



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 09:05 PM UTC

PDB ID : 9EUF / pdb_00009euf
EMDB ID : EMD-19968
Title : Cryo-EM structure of Staphylococcus aureus bacteriophage phi812 baseplate in the pre-contraction state - complete
Authors : Binovsky, J.; Siborova, M.; Baska, R.; Pichel-Beleiro, A.; Skubnik, K.; Novacek, J.; Benesik, M.; van Raaij, M.J.; Plevka, P.
Deposited on : 2024-03-27
Resolution : 7.30 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

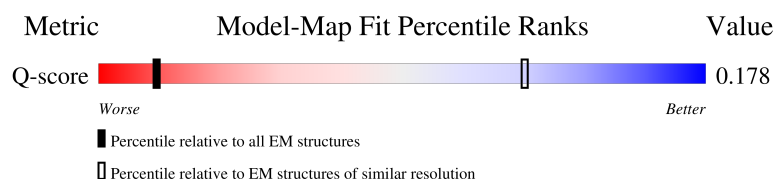
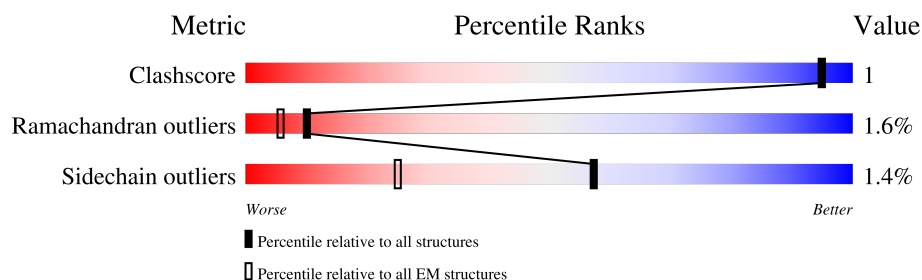
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 7.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	436 (6.80 - 7.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	1152	
1	1	1152	
1	2	1152	
1	3	1152	

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Mol	Chain	Length	Quality of chain
1	4	1152	39% 89% 5% 6%
1	h	1152	33% 89% 5% 6%
1	i	1152	34% 88% 6% 6%
1	j	1152	37% 88% 6% 6%
1	k	1152	65% 88% 6% 6%
1	l	1152	67% 89% 5% 6%
1	m	1152	68% 89% 5% 6%
1	z	1152	35% 89% 5% 6%
2	5	458	35% 99% .
2	6	458	38% 99% .
2	7	458	40% 99% .
2	n	458	33% 100%
2	o	458	35% 100%
2	p	458	38% 100%
3	8	640	31% 99% .
3	9	640	42% 100%
3	AA	640	44% 99% .
3	q	640	57% 99% .
3	r	640	63% 100%
3	s	640	60% 98% .
4	A	295	9% 90% 5% 5%
5	B	848	. 32% . 63%
6	C	348	13% 95% 5%
6	D	348	10% 94% 6%
6	I	348	14% 87% 12%

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Mol	Chain	Length	Quality of chain
6	K	348	
7	E	808	
8	F	174	
8	G	174	
9	H	1019	
9	J	1019	
10	L	234	
10	O	234	
11	M	263	
11	N	263	
12	P	587	
12	Q	587	
12	T	587	
12	U	587	
12	X	587	
12	Y	587	
13	R	142	
13	S	142	
13	V	142	
13	W	142	
13	Z	142	
13	a	142	
14	b	194	
14	c	194	
14	d	194	

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Mol	Chain	Length	Quality of chain
14	e	194	63% 88% 9%
14	f	194	72% 85% 5% 9%
14	g	194	81% 85% 5% 9%
14	t	194	12% 86% 5% 9%
14	u	194	22% 87% • 9%
14	v	194	37% 83% 7% • 9%
14	w	194	52% 86% 5% 9%
14	x	194	60% 85% 6% 9%
14	y	194	74% 87% • • 9%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 224293 atoms, of which 63816 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 DUF4815 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	1082	Total 4475	C 2164	H 146	N 1082	O 1083	0	0
1	1	1082	Total 4475	C 2164	H 146	N 1082	O 1083	0	0
1	2	1082	Total 4475	C 2164	H 146	N 1082	O 1083	0	0
1	3	1082	Total 4475	C 2164	H 146	N 1082	O 1083	0	0
1	4	1082	Total 4475	C 2164	H 146	N 1082	O 1083	0	0
1	h	1082	Total 4475	C 2164	H 146	N 1082	O 1083	0	0
1	i	1082	Total 4474	C 2163	H 146	N 1082	O 1083	0	0
1	j	1082	Total 4475	C 2164	H 146	N 1082	O 1083	0	0
1	k	1082	Total 4475	C 2164	H 146	N 1082	O 1083	0	0
1	l	1082	Total 4475	C 2164	H 146	N 1082	O 1083	0	0
1	m	1082	Total 4475	C 2164	H 146	N 1082	O 1083	0	0
1	z	1082	Total 4474	C 2164	H 146	N 1081	O 1083	0	0

- Molecule 2 is a protein called Receptor binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	458	Total 1909	C 916	H 76	N 458	O 459	0	0
2	6	458	Total 1909	C 916	H 76	N 458	O 459	0	0
2	7	458	Total 1909	C 916	H 76	N 458	O 459	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	n	458	Total	C	H	N	O	0	0
			1909	916	76	458	459		
2	o	458	Total	C	H	N	O	0	0
			1909	916	76	458	459		
2	p	458	Total	C	H	N	O	0	0
			1909	916	76	458	459		

- Molecule 3 is a protein called CBM-cenC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	640	Total	C	H	N	O	0	0
			2647	1280	86	640	641		
3	9	640	Total	C	H	N	O	0	0
			2647	1280	86	640	641		
3	AA	640	Total	C	H	N	O	0	0
			2647	1280	86	640	641		
3	q	640	Total	C	H	N	O	0	0
			2647	1280	86	640	641		
3	r	640	Total	C	H	N	O	0	0
			2647	1280	86	640	641		
3	s	640	Total	C	H	N	O	0	0
			2647	1280	86	640	641		

- Molecule 4 is a protein called NlpC/P60 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	280	Total	C	H	N	O S	0	0
			2746	1087	971	319	364 5		

- Molecule 5 is a protein called GP-PDE domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	310	Total	C	H	N	O S	0	0
			4309	1560	1839	401	502 7		

- Molecule 6 is a protein called Baseplate component.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	348	Total	C	H	N	O S	0	0
			4866	1734	2106	459	560 7		
6	D	348	Total	C	H	N	O S	0	0
			4866	1734	2106	459	560 7		

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Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	347	Total	C	H	N	O	S	0	0
			4850	1729	2098	458	559	6		
6	K	347	Total	C	H	N	O	S	0	0
			4850	1729	2098	458	559	6		

- Molecule 7 is a protein called Peptidase C51 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	E	722	Total	C	H	N	O	S	0	0
			10233	3724	4404	979	1106	20		

- Molecule 8 is a protein called Baseplate component.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	F	154	Total	C	H	N	O	S	0	0
			2240	803	992	200	241	4		
8	G	153	Total	C	H	N	O	S	0	0
			2229	799	989	198	239	4		

- Molecule 9 is a protein called TmpF.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	H	297	Total	C	H	N	O	S	0	0
			2316	933	678	345	359	1		
9	J	297	Total	C	H	N	O	S	0	0
			2316	933	678	345	359	1		

- Molecule 10 is a protein called Baseplate wedge subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	212	Total	C	H	N	O	S	0	0
			2977	1060	1283	290	339	5		
10	O	212	Total	C	H	N	O	S	0	0
			2977	1060	1283	290	339	5		

- Molecule 11 is a protein called Putative baseplate component.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	238	Total	C	H	N	O	S	0	0
			3262	1164	1384	335	375	4		
11	N	238	Total	C	H	N	O	S	0	0
			3262	1164	1384	335	375	4		

- Molecule 12 is a protein called Major tail sheath protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	P	538	Total	C	H	N	O	S	0	0
			7407	2646	3207	711	836	7		
12	Q	538	Total	C	H	N	O	S	0	0
			7407	2646	3207	711	836	7		
12	T	536	Total	C	H	N	O	S	0	0
			7389	2640	3200	711	831	7		
12	U	536	Total	C	H	N	O	S	0	0
			7389	2640	3200	711	831	7		
12	X	531	Total	C	H	N	O	S	0	0
			7322	2617	3171	704	823	7		
12	Y	531	Total	C	H	N	O	S	0	0
			7322	2617	3171	704	823	7		

- Molecule 13 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	R	139	Total	C	H	N	O	S	0	0
			1924	685	833	183	219	4		
13	S	139	Total	C	H	N	O	S	0	0
			1924	685	833	183	219	4		
13	V	139	Total	C	H	N	O	S	0	0
			1924	685	833	183	219	4		
13	W	139	Total	C	H	N	O	S	0	0
			1924	685	833	183	219	4		
13	Z	139	Total	C	H	N	O	S	0	0
			1924	685	833	183	219	4		
13	a	139	Total	C	H	N	O	S	0	0
			1924	685	833	183	219	4		

- Molecule 14 is a protein called Baseplate protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	b	176	Total	C	H	N	O	S	0	0
			2428	873	1051	226	277	1		
14	c	176	Total	C	H	N	O	S	0	0
			2432	874	1054	226	277	1		
14	d	176	Total	C	H	N	O	S	0	0
			2432	874	1054	226	277	1		
14	e	176	Total	C	H	N	O	S	0	0
			2432	874	1054	226	277	1		
14	f	176	Total	C	H	N	O	S	0	0
			2432	874	1054	226	277	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
14	g	176	Total	C	H	N	O	S	0	0
			2432	874	1054	226	277	1		
14	t	176	Total	C	H	N	O	S	0	0
			2432	874	1054	226	277	1		
14	u	176	Total	C	H	N	O	S	0	0
			2432	874	1054	226	277	1		
14	v	176	Total	C	H	N	O	S	0	0
			2432	874	1054	226	277	1		
14	w	176	Total	C	H	N	O	S	0	0
			2432	874	1054	226	277	1		
14	x	176	Total	C	H	N	O	S	0	0
			2432	874	1054	226	277	1		
14	y	176	Total	C	H	N	O	S	0	0
			2432	874	1054	226	277	1		

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	174	ASP	-	expression tag	UNP A0A0U1WGQ5
b	175	PRO	-	expression tag	UNP A0A0U1WGQ5
b	176	ASN	-	expression tag	UNP A0A0U1WGQ5
b	177	SER	-	expression tag	UNP A0A0U1WGQ5
b	178	SER	-	expression tag	UNP A0A0U1WGQ5
b	179	SER	-	expression tag	UNP A0A0U1WGQ5
b	180	VAL	-	expression tag	UNP A0A0U1WGQ5
b	181	ASP	-	expression tag	UNP A0A0U1WGQ5
b	182	LYS	-	expression tag	UNP A0A0U1WGQ5
b	183	LEU	-	expression tag	UNP A0A0U1WGQ5
b	184	ALA	-	expression tag	UNP A0A0U1WGQ5
b	185	ALA	-	expression tag	UNP A0A0U1WGQ5
b	186	ALA	-	expression tag	UNP A0A0U1WGQ5
b	187	LEU	-	expression tag	UNP A0A0U1WGQ5
b	188	GLU	-	expression tag	UNP A0A0U1WGQ5
b	189	HIS	-	expression tag	UNP A0A0U1WGQ5
b	190	HIS	-	expression tag	UNP A0A0U1WGQ5
b	191	HIS	-	expression tag	UNP A0A0U1WGQ5
b	192	HIS	-	expression tag	UNP A0A0U1WGQ5
b	193	HIS	-	expression tag	UNP A0A0U1WGQ5
b	194	HIS	-	expression tag	UNP A0A0U1WGQ5
c	174	ASP	-	expression tag	UNP A0A0U1WGQ5
c	175	PRO	-	expression tag	UNP A0A0U1WGQ5
c	176	ASN	-	expression tag	UNP A0A0U1WGQ5
c	177	SER	-	expression tag	UNP A0A0U1WGQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
c	178	SER	-	expression tag	UNP A0A0U1WGGQ5
c	179	SER	-	expression tag	UNP A0A0U1WGGQ5
c	180	VAL	-	expression tag	UNP A0A0U1WGGQ5
c	181	ASP	-	expression tag	UNP A0A0U1WGGQ5
c	182	LYS	-	expression tag	UNP A0A0U1WGGQ5
c	183	LEU	-	expression tag	UNP A0A0U1WGGQ5
c	184	ALA	-	expression tag	UNP A0A0U1WGGQ5
c	185	ALA	-	expression tag	UNP A0A0U1WGGQ5
c	186	ALA	-	expression tag	UNP A0A0U1WGGQ5
c	187	LEU	-	expression tag	UNP A0A0U1WGGQ5
c	188	GLU	-	expression tag	UNP A0A0U1WGGQ5
c	189	HIS	-	expression tag	UNP A0A0U1WGGQ5
c	190	HIS	-	expression tag	UNP A0A0U1WGGQ5
c	191	HIS	-	expression tag	UNP A0A0U1WGGQ5
c	192	HIS	-	expression tag	UNP A0A0U1WGGQ5
c	193	HIS	-	expression tag	UNP A0A0U1WGGQ5
c	194	HIS	-	expression tag	UNP A0A0U1WGGQ5
d	174	ASP	-	expression tag	UNP A0A0U1WGGQ5
d	175	PRO	-	expression tag	UNP A0A0U1WGGQ5
d	176	ASN	-	expression tag	UNP A0A0U1WGGQ5
d	177	SER	-	expression tag	UNP A0A0U1WGGQ5
d	178	SER	-	expression tag	UNP A0A0U1WGGQ5
d	179	SER	-	expression tag	UNP A0A0U1WGGQ5
d	180	VAL	-	expression tag	UNP A0A0U1WGGQ5
d	181	ASP	-	expression tag	UNP A0A0U1WGGQ5
d	182	LYS	-	expression tag	UNP A0A0U1WGGQ5
d	183	LEU	-	expression tag	UNP A0A0U1WGGQ5
d	184	ALA	-	expression tag	UNP A0A0U1WGGQ5
d	185	ALA	-	expression tag	UNP A0A0U1WGGQ5
d	186	ALA	-	expression tag	UNP A0A0U1WGGQ5
d	187	LEU	-	expression tag	UNP A0A0U1WGGQ5
d	188	GLU	-	expression tag	UNP A0A0U1WGGQ5
d	189	HIS	-	expression tag	UNP A0A0U1WGGQ5
d	190	HIS	-	expression tag	UNP A0A0U1WGGQ5
d	191	HIS	-	expression tag	UNP A0A0U1WGGQ5
d	192	HIS	-	expression tag	UNP A0A0U1WGGQ5
d	193	HIS	-	expression tag	UNP A0A0U1WGGQ5
d	194	HIS	-	expression tag	UNP A0A0U1WGGQ5
e	174	ASP	-	expression tag	UNP A0A0U1WGGQ5
e	175	PRO	-	expression tag	UNP A0A0U1WGGQ5
e	176	ASN	-	expression tag	UNP A0A0U1WGGQ5
e	177	SER	-	expression tag	UNP A0A0U1WGGQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
e	178	SER	-	expression tag	UNP A0A0U1WGGQ5
e	179	SER	-	expression tag	UNP A0A0U1WGGQ5
e	180	VAL	-	expression tag	UNP A0A0U1WGGQ5
e	181	ASP	-	expression tag	UNP A0A0U1WGGQ5
e	182	LYS	-	expression tag	UNP A0A0U1WGGQ5
e	183	LEU	-	expression tag	UNP A0A0U1WGGQ5
e	184	ALA	-	expression tag	UNP A0A0U1WGGQ5
e	185	ALA	-	expression tag	UNP A0A0U1WGGQ5
e	186	ALA	-	expression tag	UNP A0A0U1WGGQ5
e	187	LEU	-	expression tag	UNP A0A0U1WGGQ5
e	188	GLU	-	expression tag	UNP A0A0U1WGGQ5
e	189	HIS	-	expression tag	UNP A0A0U1WGGQ5
e	190	HIS	-	expression tag	UNP A0A0U1WGGQ5
e	191	HIS	-	expression tag	UNP A0A0U1WGGQ5
e	192	HIS	-	expression tag	UNP A0A0U1WGGQ5
e	193	HIS	-	expression tag	UNP A0A0U1WGGQ5
e	194	HIS	-	expression tag	UNP A0A0U1WGGQ5
f	174	ASP	-	expression tag	UNP A0A0U1WGGQ5
f	175	PRO	-	expression tag	UNP A0A0U1WGGQ5
f	176	ASN	-	expression tag	UNP A0A0U1WGGQ5
f	177	SER	-	expression tag	UNP A0A0U1WGGQ5
f	178	SER	-	expression tag	UNP A0A0U1WGGQ5
f	179	SER	-	expression tag	UNP A0A0U1WGGQ5
f	180	VAL	-	expression tag	UNP A0A0U1WGGQ5
f	181	ASP	-	expression tag	UNP A0A0U1WGGQ5
f	182	LYS	-	expression tag	UNP A0A0U1WGGQ5
f	183	LEU	-	expression tag	UNP A0A0U1WGGQ5
f	184	ALA	-	expression tag	UNP A0A0U1WGGQ5
f	185	ALA	-	expression tag	UNP A0A0U1WGGQ5
f	186	ALA	-	expression tag	UNP A0A0U1WGGQ5
f	187	LEU	-	expression tag	UNP A0A0U1WGGQ5
f	188	GLU	-	expression tag	UNP A0A0U1WGGQ5
f	189	HIS	-	expression tag	UNP A0A0U1WGGQ5
f	190	HIS	-	expression tag	UNP A0A0U1WGGQ5
f	191	HIS	-	expression tag	UNP A0A0U1WGGQ5
f	192	HIS	-	expression tag	UNP A0A0U1WGGQ5
f	193	HIS	-	expression tag	UNP A0A0U1WGGQ5
f	194	HIS	-	expression tag	UNP A0A0U1WGGQ5
g	174	ASP	-	expression tag	UNP A0A0U1WGGQ5
g	175	PRO	-	expression tag	UNP A0A0U1WGGQ5
g	176	ASN	-	expression tag	UNP A0A0U1WGGQ5
g	177	SER	-	expression tag	UNP A0A0U1WGGQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
g	178	SER	-	expression tag	UNP A0A0U1WGGQ5
g	179	SER	-	expression tag	UNP A0A0U1WGGQ5
g	180	VAL	-	expression tag	UNP A0A0U1WGGQ5
g	181	ASP	-	expression tag	UNP A0A0U1WGGQ5
g	182	LYS	-	expression tag	UNP A0A0U1WGGQ5
g	183	LEU	-	expression tag	UNP A0A0U1WGGQ5
g	184	ALA	-	expression tag	UNP A0A0U1WGGQ5
g	185	ALA	-	expression tag	UNP A0A0U1WGGQ5
g	186	ALA	-	expression tag	UNP A0A0U1WGGQ5
g	187	LEU	-	expression tag	UNP A0A0U1WGGQ5
g	188	GLU	-	expression tag	UNP A0A0U1WGGQ5
g	189	HIS	-	expression tag	UNP A0A0U1WGGQ5
g	190	HIS	-	expression tag	UNP A0A0U1WGGQ5
g	191	HIS	-	expression tag	UNP A0A0U1WGGQ5
g	192	HIS	-	expression tag	UNP A0A0U1WGGQ5
g	193	HIS	-	expression tag	UNP A0A0U1WGGQ5
g	194	HIS	-	expression tag	UNP A0A0U1WGGQ5
t	174	ASP	-	expression tag	UNP A0A0U1WGGQ5
t	175	PRO	-	expression tag	UNP A0A0U1WGGQ5
t	176	ASN	-	expression tag	UNP A0A0U1WGGQ5
t	177	SER	-	expression tag	UNP A0A0U1WGGQ5
t	178	SER	-	expression tag	UNP A0A0U1WGGQ5
t	179	SER	-	expression tag	UNP A0A0U1WGGQ5
t	180	VAL	-	expression tag	UNP A0A0U1WGGQ5
t	181	ASP	-	expression tag	UNP A0A0U1WGGQ5
t	182	LYS	-	expression tag	UNP A0A0U1WGGQ5
t	183	LEU	-	expression tag	UNP A0A0U1WGGQ5
t	184	ALA	-	expression tag	UNP A0A0U1WGGQ5
t	185	ALA	-	expression tag	UNP A0A0U1WGGQ5
t	186	ALA	-	expression tag	UNP A0A0U1WGGQ5
t	187	LEU	-	expression tag	UNP A0A0U1WGGQ5
t	188	GLU	-	expression tag	UNP A0A0U1WGGQ5
t	189	HIS	-	expression tag	UNP A0A0U1WGGQ5
t	190	HIS	-	expression tag	UNP A0A0U1WGGQ5
t	191	HIS	-	expression tag	UNP A0A0U1WGGQ5
t	192	HIS	-	expression tag	UNP A0A0U1WGGQ5
t	193	HIS	-	expression tag	UNP A0A0U1WGGQ5
t	194	HIS	-	expression tag	UNP A0A0U1WGGQ5
u	174	ASP	-	expression tag	UNP A0A0U1WGGQ5
u	175	PRO	-	expression tag	UNP A0A0U1WGGQ5
u	176	ASN	-	expression tag	UNP A0A0U1WGGQ5
u	177	SER	-	expression tag	UNP A0A0U1WGGQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
u	178	SER	-	expression tag	UNP A0A0U1WGG5
u	179	SER	-	expression tag	UNP A0A0U1WGG5
u	180	VAL	-	expression tag	UNP A0A0U1WGG5
u	181	ASP	-	expression tag	UNP A0A0U1WGG5
u	182	LYS	-	expression tag	UNP A0A0U1WGG5
u	183	LEU	-	expression tag	UNP A0A0U1WGG5
u	184	ALA	-	expression tag	UNP A0A0U1WGG5
u	185	ALA	-	expression tag	UNP A0A0U1WGG5
u	186	ALA	-	expression tag	UNP A0A0U1WGG5
u	187	LEU	-	expression tag	UNP A0A0U1WGG5
u	188	GLU	-	expression tag	UNP A0A0U1WGG5
u	189	HIS	-	expression tag	UNP A0A0U1WGG5
u	190	HIS	-	expression tag	UNP A0A0U1WGG5
u	191	HIS	-	expression tag	UNP A0A0U1WGG5
u	192	HIS	-	expression tag	UNP A0A0U1WGG5
u	193	HIS	-	expression tag	UNP A0A0U1WGG5
u	194	HIS	-	expression tag	UNP A0A0U1WGG5
v	174	ASP	-	expression tag	UNP A0A0U1WGG5
v	175	PRO	-	expression tag	UNP A0A0U1WGG5
v	176	ASN	-	expression tag	UNP A0A0U1WGG5
v	177	SER	-	expression tag	UNP A0A0U1WGG5
v	178	SER	-	expression tag	UNP A0A0U1WGG5
v	179	SER	-	expression tag	UNP A0A0U1WGG5
v	180	VAL	-	expression tag	UNP A0A0U1WGG5
v	181	ASP	-	expression tag	UNP A0A0U1WGG5
v	182	LYS	-	expression tag	UNP A0A0U1WGG5
v	183	LEU	-	expression tag	UNP A0A0U1WGG5
v	184	ALA	-	expression tag	UNP A0A0U1WGG5
v	185	ALA	-	expression tag	UNP A0A0U1WGG5
v	186	ALA	-	expression tag	UNP A0A0U1WGG5
v	187	LEU	-	expression tag	UNP A0A0U1WGG5
v	188	GLU	-	expression tag	UNP A0A0U1WGG5
v	189	HIS	-	expression tag	UNP A0A0U1WGG5
v	190	HIS	-	expression tag	UNP A0A0U1WGG5
v	191	HIS	-	expression tag	UNP A0A0U1WGG5
v	192	HIS	-	expression tag	UNP A0A0U1WGG5
v	193	HIS	-	expression tag	UNP A0A0U1WGG5
v	194	HIS	-	expression tag	UNP A0A0U1WGG5
w	174	ASP	-	expression tag	UNP A0A0U1WGG5
w	175	PRO	-	expression tag	UNP A0A0U1WGG5
w	176	ASN	-	expression tag	UNP A0A0U1WGG5
w	177	SER	-	expression tag	UNP A0A0U1WGG5

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Chain	Residue	Modelled	Actual	Comment	Reference
w	178	SER	-	expression tag	UNP A0A0U1WGGQ5
w	179	SER	-	expression tag	UNP A0A0U1WGGQ5
w	180	VAL	-	expression tag	UNP A0A0U1WGGQ5
w	181	ASP	-	expression tag	UNP A0A0U1WGGQ5
w	182	LYS	-	expression tag	UNP A0A0U1WGGQ5
w	183	LEU	-	expression tag	UNP A0A0U1WGGQ5
w	184	ALA	-	expression tag	UNP A0A0U1WGGQ5
w	185	ALA	-	expression tag	UNP A0A0U1WGGQ5
w	186	ALA	-	expression tag	UNP A0A0U1WGGQ5
w	187	LEU	-	expression tag	UNP A0A0U1WGGQ5
w	188	GLU	-	expression tag	UNP A0A0U1WGGQ5
w	189	HIS	-	expression tag	UNP A0A0U1WGGQ5
w	190	HIS	-	expression tag	UNP A0A0U1WGGQ5
w	191	HIS	-	expression tag	UNP A0A0U1WGGQ5
w	192	HIS	-	expression tag	UNP A0A0U1WGGQ5
w	193	HIS	-	expression tag	UNP A0A0U1WGGQ5
w	194	HIS	-	expression tag	UNP A0A0U1WGGQ5
x	174	ASP	-	expression tag	UNP A0A0U1WGGQ5
x	175	PRO	-	expression tag	UNP A0A0U1WGGQ5
x	176	ASN	-	expression tag	UNP A0A0U1WGGQ5
x	177	SER	-	expression tag	UNP A0A0U1WGGQ5
x	178	SER	-	expression tag	UNP A0A0U1WGGQ5
x	179	SER	-	expression tag	UNP A0A0U1WGGQ5
x	180	VAL	-	expression tag	UNP A0A0U1WGGQ5
x	181	ASP	-	expression tag	UNP A0A0U1WGGQ5
x	182	LYS	-	expression tag	UNP A0A0U1WGGQ5
x	183	LEU	-	expression tag	UNP A0A0U1WGGQ5
x	184	ALA	-	expression tag	UNP A0A0U1WGGQ5
x	185	ALA	-	expression tag	UNP A0A0U1WGGQ5
x	186	ALA	-	expression tag	UNP A0A0U1WGGQ5
x	187	LEU	-	expression tag	UNP A0A0U1WGGQ5
x	188	GLU	-	expression tag	UNP A0A0U1WGGQ5
x	189	HIS	-	expression tag	UNP A0A0U1WGGQ5
x	190	HIS	-	expression tag	UNP A0A0U1WGGQ5
x	191	HIS	-	expression tag	UNP A0A0U1WGGQ5
x	192	HIS	-	expression tag	UNP A0A0U1WGGQ5
x	193	HIS	-	expression tag	UNP A0A0U1WGGQ5
x	194	HIS	-	expression tag	UNP A0A0U1WGGQ5
y	174	ASP	-	expression tag	UNP A0A0U1WGGQ5
y	175	PRO	-	expression tag	UNP A0A0U1WGGQ5
y	176	ASN	-	expression tag	UNP A0A0U1WGGQ5
y	177	SER	-	expression tag	UNP A0A0U1WGGQ5

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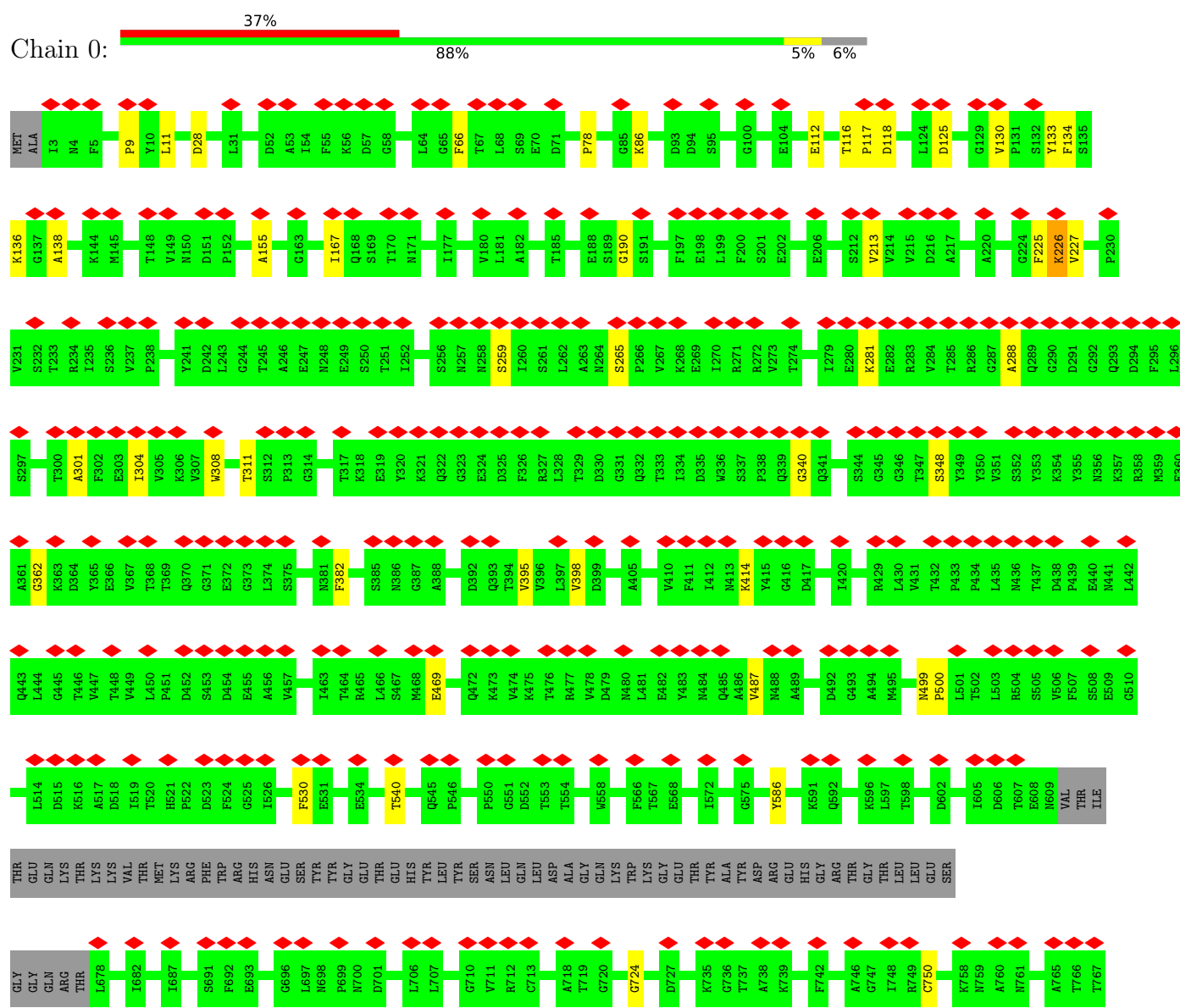
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Chain	Residue	Modelled	Actual	Comment	Reference
y	178	SER	-	expression tag	UNP A0A0U1WGQ5
y	179	SER	-	expression tag	UNP A0A0U1WGQ5
y	180	VAL	-	expression tag	UNP A0A0U1WGQ5
y	181	ASP	-	expression tag	UNP A0A0U1WGQ5
y	182	LYS	-	expression tag	UNP A0A0U1WGQ5
y	183	LEU	-	expression tag	UNP A0A0U1WGQ5
y	184	ALA	-	expression tag	UNP A0A0U1WGQ5
y	185	ALA	-	expression tag	UNP A0A0U1WGQ5
y	186	ALA	-	expression tag	UNP A0A0U1WGQ5
y	187	LEU	-	expression tag	UNP A0A0U1WGQ5
y	188	GLU	-	expression tag	UNP A0A0U1WGQ5
y	189	HIS	-	expression tag	UNP A0A0U1WGQ5
y	190	HIS	-	expression tag	UNP A0A0U1WGQ5
y	191	HIS	-	expression tag	UNP A0A0U1WGQ5
y	192	HIS	-	expression tag	UNP A0A0U1WGQ5
y	193	HIS	-	expression tag	UNP A0A0U1WGQ5
y	194	HIS	-	expression tag	UNP A0A0U1WGQ5

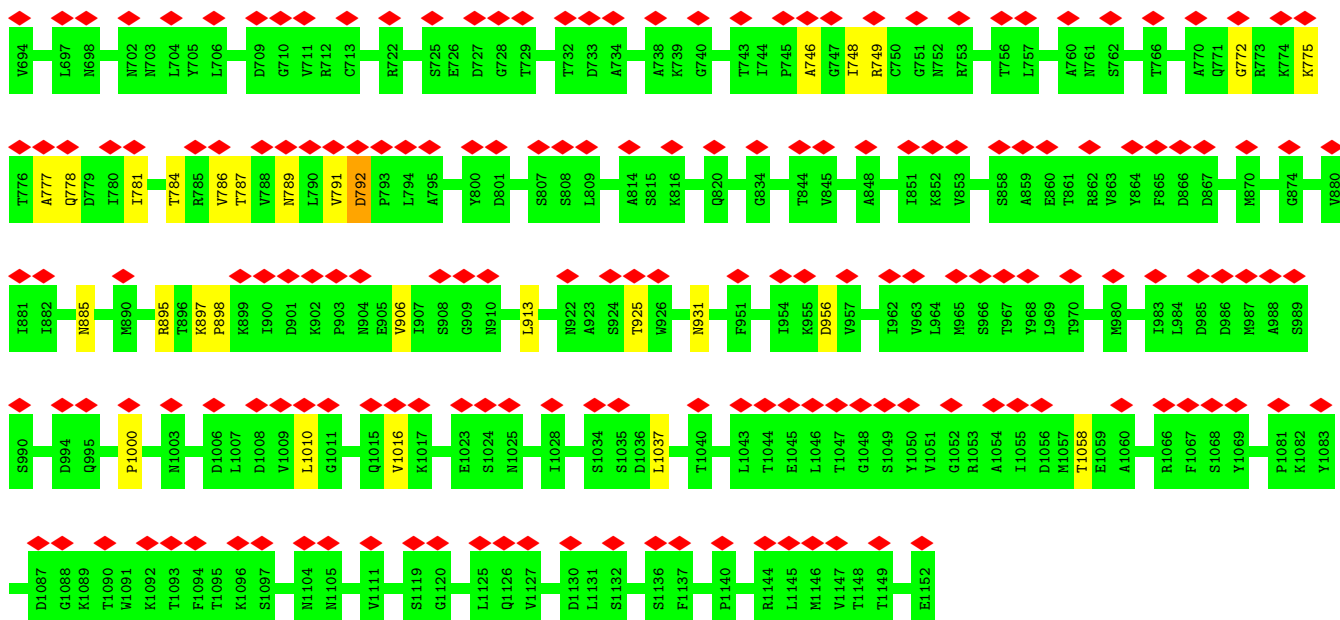
3 Residue-property plots

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.

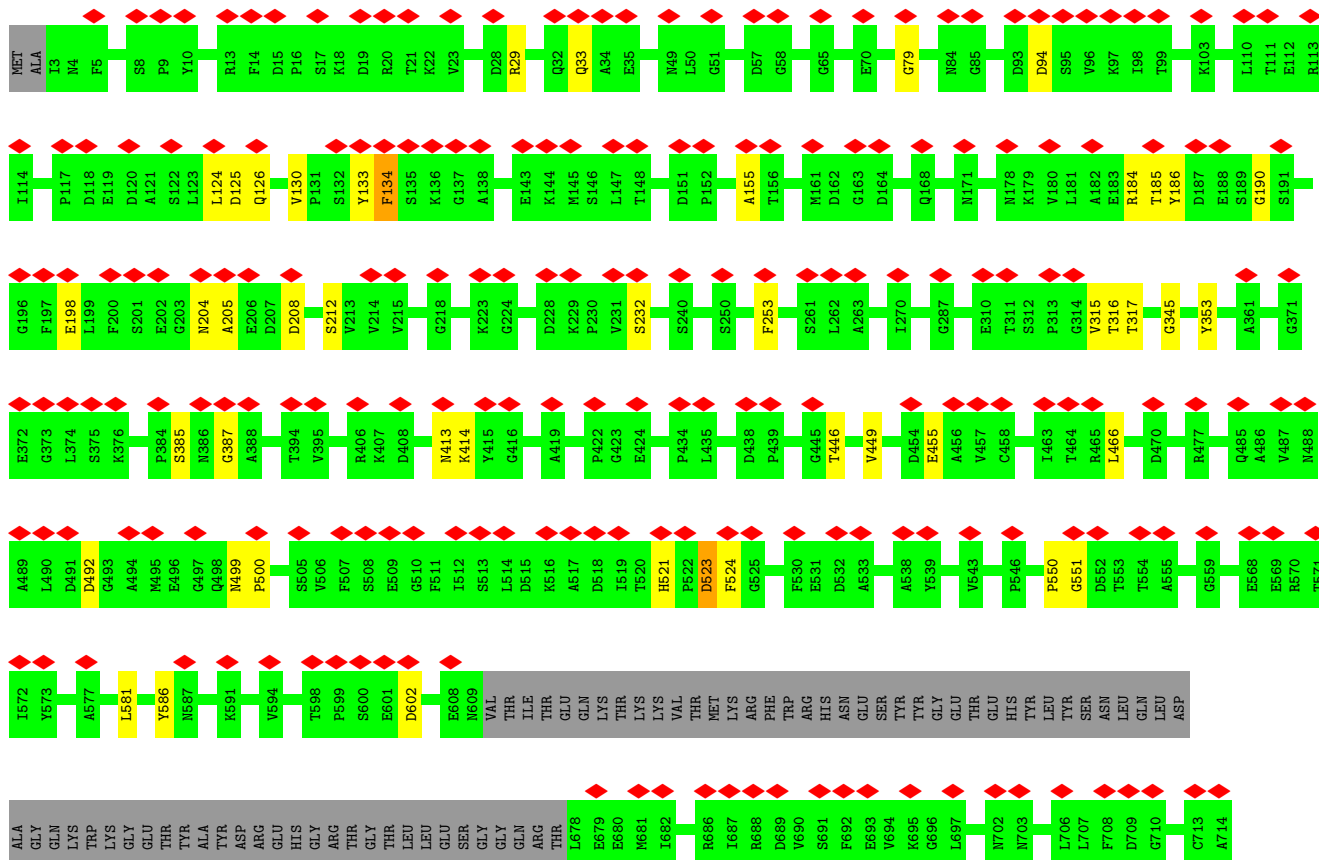
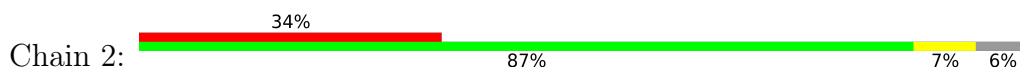
- Molecule 1: DUF4815 domain-containing protein

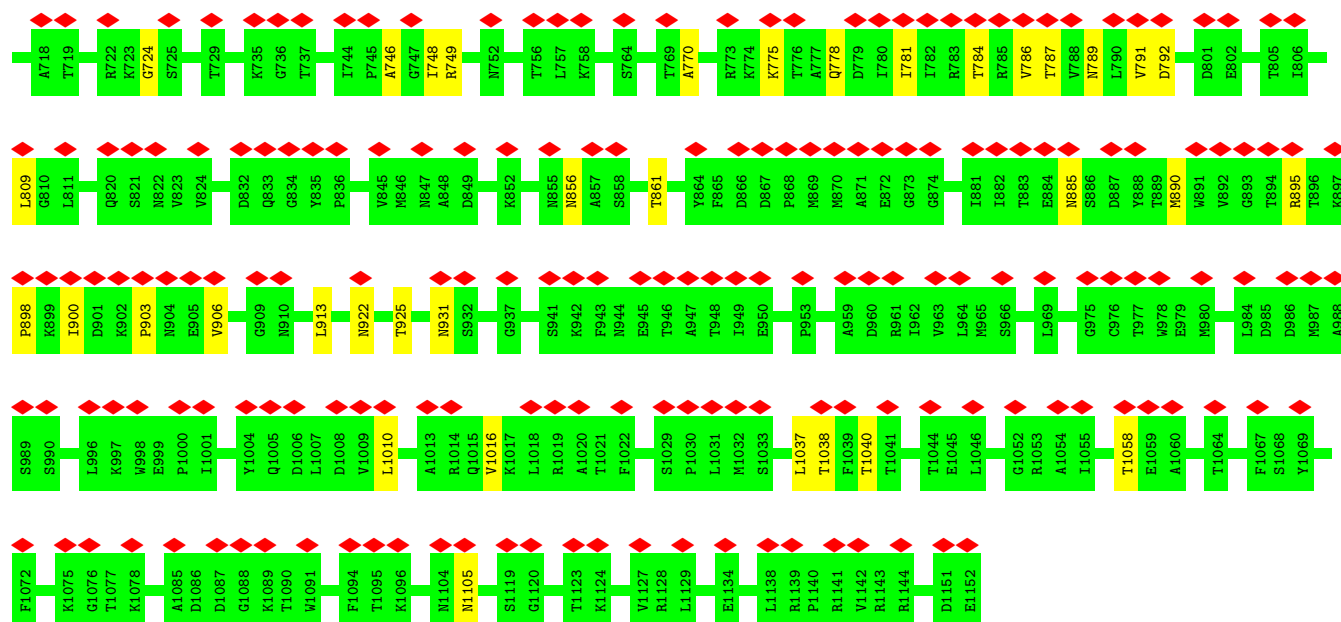




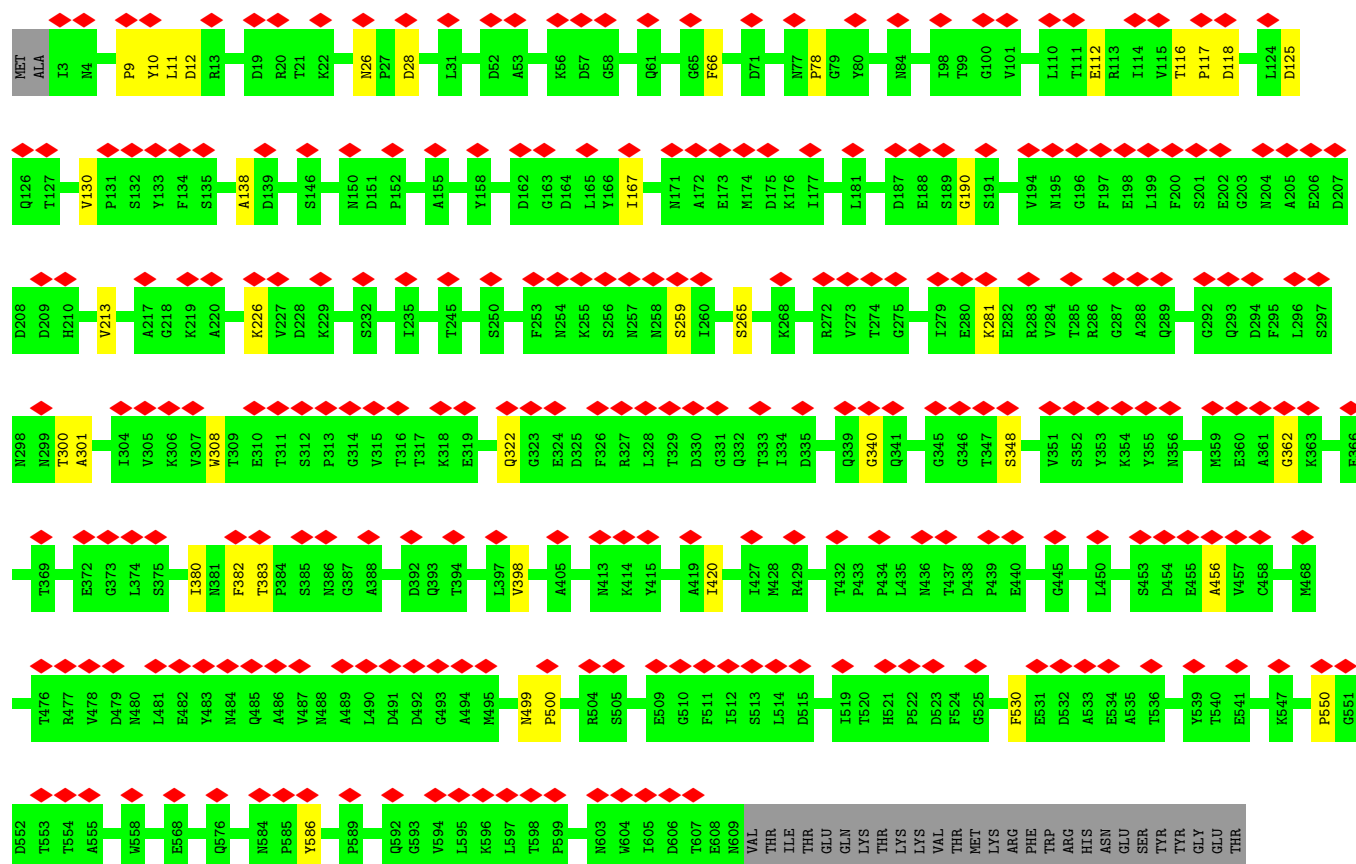
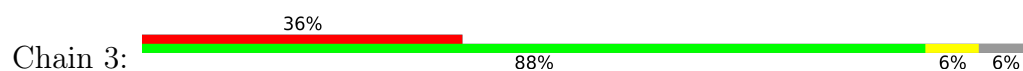


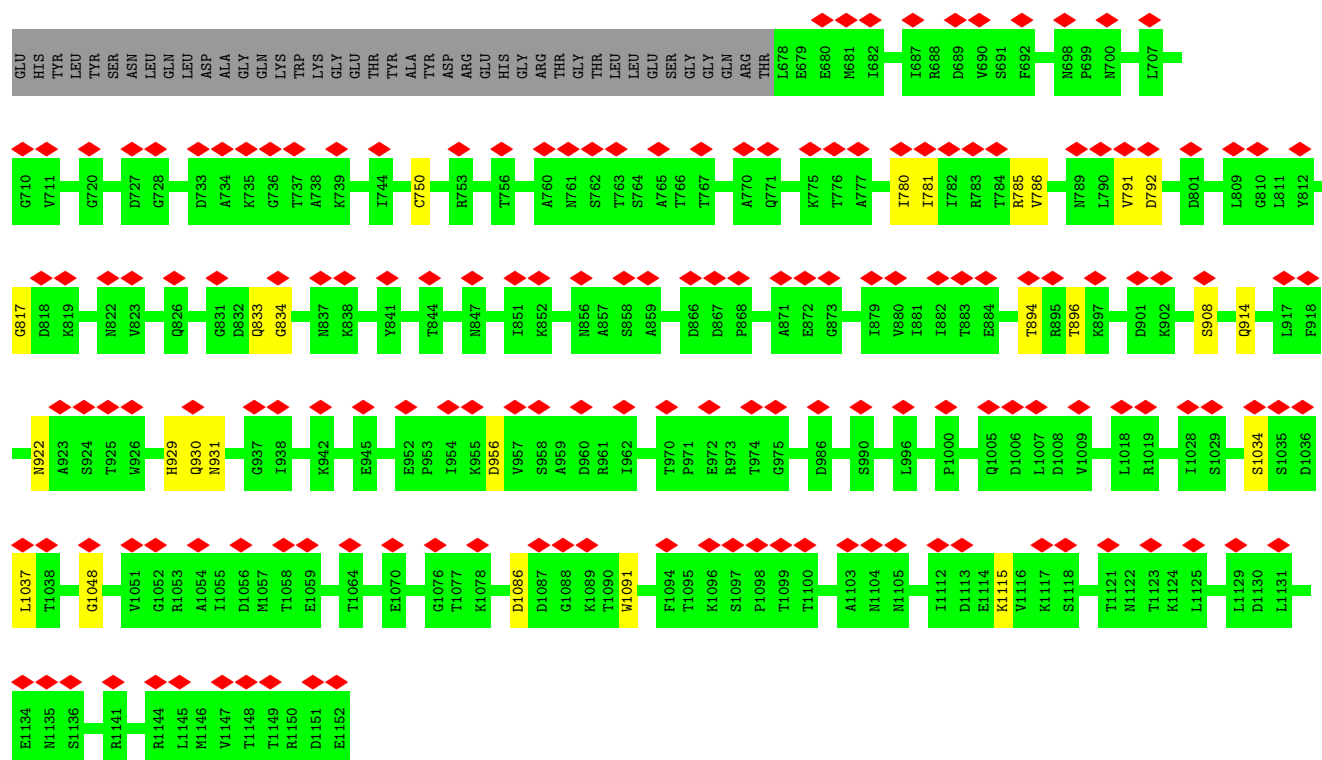
• Molecule 1: DUF4815 domain-containing protein



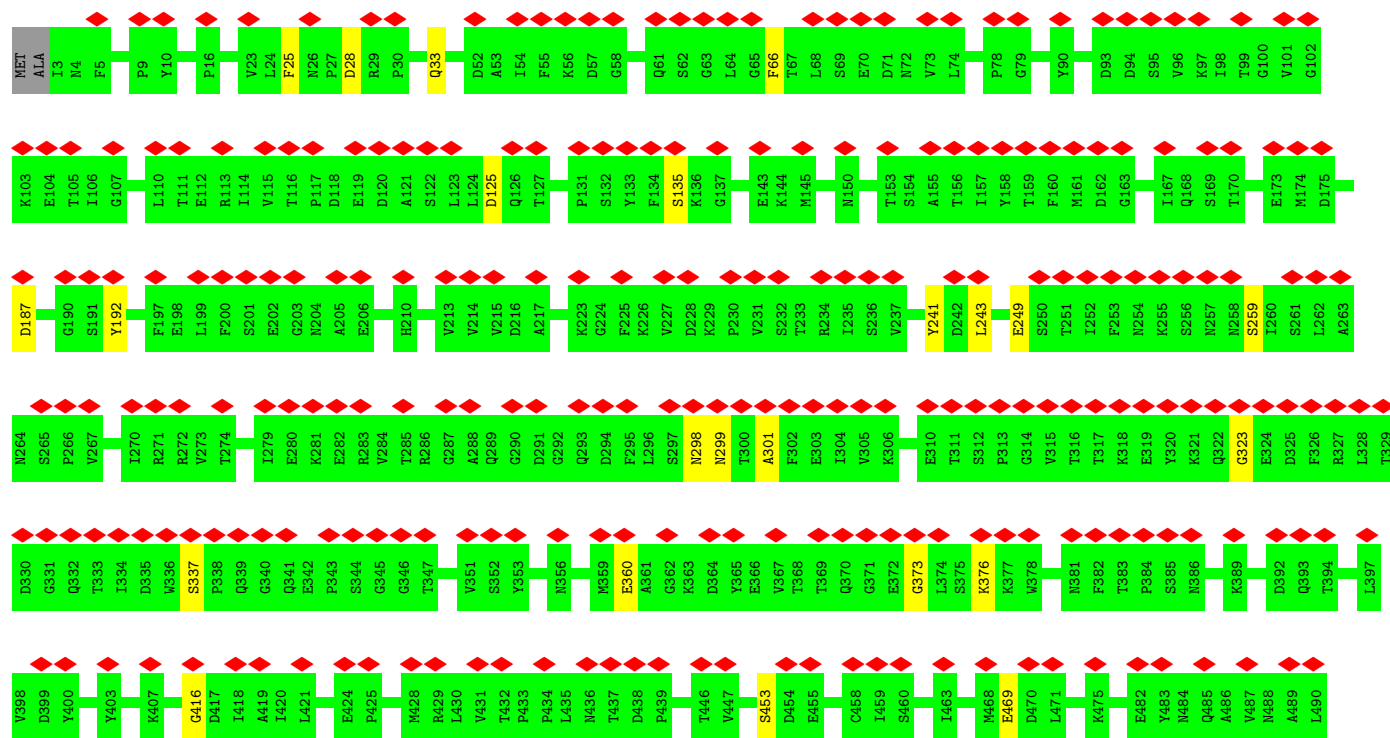
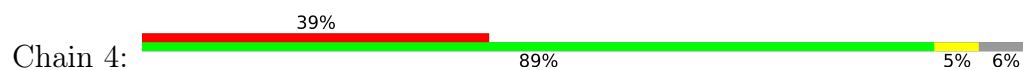


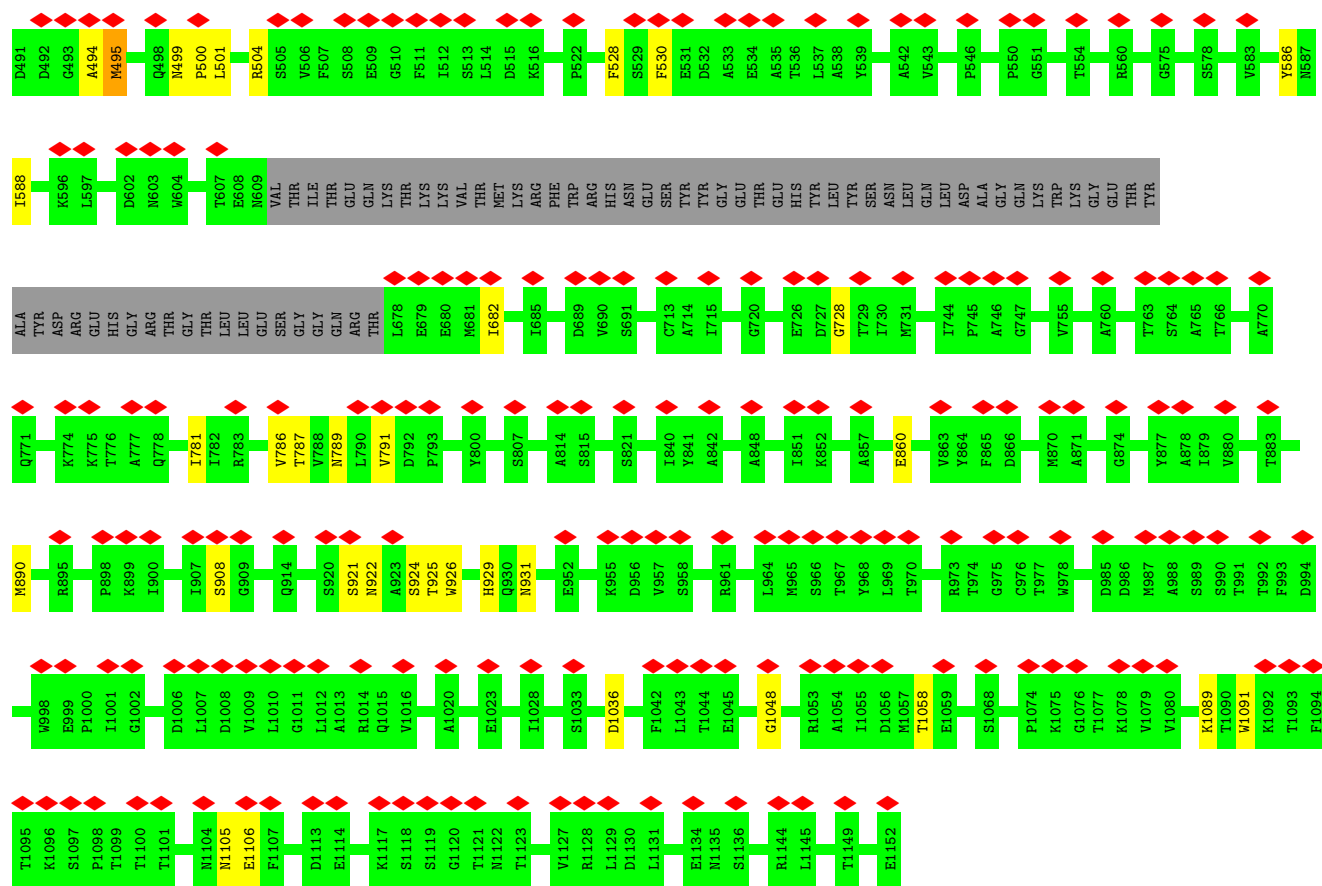
• Molecule 1: DUF4815 domain-containing protein



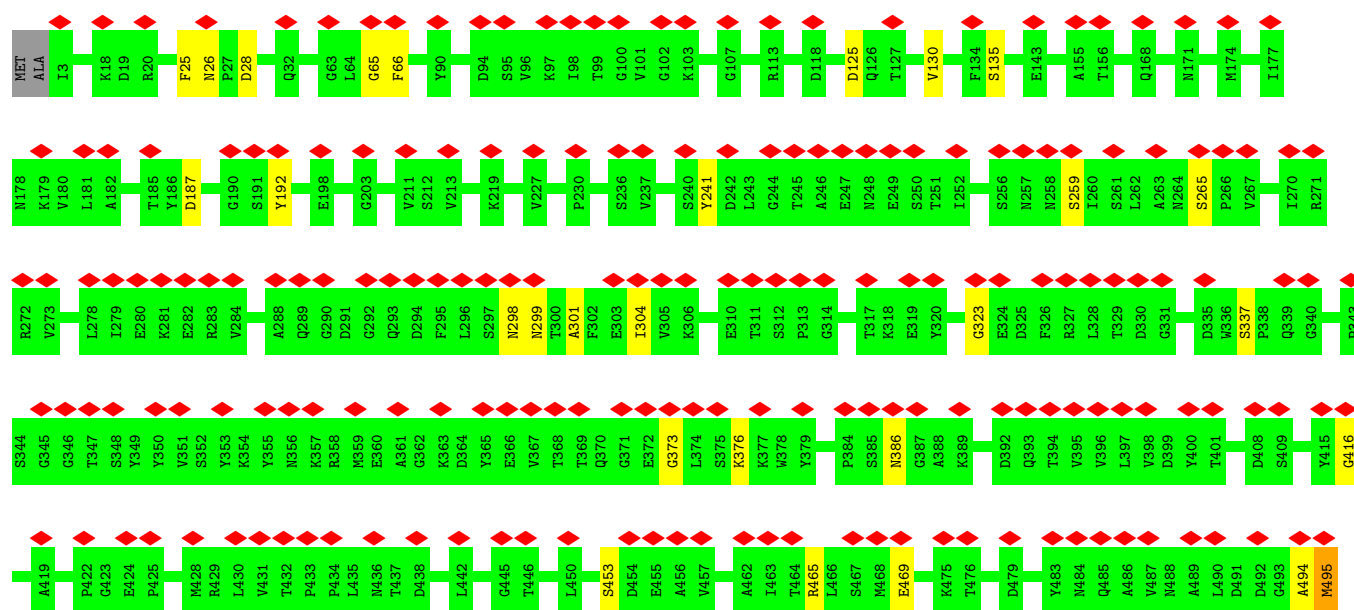
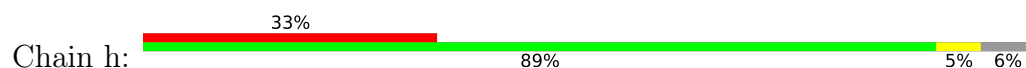


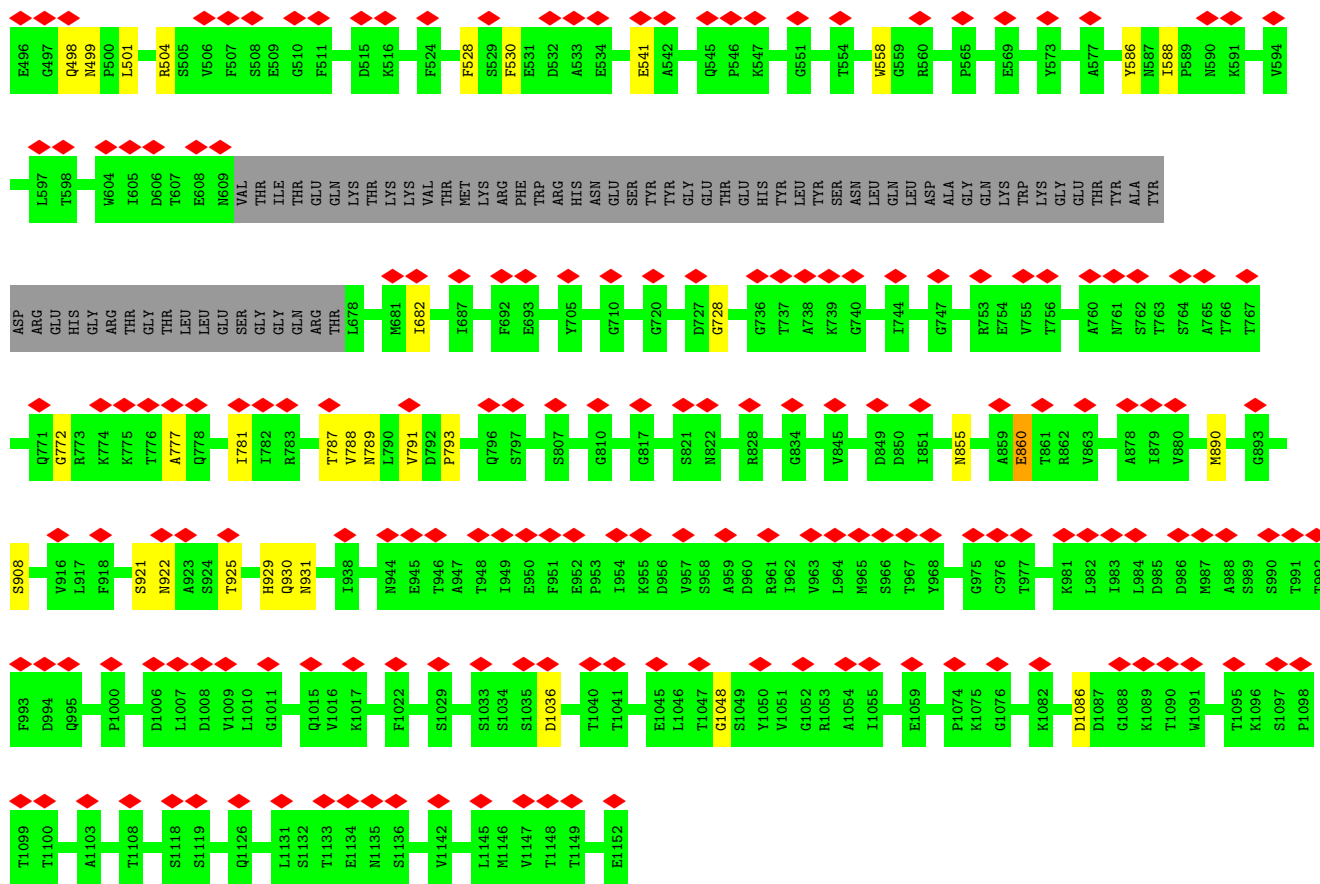
• Molecule 1: DUF4815 domain-containing protein



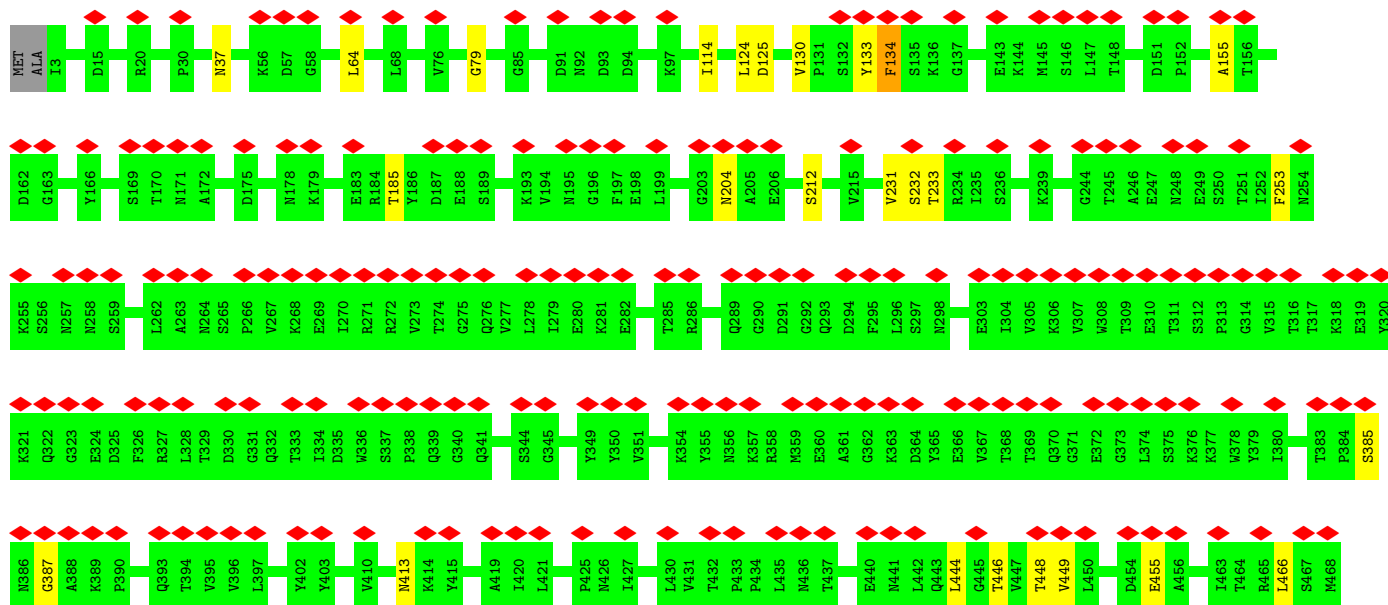
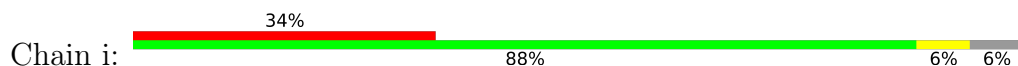


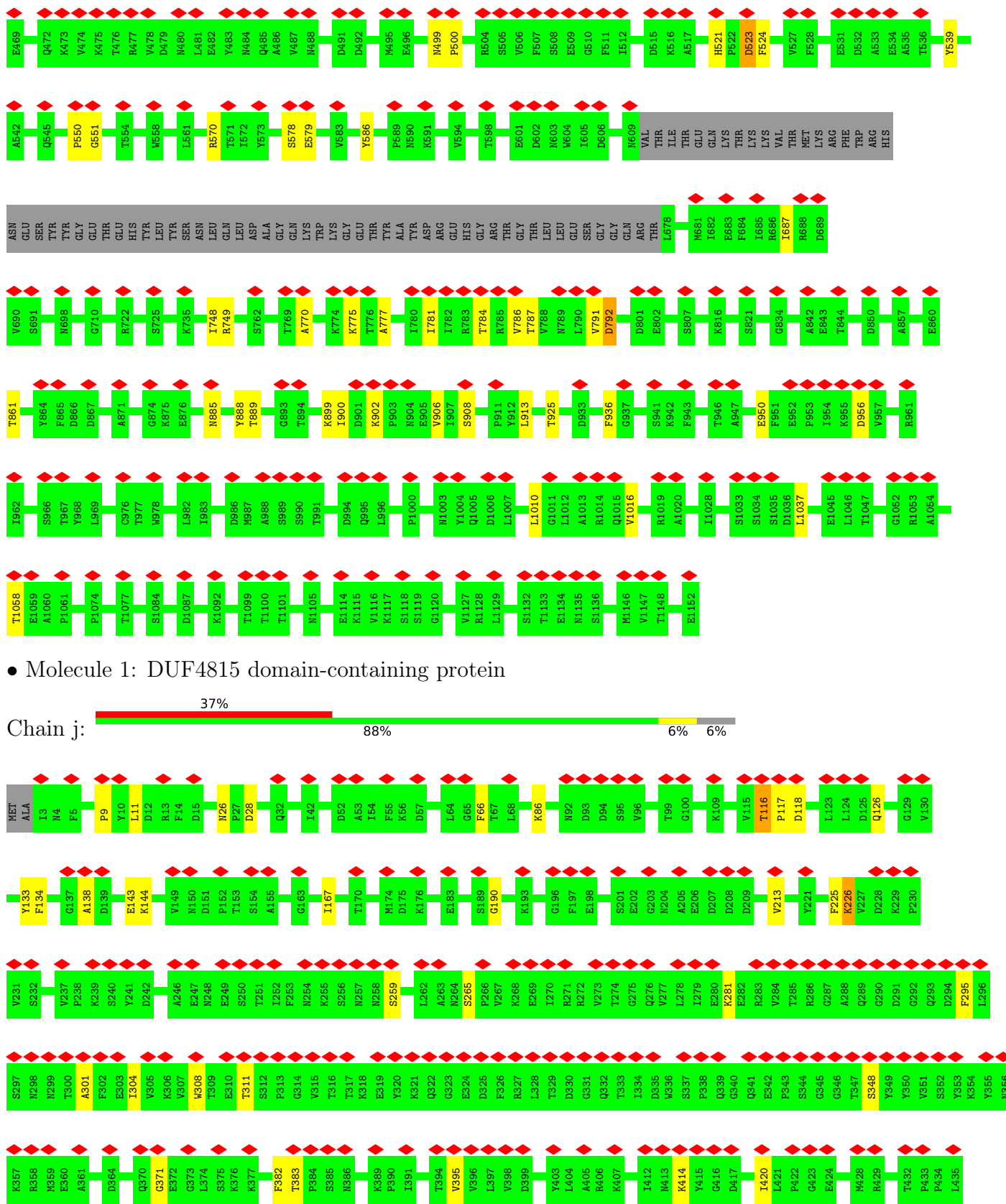
• Molecule 1: DUF4815 domain-containing protein

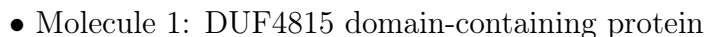




• Molecule 1: DUF4815 domain-containing protein

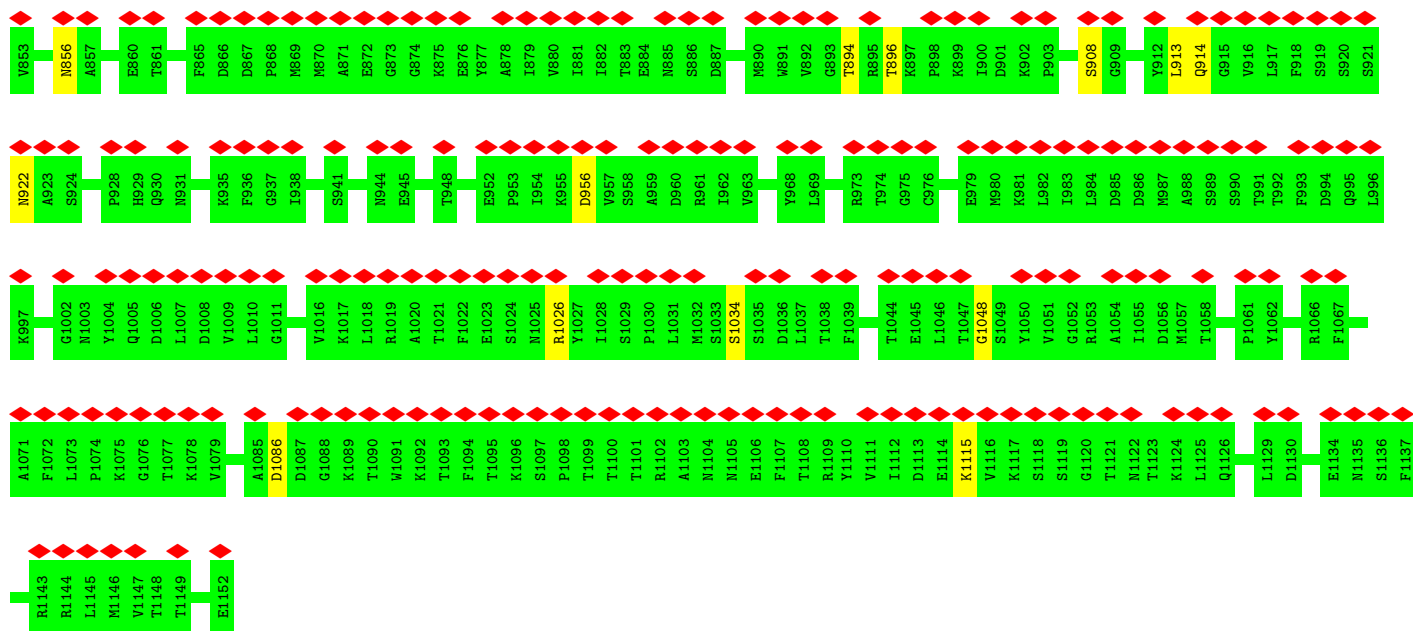




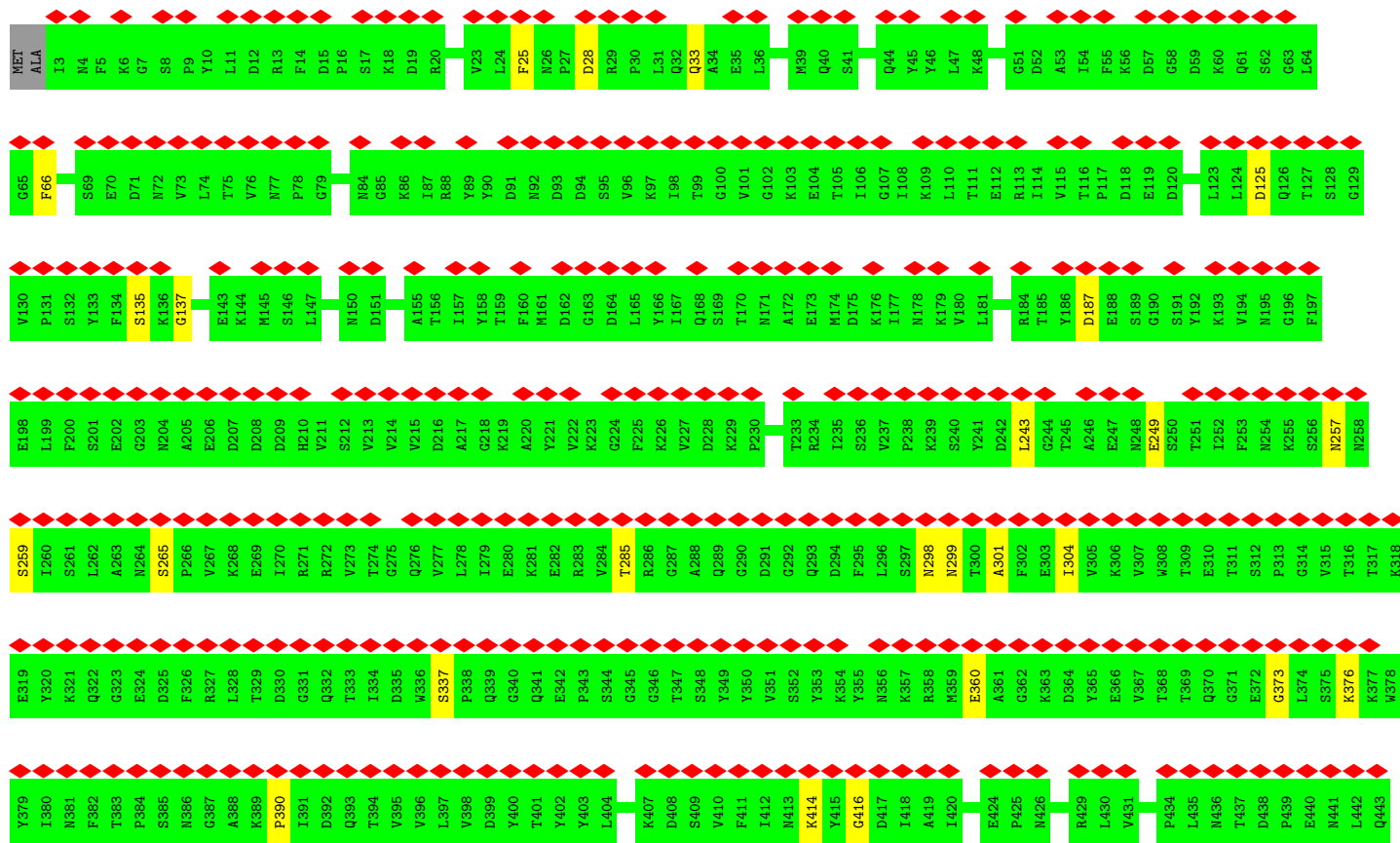
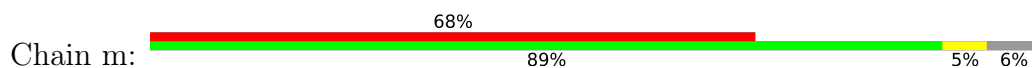


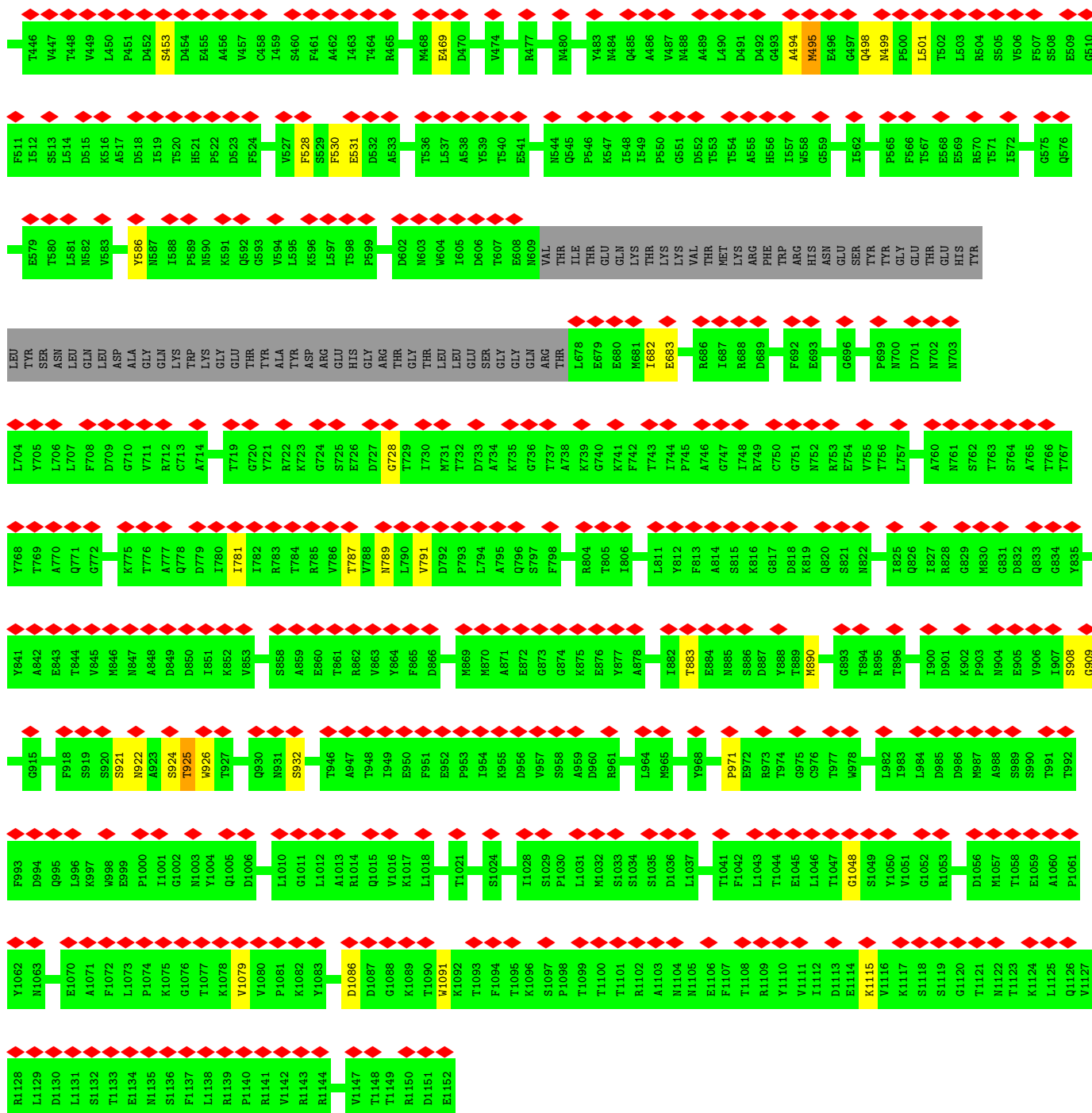
Response	Percentage
U.S. is a threat to my country's security	67%
U.S. is not a threat to my country's security	89%
Don't know	5%
No answer	6%





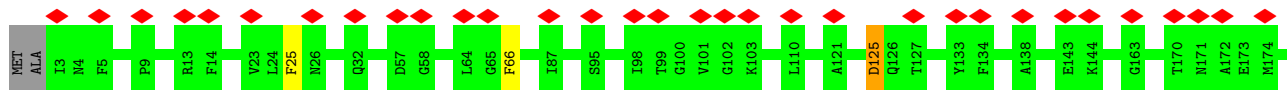
• Molecule 1: DUF4815 domain-containing protein

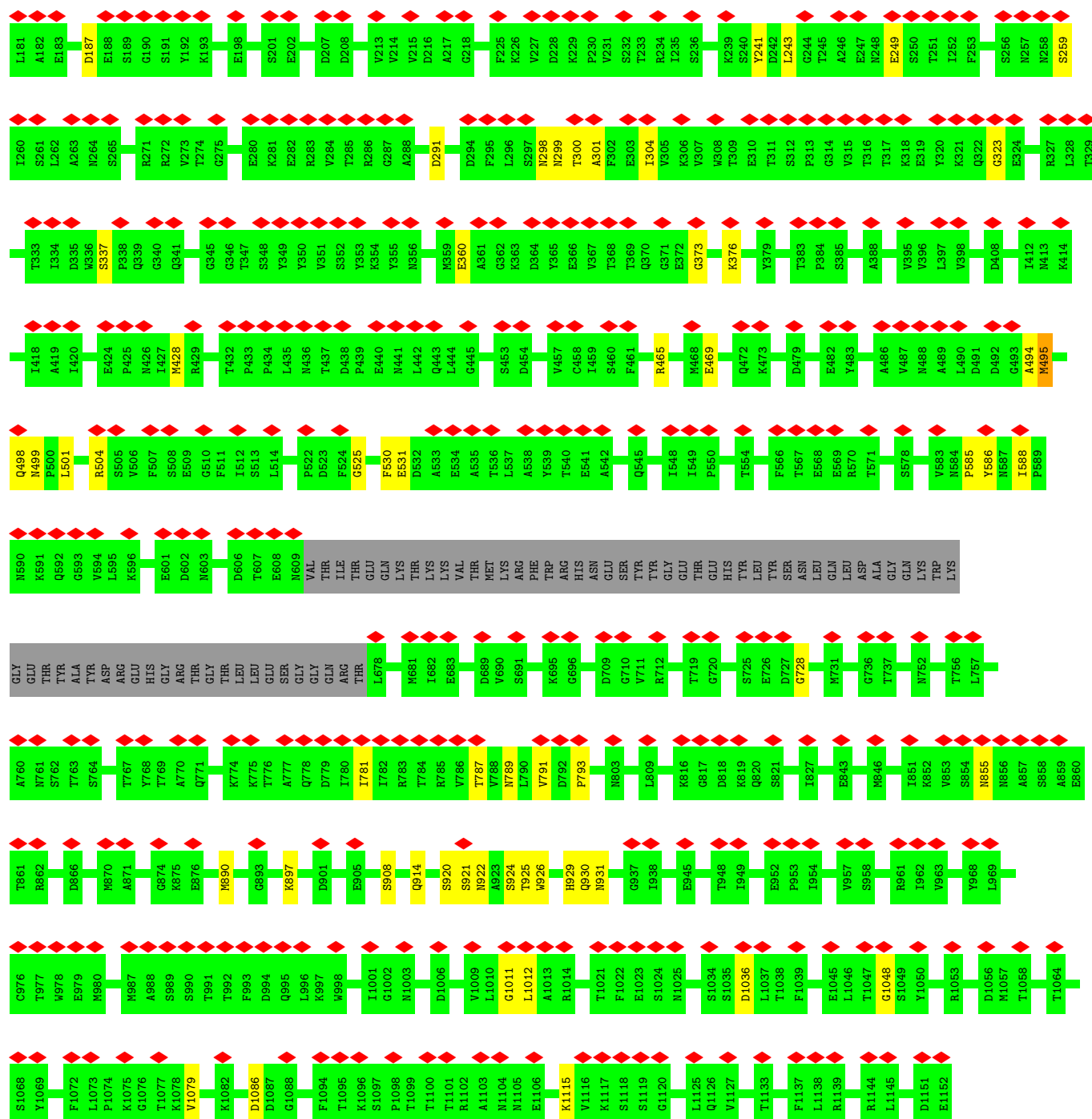




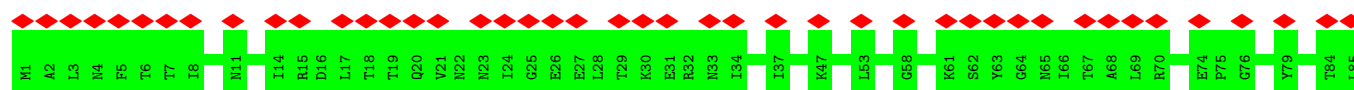
- Molecule 1: DUF4815 domain-containing protein

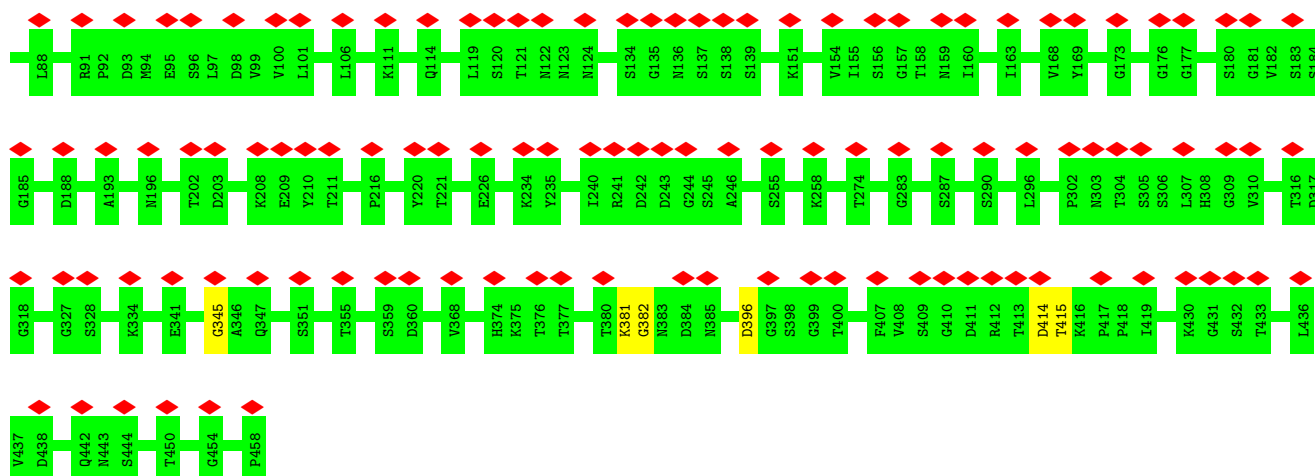
Chain z: 35% 89% 5% 6%



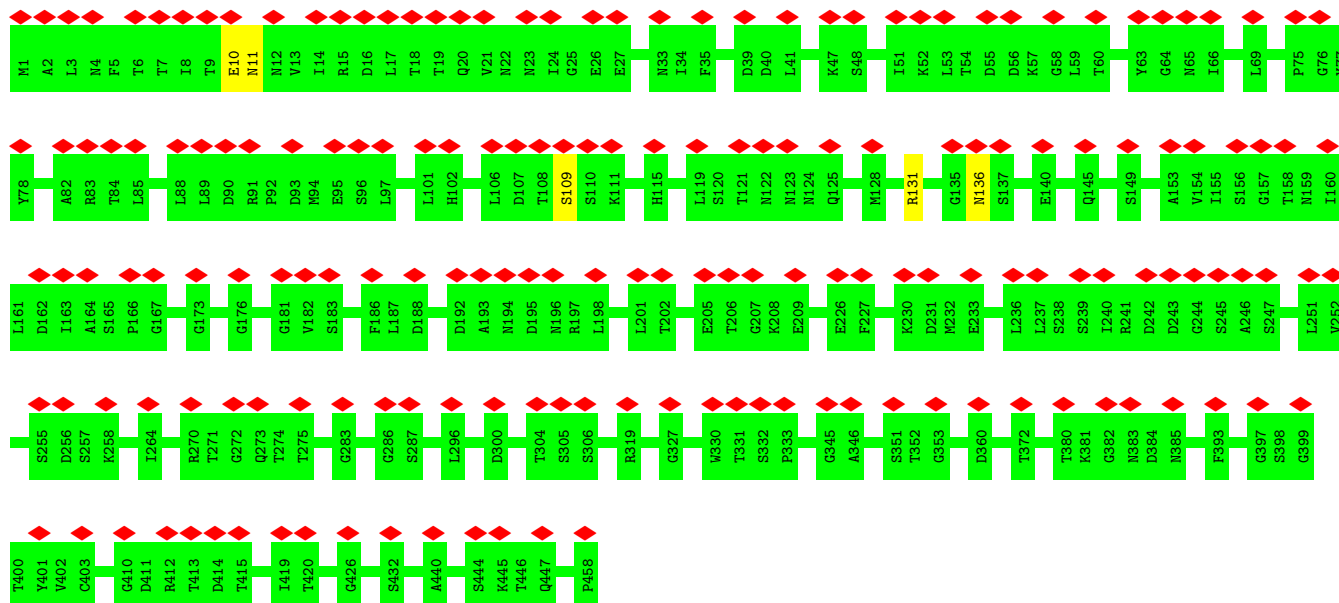


• Molecule 2: Receptor binding protein

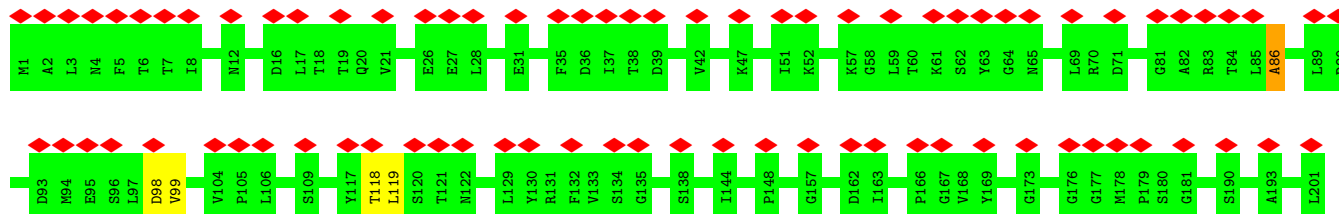


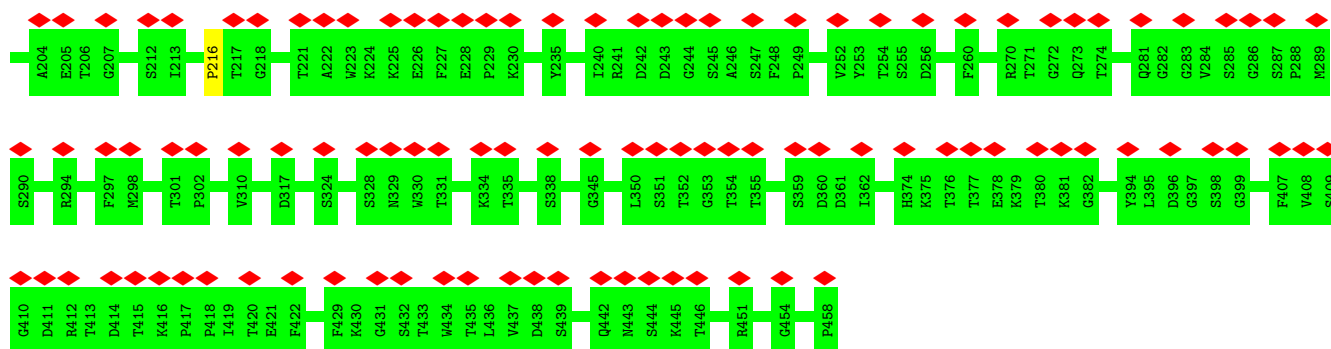


• Molecule 2: Receptor binding protein

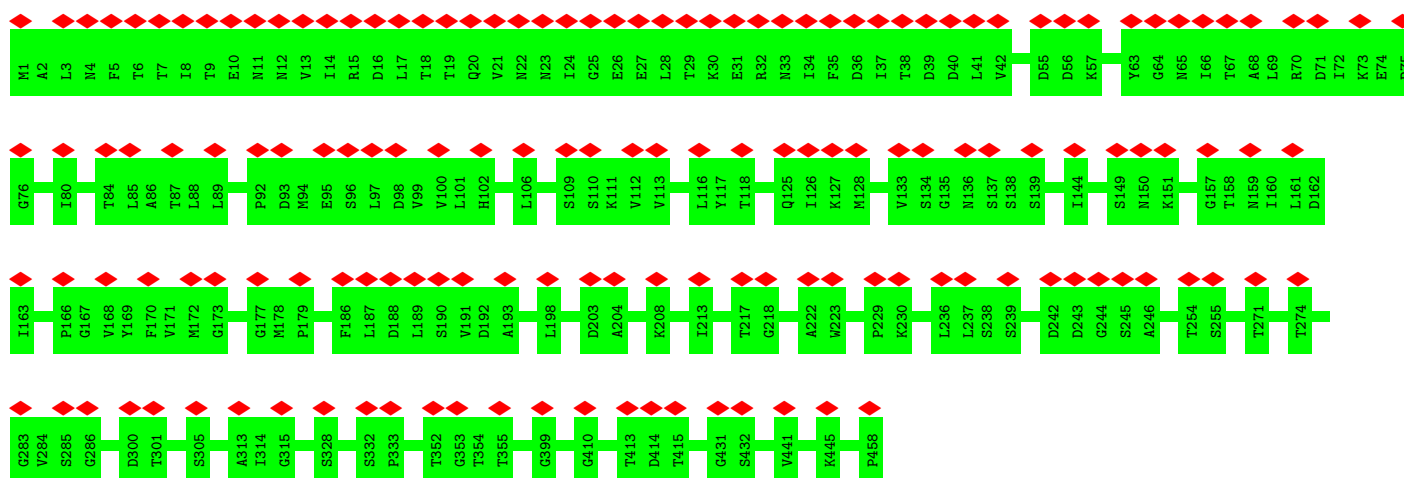


• Molecule 2: Receptor binding protein

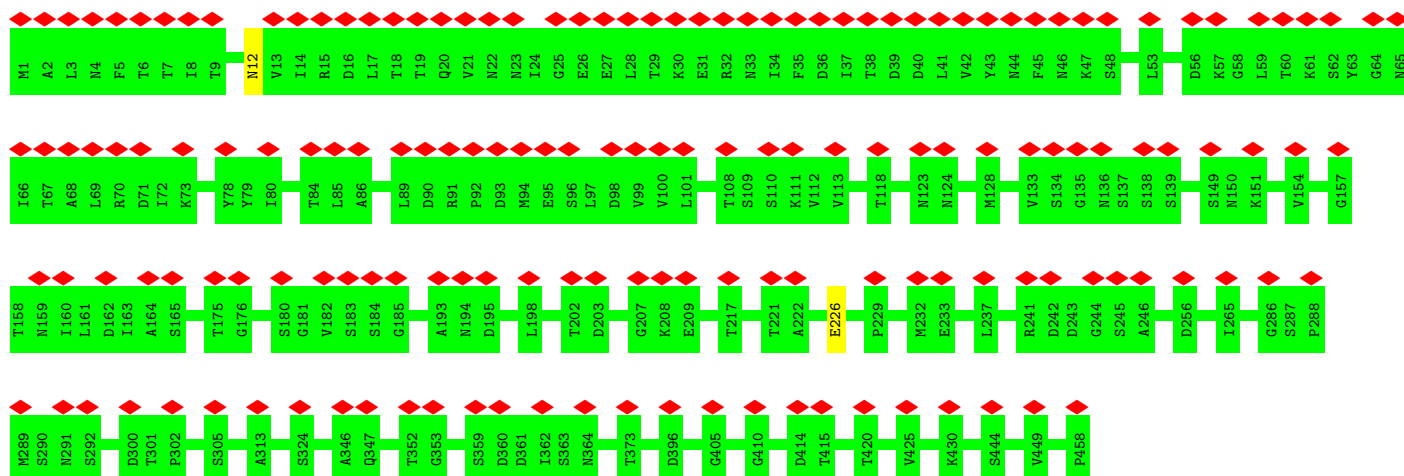




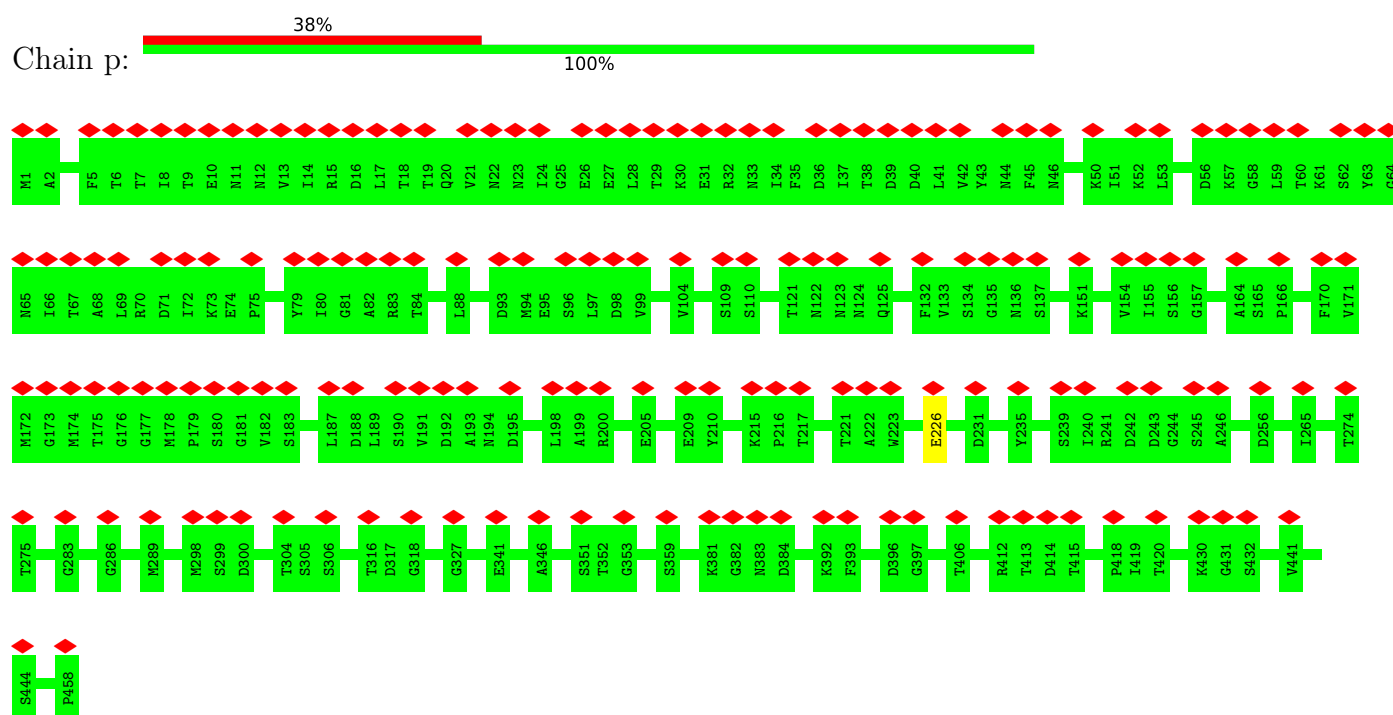
• Molecule 2: Receptor binding protein



• Molecule 2: Receptor binding protein



• Molecule 2: Receptor binding protein

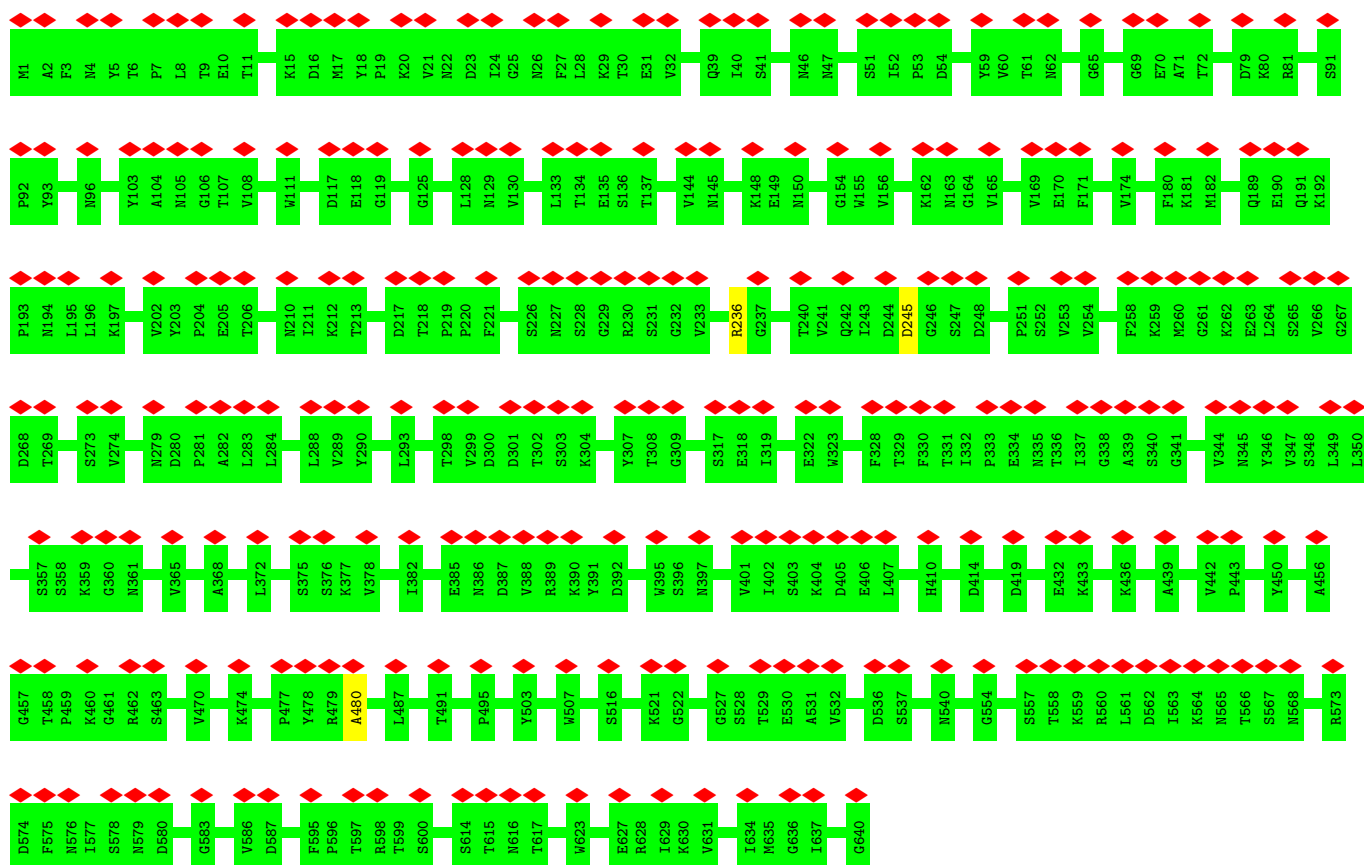


• Molecule 3: CBM-cenC domain-containing protein

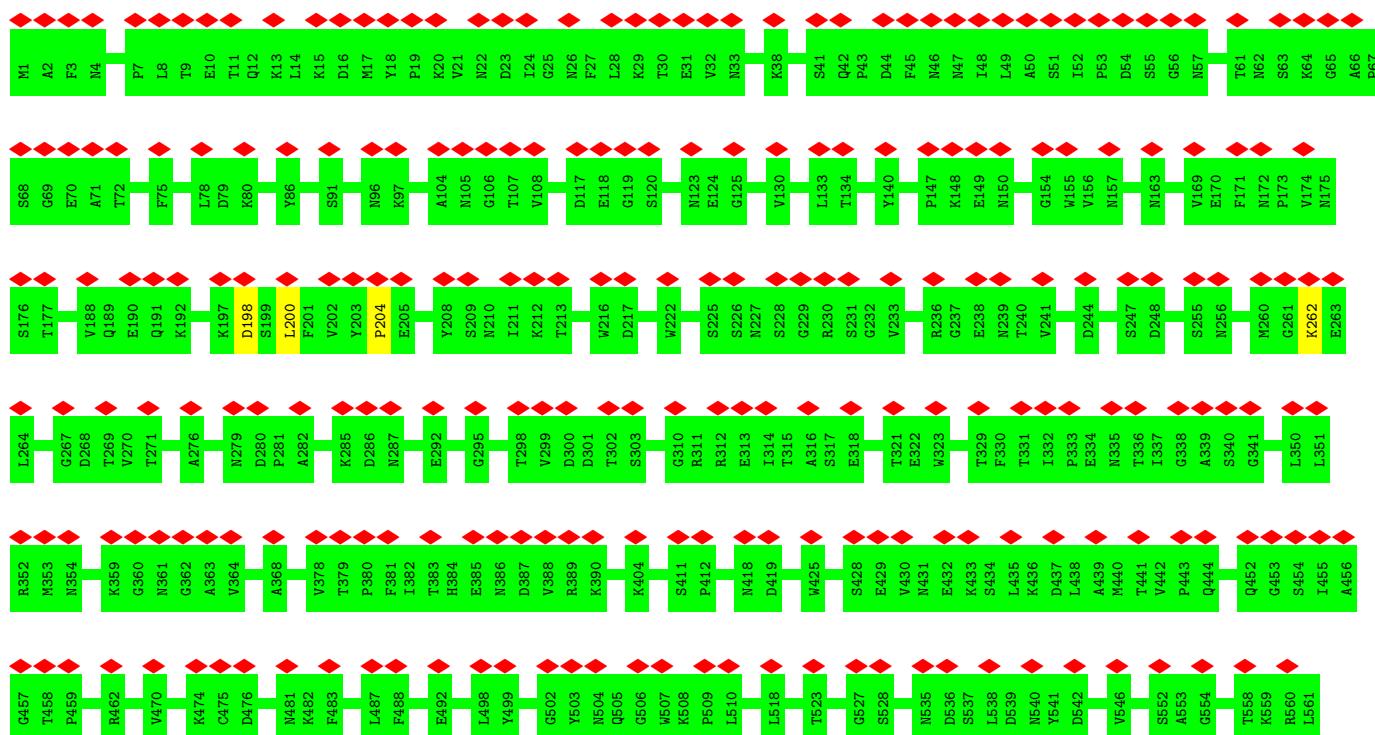


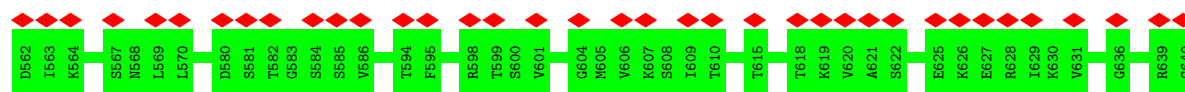
• Molecule 3: CBM-cenC domain-containing protein





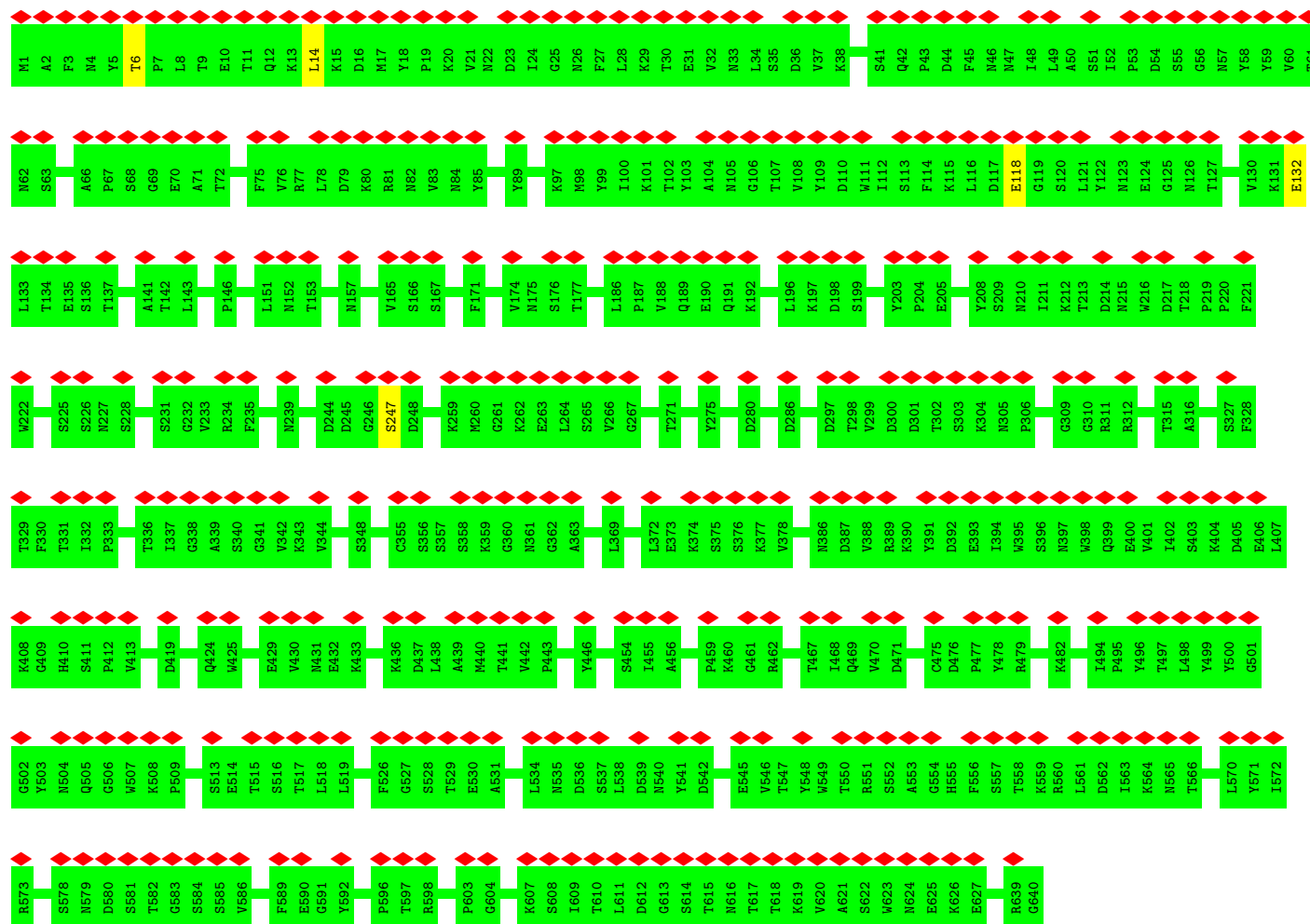
• Molecule 3: CBM-cenC domain-containing protein





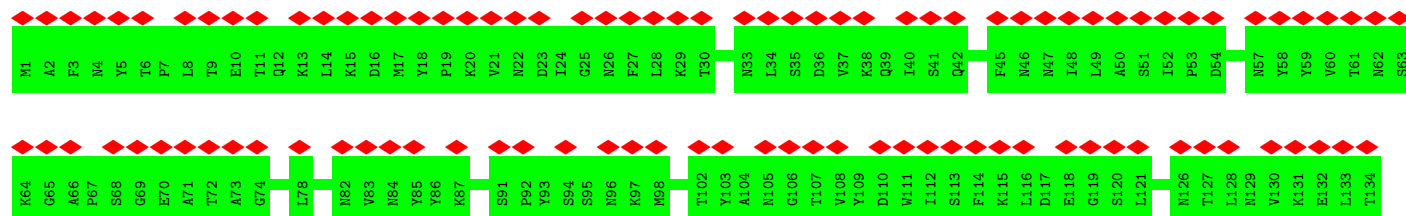
• Molecule 3: CBM-cenC domain-containing protein

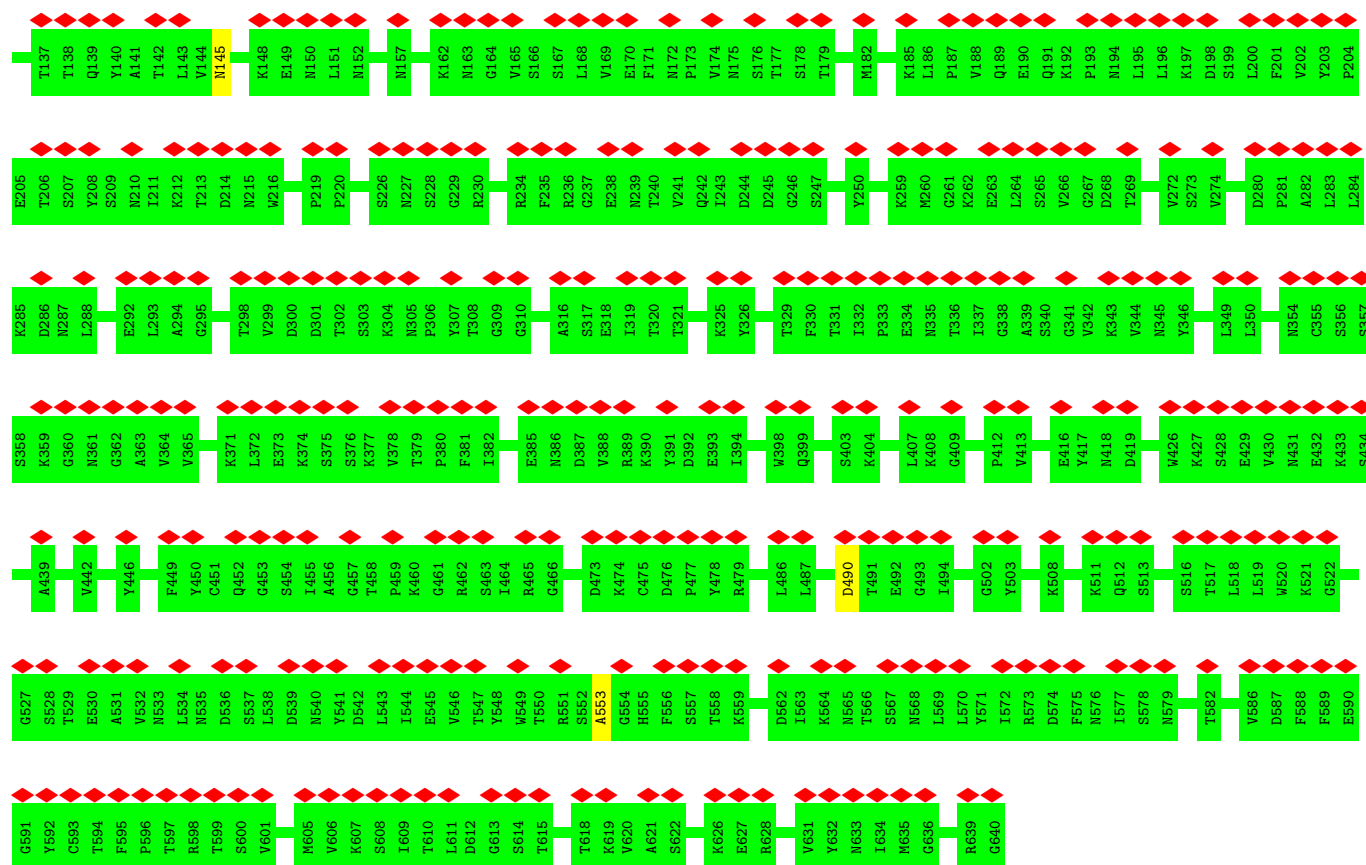
Chain q: 57% 99%



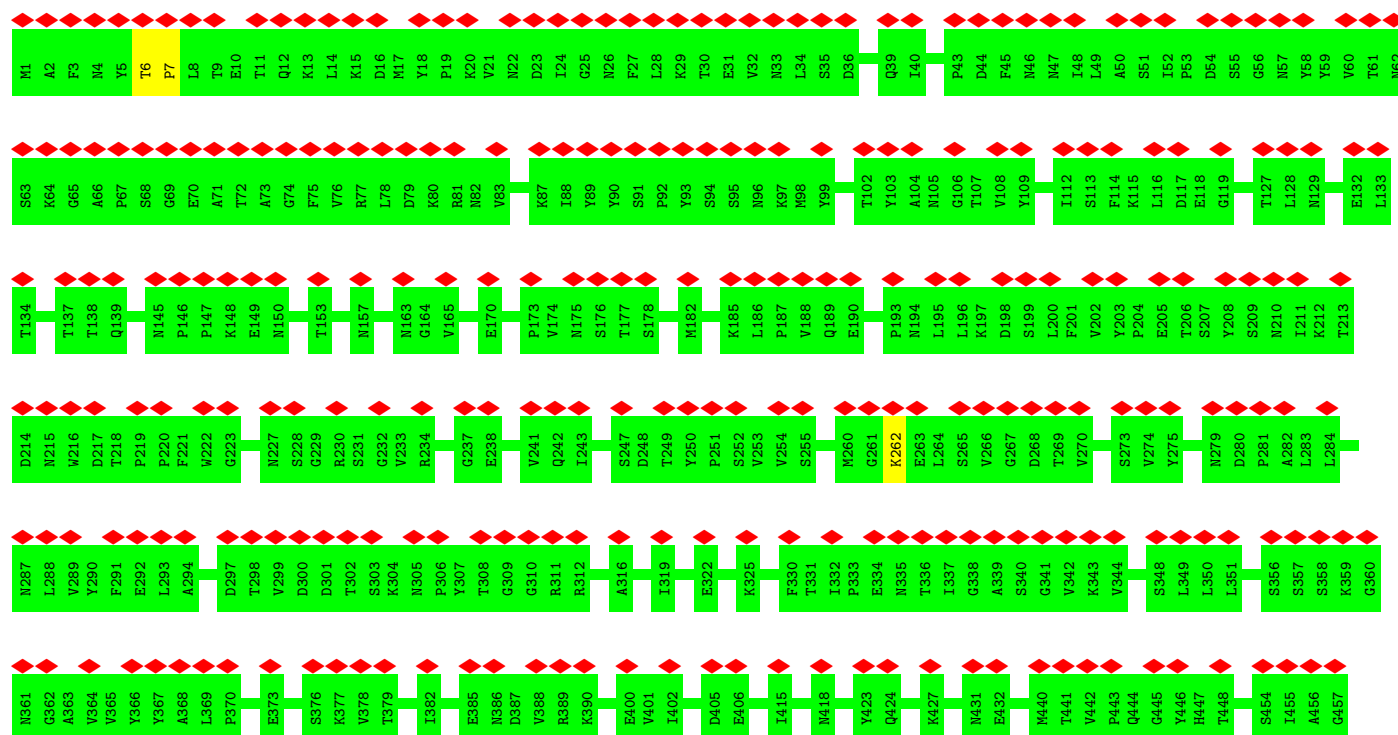
• Molecule 3: CBM-cenC domain-containing protein

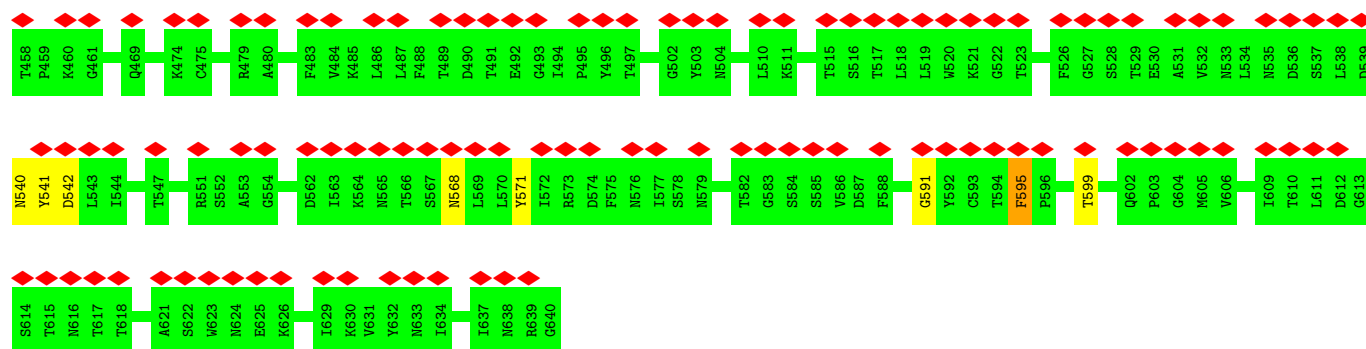
Chain r: 63% 100%



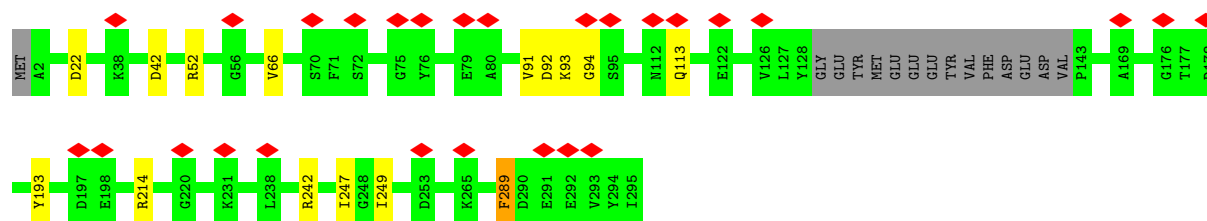


• Molecule 3: CBM-cenC domain-containing protein

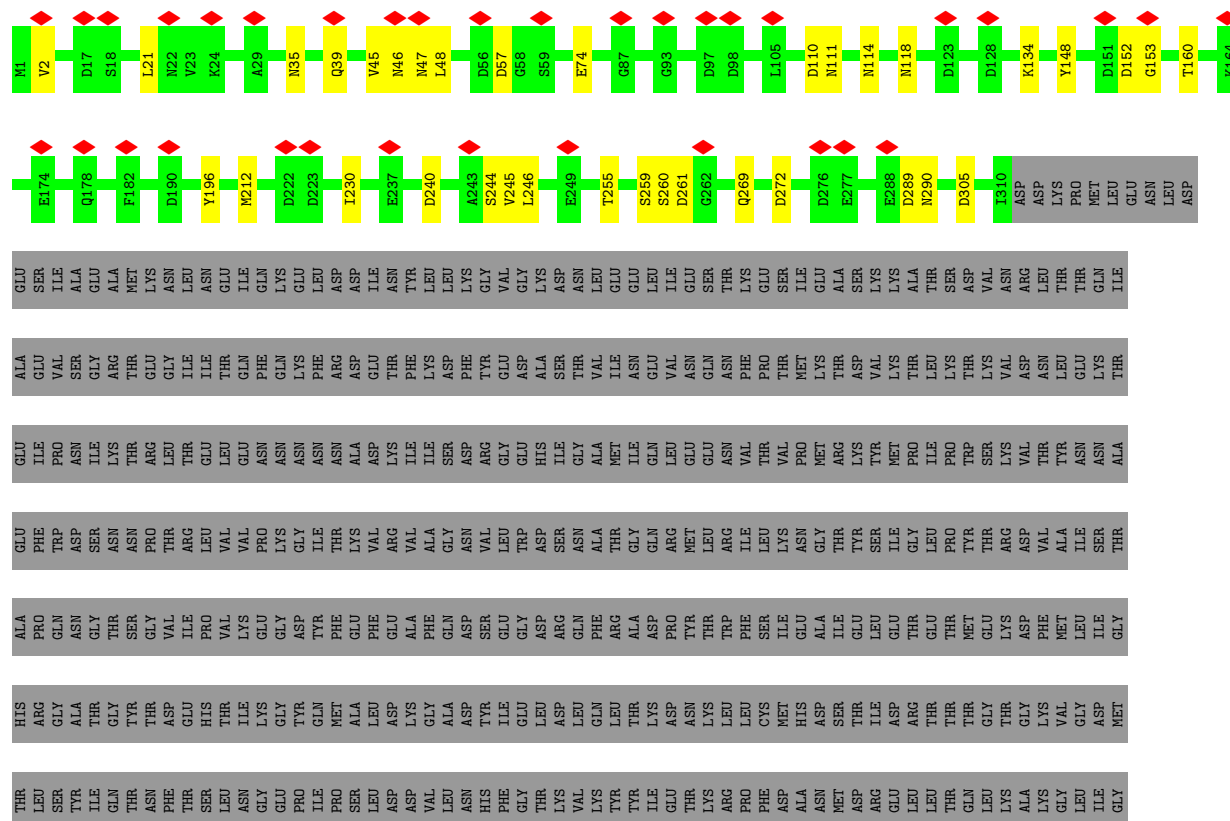




• Molecule 4: NlpC/P60 domain-containing protein

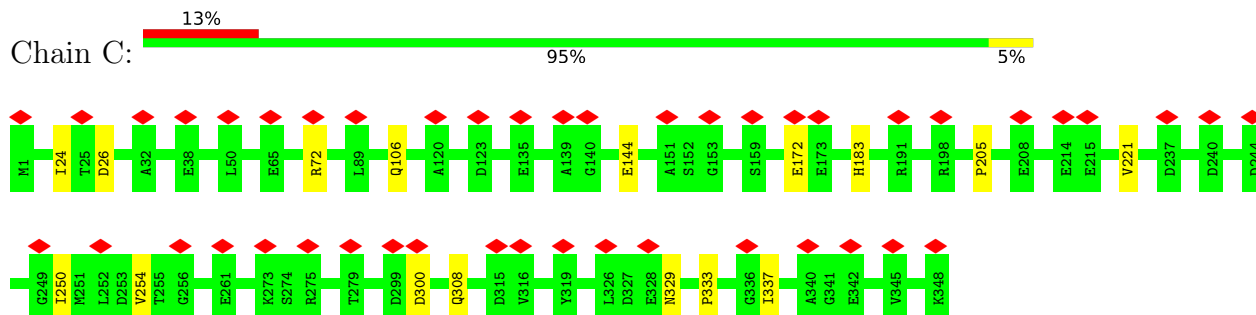


• Molecule 5: GP-PDE domain-containing protein

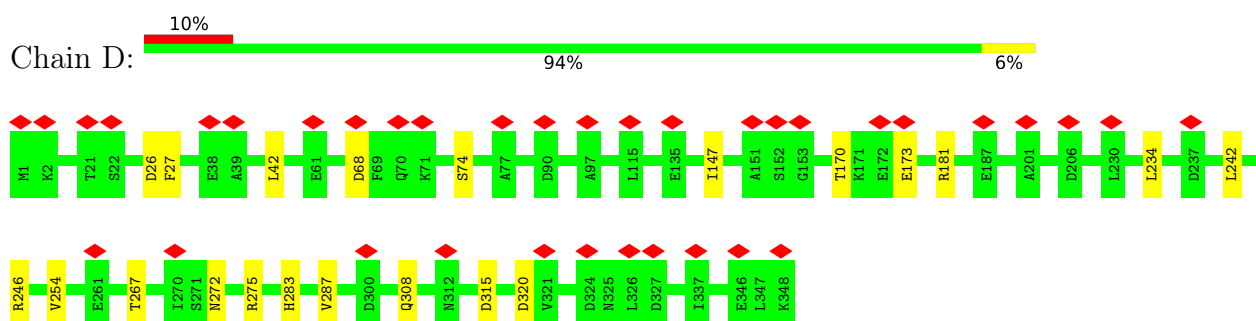


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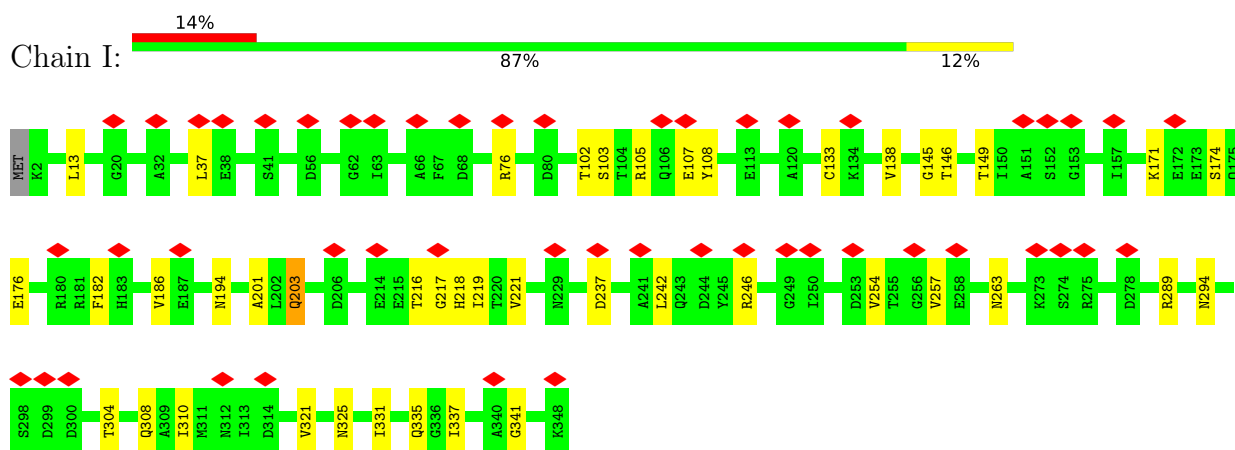
• Molecule 6: Baseplate component



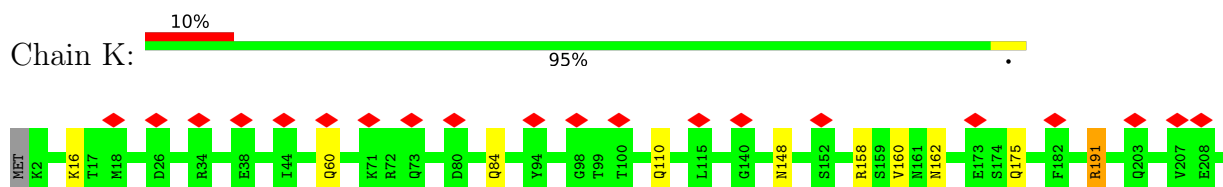
• Molecule 6: Baseplate component

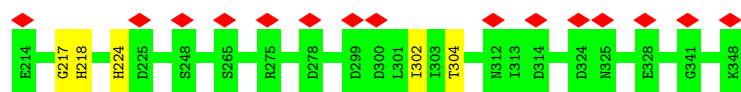


• Molecule 6: Baseplate component

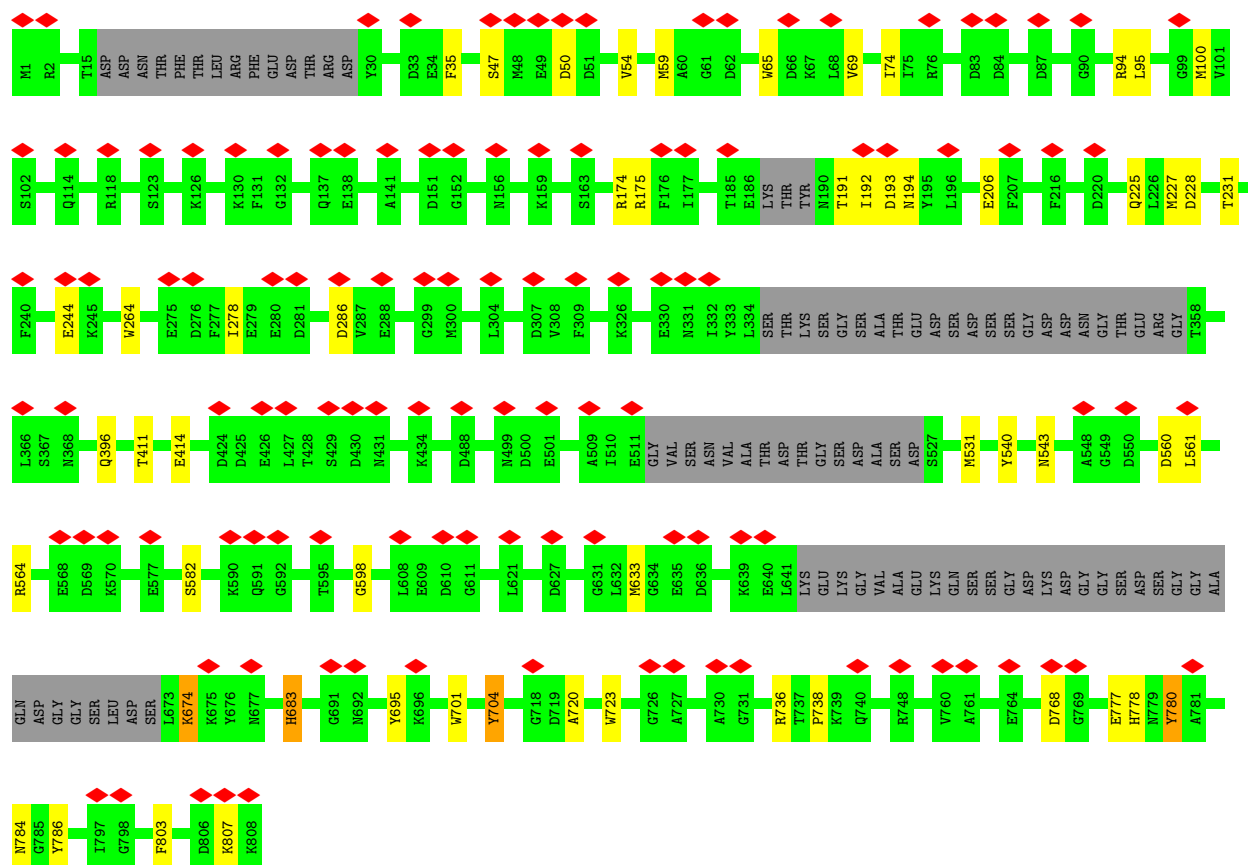
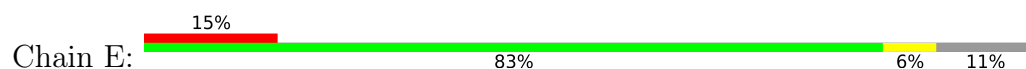


• Molecule 6: Baseplate component

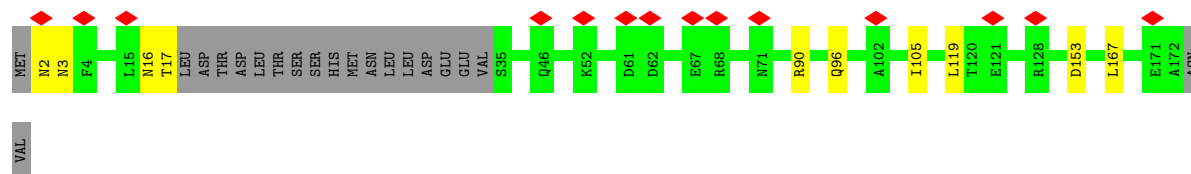
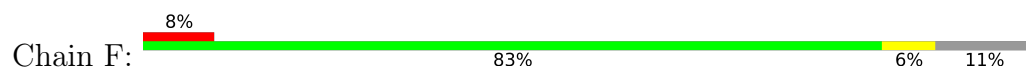




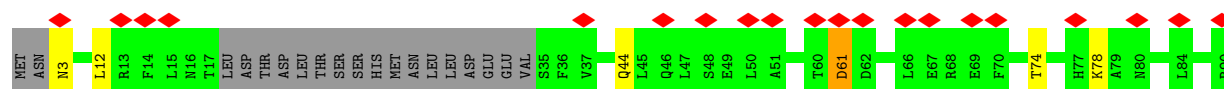
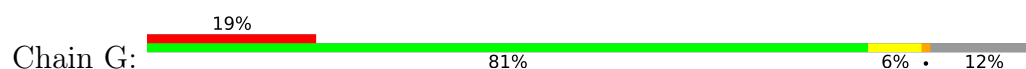
• Molecule 7: Peptidase C51 domain-containing protein



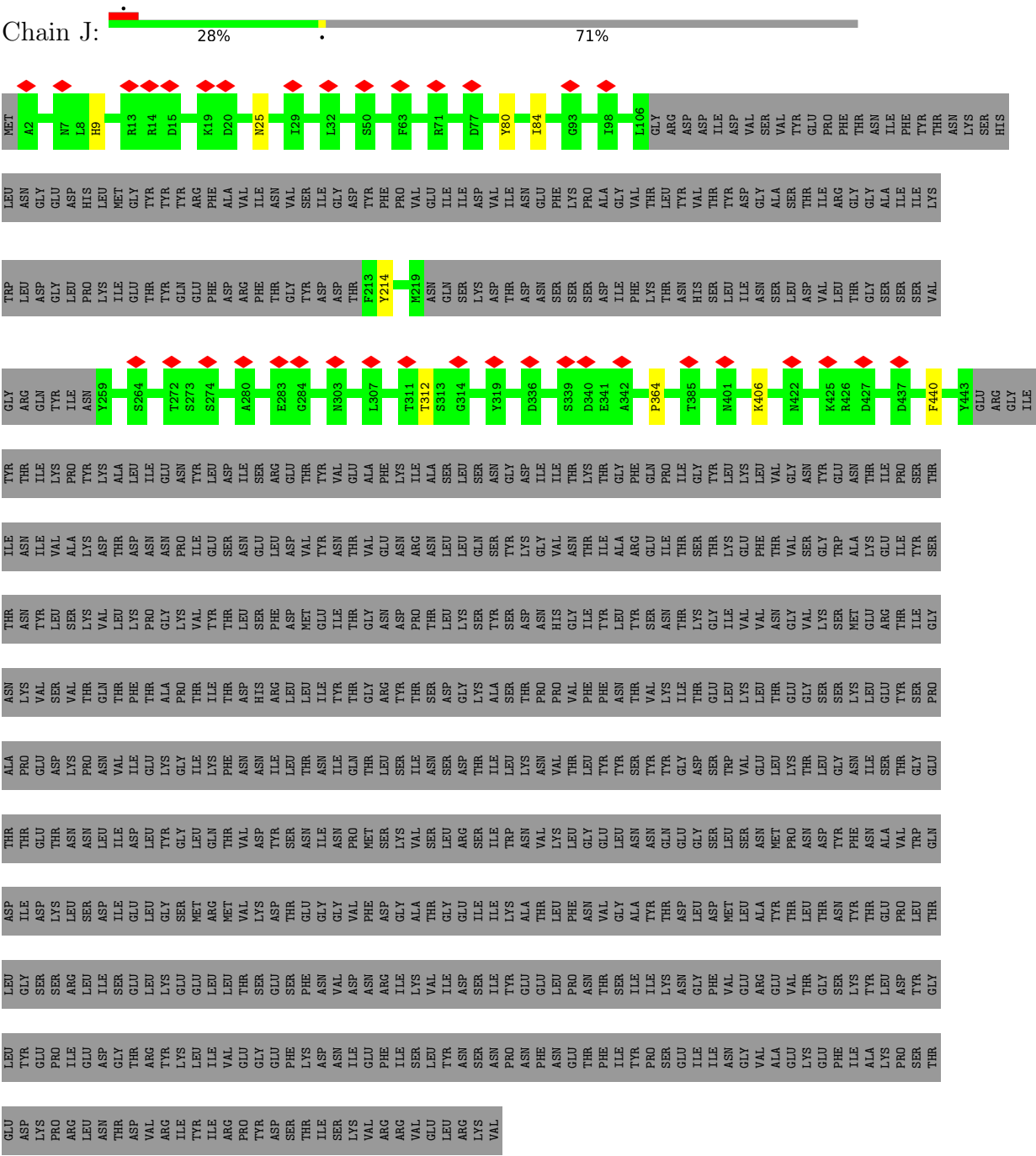
• Molecule 8: Baseplate component



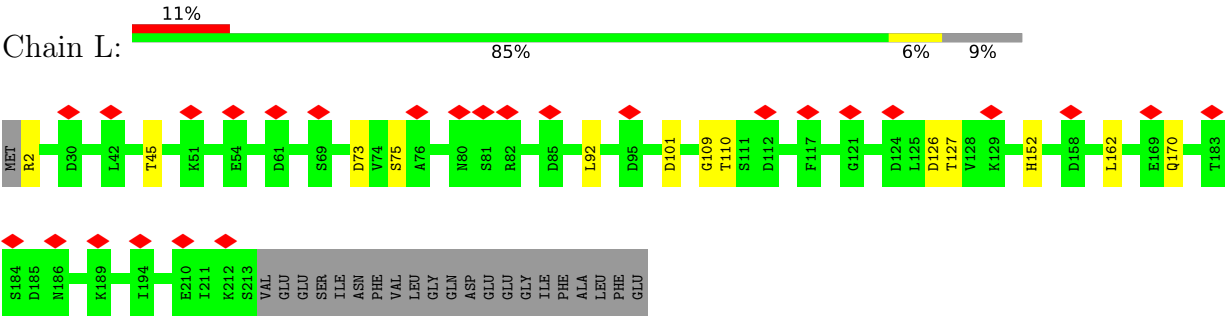
• Molecule 8: Baseplate component



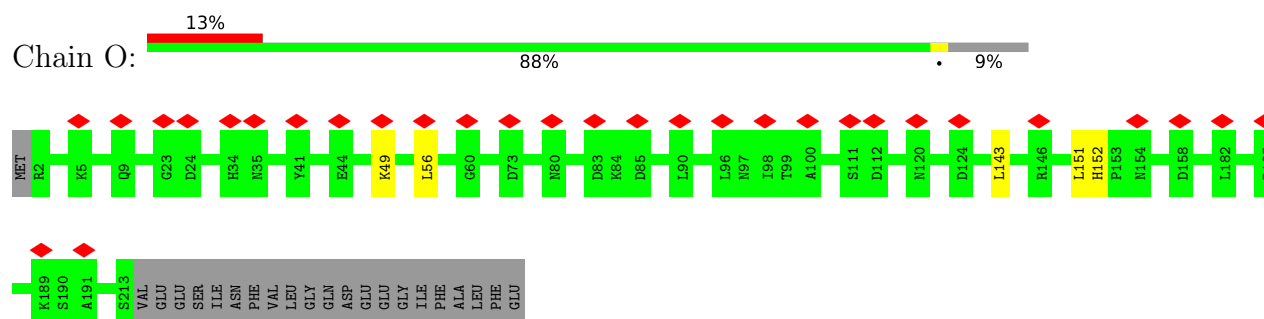




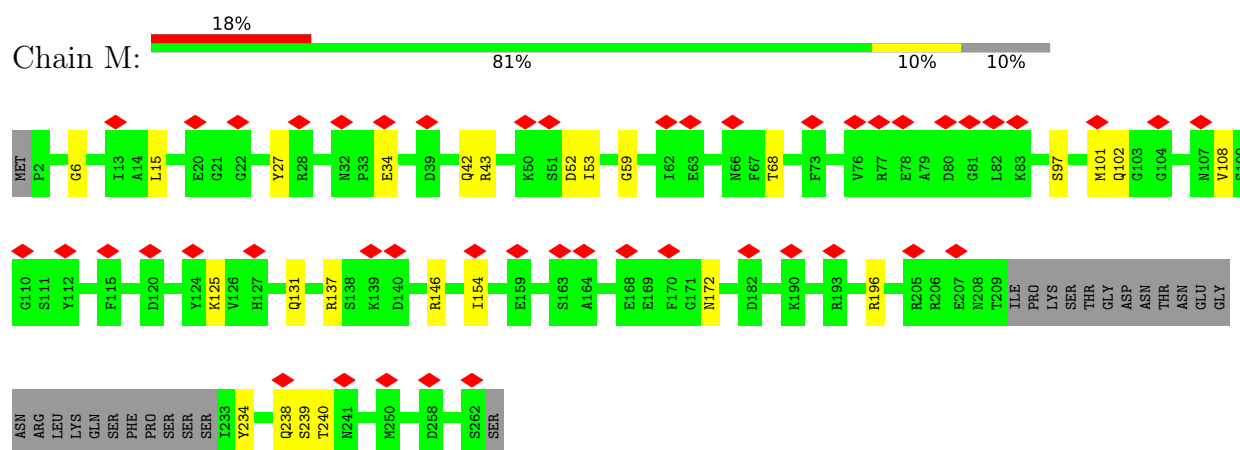
• Molecule 10: Baseplate wedge subunit



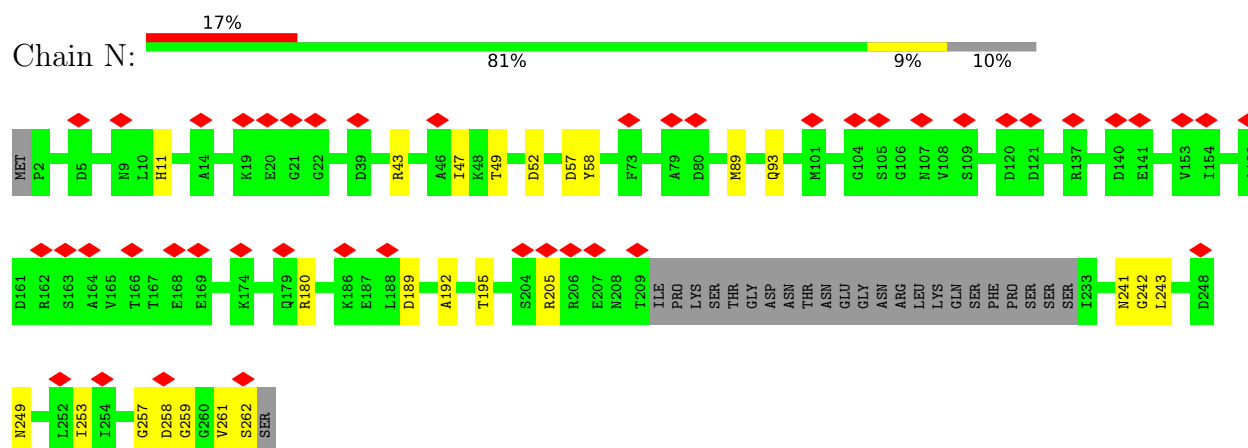
- Molecule 10: Baseplate wedge subunit



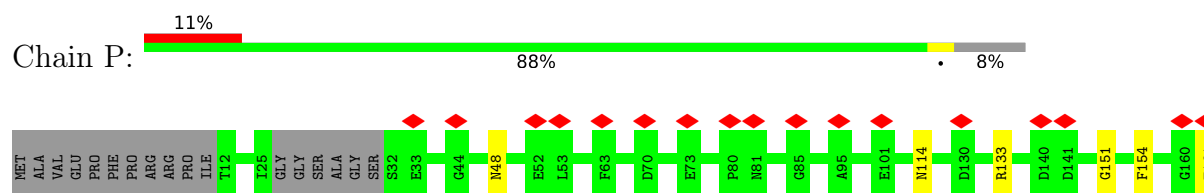
- Molecule 11: Putative baseplate component

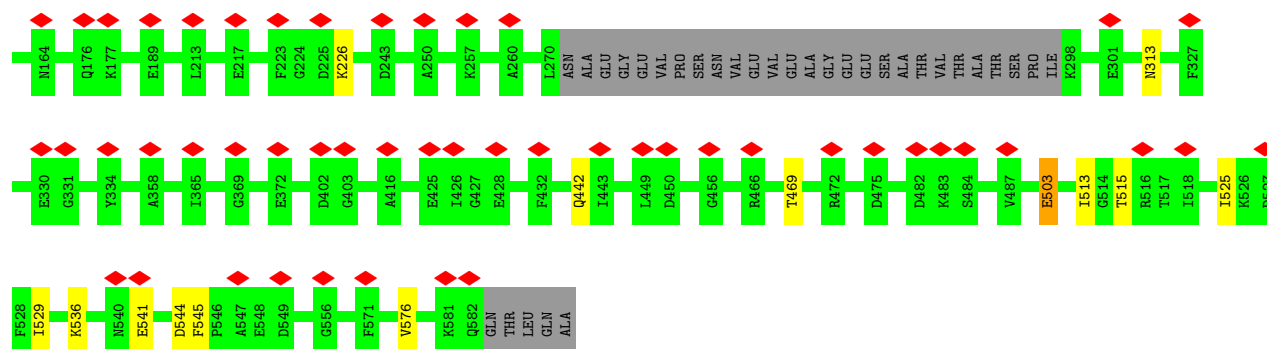


- Molecule 11: Putative baseplate component



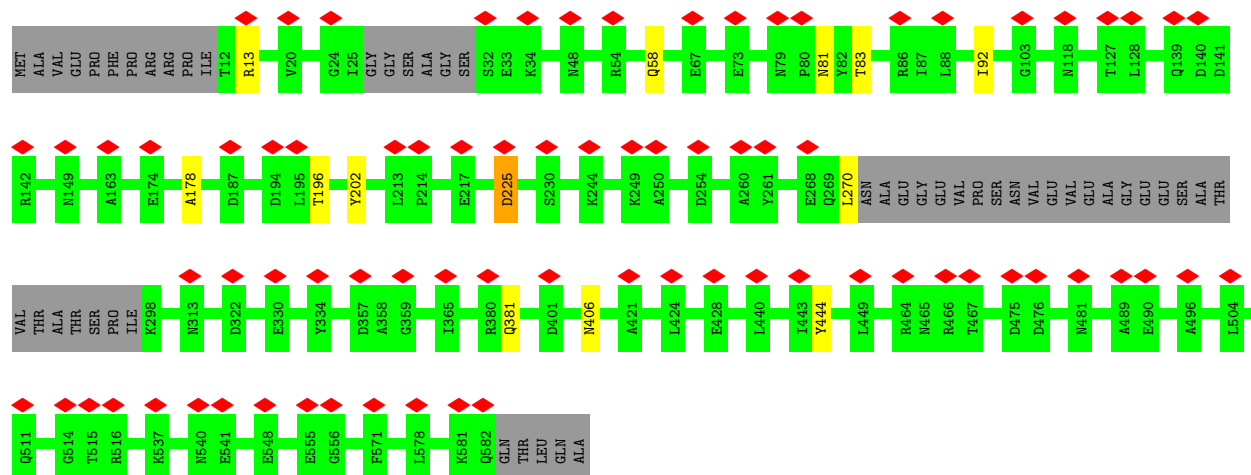
- Molecule 12: Major tail sheath protein





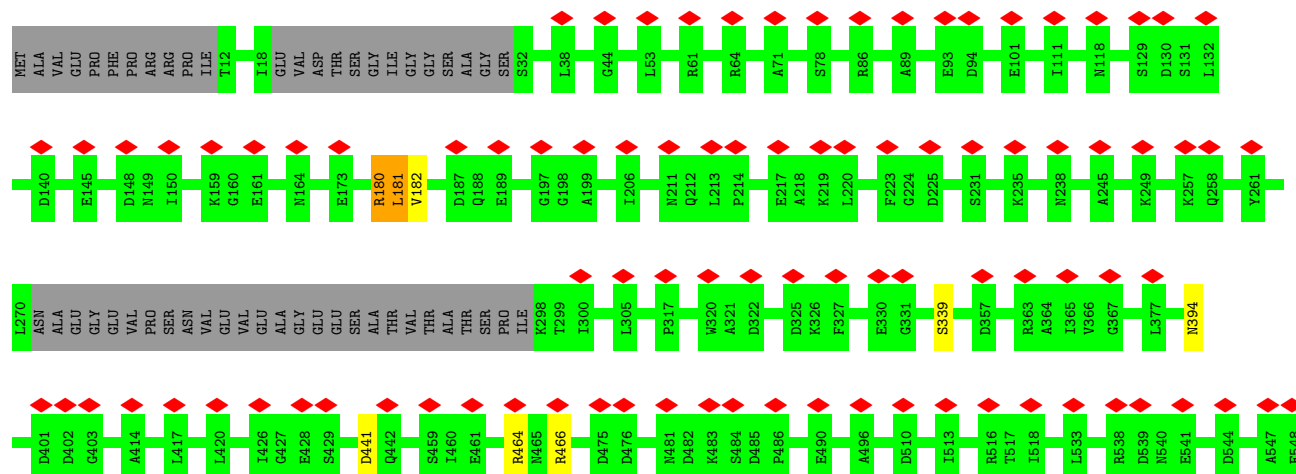
• Molecule 12: Major tail sheath protein

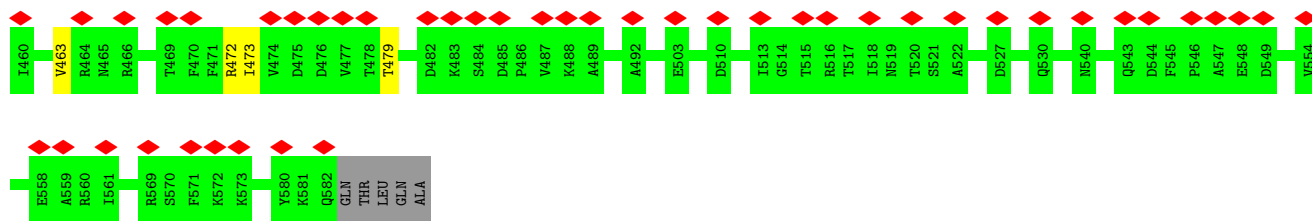
Chain Q: 13% 89% 8%



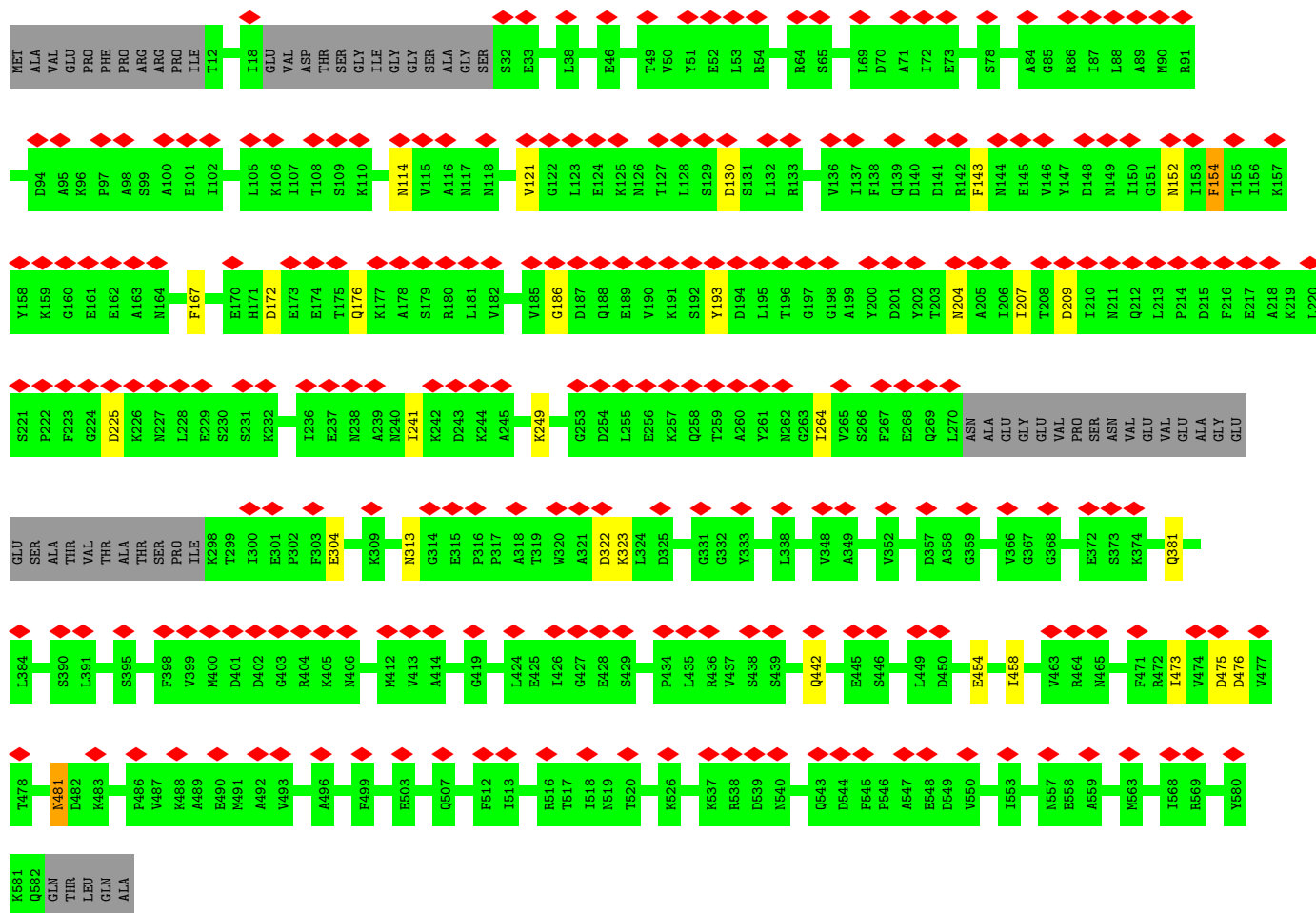
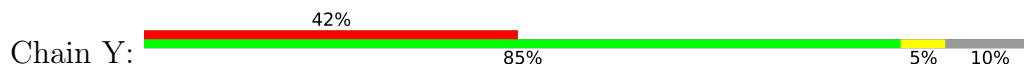
• Molecule 12: Major tail sheath protein

Chain T: 17% 90% 9%

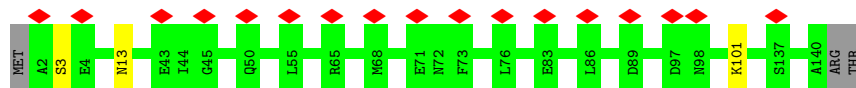




• Molecule 12: Major tail sheath protein

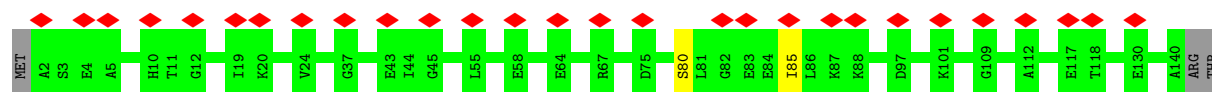


• Molecule 13: Capsid protein

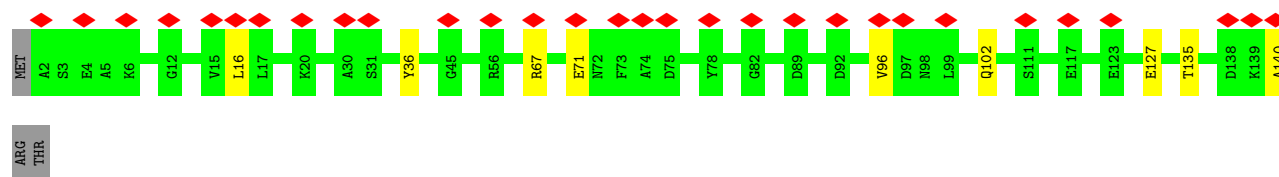


• Molecule 13: Capsid protein

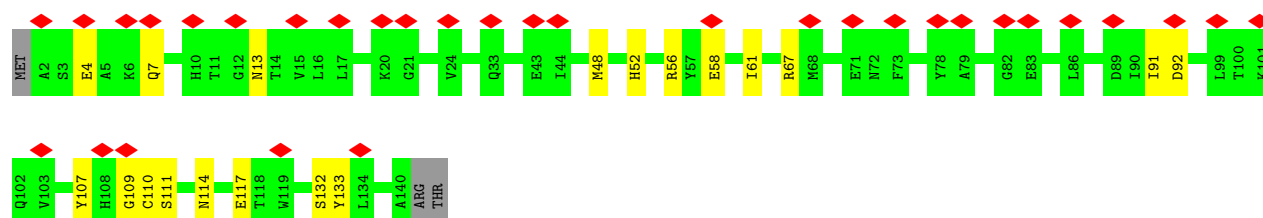
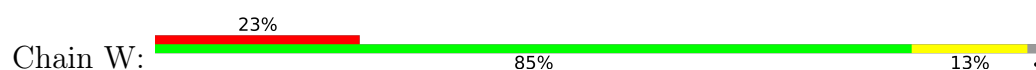




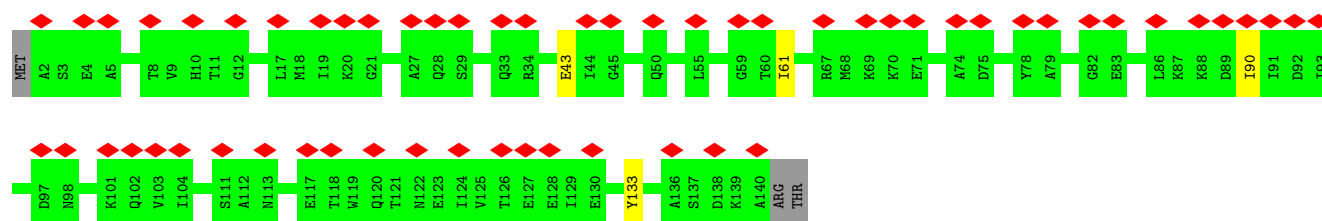
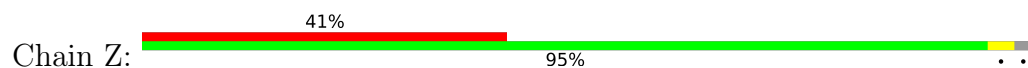
- Molecule 13: Capsid protein



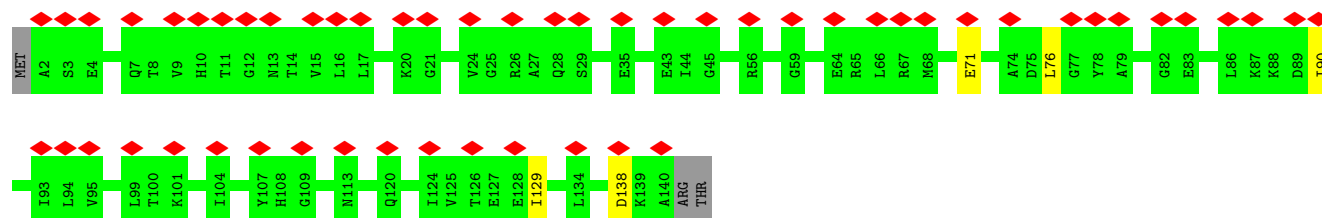
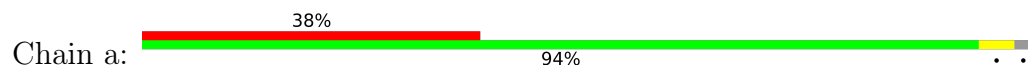
- Molecule 13: Capsid protein



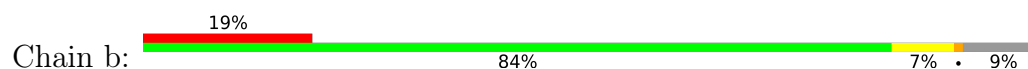
- Molecule 13: Capsid protein

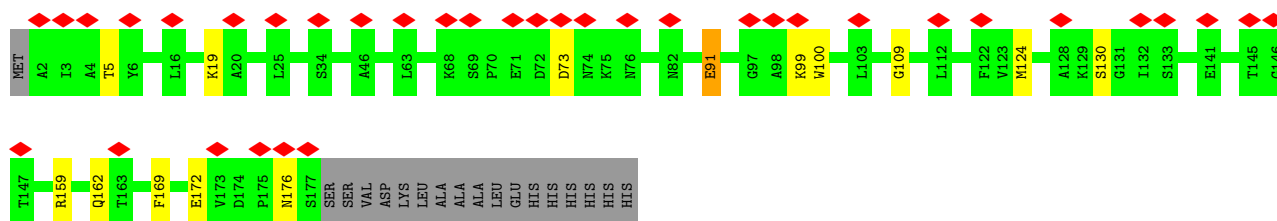


- Molecule 13: Capsid protein

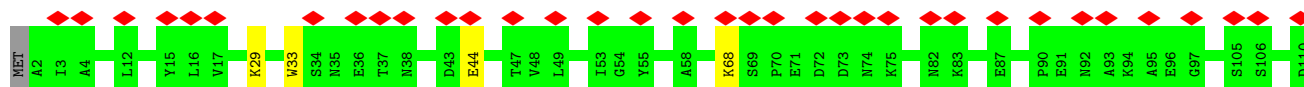
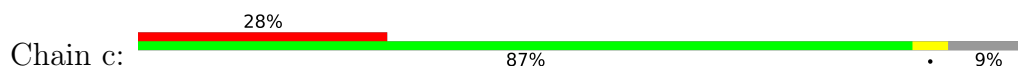


- Molecule 14: Baseplate protein

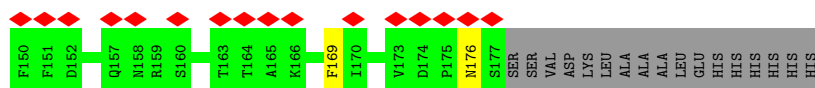
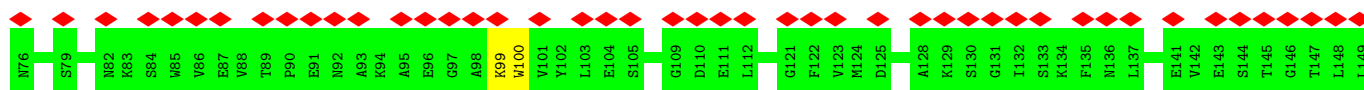
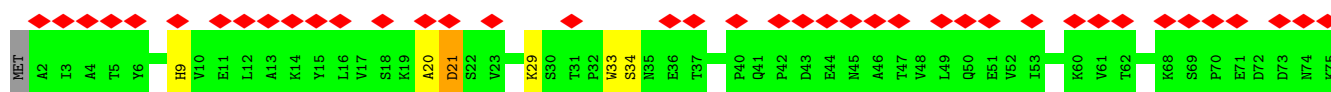
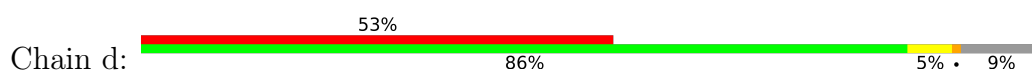




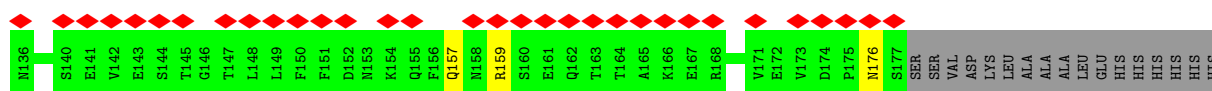
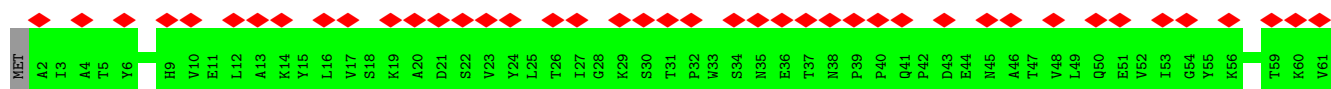
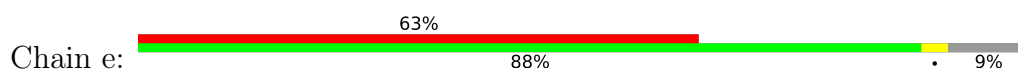
• Molecule 14: Baseplate protein



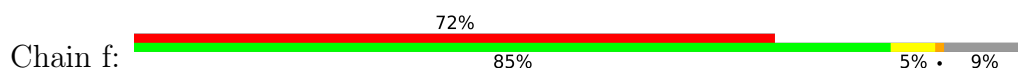
• Molecule 14: Baseplate protein



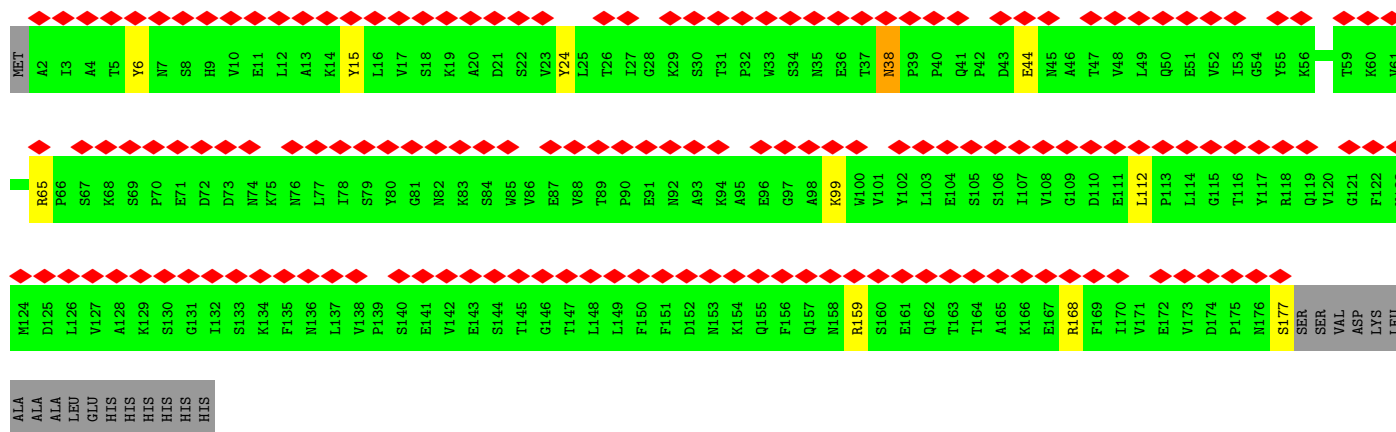
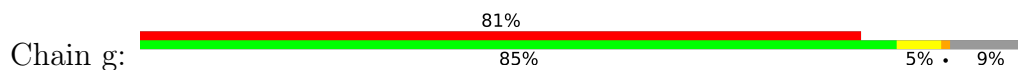
• Molecule 14: Baseplate protein



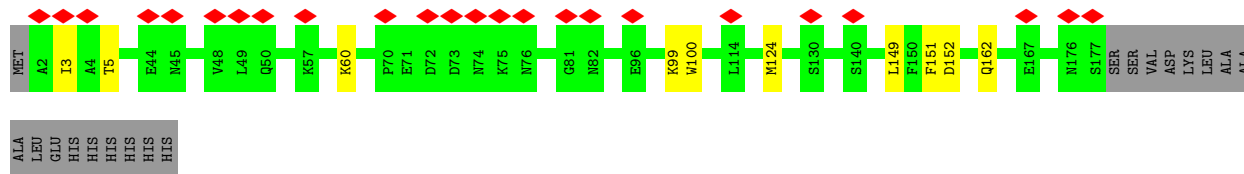
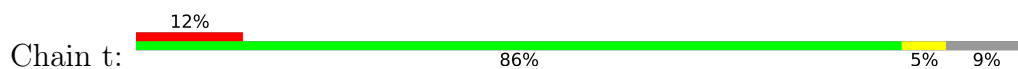
• Molecule 14: Baseplate protein



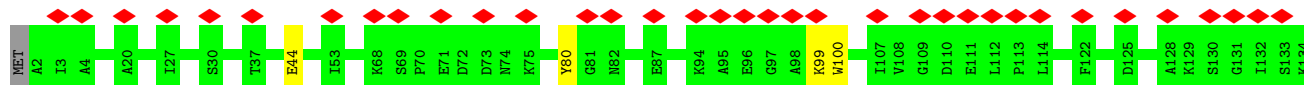
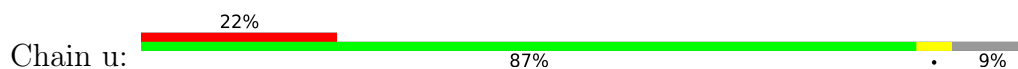
• Molecule 14: Baseplate protein

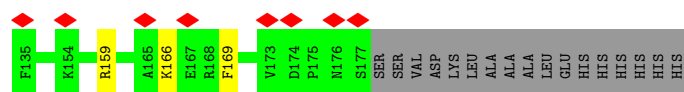


• Molecule 14: Baseplate protein

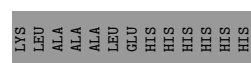
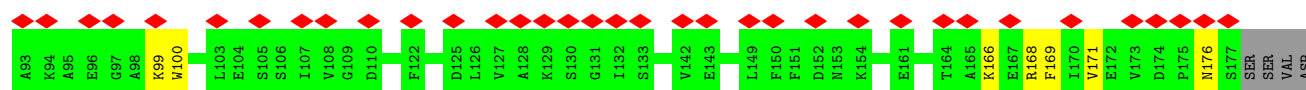
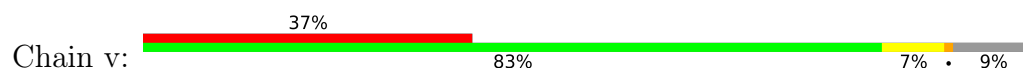


• Molecule 14: Baseplate protein

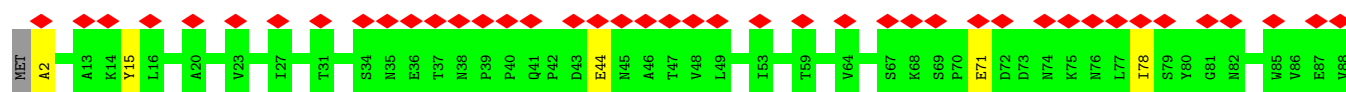
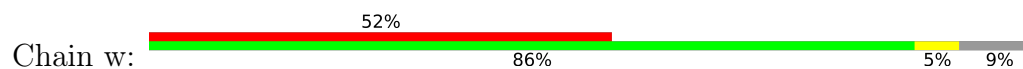




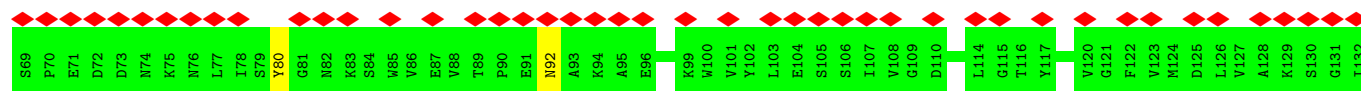
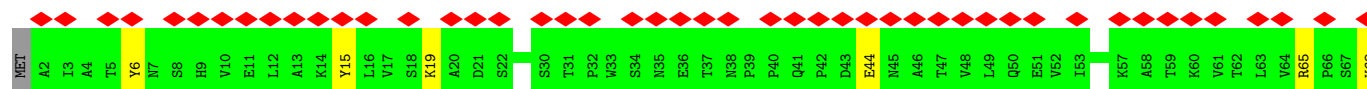
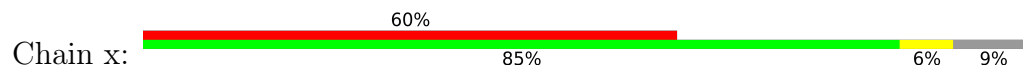
• Molecule 14: Baseplate protein



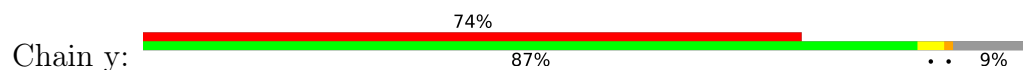
• Molecule 14: Baseplate protein



• Molecule 14: Baseplate protein



• Molecule 14: Baseplate protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	9705	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	903.00006, 903.00006, 903.00006	wwPDB
Map dimensions	840, 840, 840	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.075, 1.075, 1.075	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	0	0.95	0/4327	1.65	36/5404 (0.7%)
1	1	0.99	2/4327 (0.0%)	1.72	59/5404 (1.1%)
1	2	0.96	0/4327	1.71	53/5404 (1.0%)
1	3	0.95	0/4327	1.66	33/5404 (0.6%)
1	4	0.94	1/4327 (0.0%)	1.64	35/5404 (0.6%)
1	h	0.94	1/4327 (0.0%)	1.66	39/5404 (0.7%)
1	i	0.97	1/4324 (0.0%)	1.70	50/5399 (0.9%)
1	j	0.97	0/4327	1.69	45/5404 (0.8%)
1	k	0.98	0/4327	1.69	50/5404 (0.9%)
1	l	0.92	0/4327	1.65	44/5404 (0.8%)
1	m	0.93	0/4327	1.63	41/5404 (0.8%)
1	z	0.95	0/4325	1.66	42/5400 (0.8%)
2	5	0.75	0/1832	1.27	0/2287
2	6	0.82	0/1832	1.33	1/2287 (0.0%)
2	7	0.83	0/1832	1.37	7/2287 (0.3%)
2	n	0.74	0/1832	1.21	0/2287
2	o	0.78	0/1832	1.26	1/2287 (0.0%)
2	p	0.77	0/1832	1.23	0/2287
3	8	0.81	0/2560	1.36	2/3197 (0.1%)
3	9	0.81	0/2560	1.30	1/3197 (0.0%)
3	AA	0.82	0/2560	1.33	0/3197
3	q	0.90	0/2560	1.44	5/3197 (0.2%)
3	r	0.89	0/2560	1.45	2/3197 (0.1%)
3	s	0.91	0/2560	1.42	7/3197 (0.2%)
4	A	0.63	0/1810	1.09	6/2388 (0.3%)
5	B	0.32	0/2519	0.64	0/3404
6	C	0.46	0/2803	0.75	4/3794 (0.1%)
6	D	0.40	2/2803 (0.1%)	0.63	0/3794
6	I	0.30	0/2795	0.65	0/3784
6	K	0.42	2/2795 (0.1%)	0.65	0/3784
7	E	0.45	0/5961	0.80	3/8017 (0.0%)
8	F	0.34	0/1269	0.65	1/1724 (0.1%)
8	G	0.25	0/1261	0.53	0/1713
9	H	0.64	0/1649	1.15	1/2140 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	J	0.62	0/1649	1.12	3/2140 (0.1%)
10	L	0.51	0/1722	0.89	0/2331
10	O	0.43	0/1722	0.78	0/2331
11	M	0.37	0/1907	0.77	1/2565 (0.0%)
11	N	0.44	0/1907	0.82	0/2565
12	P	0.34	0/4267	0.69	0/5760
12	Q	0.43	0/4267	0.82	1/5760 (0.0%)
12	T	0.42	0/4256	0.79	1/5745 (0.0%)
12	U	0.38	0/4256	0.72	1/5745 (0.0%)
12	X	0.29	0/4218	0.63	0/5693
12	Y	0.31	0/4218	0.64	0/5693
13	R	0.48	0/1107	0.88	4/1496 (0.3%)
13	S	0.37	0/1107	0.72	0/1496
13	V	0.49	0/1107	0.79	0/1496
13	W	0.30	0/1107	0.69	1/1496 (0.1%)
13	Z	0.39	0/1107	0.75	0/1496
13	a	0.31	0/1107	0.67	0/1496
14	b	0.72	0/1405	1.29	5/1911 (0.3%)
14	c	0.73	0/1407	1.26	1/1914 (0.1%)
14	d	0.76	0/1407	1.32	5/1914 (0.3%)
14	e	0.79	0/1407	1.30	0/1914
14	f	0.79	0/1407	1.32	3/1914 (0.2%)
14	g	0.87	0/1407	1.38	5/1914 (0.3%)
14	t	0.70	0/1407	1.22	0/1914
14	u	0.71	0/1407	1.22	1/1914 (0.1%)
14	v	0.73	0/1407	1.26	5/1914 (0.3%)
14	w	0.79	0/1407	1.30	0/1914
14	x	0.77	0/1407	1.29	5/1914 (0.3%)
14	y	0.83	0/1407	1.31	1/1914 (0.1%)
All	All	0.73	9/161849 (0.0%)	1.25	611/210554 (0.3%)

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	0	0	1
1	l	0	1
5	B	0	1
6	I	0	1
7	E	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	M	0	1
12	Q	0	1
12	T	0	1
13	V	0	1
14	e	0	1
14	f	0	2
14	g	0	3
14	u	0	2
14	v	0	1
14	w	0	1
14	x	0	4
All	All	0	26

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	68	ASP	CG-OD2	-9.80	1.06	1.25
6	D	68	ASP	CG-OD1	-8.89	1.08	1.25
6	K	191	ARG	NE-CZ	-6.41	1.25	1.33
6	K	191	ARG	CZ-NH2	-5.70	1.26	1.33
1	1	786	VAL	CA-C	5.26	1.58	1.52

The worst 5 of 611 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	265	SER	N-CA-C	12.52	119.49	108.22
1	2	786	VAL	N-CA-C	11.90	124.65	107.75
1	1	786	VAL	N-CA-C	11.44	124.59	108.23
1	k	784	THR	N-CA-C	11.17	129.31	108.65
1	l	265	SER	N-CA-C	11.10	118.12	108.13

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	382	PHE	Peptide
5	B	196	TYR	Sidechain
7	E	175	ARG	Sidechain
7	E	695	TYR	Sidechain
7	E	736	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4329	146	1177	11	0
1	1	4329	146	1177	2	0
1	2	4329	146	1177	6	0
1	3	4329	146	1177	2	0
1	4	4329	146	1177	2	0
1	h	4329	146	1177	1	0
1	i	4328	146	1176	5	0
1	j	4329	146	1177	5	0
1	k	4329	146	1177	4	0
1	l	4329	146	1177	1	0
1	m	4329	146	1177	1	0
1	z	4328	146	1176	3	0
2	5	1833	76	519	12	0
2	6	1833	76	520	4	0
2	7	1833	76	520	0	0
2	n	1833	76	520	0	0
2	o	1833	76	520	0	0
2	p	1833	76	520	0	0
3	8	2561	86	700	0	0
3	9	2561	86	700	0	0
3	AA	2561	86	700	1	0
3	q	2561	86	700	0	0
3	r	2561	86	700	0	0
3	s	2561	86	700	0	0
4	A	1775	971	1348	5	0
5	B	2470	1839	2394	23	0
6	C	2760	2106	2729	6	0
6	D	2760	2106	2727	10	0
6	I	2752	2098	2716	34	0
6	K	2752	2098	2717	17	0
7	E	5829	4404	5742	30	0
8	F	1248	992	1257	5	0
8	G	1240	989	1251	10	0
9	H	1638	678	1076	2	0
9	J	1638	678	1076	3	0
10	L	1694	1283	1663	4	0
10	O	1694	1283	1663	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	1878	1384	1844	13	0
11	N	1878	1384	1844	14	0
12	P	4200	3207	4155	10	0
12	Q	4200	3207	4156	2	0
12	T	4189	3200	4150	3	0
12	U	4189	3200	4150	4	0
12	X	4151	3171	4111	9	0
12	Y	4151	3171	4111	16	0
13	R	1091	833	1081	0	0
13	S	1091	833	1081	0	0
13	V	1091	833	1081	2	0
13	W	1091	833	1081	7	0
13	Z	1091	833	1081	0	0
13	a	1091	833	1081	0	0
14	b	1377	1051	1357	5	0
14	c	1378	1054	1361	2	0
14	d	1378	1054	1361	3	0
14	e	1378	1054	1361	1	0
14	f	1378	1054	1361	2	0
14	g	1378	1054	1361	2	0
14	t	1378	1054	1361	2	0
14	u	1378	1054	1361	2	0
14	v	1378	1054	1361	14	0
14	w	1378	1054	1361	11	0
14	x	1378	1054	1361	5	0
14	y	1378	1054	1361	3	0
All	All	160477	63816	101135	280	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 1.

The worst 5 of 280 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:134:PHE:CA	6:K:218:HIS:HD2	1.40	1.34
1:0:134:PHE:O	6:K:218:HIS:CD2	1.88	1.25
1:0:134:PHE:O	6:K:218:HIS:NE2	1.67	1.24
6:I:217:GLY:C	1:j:134:PHE:CA	2.05	1.20
1:0:134:PHE:CA	6:K:218:HIS:CD2	2.27	1.17

There are no symmetry-related clashes.

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	0	1078/1152 (94%)	886 (82%)	157 (15%)	35 (3%)	3	21
1	1	1078/1152 (94%)	864 (80%)	181 (17%)	33 (3%)	3	22
1	2	1078/1152 (94%)	863 (80%)	170 (16%)	45 (4%)	2	17
1	3	1078/1152 (94%)	892 (83%)	146 (14%)	40 (4%)	2	20
1	4	1078/1152 (94%)	902 (84%)	145 (14%)	31 (3%)	3	23
1	h	1078/1152 (94%)	899 (83%)	145 (14%)	34 (3%)	3	21
1	i	1076/1152 (93%)	863 (80%)	176 (16%)	37 (3%)	3	21
1	j	1078/1152 (94%)	879 (82%)	161 (15%)	38 (4%)	3	20
1	k	1078/1152 (94%)	860 (80%)	185 (17%)	33 (3%)	3	22
1	l	1078/1152 (94%)	883 (82%)	162 (15%)	33 (3%)	3	22
1	m	1078/1152 (94%)	897 (83%)	147 (14%)	34 (3%)	3	21
1	z	1076/1152 (93%)	903 (84%)	142 (13%)	31 (3%)	3	23
2	5	456/458 (100%)	439 (96%)	14 (3%)	3 (1%)	18	56
2	6	456/458 (100%)	427 (94%)	27 (6%)	2 (0%)	30	67
2	7	456/458 (100%)	427 (94%)	26 (6%)	3 (1%)	18	56
2	n	456/458 (100%)	439 (96%)	17 (4%)	0	100	100
2	o	456/458 (100%)	442 (97%)	13 (3%)	1 (0%)	43	78
2	p	456/458 (100%)	433 (95%)	22 (5%)	1 (0%)	43	78
3	8	638/640 (100%)	598 (94%)	37 (6%)	3 (0%)	24	63
3	9	638/640 (100%)	609 (96%)	27 (4%)	2 (0%)	36	72
3	AA	638/640 (100%)	608 (95%)	28 (4%)	2 (0%)	36	72
3	q	638/640 (100%)	604 (95%)	32 (5%)	2 (0%)	36	72
3	r	638/640 (100%)	606 (95%)	30 (5%)	2 (0%)	36	72
3	s	638/640 (100%)	585 (92%)	47 (7%)	6 (1%)	14	51
4	A	276/295 (94%)	242 (88%)	30 (11%)	4 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	308/848 (36%)	281 (91%)	27 (9%)	0	100	100
6	C	346/348 (99%)	330 (95%)	16 (5%)	0	100	100
6	D	346/348 (99%)	329 (95%)	17 (5%)	0	100	100
6	I	345/348 (99%)	330 (96%)	15 (4%)	0	100	100
6	K	345/348 (99%)	331 (96%)	14 (4%)	0	100	100
7	E	710/808 (88%)	659 (93%)	50 (7%)	1 (0%)	48	83
8	F	150/174 (86%)	143 (95%)	7 (5%)	0	100	100
8	G	149/174 (86%)	141 (95%)	8 (5%)	0	100	100
9	H	291/1019 (29%)	264 (91%)	26 (9%)	1 (0%)	36	72
9	J	291/1019 (29%)	260 (89%)	29 (10%)	2 (1%)	18	56
10	L	210/234 (90%)	196 (93%)	14 (7%)	0	100	100
10	O	210/234 (90%)	196 (93%)	14 (7%)	0	100	100
11	M	234/263 (89%)	216 (92%)	17 (7%)	1 (0%)	30	67
11	N	234/263 (89%)	222 (95%)	12 (5%)	0	100	100
12	P	532/587 (91%)	495 (93%)	37 (7%)	0	100	100
12	Q	532/587 (91%)	496 (93%)	35 (7%)	1 (0%)	43	78
12	T	530/587 (90%)	499 (94%)	31 (6%)	0	100	100
12	U	530/587 (90%)	499 (94%)	30 (6%)	1 (0%)	43	78
12	X	525/587 (89%)	488 (93%)	34 (6%)	3 (1%)	21	59
12	Y	525/587 (89%)	487 (93%)	37 (7%)	1 (0%)	43	78
13	R	137/142 (96%)	128 (93%)	9 (7%)	0	100	100
13	S	137/142 (96%)	126 (92%)	11 (8%)	0	100	100
13	V	137/142 (96%)	132 (96%)	5 (4%)	0	100	100
13	W	137/142 (96%)	133 (97%)	4 (3%)	0	100	100
13	Z	137/142 (96%)	133 (97%)	4 (3%)	0	100	100
13	a	137/142 (96%)	131 (96%)	5 (4%)	1 (1%)	18	56
14	b	174/194 (90%)	165 (95%)	8 (5%)	1 (1%)	21	59
14	c	174/194 (90%)	166 (95%)	8 (5%)	0	100	100
14	d	174/194 (90%)	168 (97%)	5 (3%)	1 (1%)	21	59
14	e	174/194 (90%)	164 (94%)	9 (5%)	1 (1%)	21	59
14	f	174/194 (90%)	169 (97%)	4 (2%)	1 (1%)	21	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	g	174/194 (90%)	171 (98%)	3 (2%)	0	100	100
14	t	174/194 (90%)	163 (94%)	10 (6%)	1 (1%)	21	59
14	u	174/194 (90%)	169 (97%)	5 (3%)	0	100	100
14	v	174/194 (90%)	171 (98%)	3 (2%)	0	100	100
14	w	174/194 (90%)	165 (95%)	8 (5%)	1 (1%)	21	59
14	x	174/194 (90%)	169 (97%)	5 (3%)	0	100	100
14	y	174/194 (90%)	168 (97%)	5 (3%)	1 (1%)	21	59
All	All	30025/33837 (89%)	26703 (89%)	2848 (10%)	474 (2%)	10	38

5 of 474 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	226	LYS
1	0	301	ALA
1	0	500	PRO
1	0	781	ILE
1	0	786	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	
4	A	136/271 (50%)	134 (98%)	2 (2%)	57	72
5	B	279/758 (37%)	279 (100%)	0	100	100
6	C	311/311 (100%)	308 (99%)	3 (1%)	68	78
6	D	311/311 (100%)	307 (99%)	4 (1%)	61	74
6	I	310/311 (100%)	308 (99%)	2 (1%)	78	83
6	K	310/311 (100%)	309 (100%)	1 (0%)	86	86
7	E	628/695 (90%)	621 (99%)	7 (1%)	65	76
8	F	144/164 (88%)	143 (99%)	1 (1%)	76	81
8	G	143/164 (87%)	141 (99%)	2 (1%)	59	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	H	95/928 (10%)	93 (98%)	2 (2%)	47	65
9	J	95/928 (10%)	94 (99%)	1 (1%)	65	76
10	L	190/209 (91%)	185 (97%)	5 (3%)	40	62
10	O	190/209 (91%)	187 (98%)	3 (2%)	55	70
11	M	205/228 (90%)	205 (100%)	0	100	100
11	N	205/228 (90%)	204 (100%)	1 (0%)	81	83
12	P	458/495 (92%)	451 (98%)	7 (2%)	57	72
12	Q	458/495 (92%)	449 (98%)	9 (2%)	48	66
12	T	456/495 (92%)	454 (100%)	2 (0%)	84	84
12	U	456/495 (92%)	450 (99%)	6 (1%)	61	74
12	X	452/495 (91%)	444 (98%)	8 (2%)	51	68
12	Y	452/495 (91%)	447 (99%)	5 (1%)	65	76
13	R	119/122 (98%)	118 (99%)	1 (1%)	73	80
13	S	119/122 (98%)	117 (98%)	2 (2%)	53	69
13	V	119/122 (98%)	115 (97%)	4 (3%)	32	54
13	W	119/122 (98%)	115 (97%)	4 (3%)	32	54
13	Z	119/122 (98%)	115 (97%)	4 (3%)	32	54
13	a	119/122 (98%)	115 (97%)	4 (3%)	32	54
14	b	155/171 (91%)	152 (98%)	3 (2%)	50	67
14	c	156/171 (91%)	152 (97%)	4 (3%)	40	62
14	d	156/171 (91%)	154 (99%)	2 (1%)	61	74
14	e	156/171 (91%)	154 (99%)	2 (1%)	61	74
14	f	156/171 (91%)	153 (98%)	3 (2%)	50	67
14	g	156/171 (91%)	153 (98%)	3 (2%)	50	67
14	t	156/171 (91%)	150 (96%)	6 (4%)	29	50
14	u	156/171 (91%)	155 (99%)	1 (1%)	78	83
14	v	156/171 (91%)	153 (98%)	3 (2%)	50	67
14	w	156/171 (91%)	154 (99%)	2 (1%)	61	74
14	x	156/171 (91%)	154 (99%)	2 (1%)	61	74
14	y	156/171 (91%)	153 (98%)	3 (2%)	50	67
All	All	8869/11780 (75%)	8745 (99%)	124 (1%)	57	72

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	U	185	VAL
14	t	151	PHE
12	X	154	PHE
14	t	124	MET
14	w	157	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
12	X	442	GLN
14	u	158	ASN
12	Y	530	GLN
14	f	50	GLN
14	x	9	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

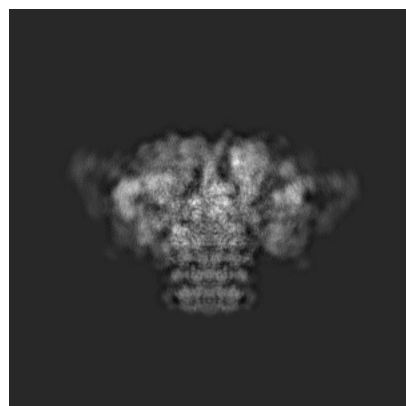
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19968. These allow visual inspection of the internal detail of the map and identification of artifacts.

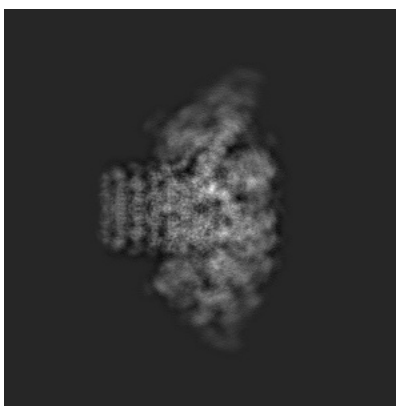
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

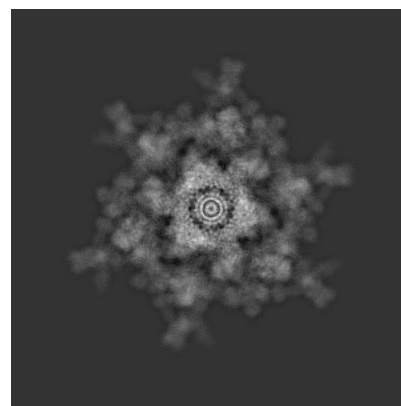
6.1.1 Primary map



X



Y

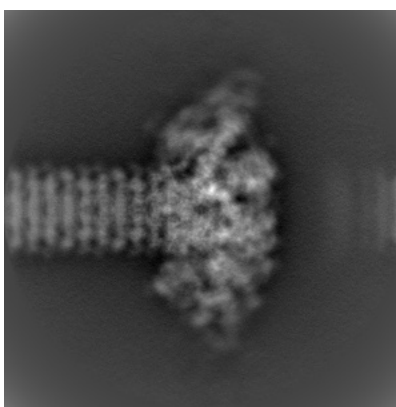


Z

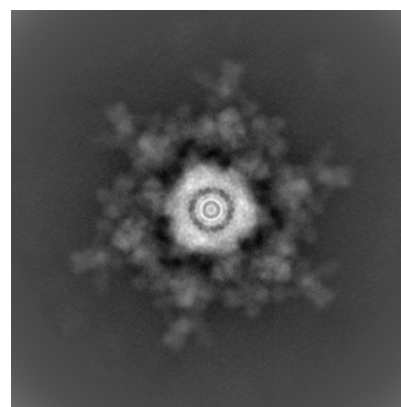
6.1.2 Raw map



X



Y

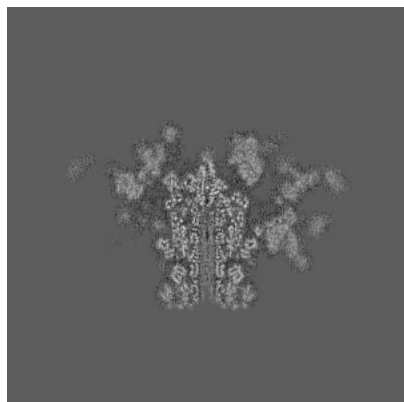


Z

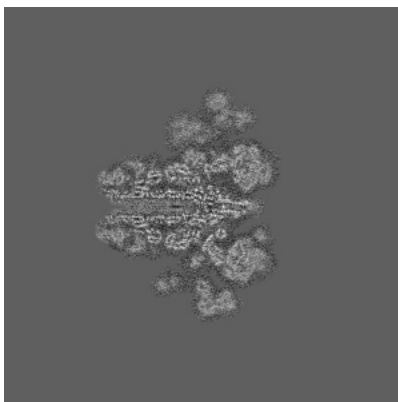
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

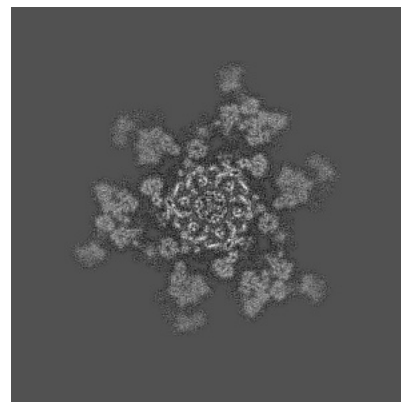
6.2.1 Primary map



X Index: 420

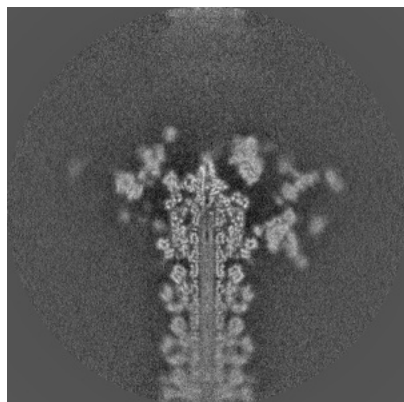


Y Index: 420

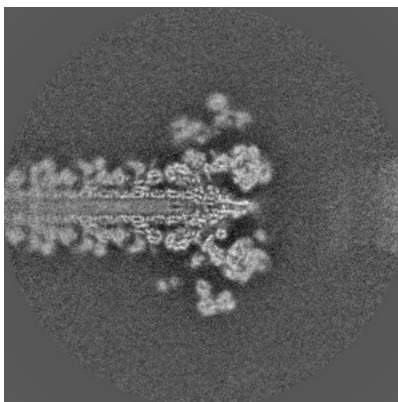


Z Index: 420

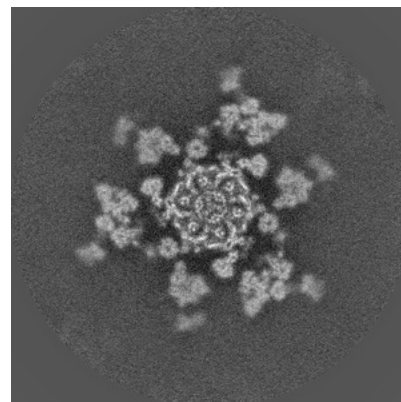
6.2.2 Raw map



X Index: 420



Y Index: 420

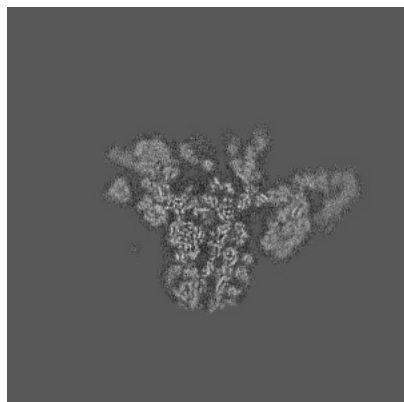


Z Index: 420

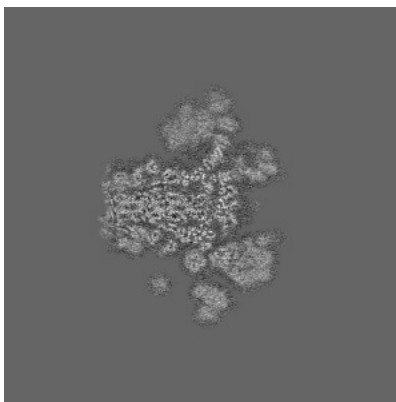
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

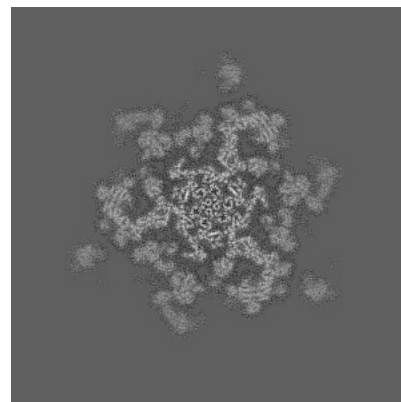
6.3.1 Primary map



X Index: 461

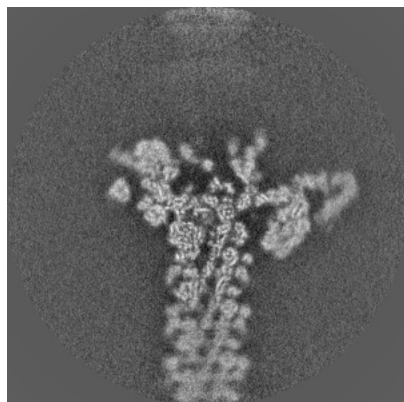


Y Index: 439

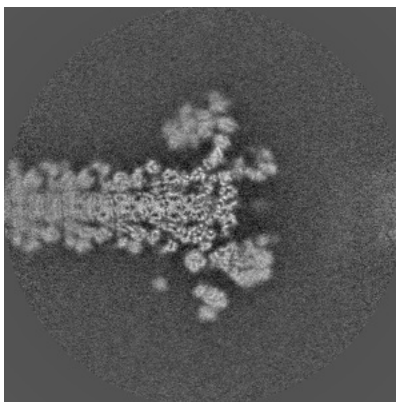


Z Index: 435

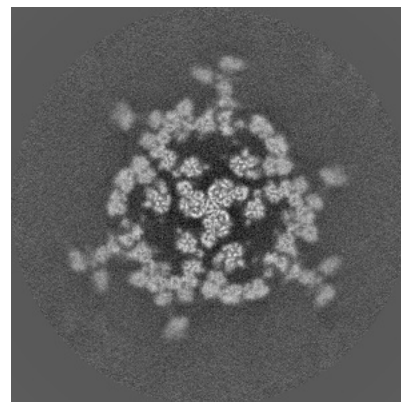
6.3.2 Raw map



X Index: 461



Y Index: 440

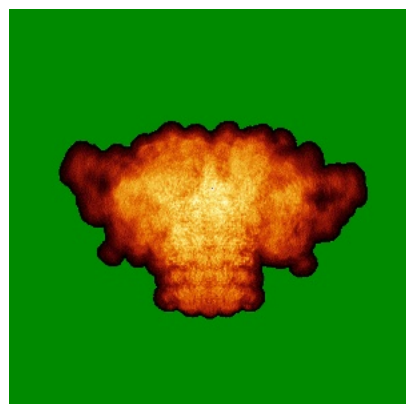


Z Index: 461

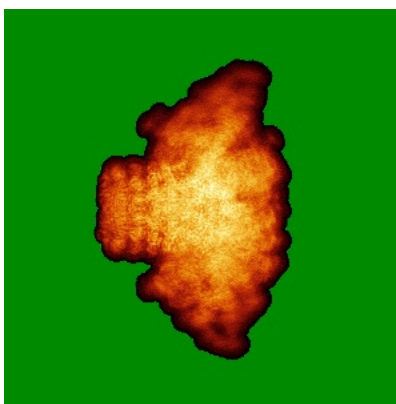
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

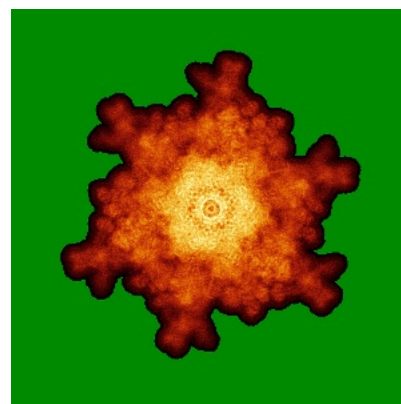
6.4.1 Primary map



X

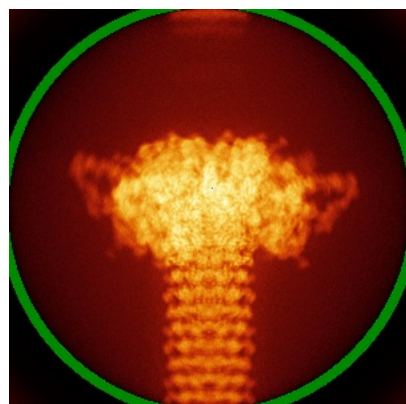


Y

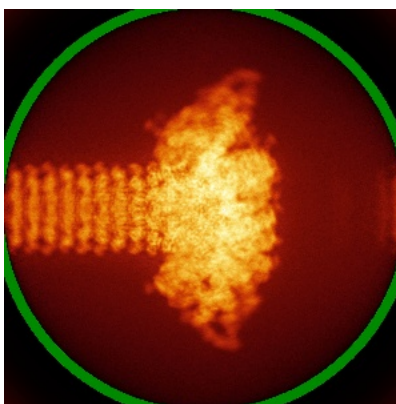


Z

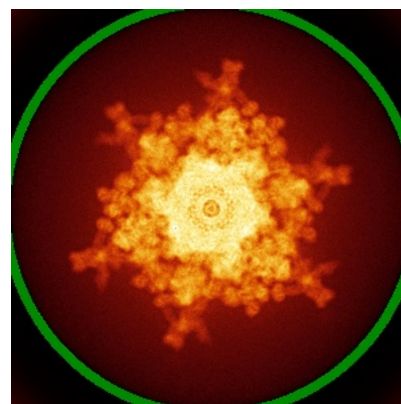
6.4.2 Raw map



X



Y

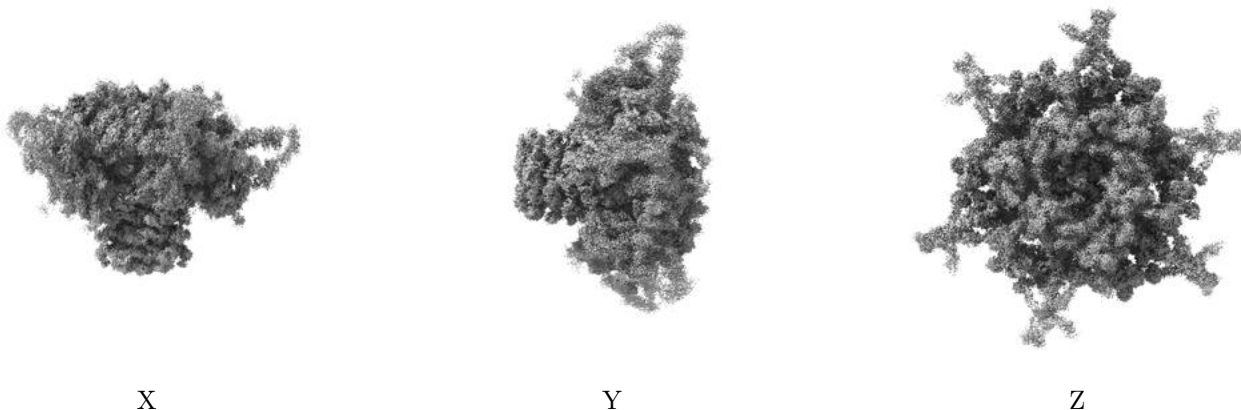


Z

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

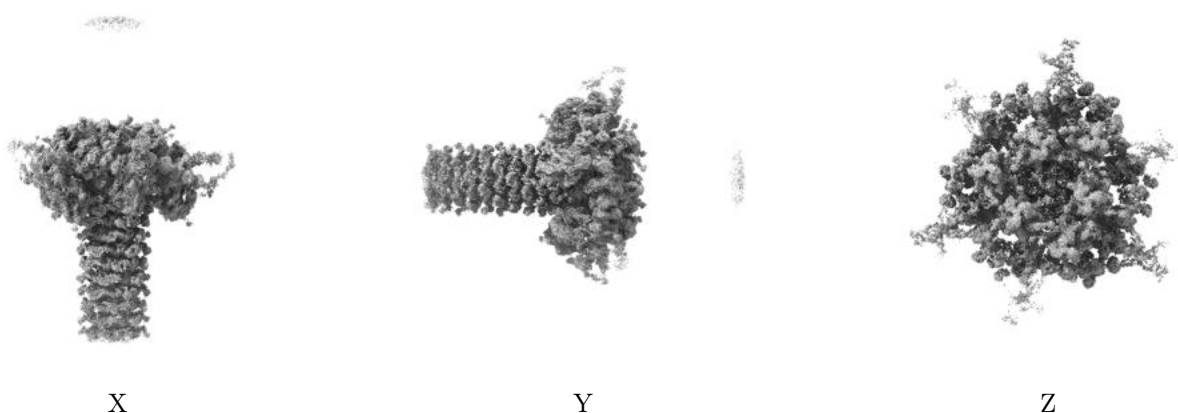
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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



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

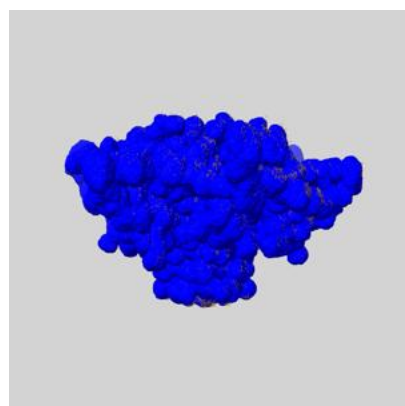
6.6 Mask visualisation [i](#)

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

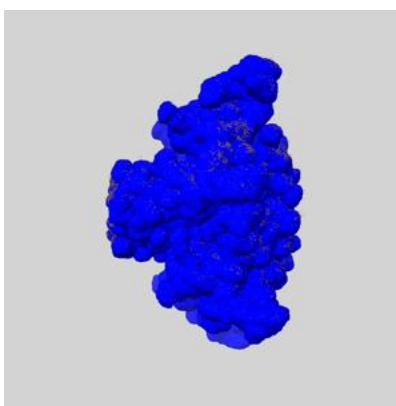
A mask typically either:

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

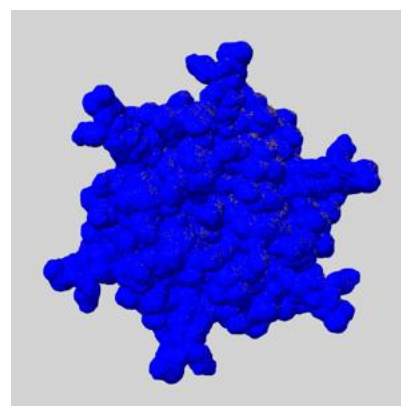
6.6.1 emd_19968_msk_1.map [i](#)



X



Y

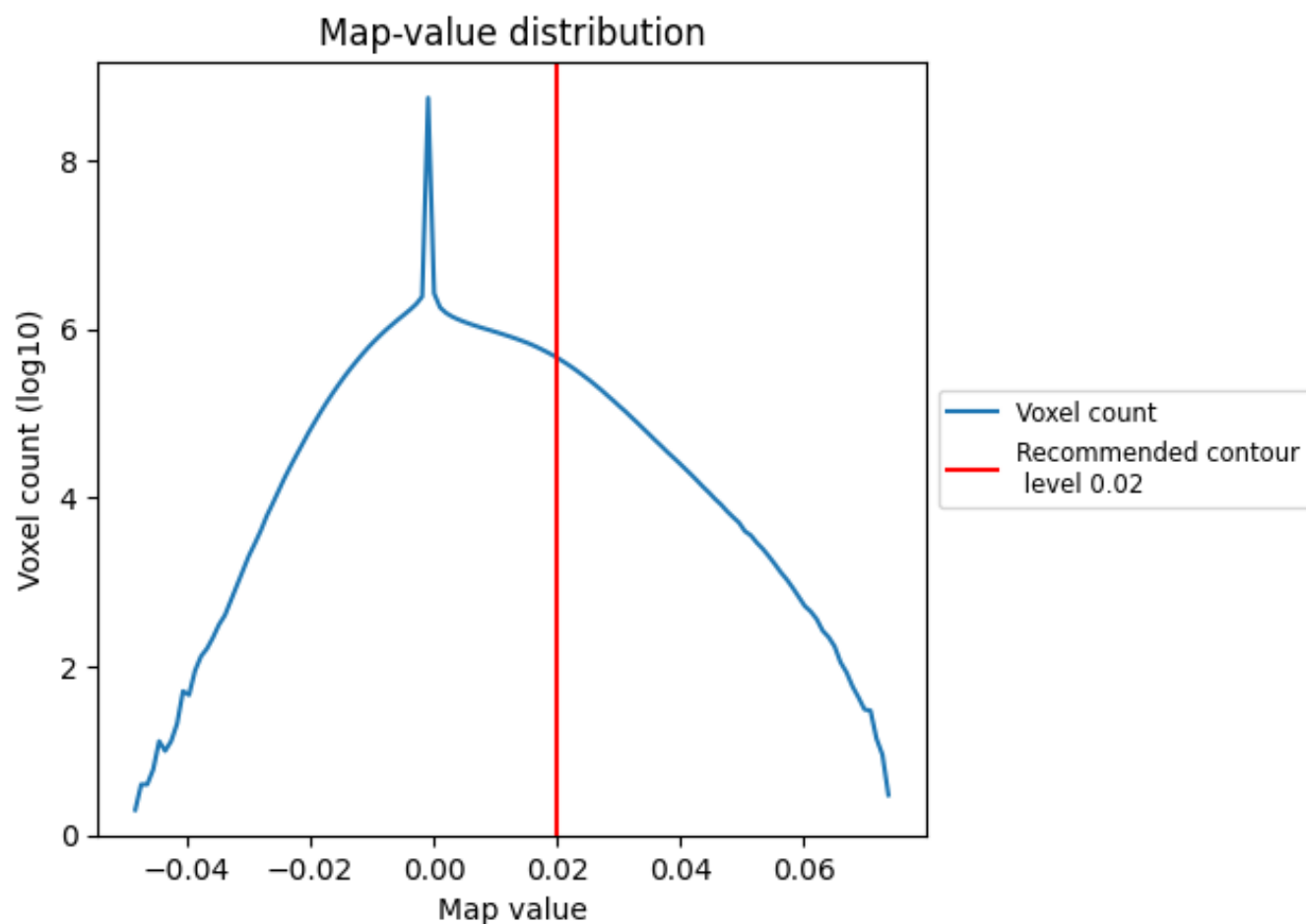


Z

7 Map analysis [i](#)

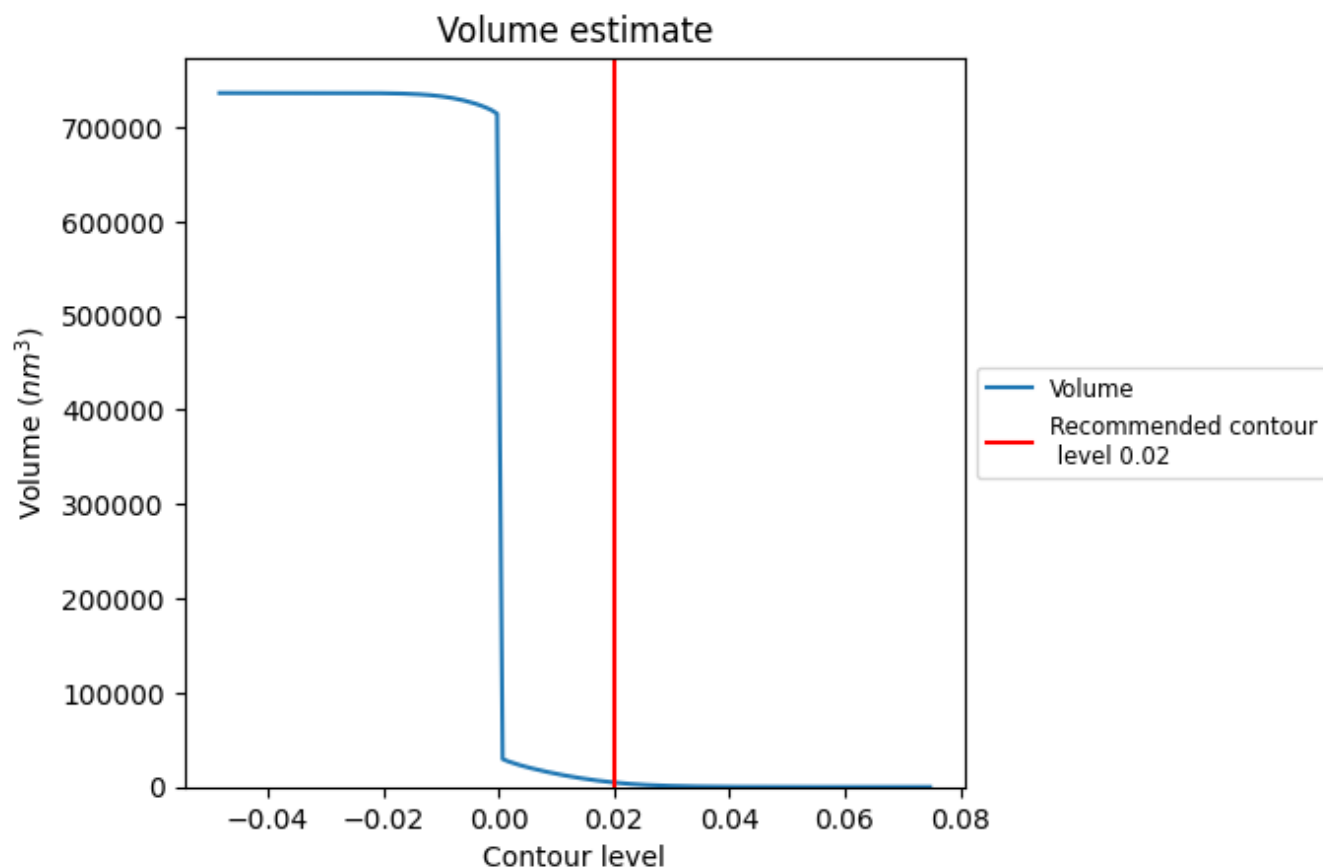
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

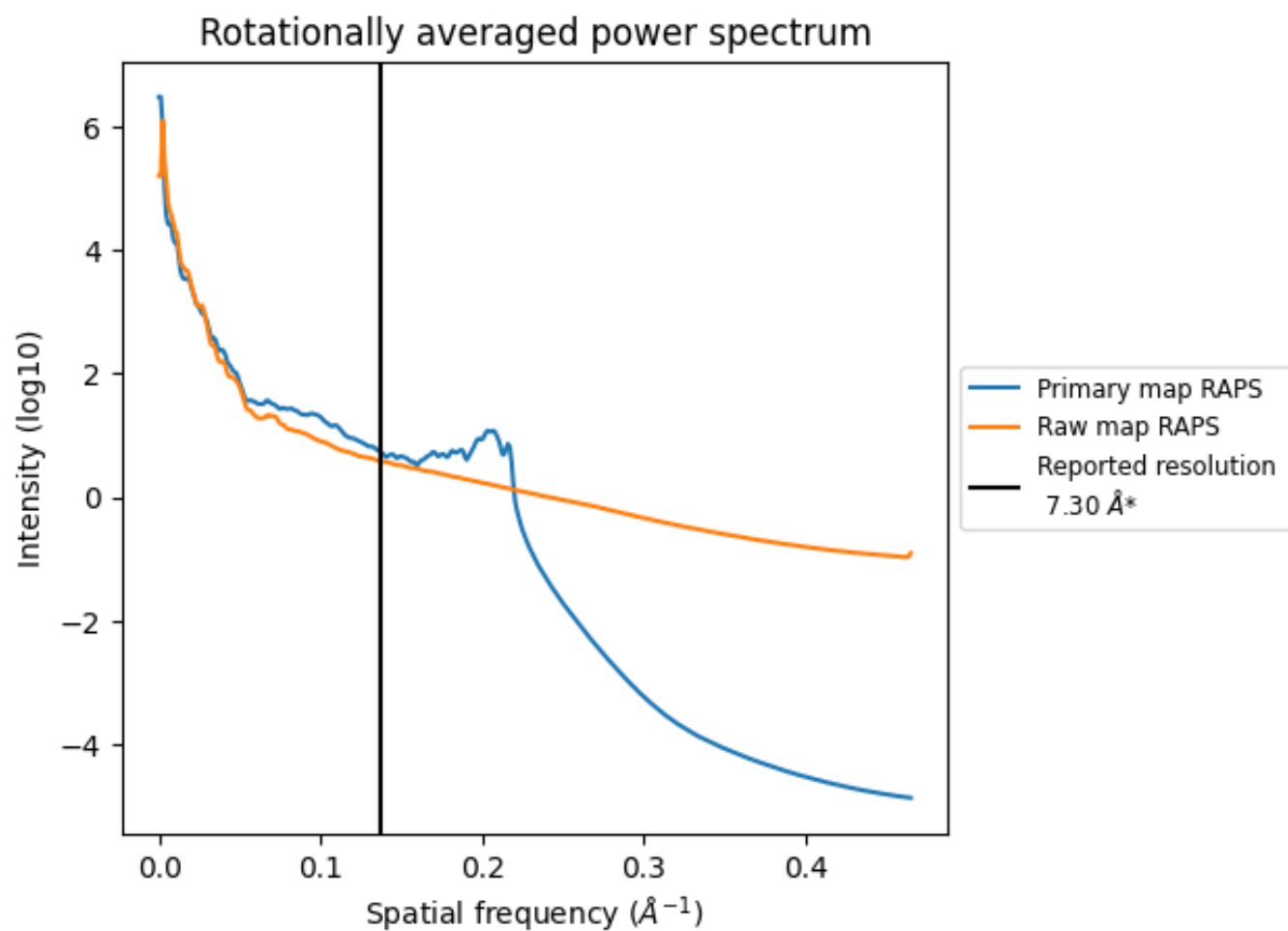
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4737 nm^3 ; this corresponds to an approximate mass of 4279 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 ⓘ

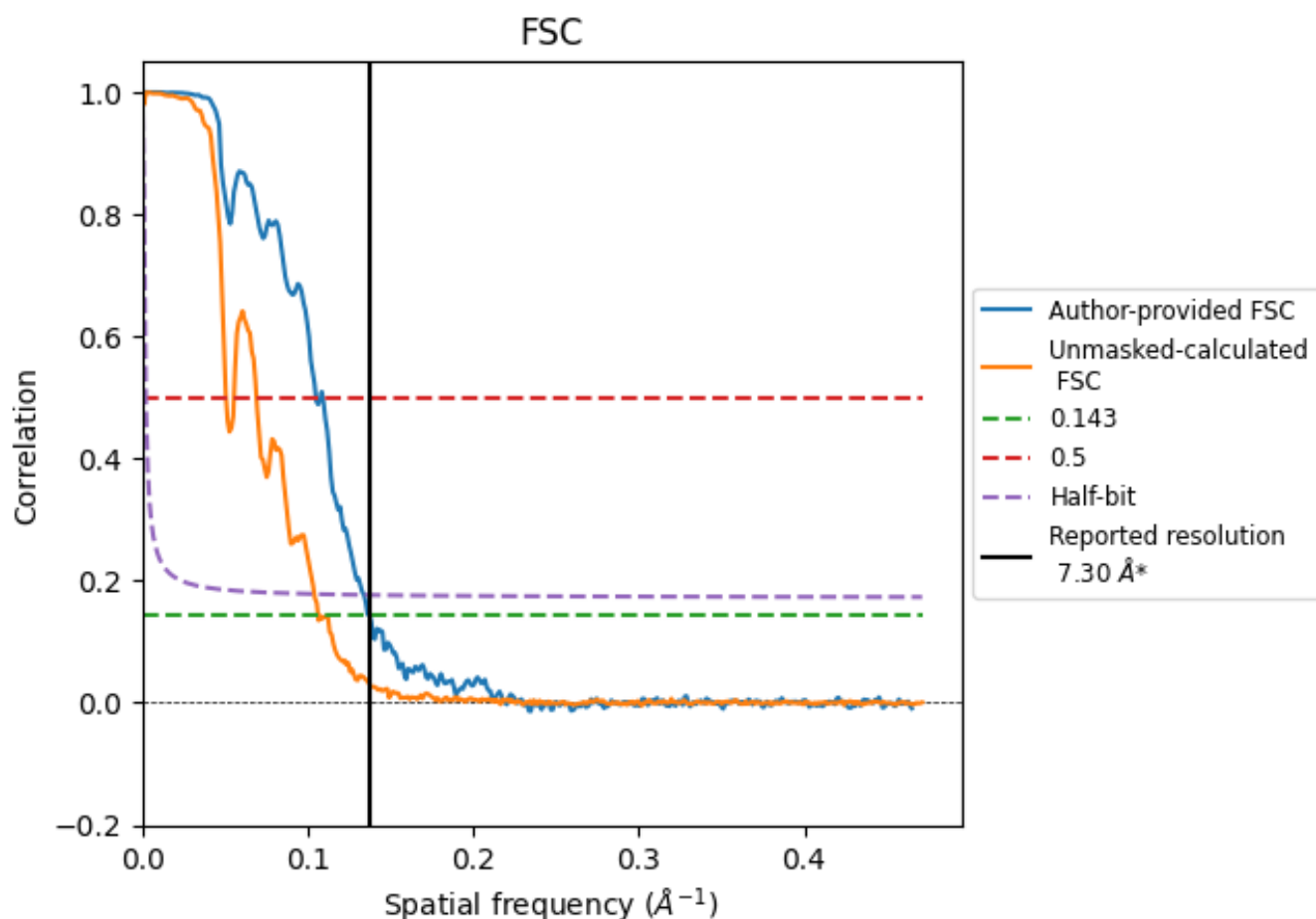


*Reported resolution corresponds to spatial frequency of 0.137 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.137 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.30	-	-
Author-provided FSC curve	7.28	9.52	7.46
Unmasked-calculated*	9.41	19.76	9.62

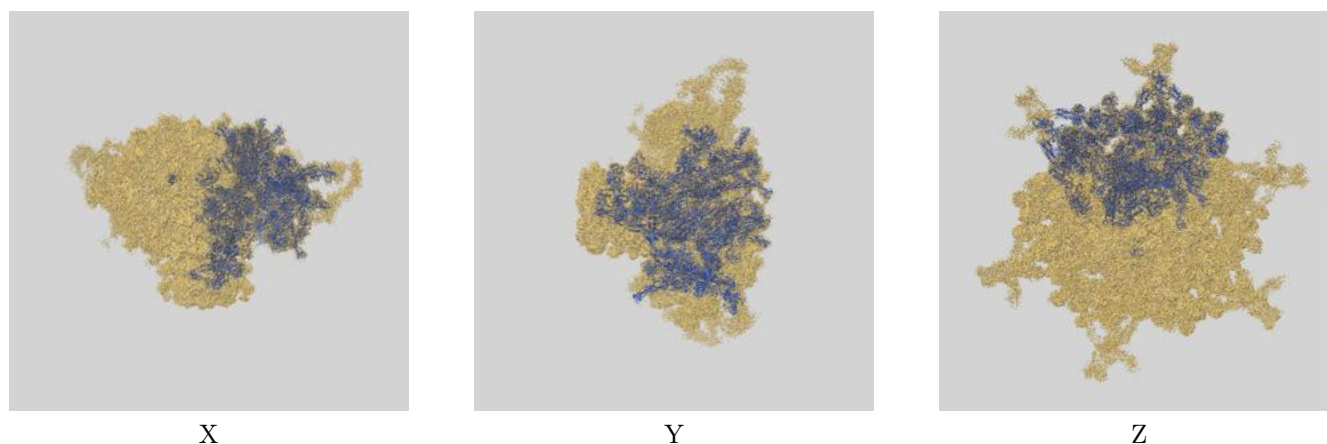
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.41 differs from the reported value 7.3 by more than 10 %

9 Map-model fit [i](#)

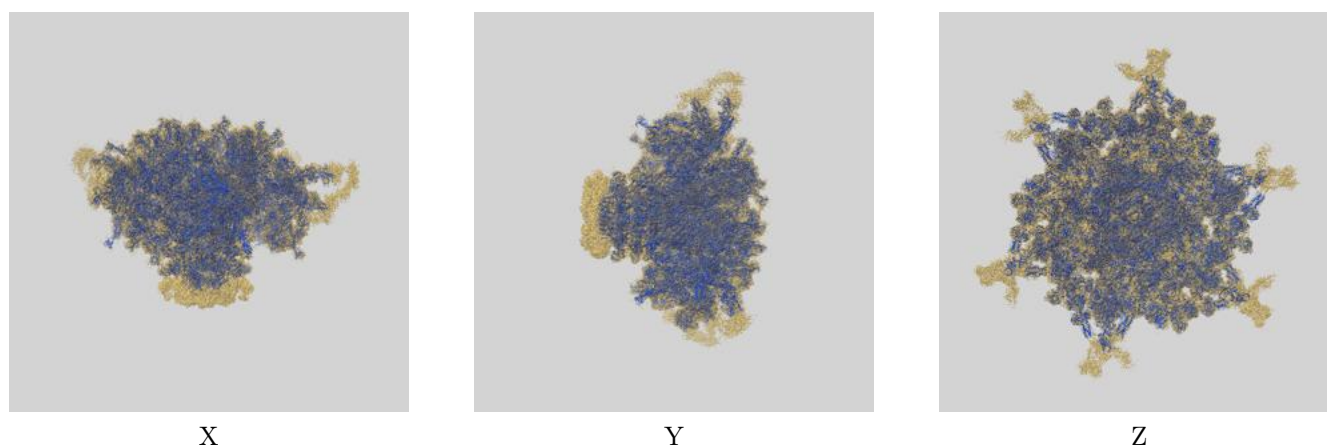
This section contains information regarding the fit between EMDB map EMD-19968 and PDB model 9EUF. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

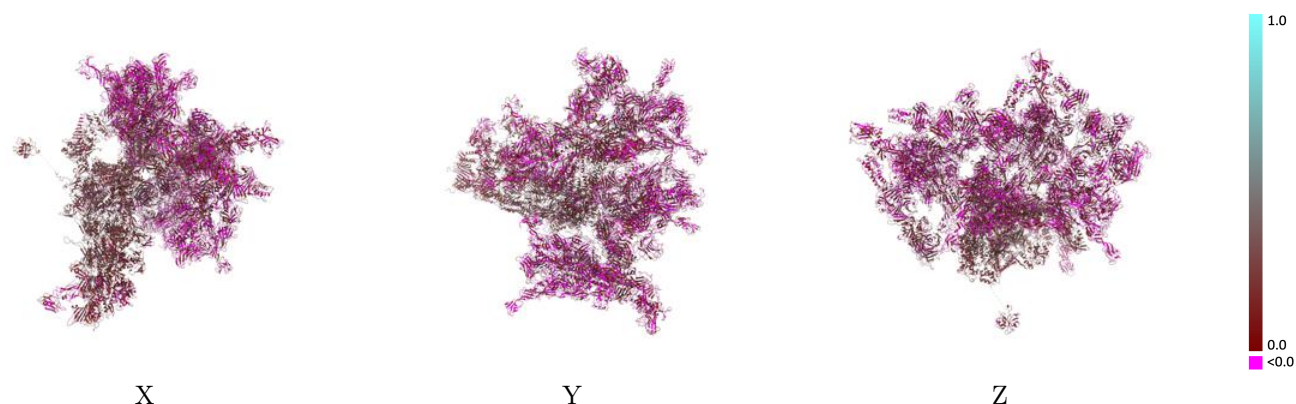


9.1.2 Map-model assembly overlay [i](#)



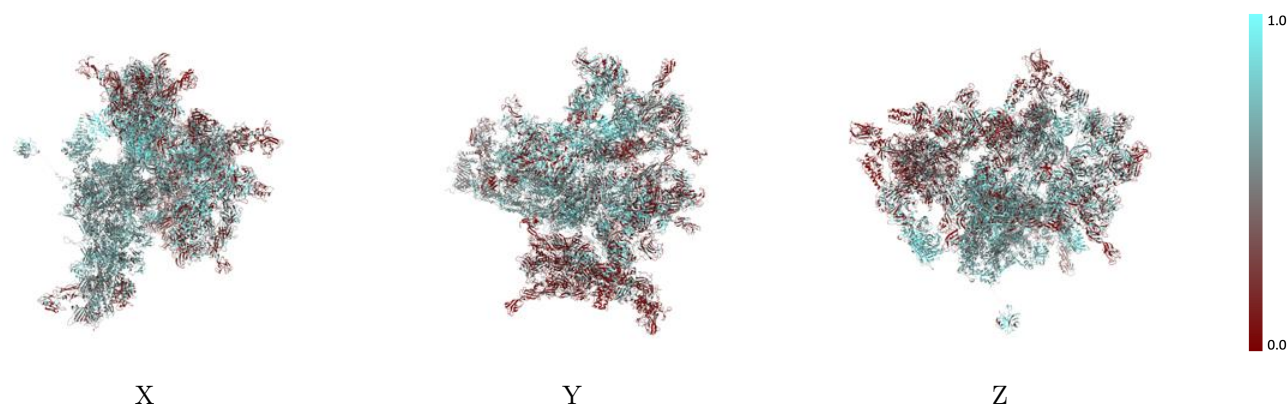
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



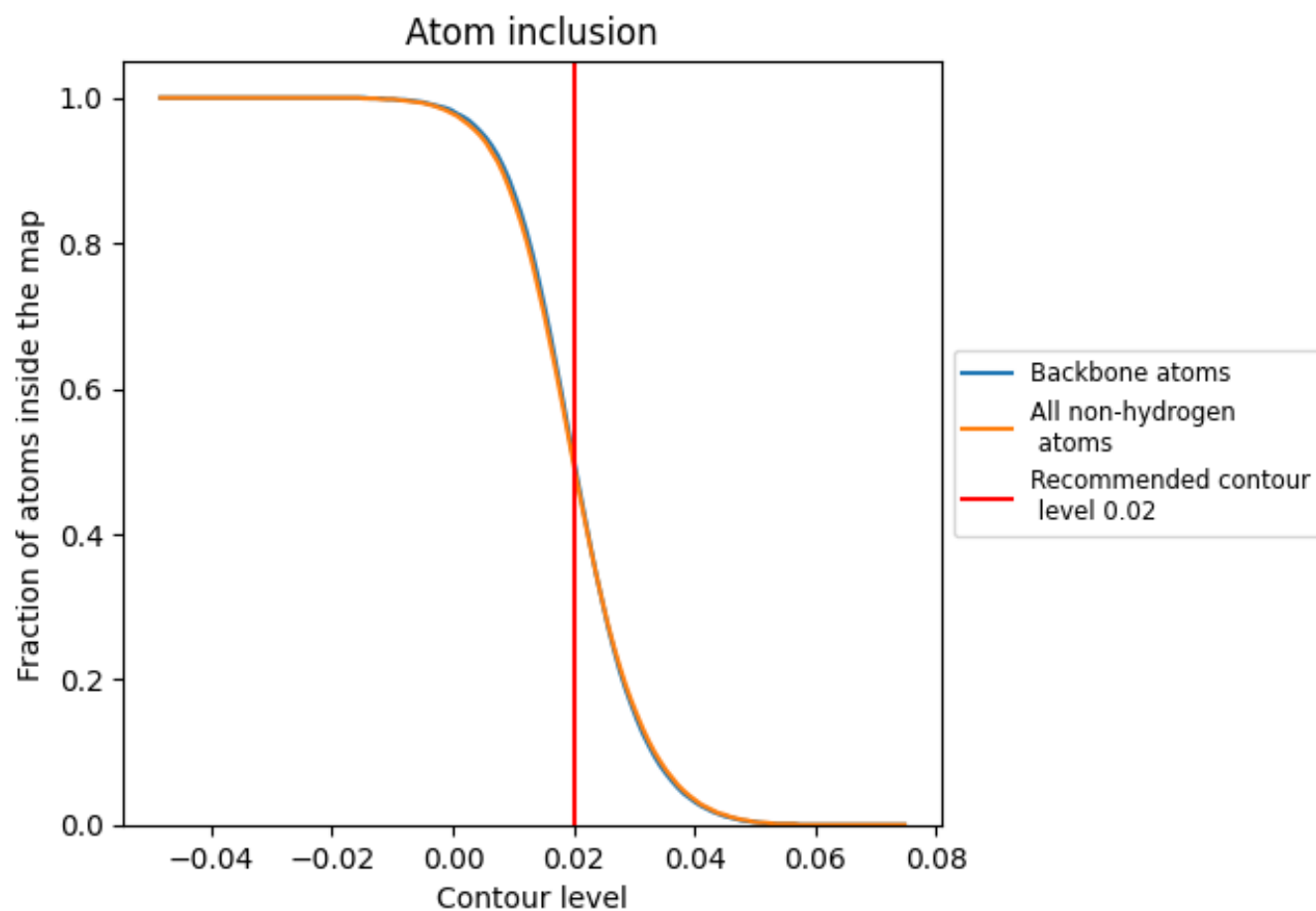
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 50% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4960	0.1780
0	0.5030	0.1100
1	0.4790	0.1170
2	0.5250	0.1210
3	0.5020	0.1270
4	0.4900	0.1260
5	0.5160	0.2190
6	0.5120	0.2090
7	0.4790	0.2000
8	0.5580	0.1790
9	0.4750	0.1290
A	0.7100	0.2660
AA	0.4620	0.1240
B	0.6330	0.2710
C	0.6110	0.2690
D	0.6310	0.2710
E	0.6010	0.2680
F	0.6130	0.2690
G	0.5810	0.2440
H	0.5970	0.2440
I	0.6060	0.2400
J	0.7020	0.2490
K	0.6230	0.2520
L	0.6010	0.2680
M	0.5650	0.2840
N	0.5710	0.2890
O	0.5960	0.2780
P	0.6120	0.2610
Q	0.6110	0.2550
R	0.5880	0.3000
S	0.5770	0.3040
T	0.5800	0.2360
U	0.6050	0.2410
V	0.5510	0.2860
W	0.5430	0.2660



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Chain	Atom inclusion	Q-score
X	 0.4260	 0.1450
Y	 0.4260	 0.1520
Z	 0.4500	 0.2240
a	 0.4630	 0.2090
b	 0.6090	 0.2360
c	 0.5210	 0.1870
d	 0.3760	 0.1490
e	 0.3080	 0.1330
f	 0.2300	 0.1040
g	 0.1470	 0.0860
h	 0.5310	 0.1260
i	 0.5400	 0.1220
j	 0.5130	 0.1070
k	 0.2460	 0.0720
l	 0.2330	 0.0690
m	 0.2270	 0.0680
n	 0.5620	 0.1790
o	 0.5500	 0.1910
p	 0.5340	 0.1830
q	 0.3610	 0.1370
r	 0.3250	 0.1230
s	 0.3180	 0.1270
t	 0.6450	 0.2500
u	 0.5920	 0.2330
v	 0.4840	 0.1820
w	 0.3780	 0.0940
x	 0.3070	 0.1400
y	 0.1770	 0.0880
z	 0.5120	 0.1170