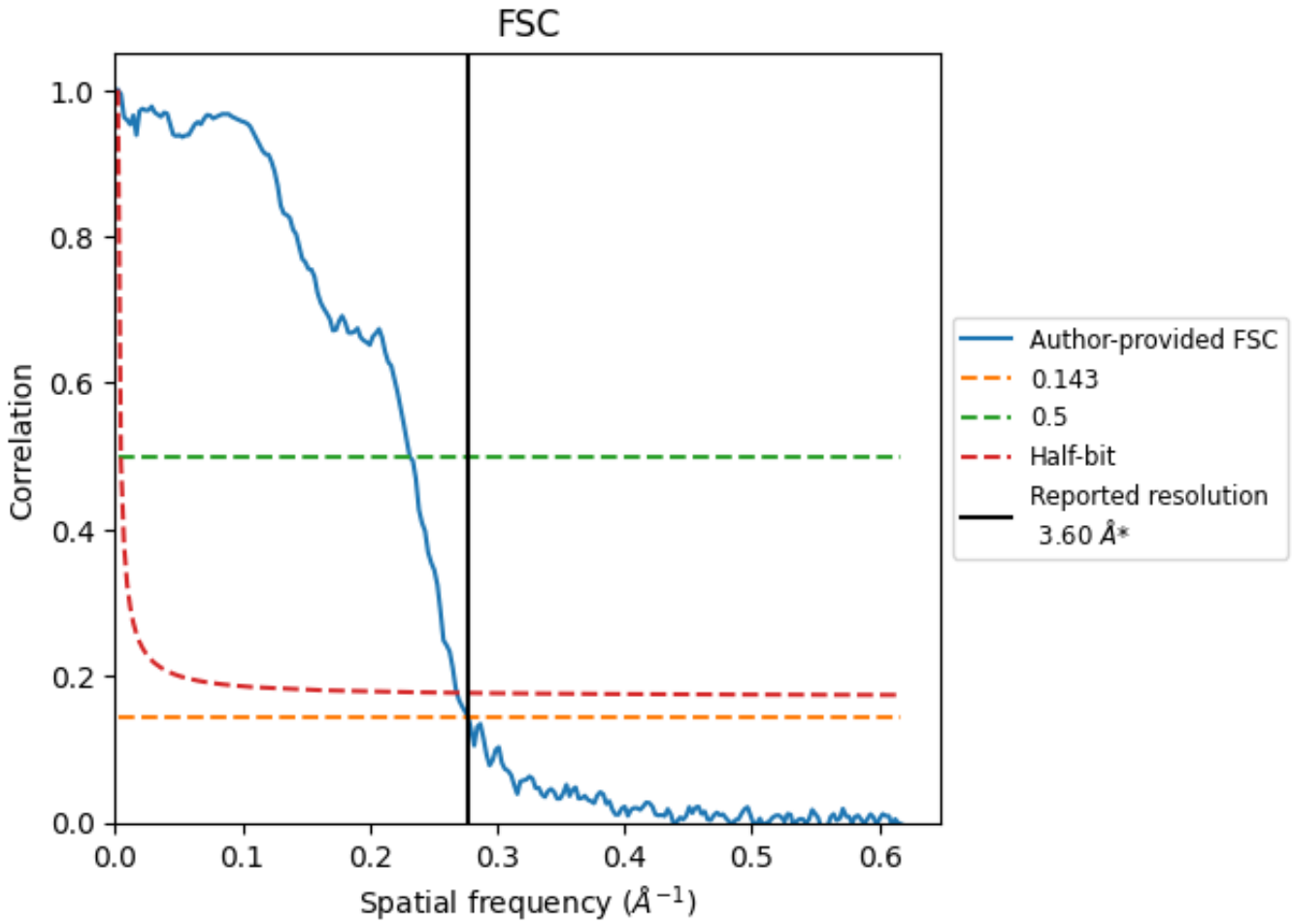


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

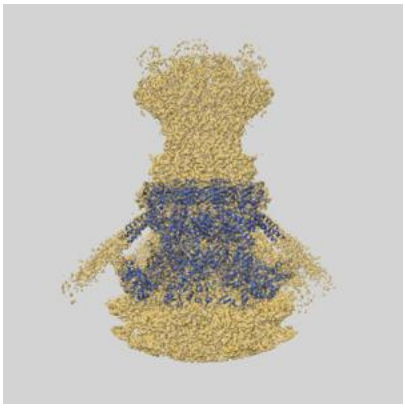
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.32	3.72
Unmasked-calculated*	-	-	-

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

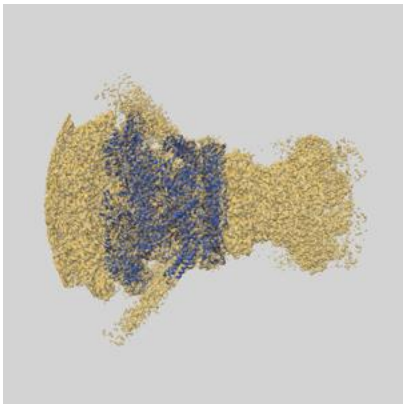
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22896 and PDB model 7KJK. Per-residue inclusion information can be found in section 3 on page 8.

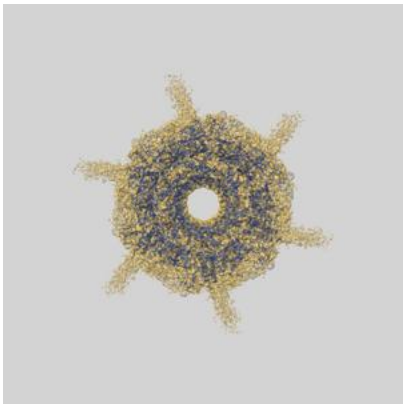
9.1 Map-model overlay



X



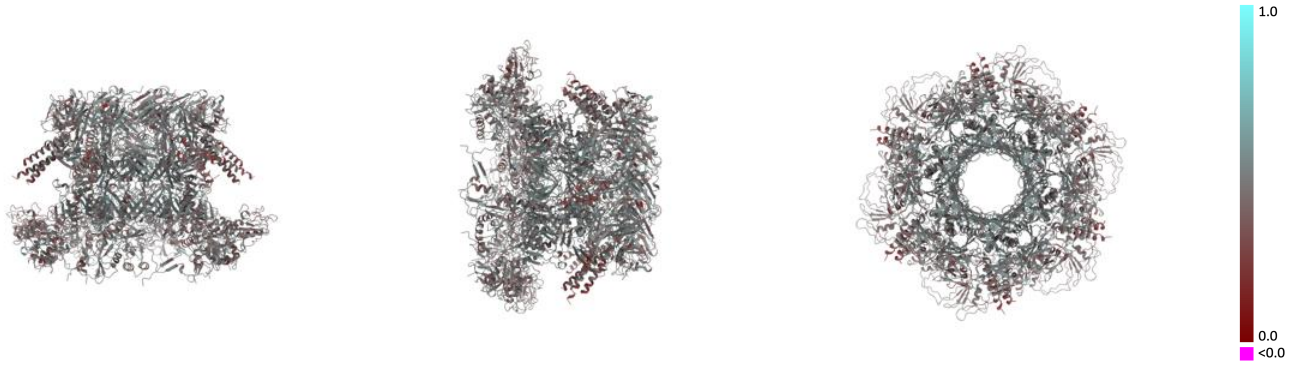
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.63 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.

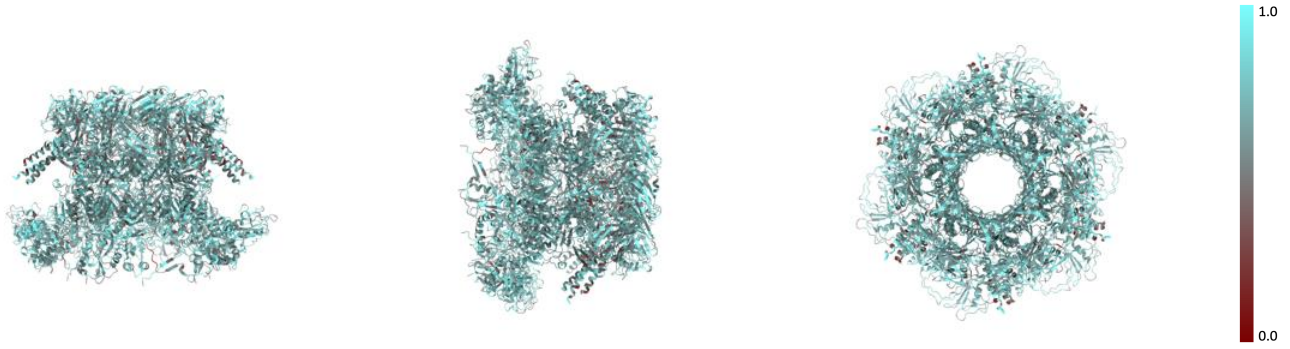
9.2 Q-score mapped to coordinate model



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.

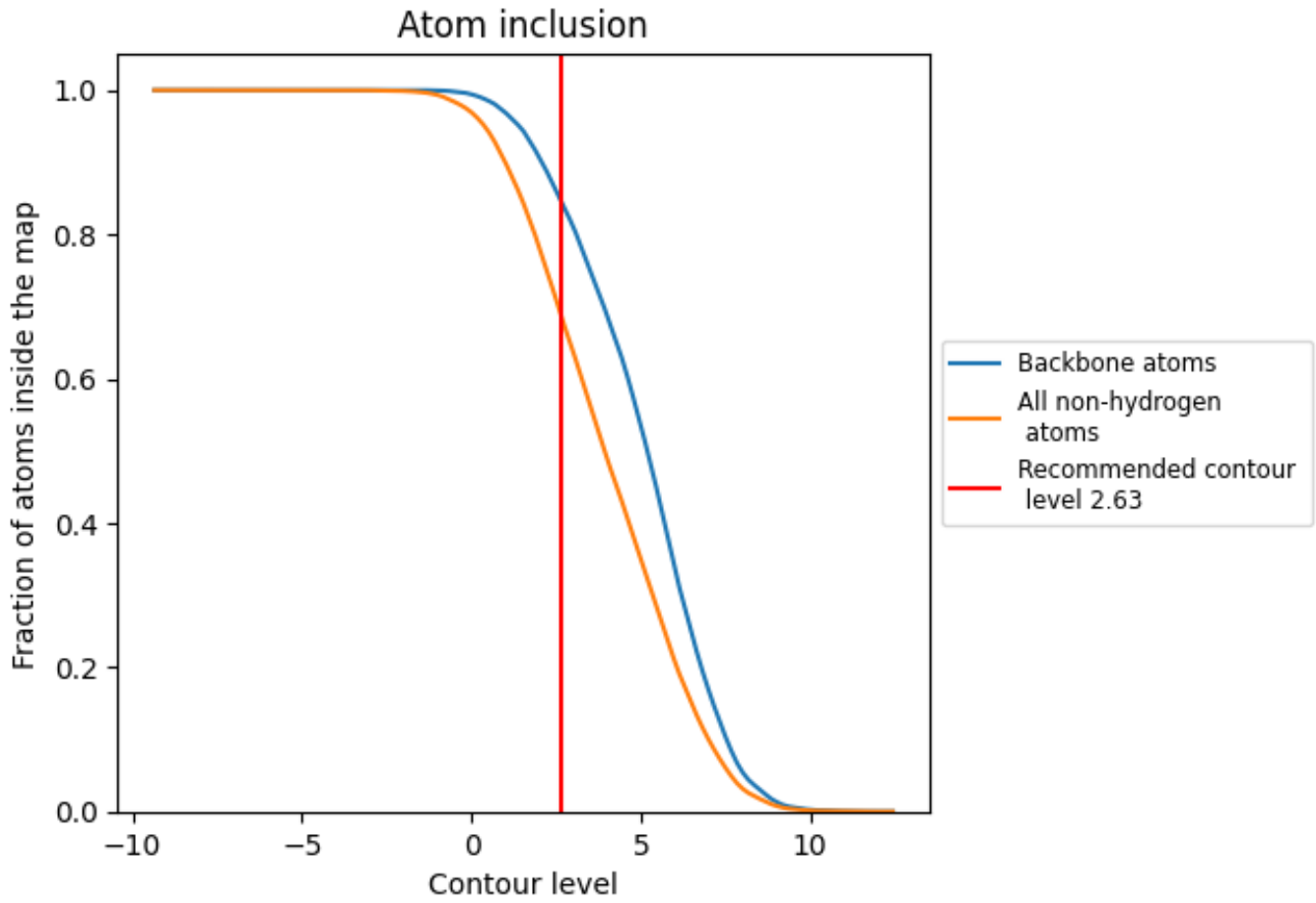
9.3 Atom inclusion mapped to coordinate model



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 (2.63).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 69% 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 (2.63) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6898	0.4600
A3	0.6998	0.4500
A4	0.6977	0.4960
A5	0.7051	0.4880
A6	0.6979	0.4540
A7	0.6993	0.4950
B3	0.6677	0.4290
B4	0.6955	0.4980
B5	0.6986	0.4870
B6	0.6973	0.4550
B7	0.7011	0.5000
C3	0.6702	0.4380
C4	0.6944	0.5000
C5	0.7059	0.4890
C6	0.6731	0.4290
C7	0.7039	0.4990
D3	0.6902	0.4440
D4	0.7076	0.4990
D5	0.7010	0.4850
D6	0.6954	0.4530
D7	0.7030	0.4980
E3	0.6677	0.4260
E4	0.6988	0.4990
E5	0.7051	0.4870
E6	0.6908	0.4500
E7	0.7011	0.4980
F3	0.6681	0.4350
F4	0.6988	0.5000
F5	0.7019	0.4870
F6	0.6957	0.4520
F7	0.7048	0.5000
G3	0.6838	0.4400
H3	0.6688	0.4250
I3	0.6627	0.4390
J3	0.6955	0.4480

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Chain	Atom inclusion	Q-score
K3	0.6624	0.4230
L3	0.6660	0.4380
M3	0.6923	0.4440
N3	0.6667	0.4240
O3	0.6660	0.4360
P3	0.6763	0.4470
Q3	0.6613	0.4310
R3	0.6638	0.4340