



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 10:03 am BST

PDB ID : 9TIC / pdb_00009tic
EMDB ID : EMD-55951
Title : Phage 812 baseplate in the pre-contraction state (C3)
Authors : Binovsky, J.; Plevka, P.
Deposited on : 2025-12-05
Resolution : 5.90 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 ⓘ symbol.

The types of validation reports are described at

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

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

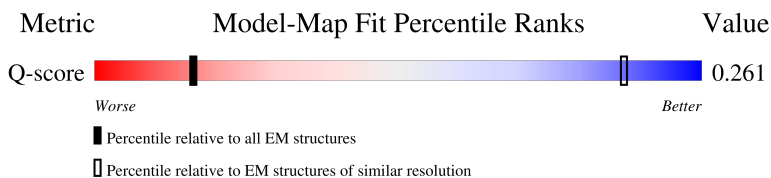
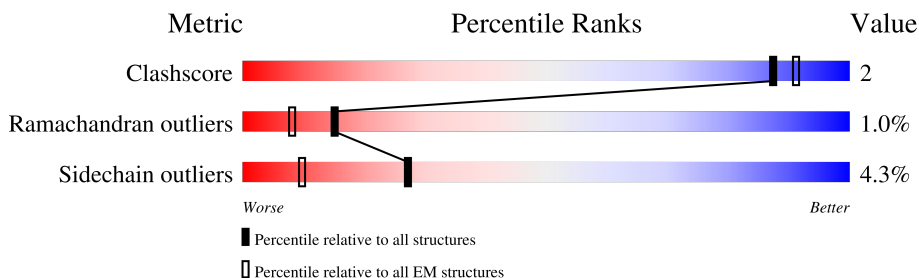
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 5.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	501 (5.40 - 6.40)

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	458	32% 94% 6%
1	8	458	30% 91% 9%
1	9	458	28% 95% 5%
1	w	458	29% 92% 7%

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Mol	Chain	Length	Quality of chain
1	x	458	25% 94% 6%
1	y	458	24% 94% 5%
2	l	173	98% 83% 14% ..
2	P	173	83% 9% 7%
2	Q	173	14% 87% 7% 6%
2	R	173	39% 85% 8% 6%
2	S	173	62% 94% ..
2	T	173	83% 83% 16% ..
2	U	173	91% 84% 13% ...
2	V	173	95% 83% 14% ..
2	W	173	99% 86% 11% ..
2	X	173	98% 87% 10% ...
2	Y	173	99% 86% 12% ...
2	Z	173	96% 82% 16% ..
2	e	173	89% 5% 6%
2	f	173	9% 89% .. 6%
2	g	173	16% 94% 6%
2	h	173	43% 94% 5% ..
2	i	173	47% 83% 5% 12%
2	j	173	76% 91% 8% ..
2	k	173	86% 85% 13% ..
2	l	173	94% 88% 10% ..
2	m	173	94% 91% 6% ...
2	n	173	92% 88% 11% .
2	o	173	85% 87% 11% ..

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Mol	Chain	Length	Quality of chain
2	p	173	
3	2	1152	
3	3	1152	
3	4	1152	
3	5	1152	
3	6	1152	
3	7	1152	
3	q	1152	
3	r	1152	
3	s	1152	
3	t	1152	
3	u	1152	
3	v	1152	
4	A	848	
5	AA	640	
5	AB	640	
5	a	640	
5	b	640	
5	c	640	
5	z	640	
6	AC	142	
6	AD	142	
6	AE	142	
6	AF	142	
6	AG	142	

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Mol	Chain	Length	Quality of chain
6	AH	142	
7	AI	587	
7	AJ	587	
7	AK	587	
7	AL	587	
7	AM	587	
7	AN	587	
8	B	295	
9	C	808	
10	D	174	
10	E	174	
11	F	263	
11	G	263	
12	H	234	
12	I	234	
13	J	348	
13	K	348	
13	L	348	
13	M	348	
14	N	1019	
14	O	1019	
15	d	124	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 256934 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 ORF68.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
1	8	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
1	9	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
1	w	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
1	x	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
1	y	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		

- Molecule 2 is a protein called ORF64.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	P	161	Total	C	N	O	S	0	0
			1266	809	207	249	1		
2	Q	163	Total	C	N	O	S	0	0
			1277	817	208	251	1		
2	R	162	Total	C	N	O	S	0	0
			1272	812	208	251	1		
2	S	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	T	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	U	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	V	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	W	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	Y	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	Z	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	e	163	Total	C	N	O	S	0	0
			1280	818	209	252	1		
2	f	162	Total	C	N	O	S	0	0
			1270	811	207	251	1		
2	g	163	Total	C	N	O	S	0	0
			1278	817	208	252	1		
2	h	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	i	152	Total	C	N	O	S	0	0
			1199	769	196	233	1		
2	j	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	k	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	l	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	m	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	n	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	o	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	p	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		

- Molecule 3 is a protein called ORF65.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	3	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	4	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	5	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	7	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	q	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	r	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	s	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	t	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	u	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	v	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		

- Molecule 4 is a protein called ORF58.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	309	Total	C	N	O	S	0	0
			2462	1555	400	501	6		

- Molecule 5 is a protein called CBM-cenC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AA	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
5	AB	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
5	a	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
5	b	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
5	c	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
5	z	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		

- Molecule 6 is a protein called ORF50.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AC	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
6	AD	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
6	AE	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
6	AF	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
6	AG	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
6	AH	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		

- Molecule 7 is a protein called ORF49.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AI	550	Total	C	N	O	S	0	0
			4284	2698	729	850	7		
7	AJ	550	Total	C	N	O	S	0	0
			4284	2698	729	850	7		
7	AK	549	Total	C	N	O	S	0	0
			4267	2684	724	852	7		
7	AL	549	Total	C	N	O	S	0	0
			4267	2684	724	852	7		
7	AM	342	Total	C	N	O	S	0	0
			2667	1678	459	523	7		
7	AN	342	Total	C	N	O	S	0	0
			2667	1678	459	523	7		

- Molecule 8 is a protein called ORF57.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	292	Total	C	N	O	S	0	0
			2424	1572	369	476	7		

- Molecule 9 is a protein called ORF56.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	725	Total	C	N	O	S	0	0
			5852	3738	984	1110	20		

- Molecule 10 is a protein called ORF60.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	160	Total	C	N	O	S	0	0
			1294	831	206	253	4		
10	E	154	Total	C	N	O	S	0	0
			1248	803	200	241	4		

- Molecule 11 is a protein called ORF59.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	238	Total	C	N	O	S	0	0
			1878	1164	335	375	4		
11	G	237	Total	C	N	O	S	0	0
			1871	1160	334	373	4		

- Molecule 12 is a protein called ORF61.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	212	Total	C	N	O	S	0	0
			1694	1060	290	339	5		
12	I	213	Total	C	N	O	S	0	0
			1701	1065	291	340	5		

- Molecule 13 is a protein called ORF62.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	348	Total	C	N	O	S	0	0
			2760	1734	459	560	7		
13	K	348	Total	C	N	O	S	0	0
			2760	1734	459	560	7		
13	L	348	Total	C	N	O	S	0	0
			2760	1734	459	560	7		
13	M	348	Total	C	N	O	S	0	0
			2760	1734	459	560	7		

- Molecule 14 is a protein called ORF63.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	721	Total	C	N	O	S	0	0
			5845	3728	945	1161	11		
14	O	721	Total	C	N	O	S	0	0
			5845	3728	945	1161	11		

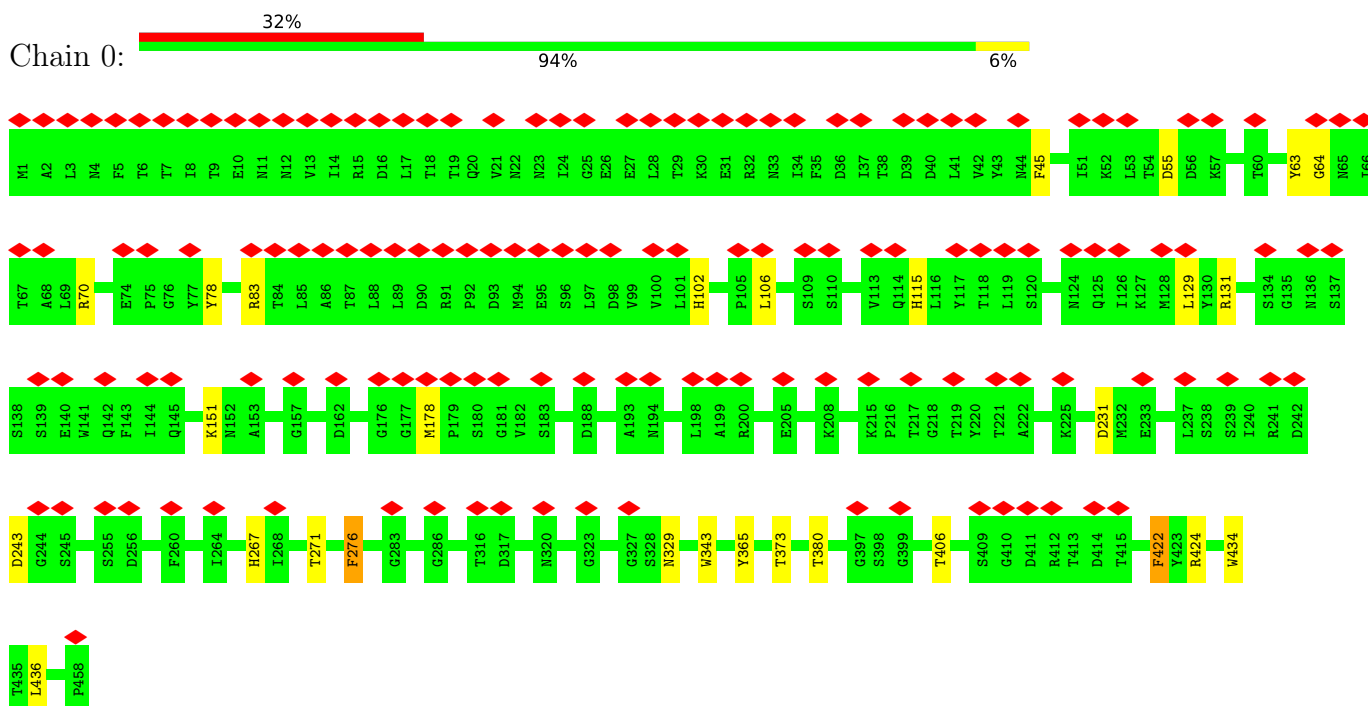
- Molecule 15 is a protein called ORF67.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	d	71	597	390	94	113	0	0

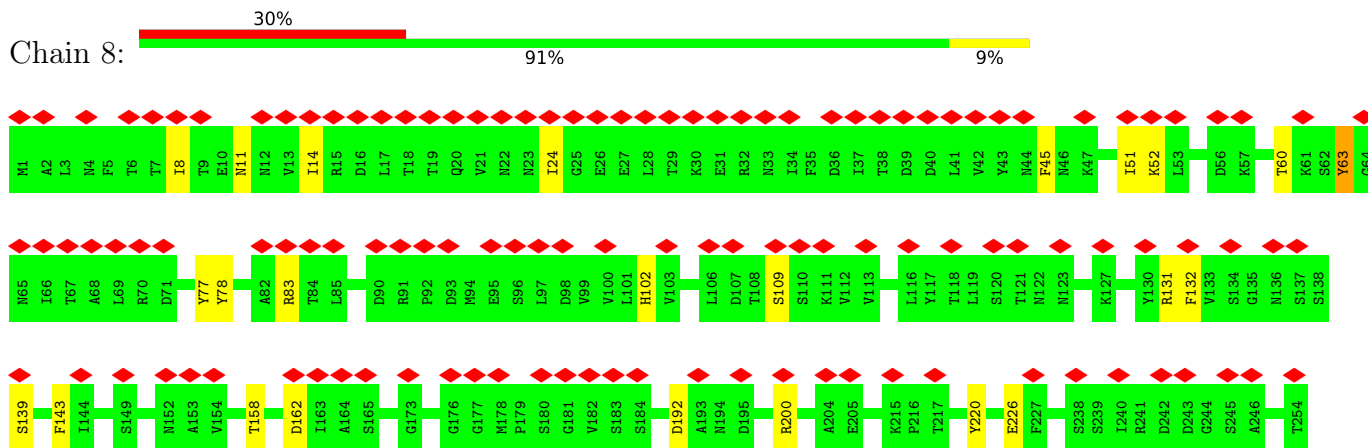
3 Residue-property plots

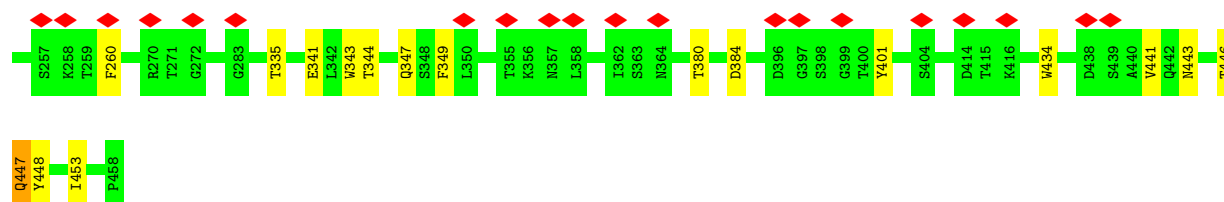
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: ORF68

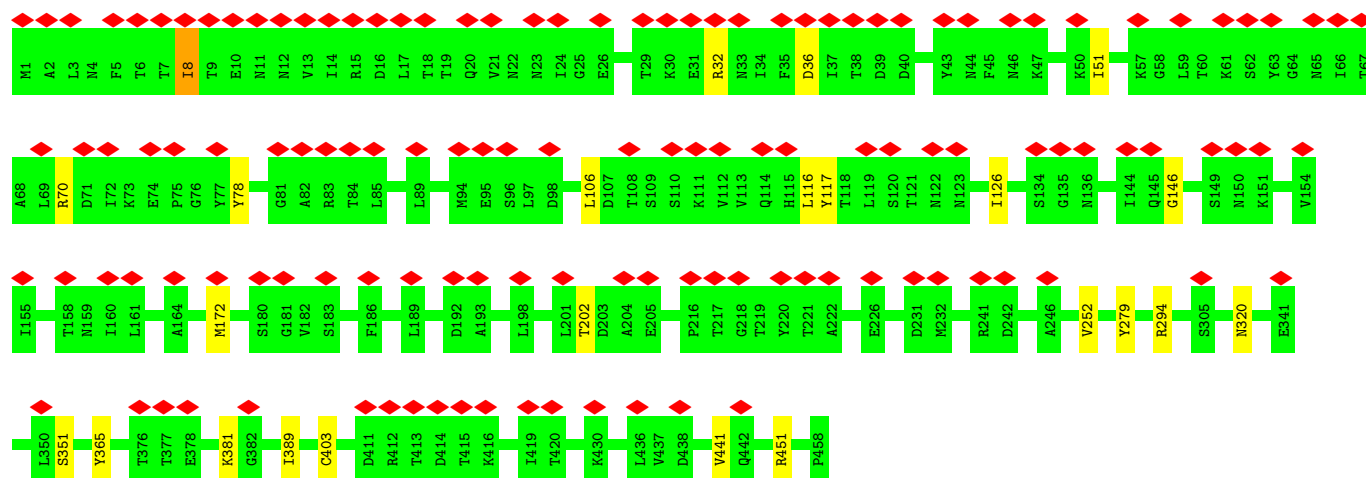


• Molecule 1: ORF68

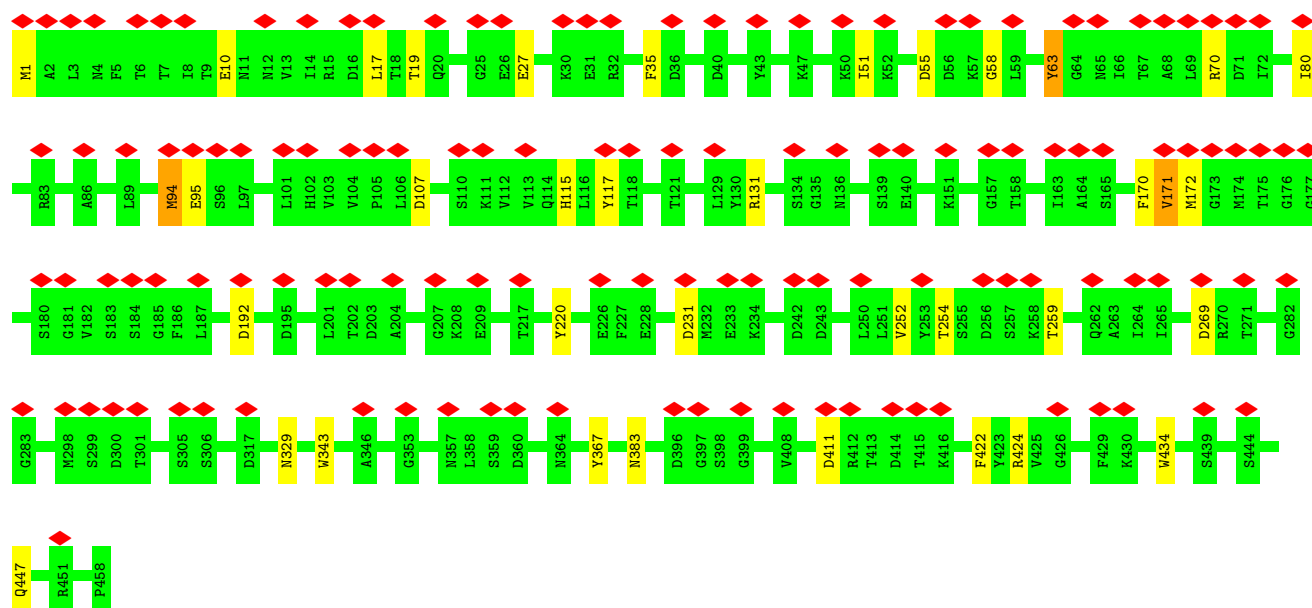
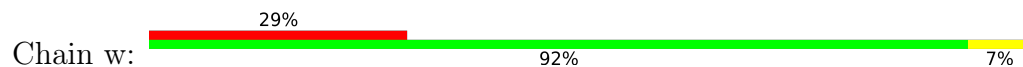




• Molecule 1: ORF68

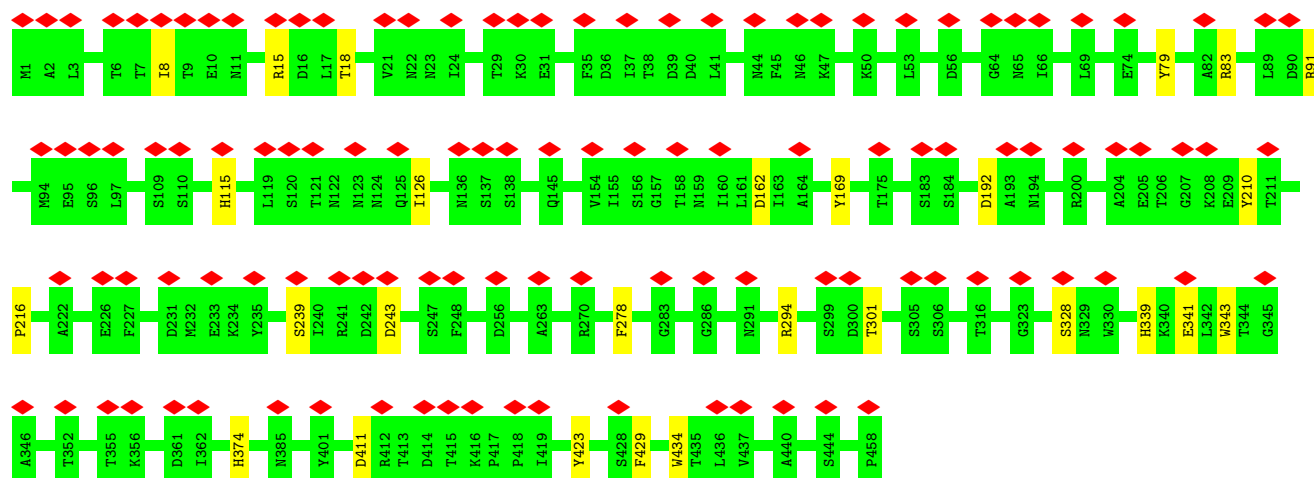


• Molecule 1: ORF68

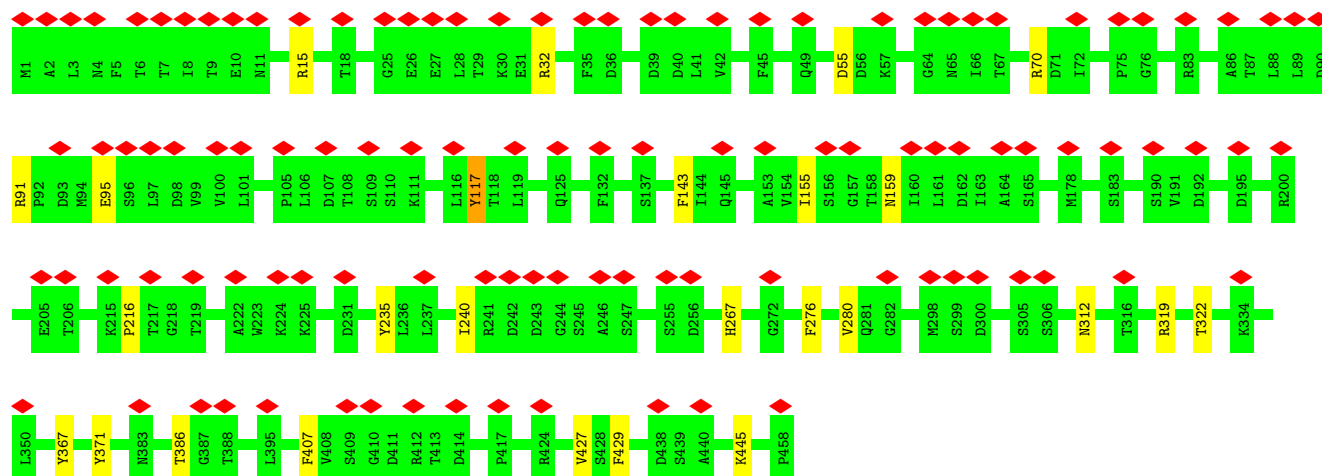


• Molecule 1: ORF68

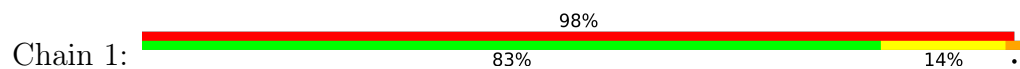




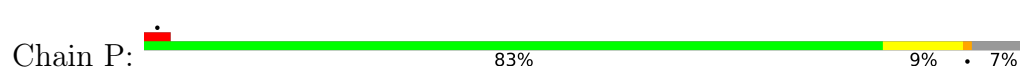
• Molecule 1: ORF68



• Molecule 2: ORF64

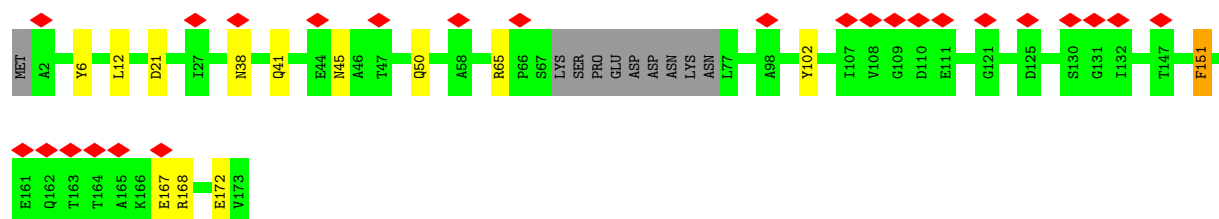
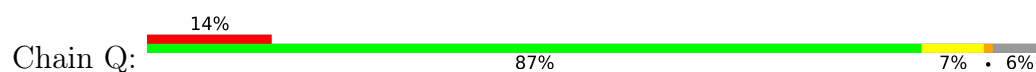


• Molecule 2: ORF64

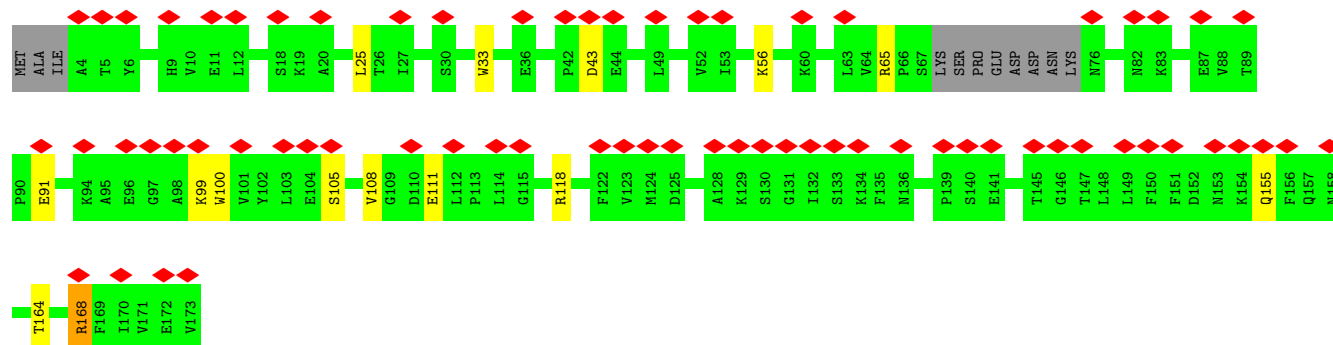
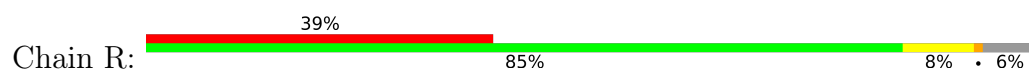




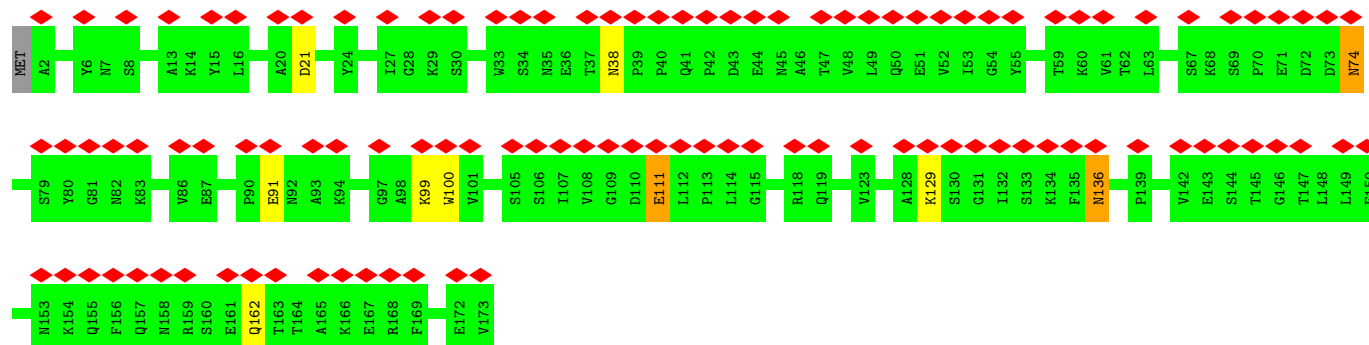
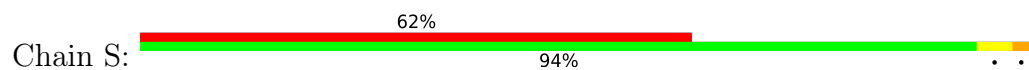
• Molecule 2: ORF64



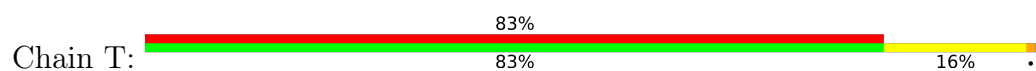
• Molecule 2: ORF64



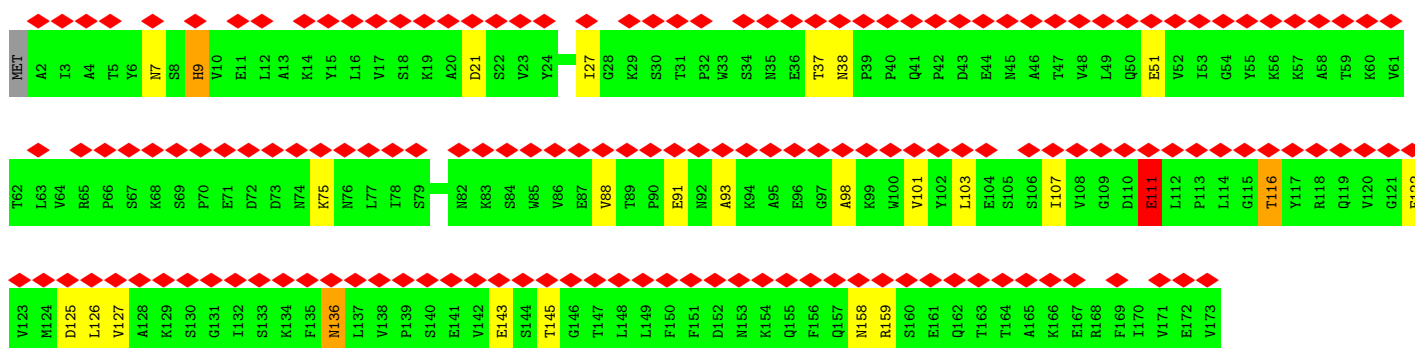
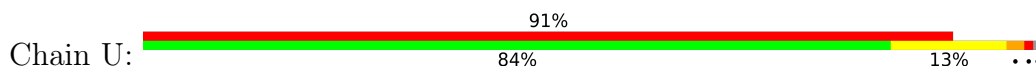
• Molecule 2: ORF64



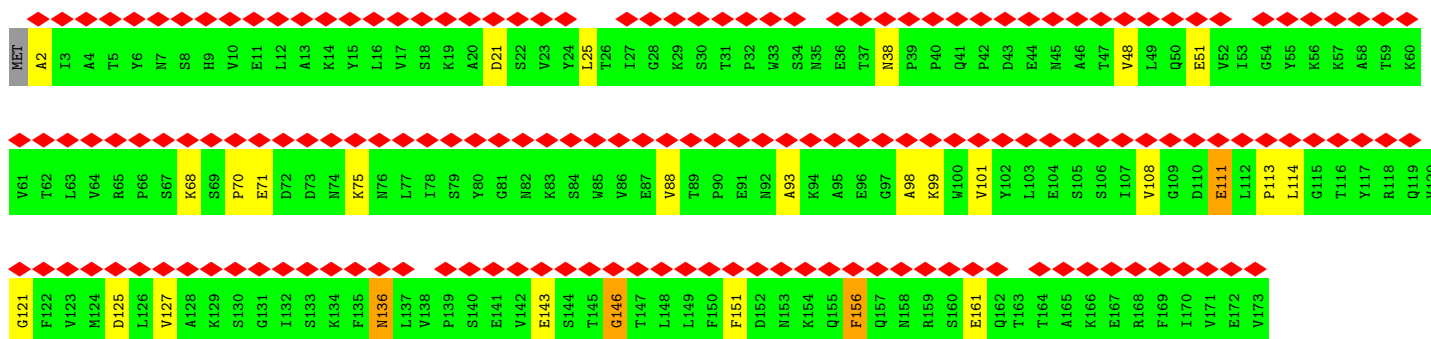
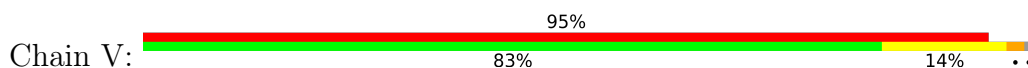
• Molecule 2: ORF64



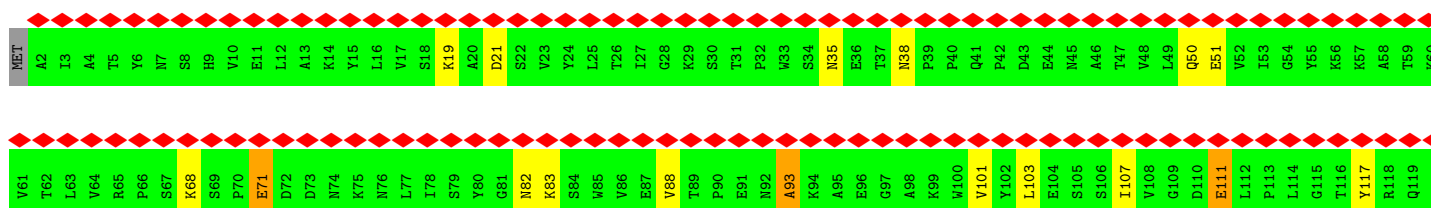
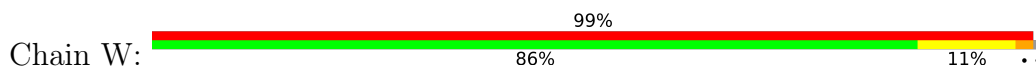
- Molecule 2: ORF64

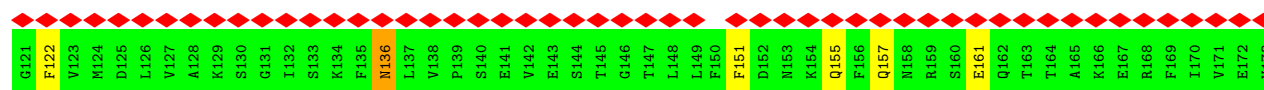


- Molecule 2: ORF64

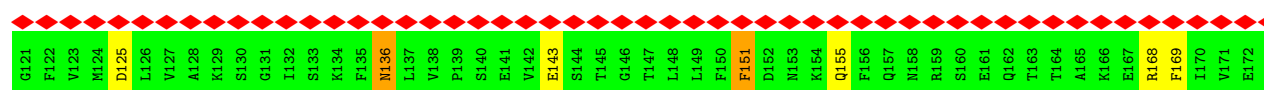
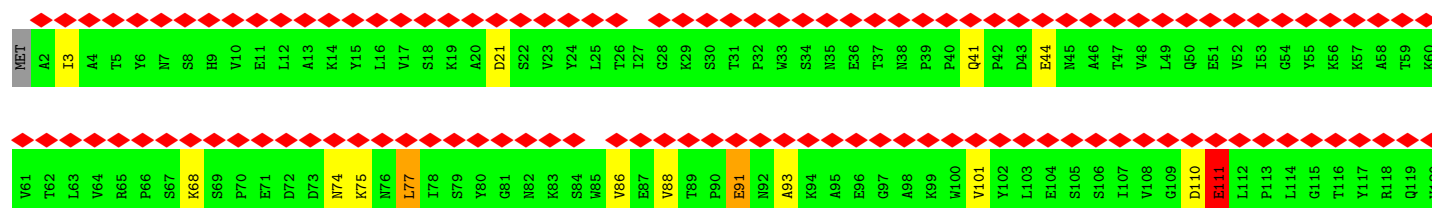
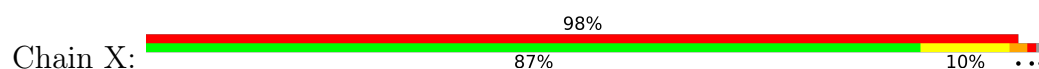


- Molecule 2: ORF64

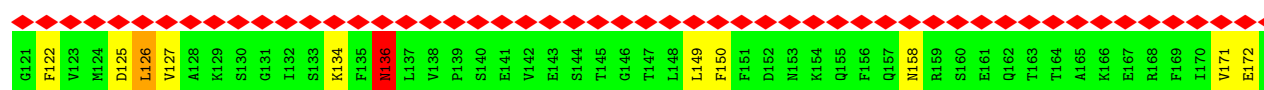
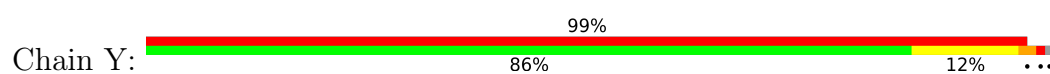




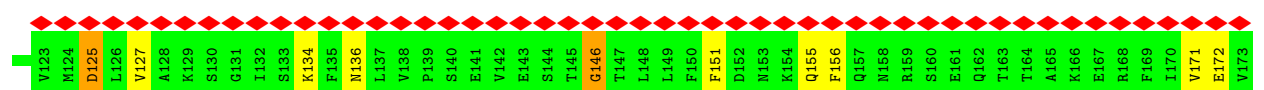
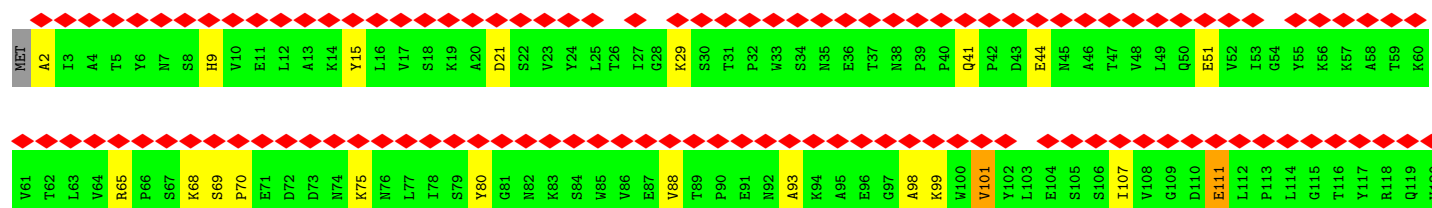
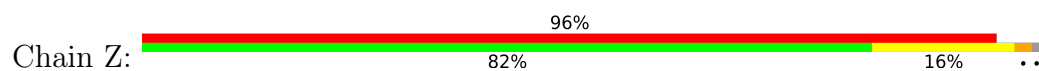
• Molecule 2: ORF64



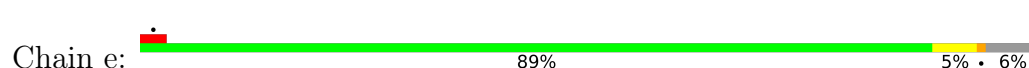
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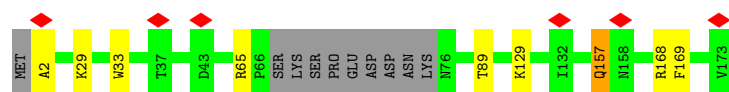


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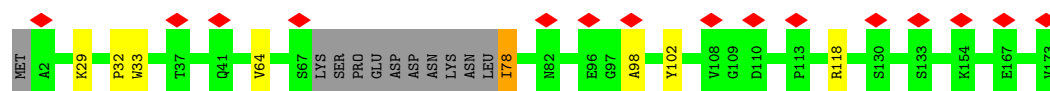
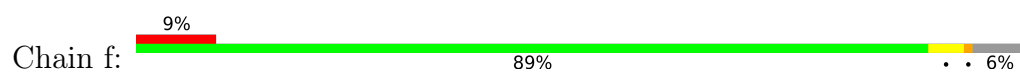


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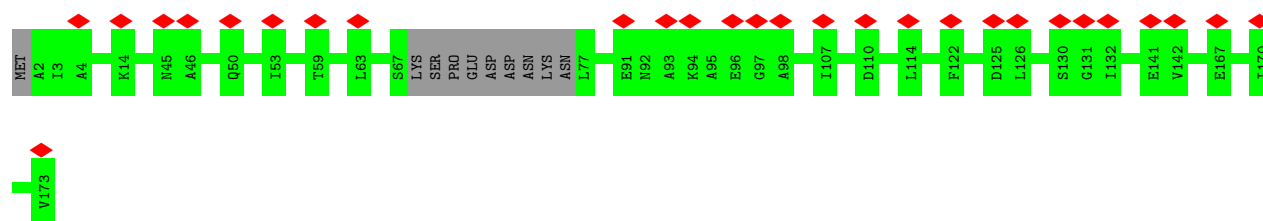




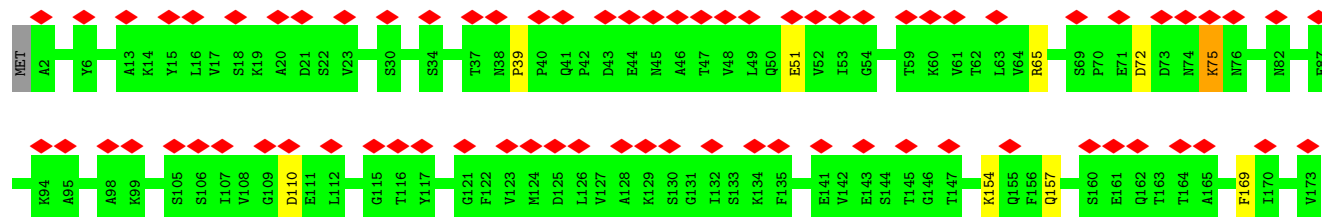
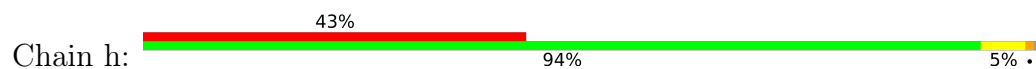
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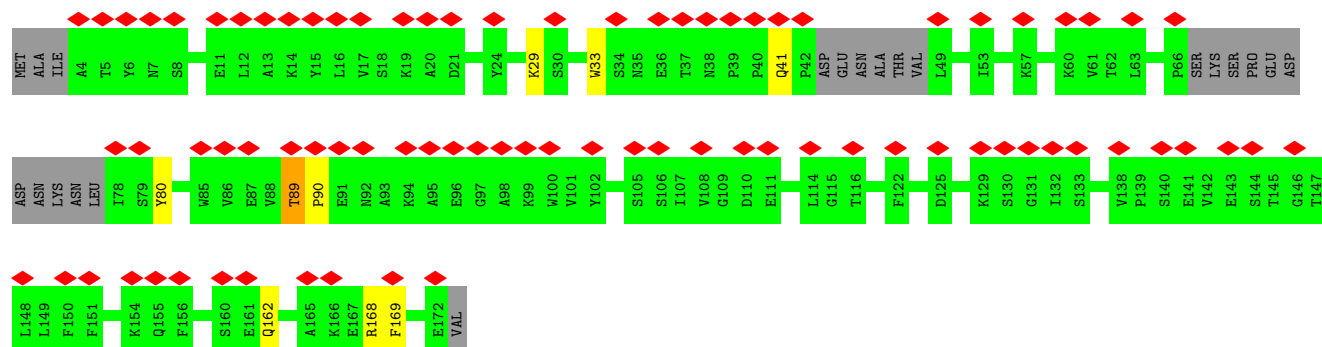
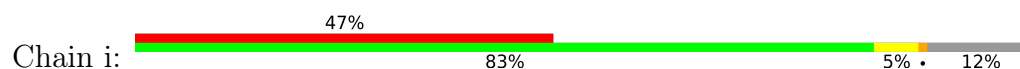
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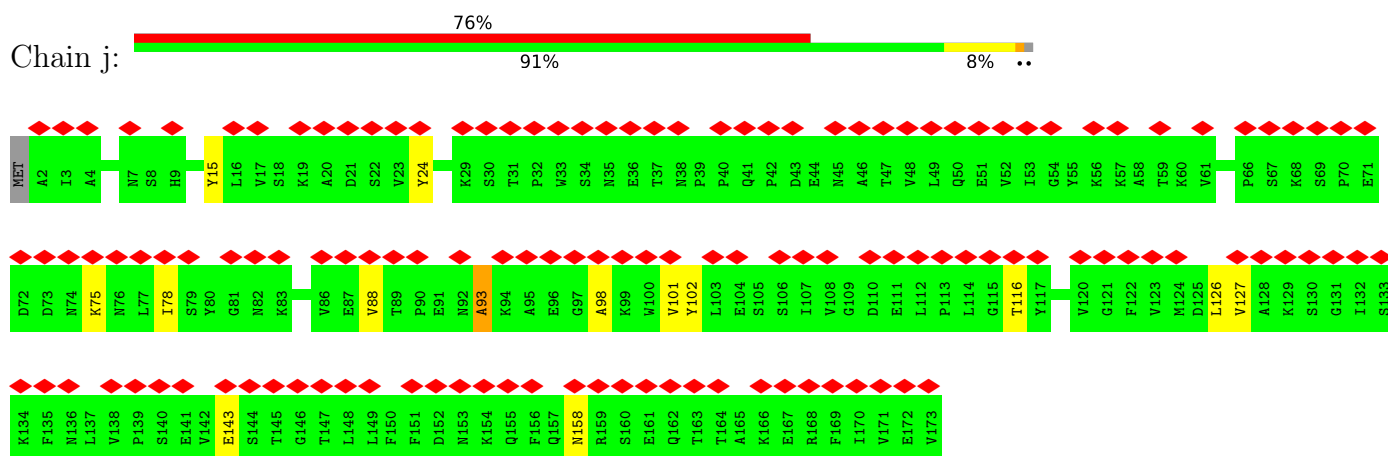
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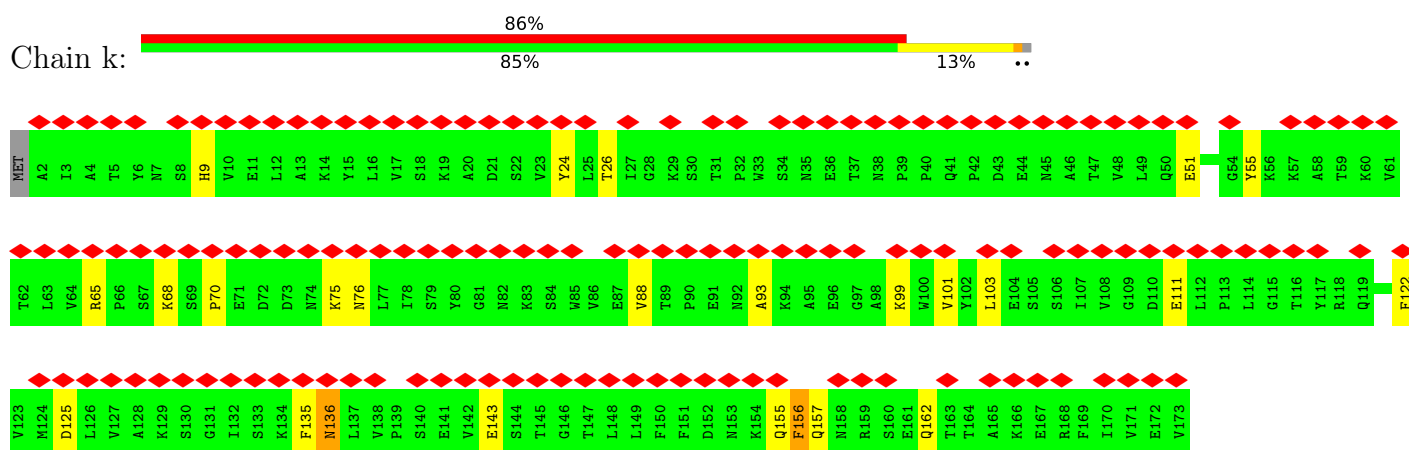
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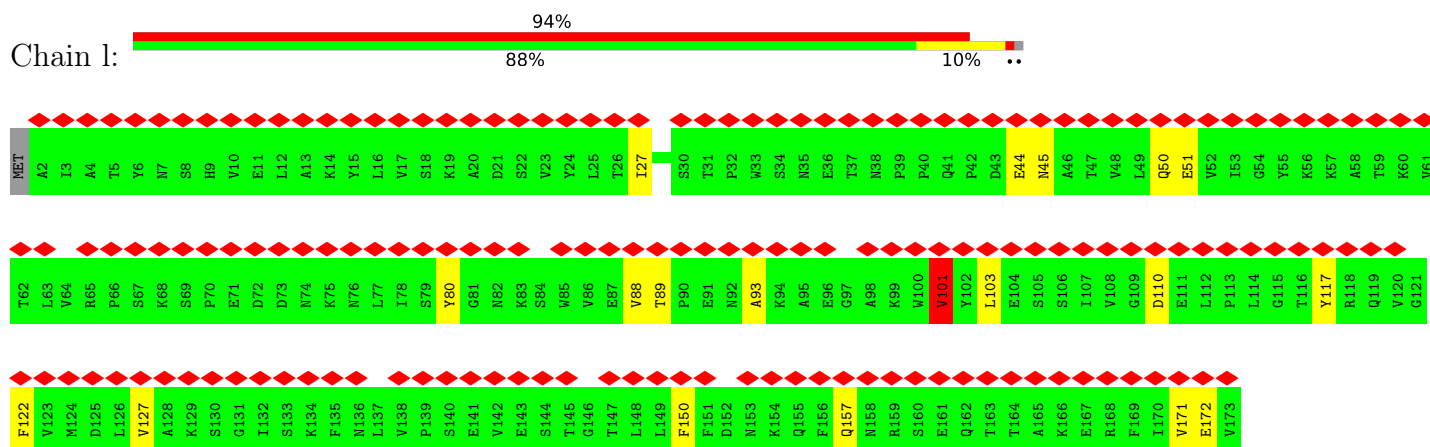
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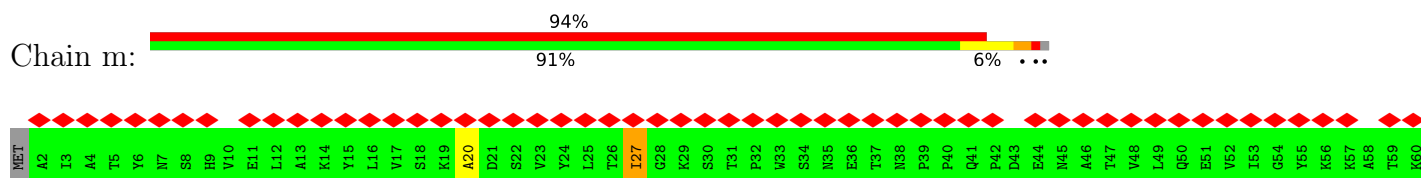
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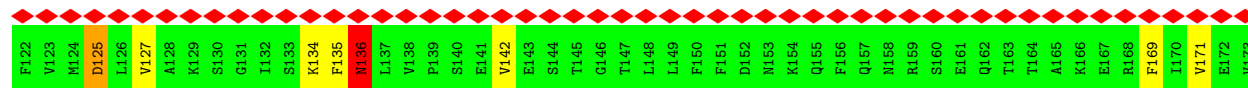
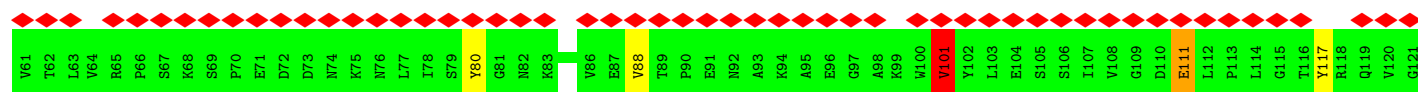


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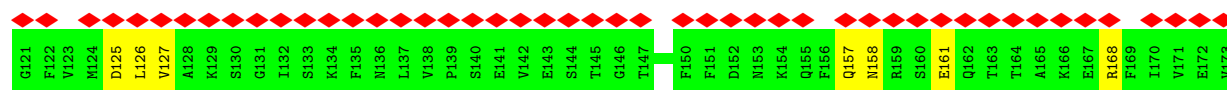
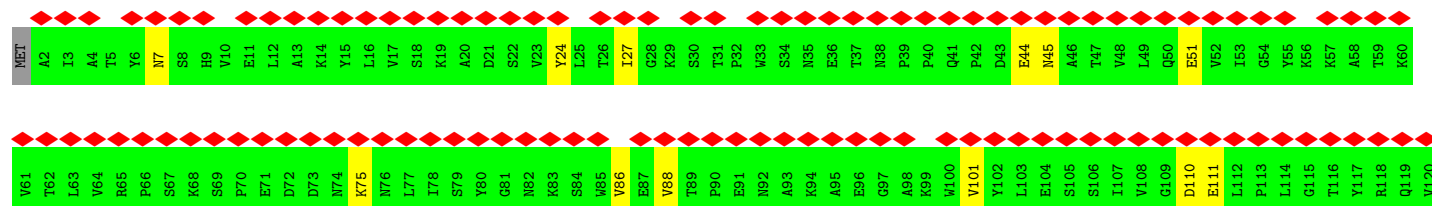
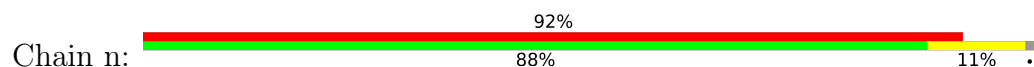


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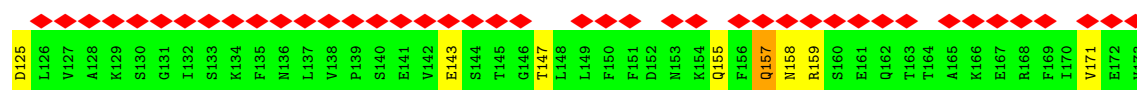
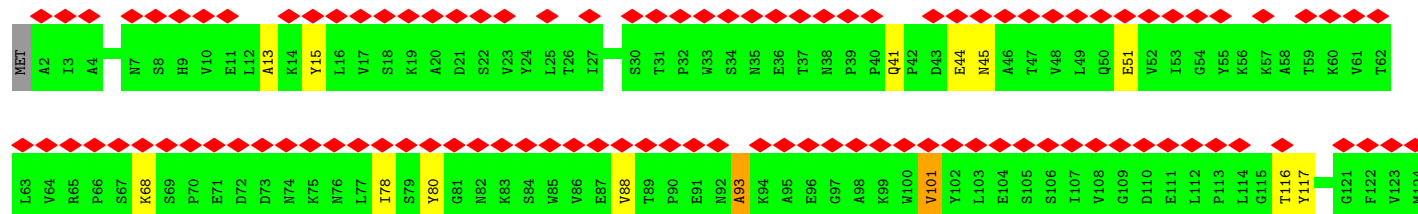
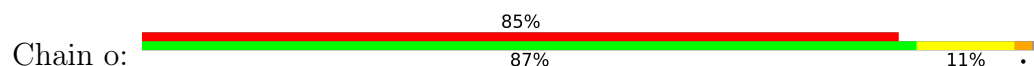




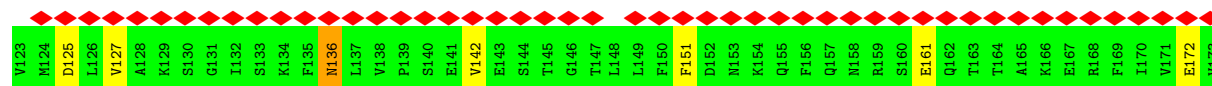
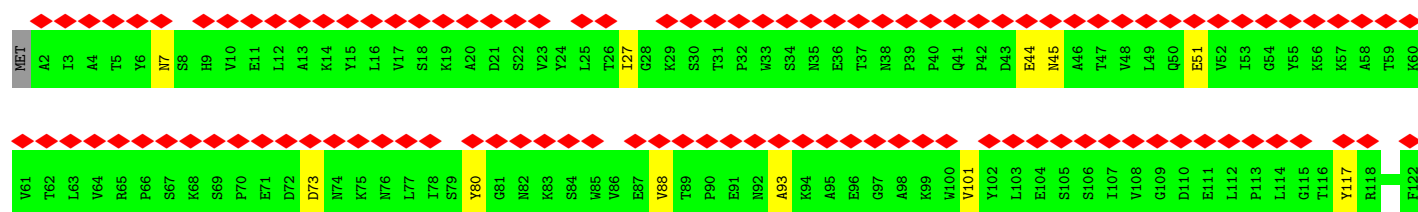
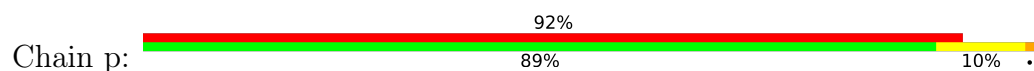
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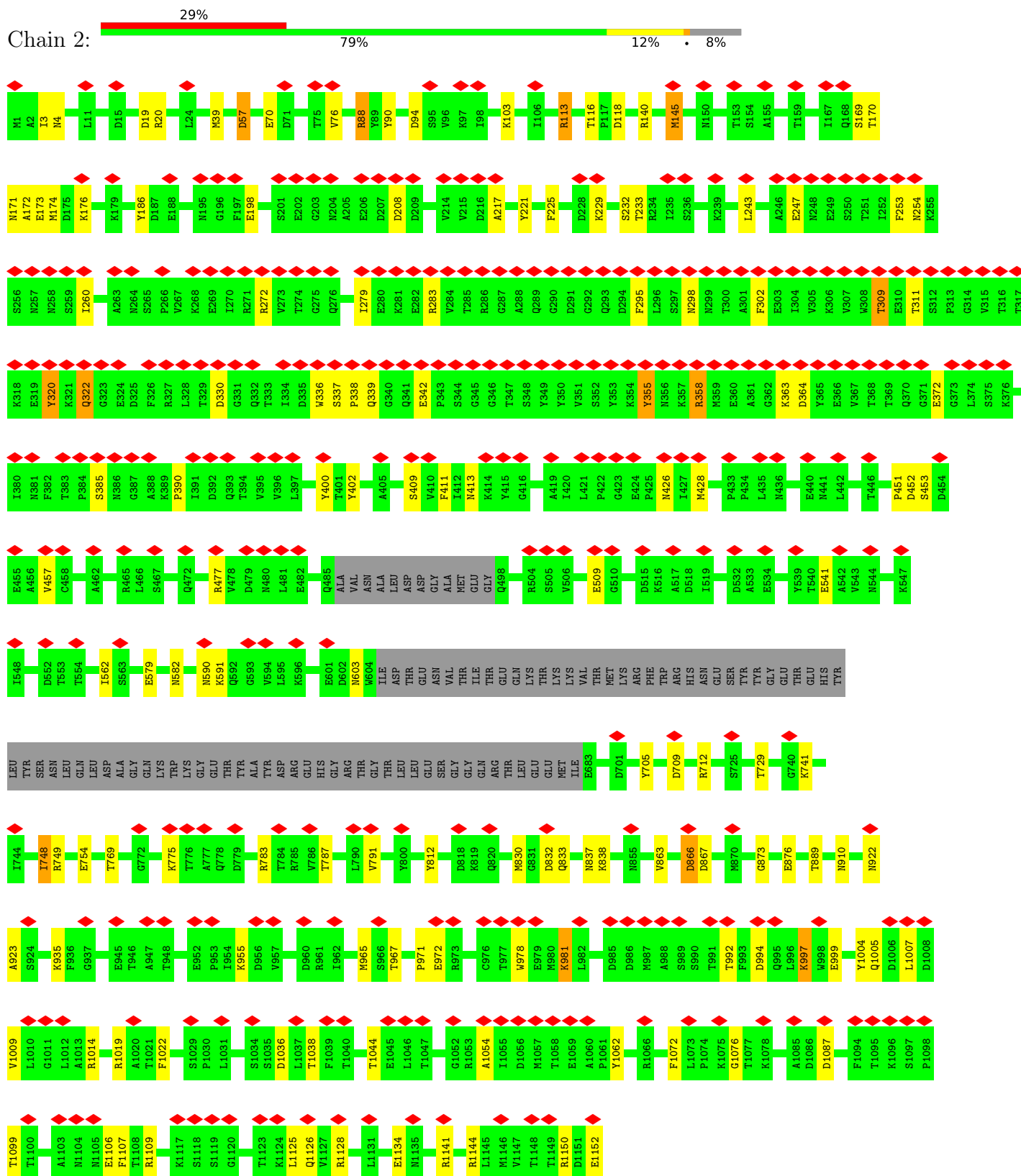
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• Molecule 2: ORF64



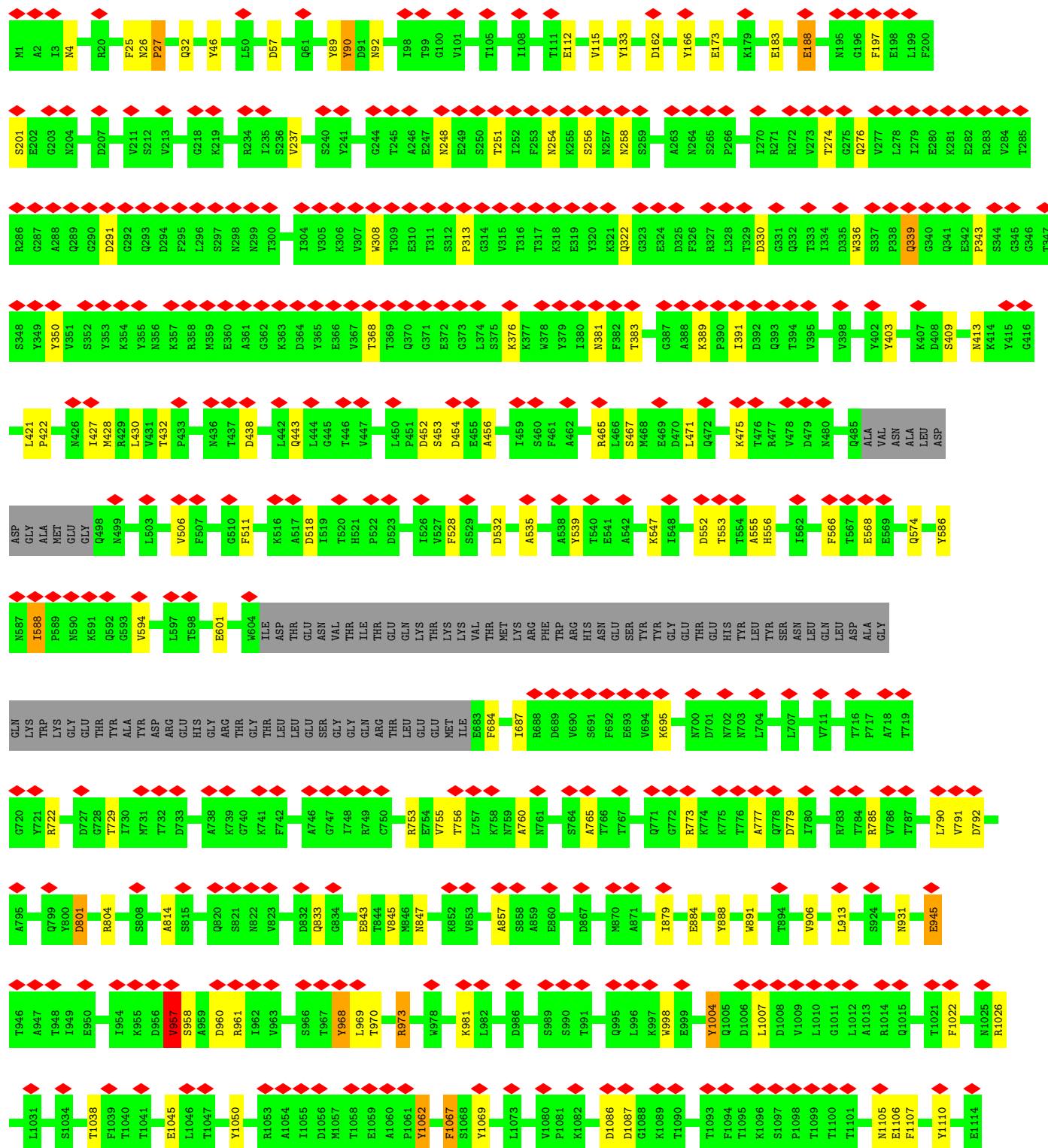
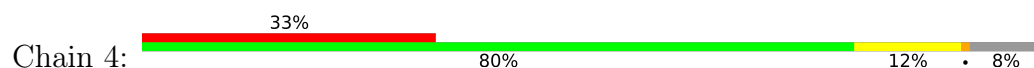
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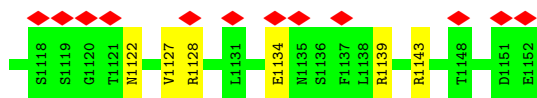


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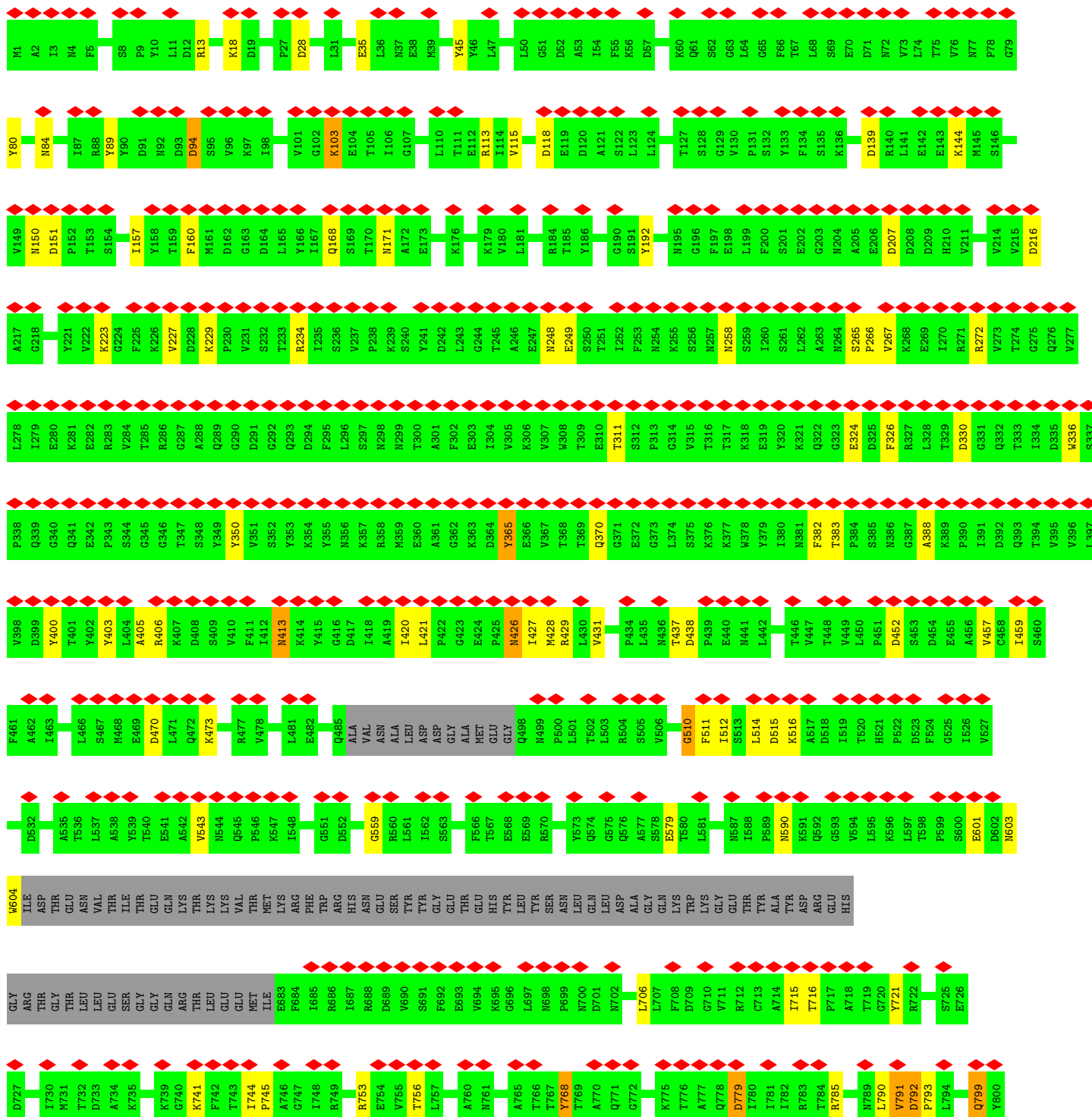
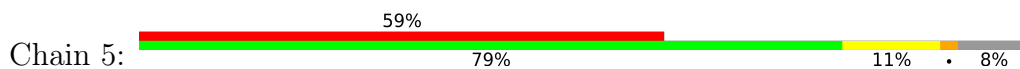


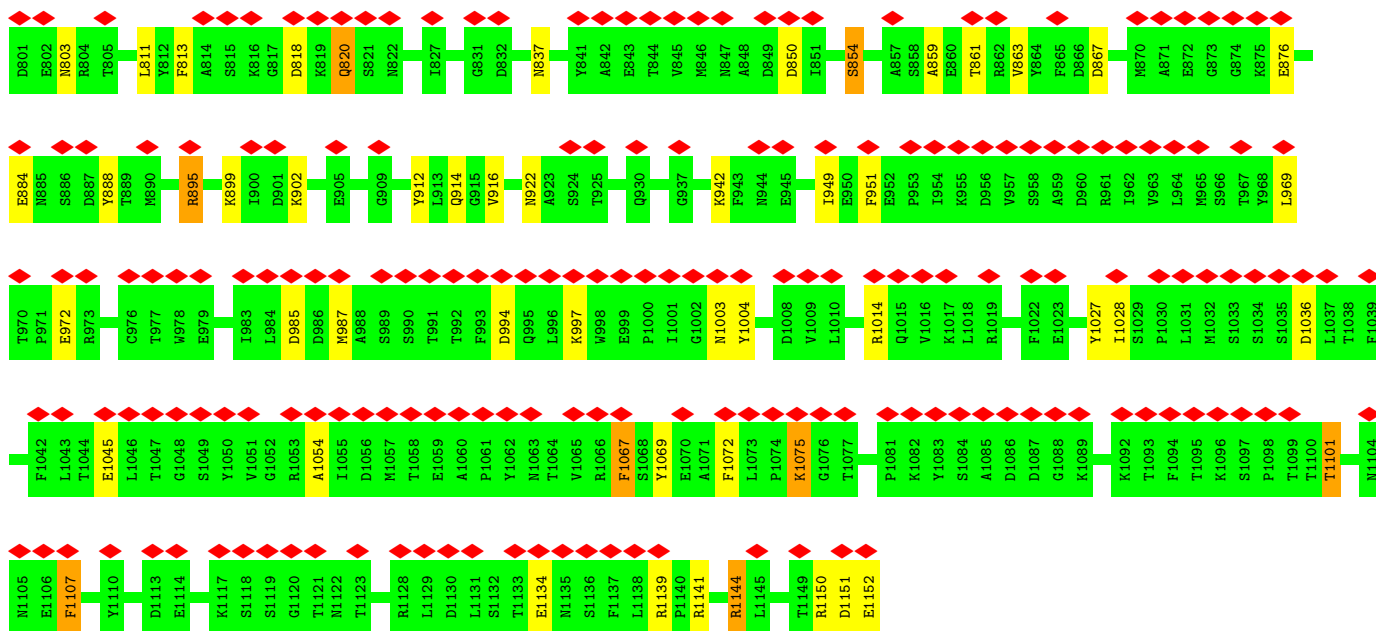
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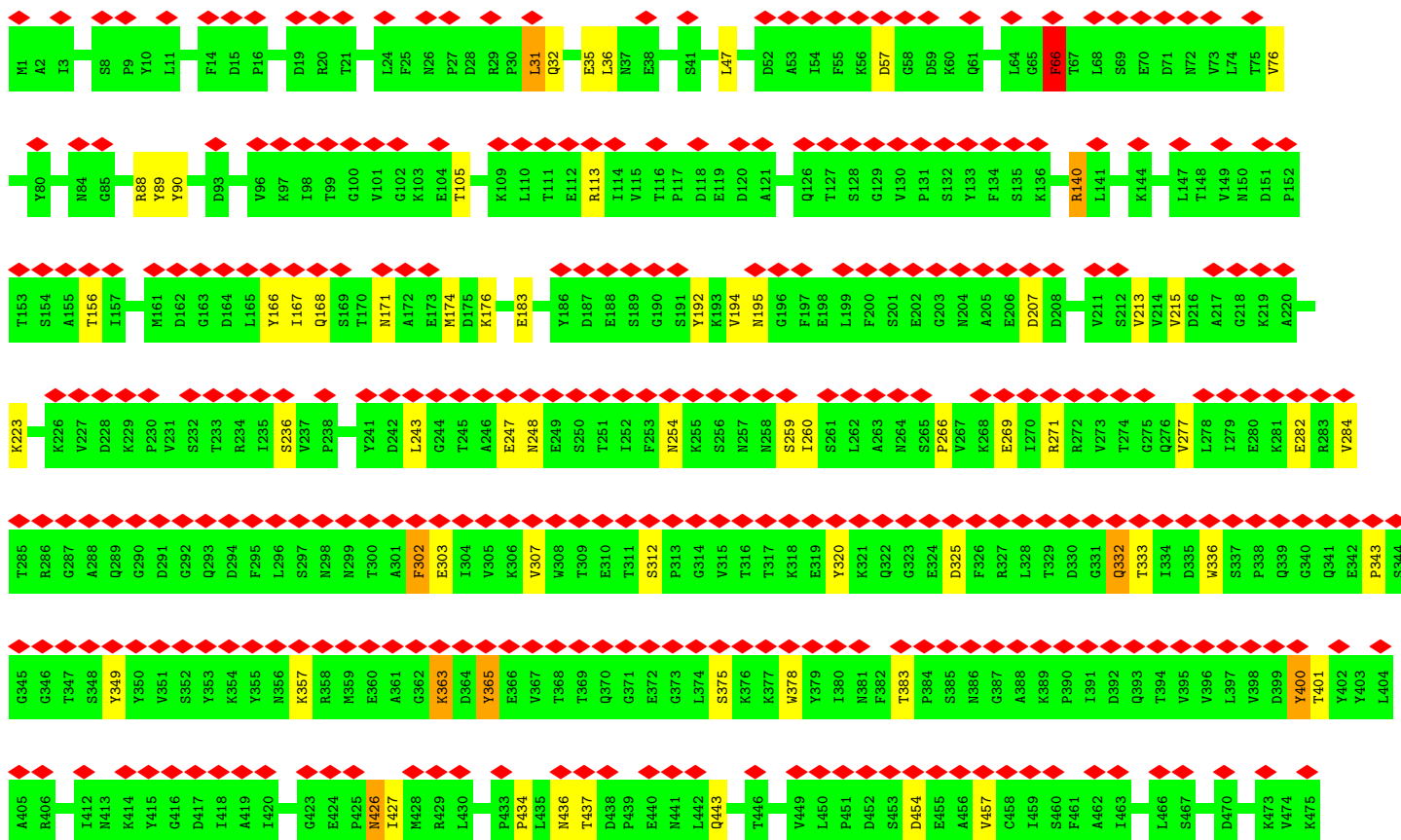
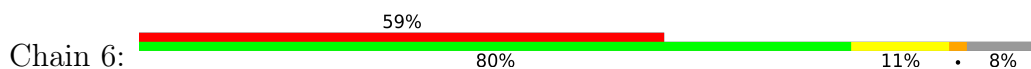


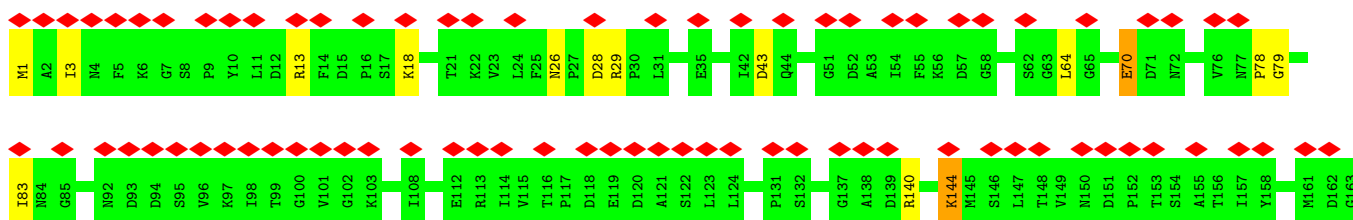
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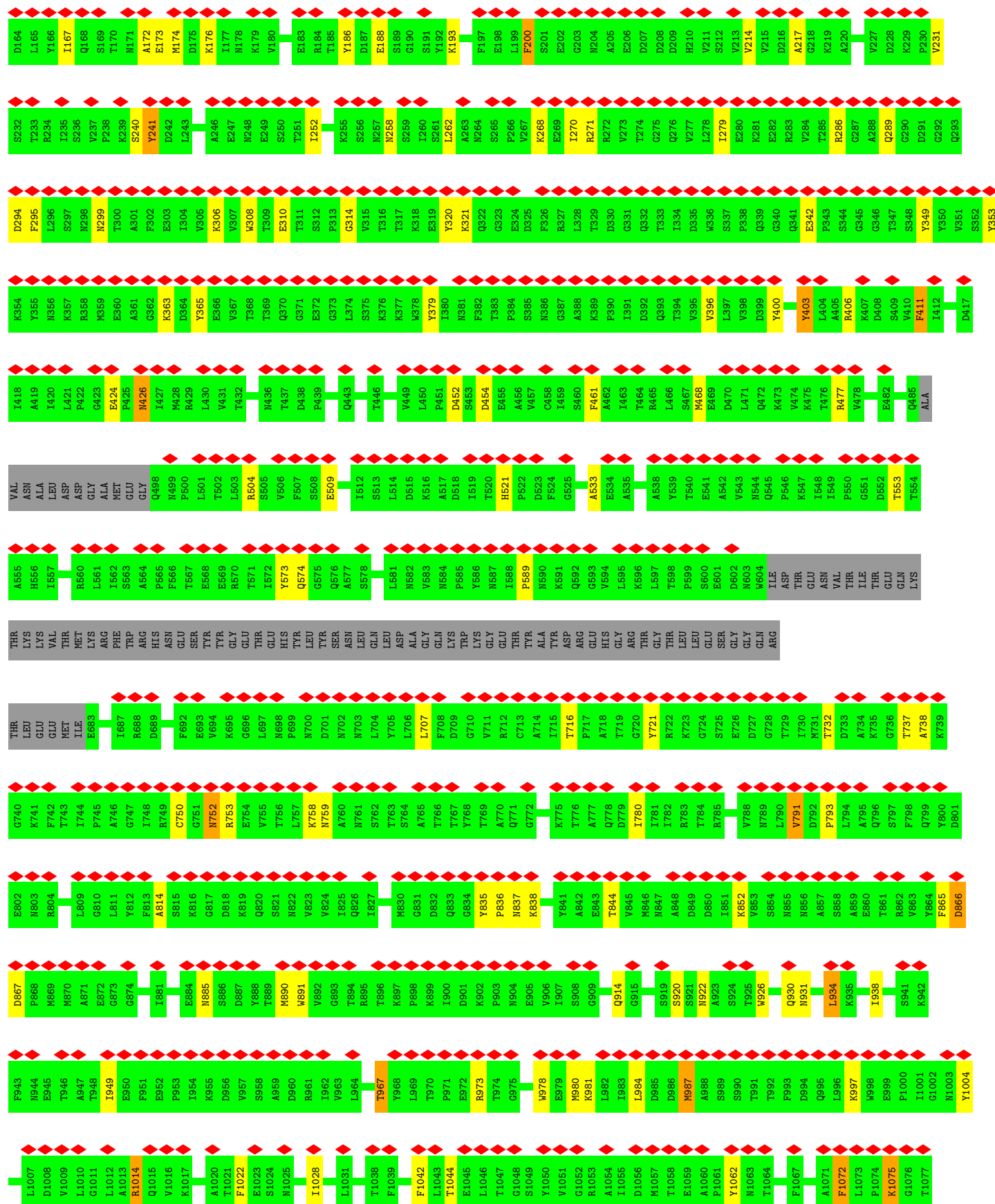




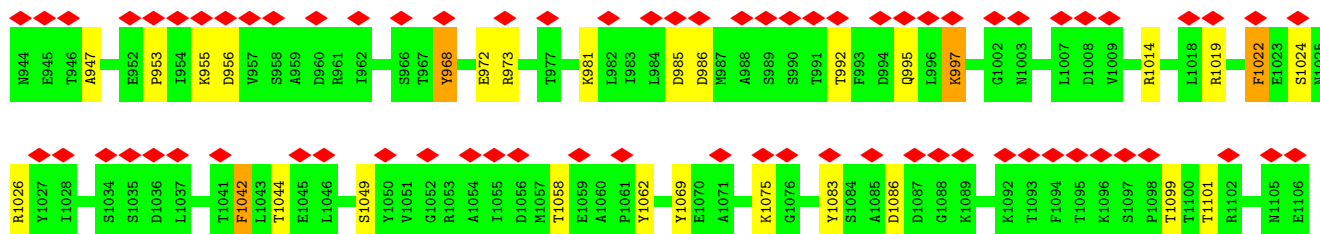
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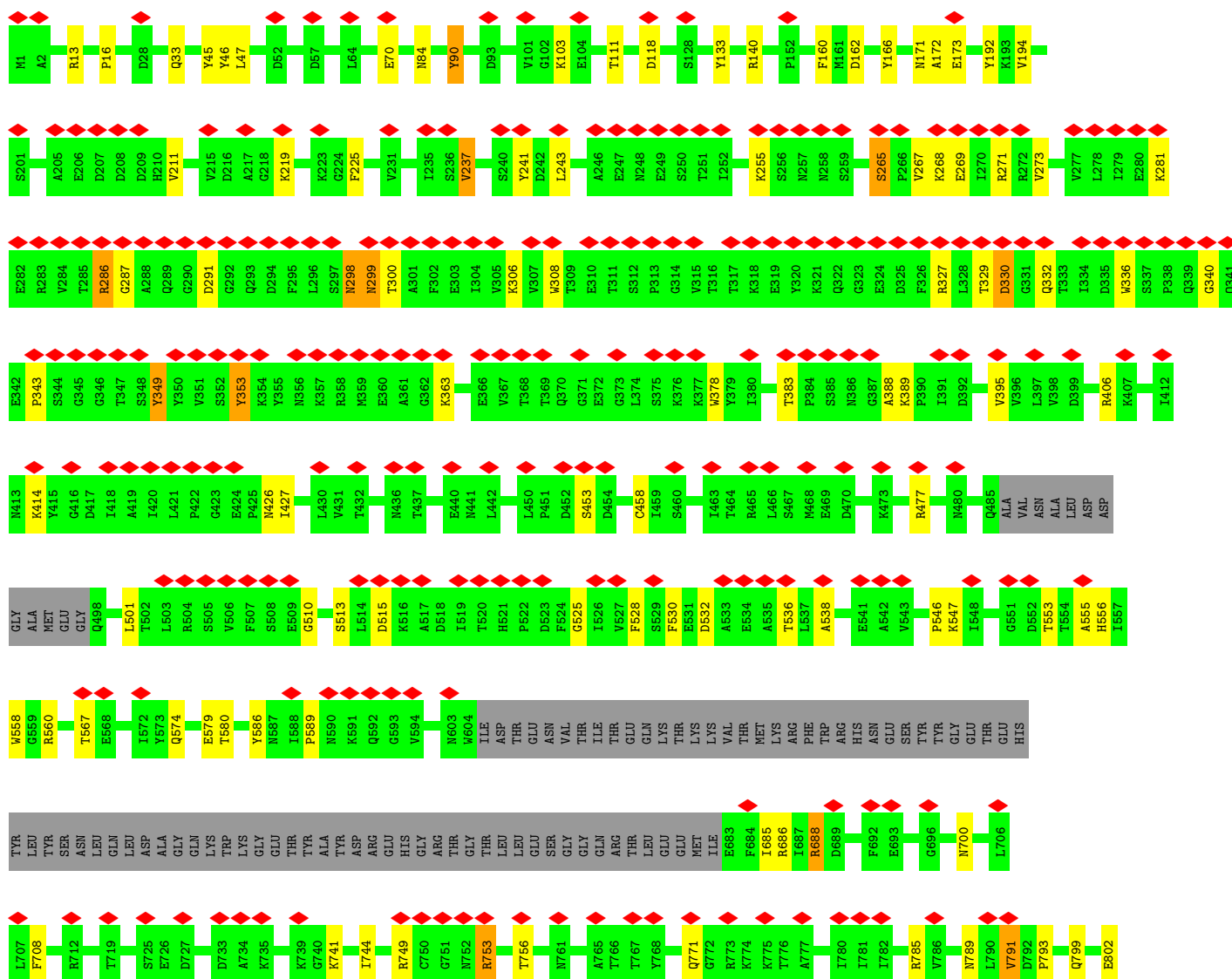
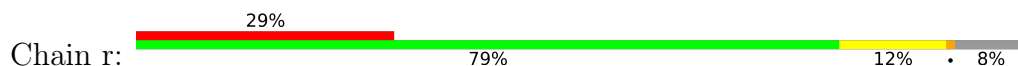


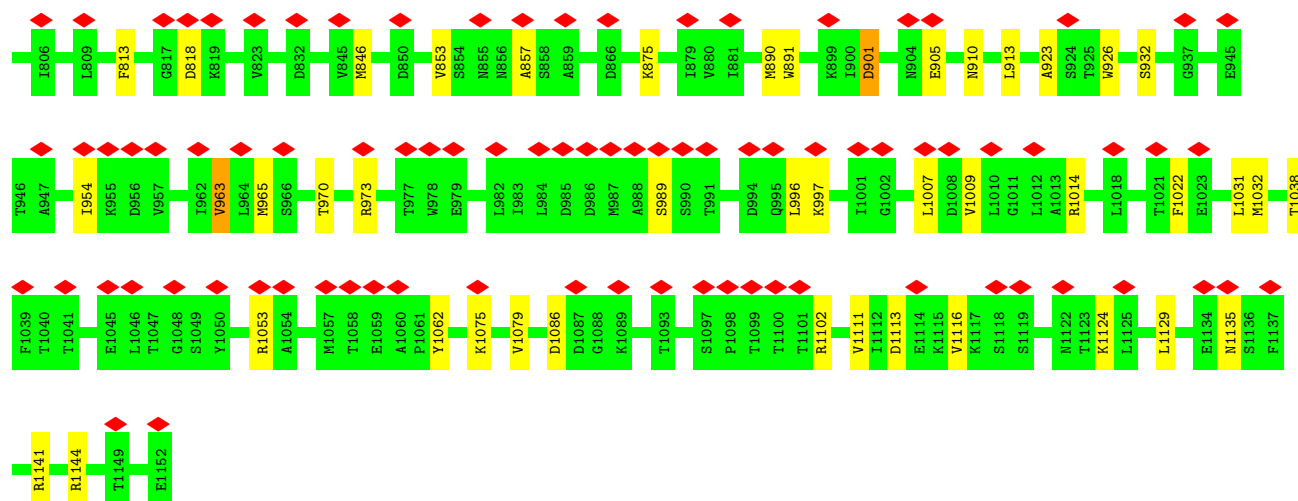




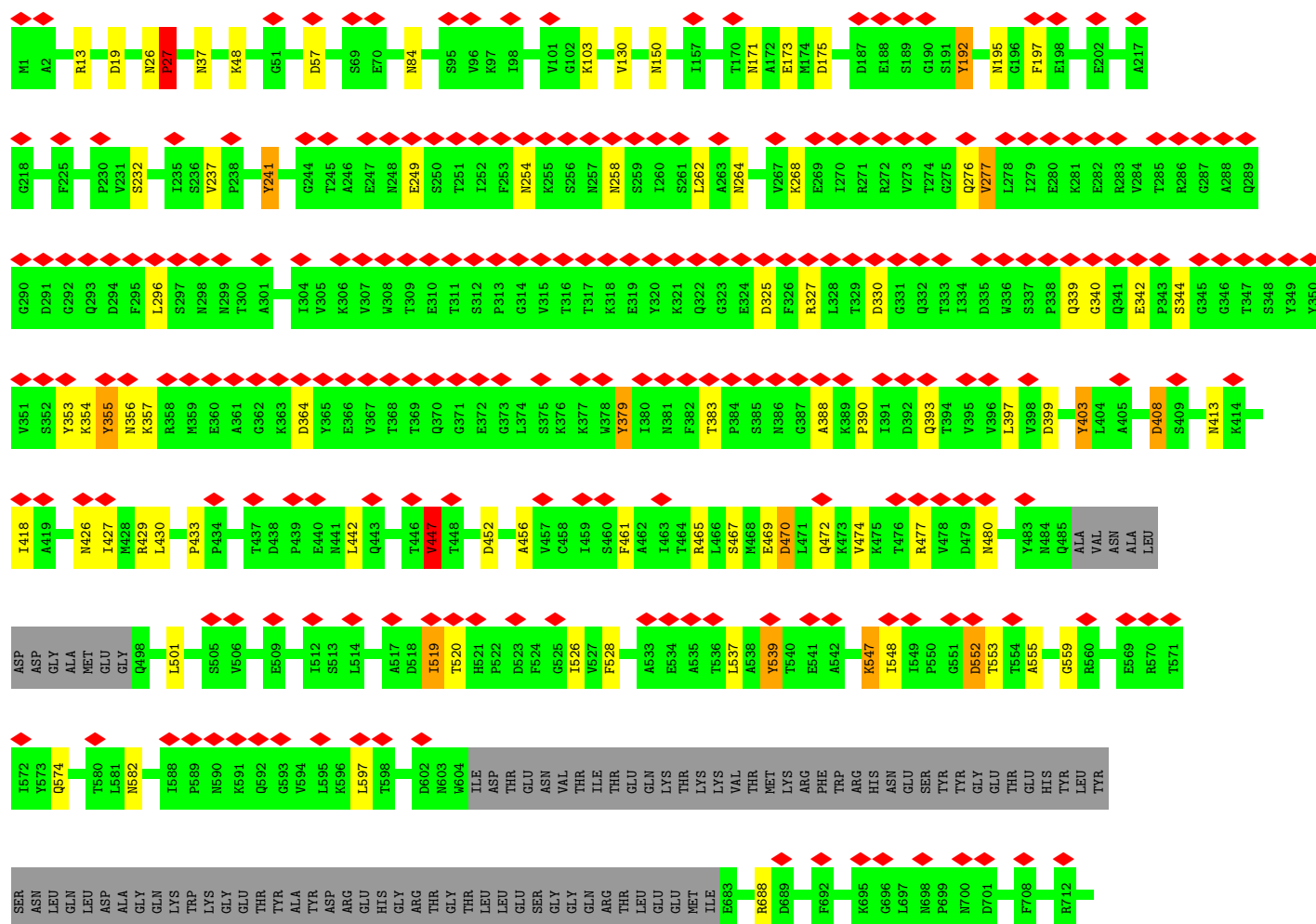
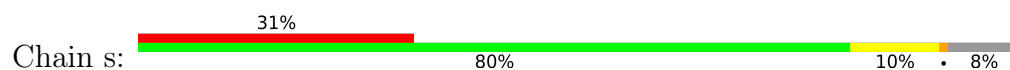


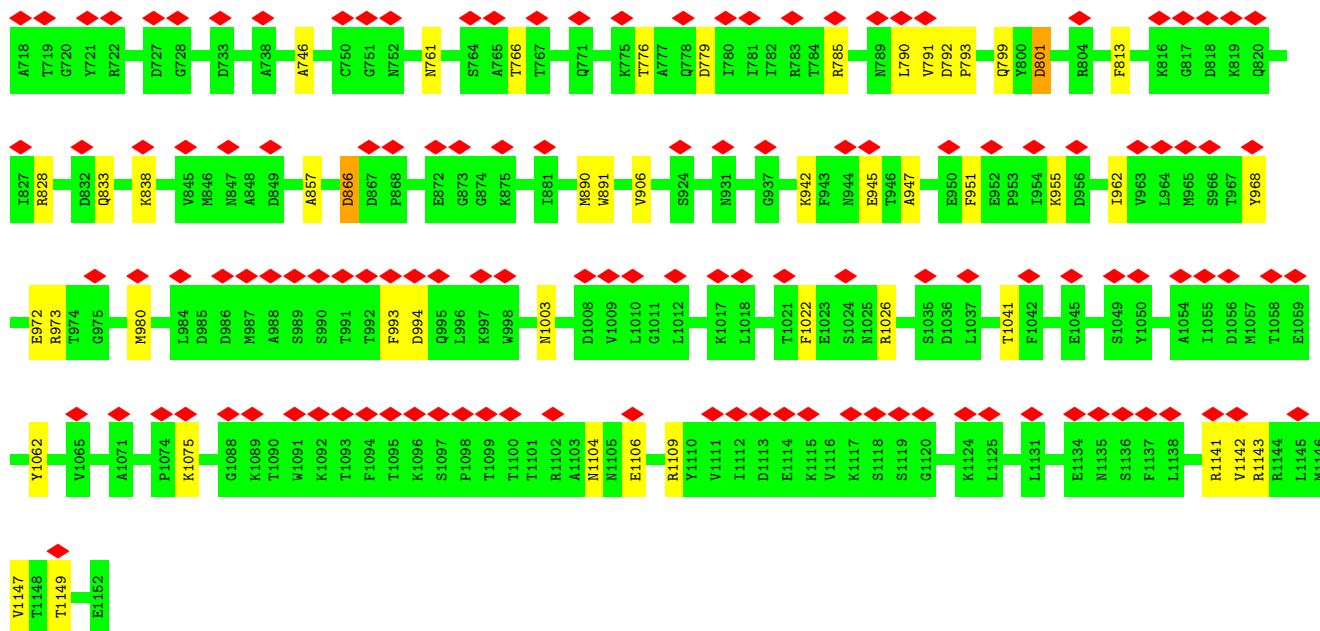
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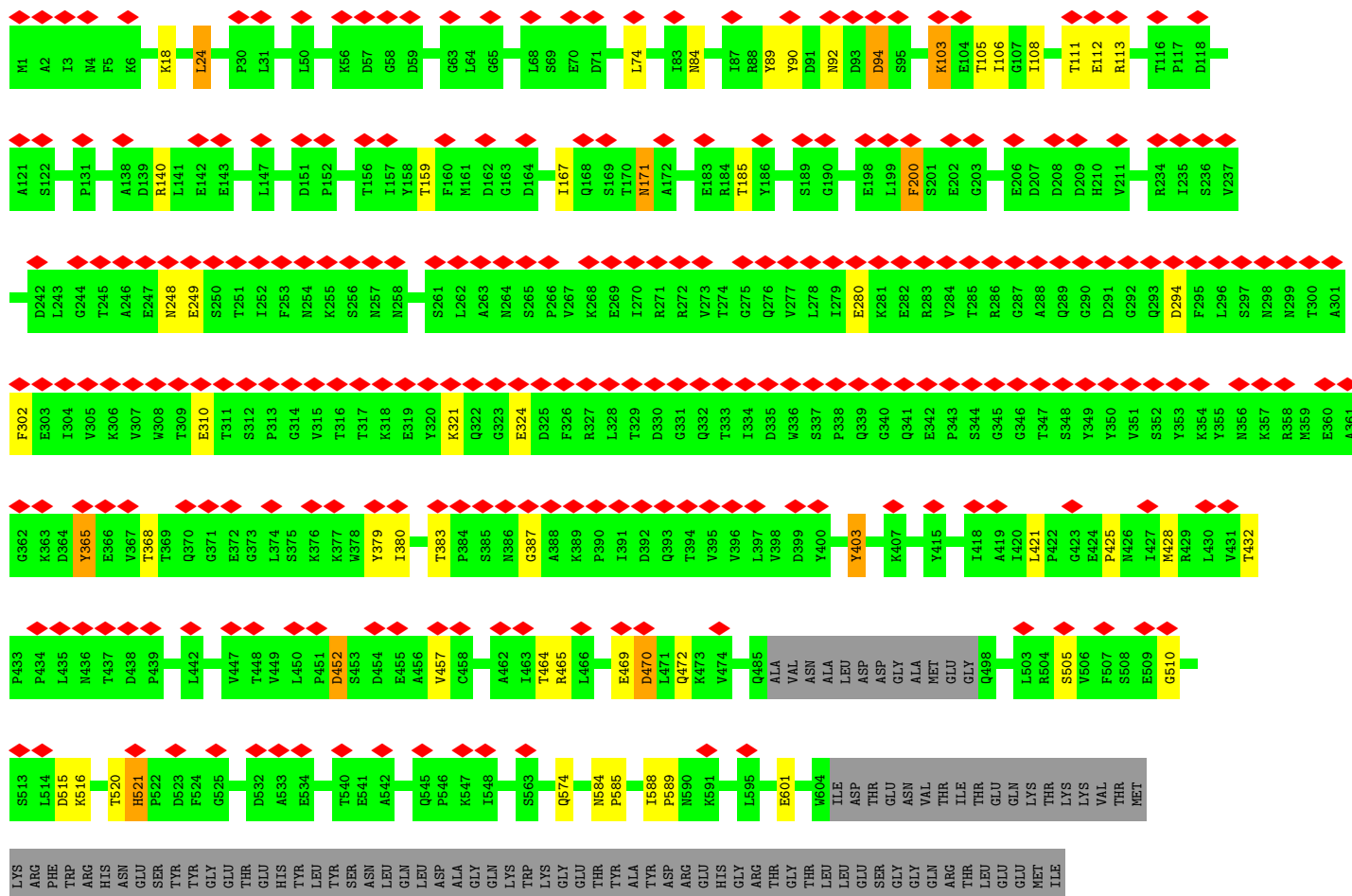
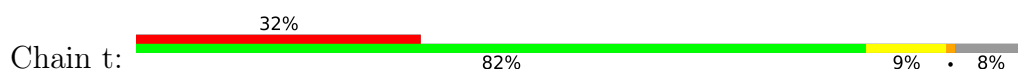


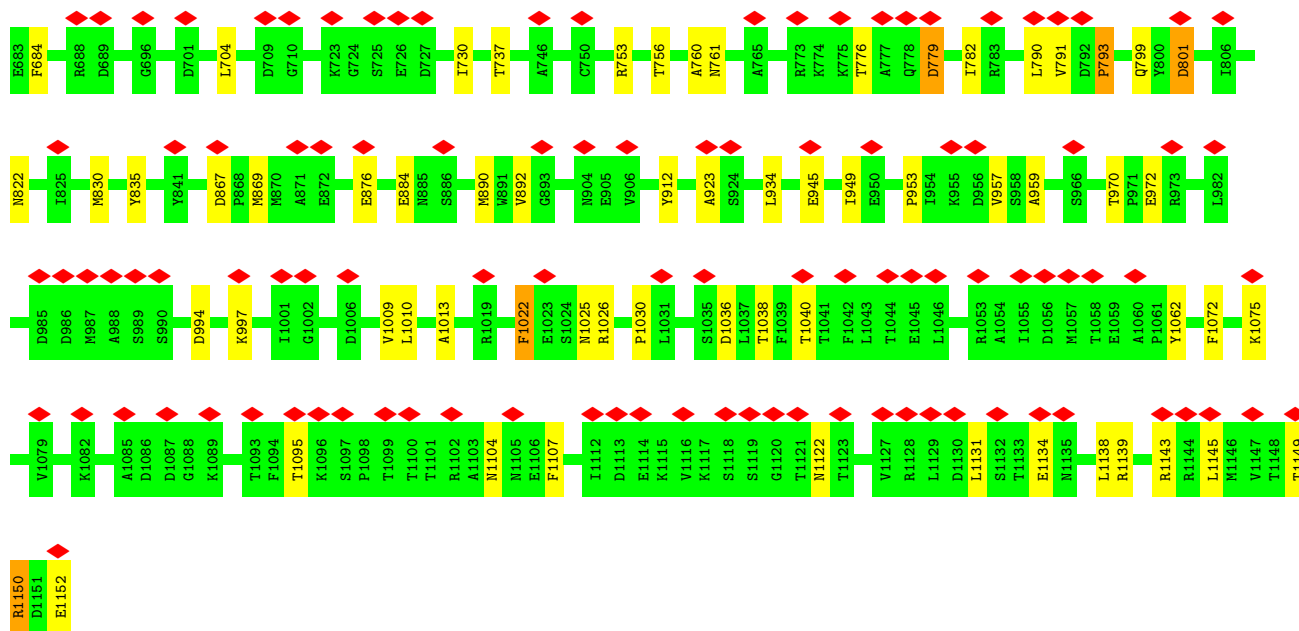
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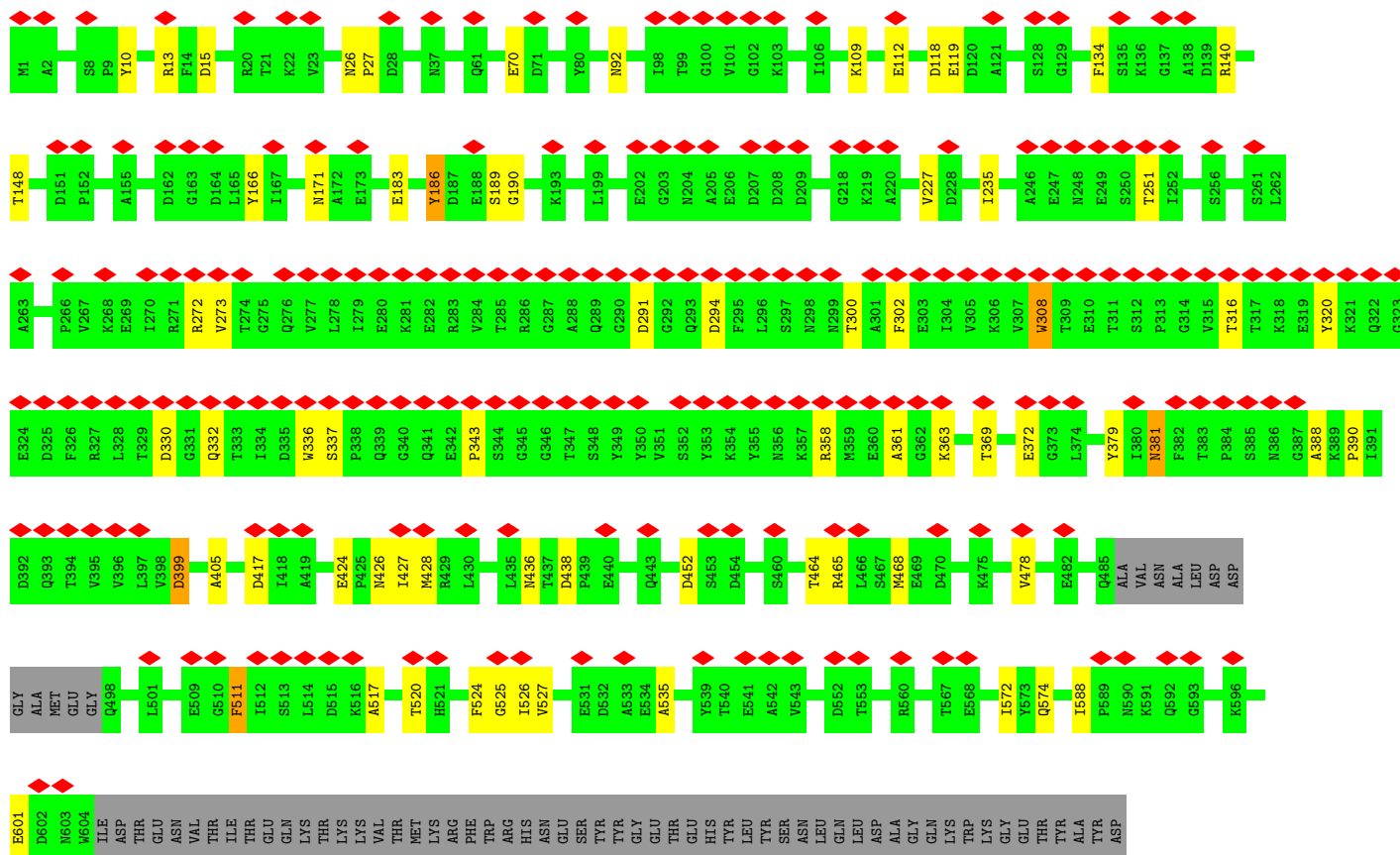
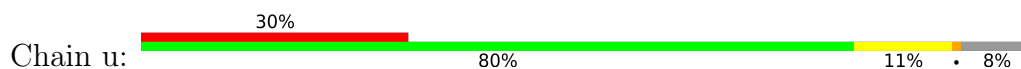


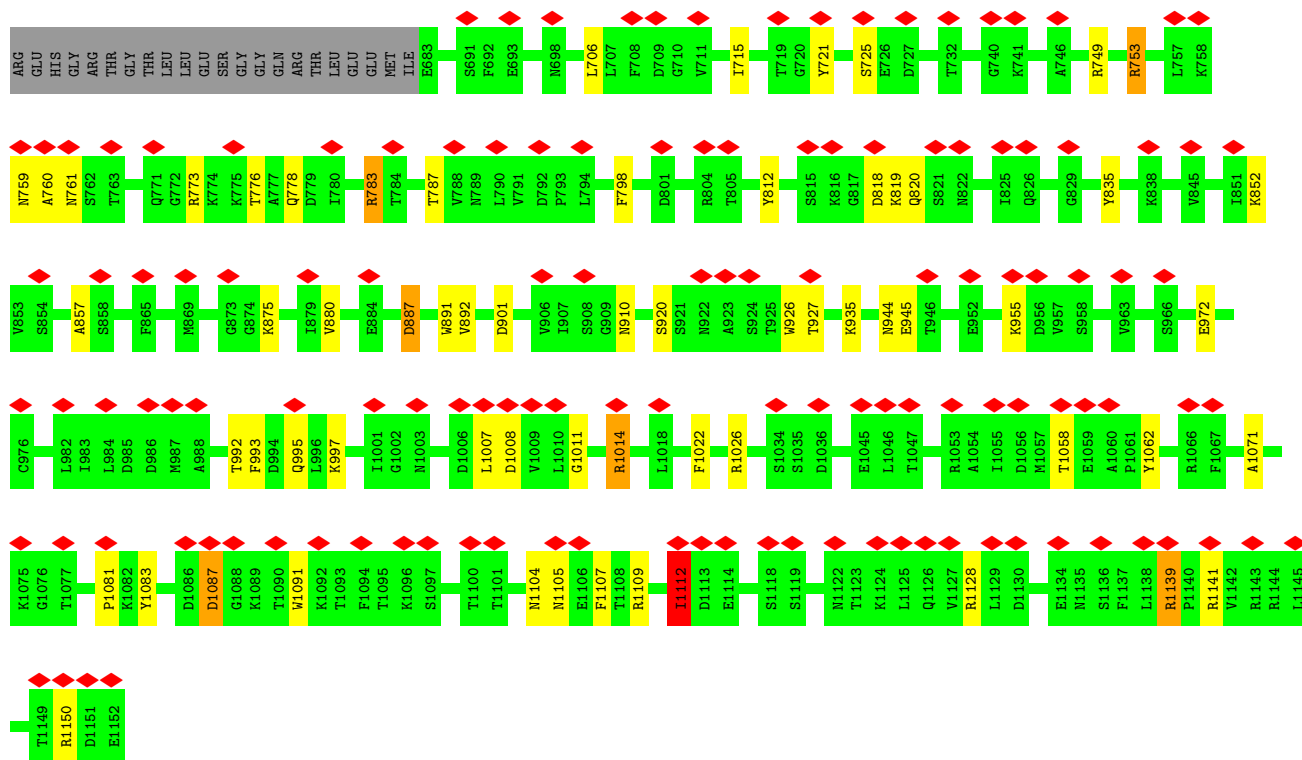
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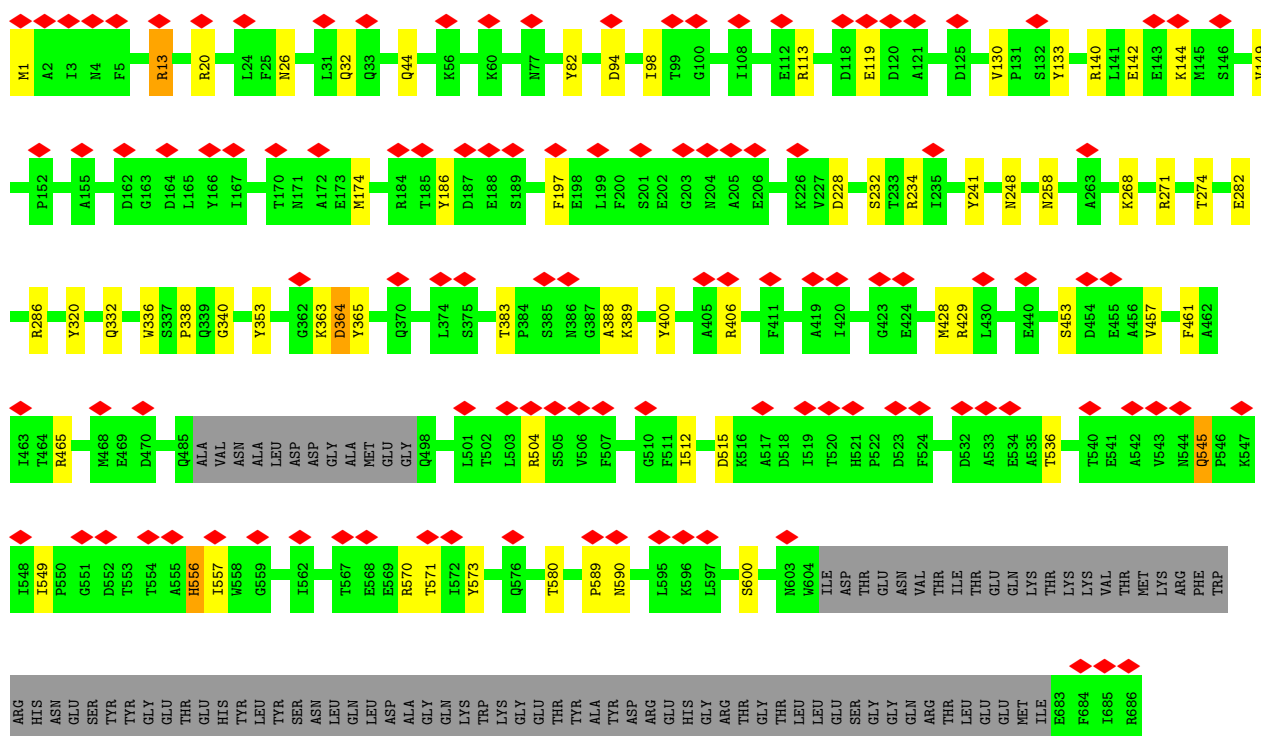
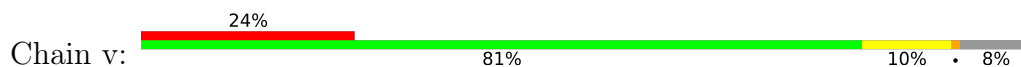


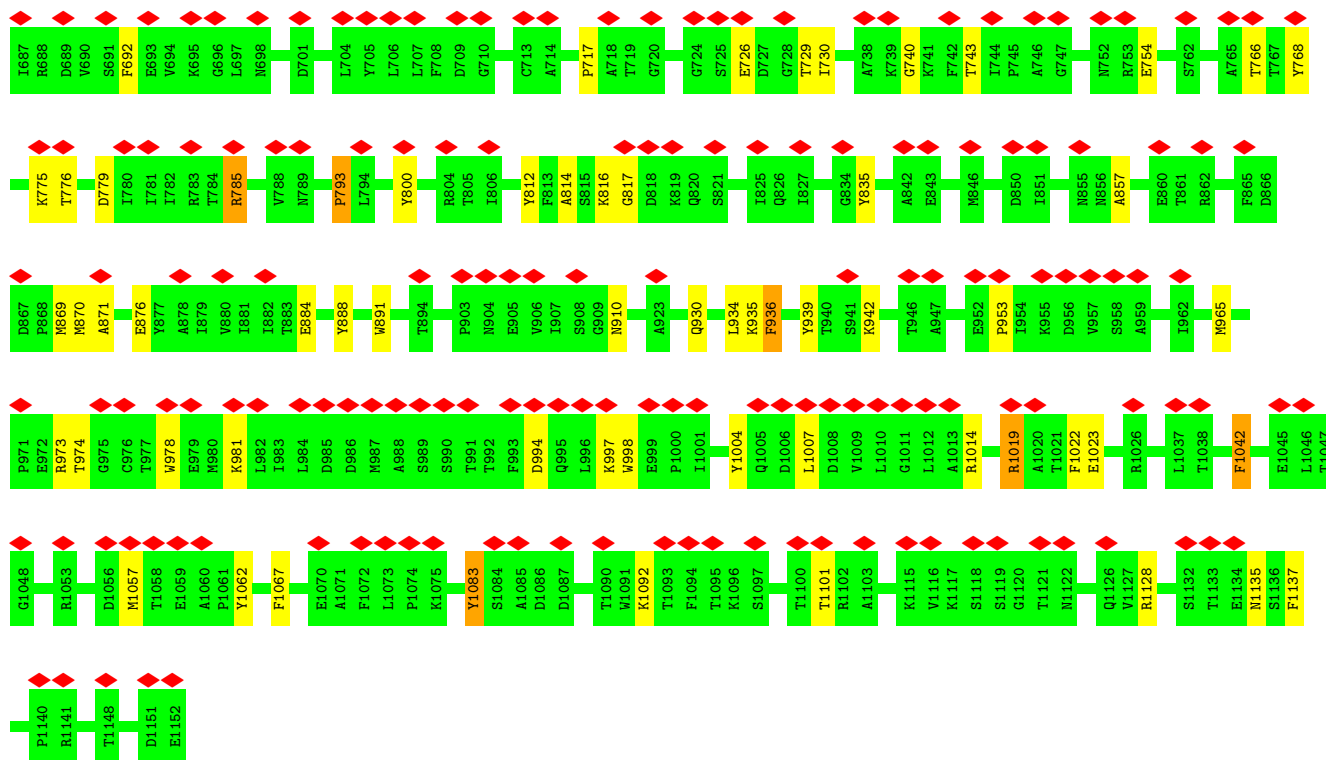
• Molecule 3: ORF65





• Molecule 3: ORF65





• Molecule 4: ORF58

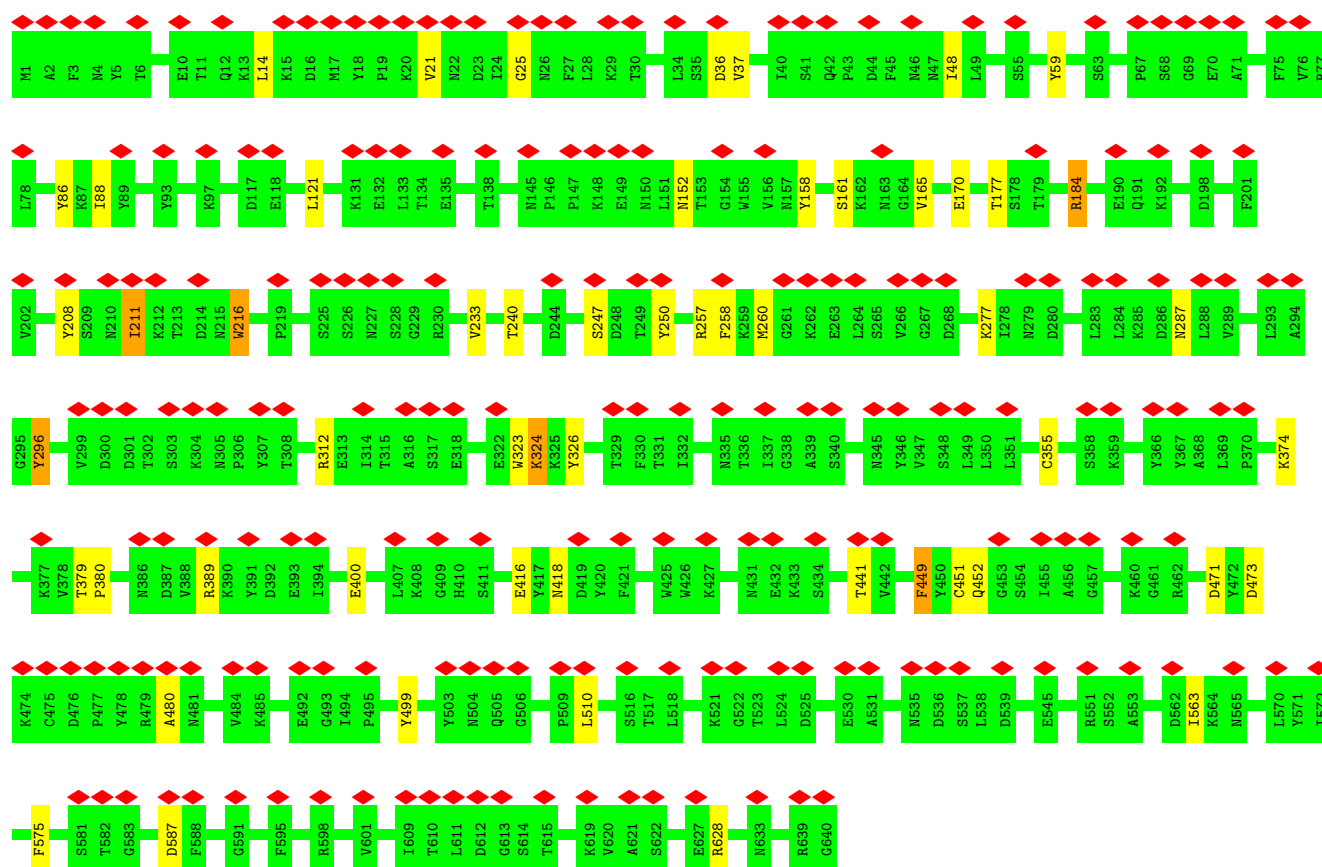
Chain A: 33% 64%

LEU	LYS	GLY	GLU	THR	SER											THR	ARG	ASP	LYS	VAL											ASN	VAL	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
LYS	ALA	GLY	ASP	ARG	LYS	THR	LYS	ASP	GLY	VAL	THR	GLY	THR	VAL	ASP	GLY	THR	ASP	GLY	THR	VAL	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR

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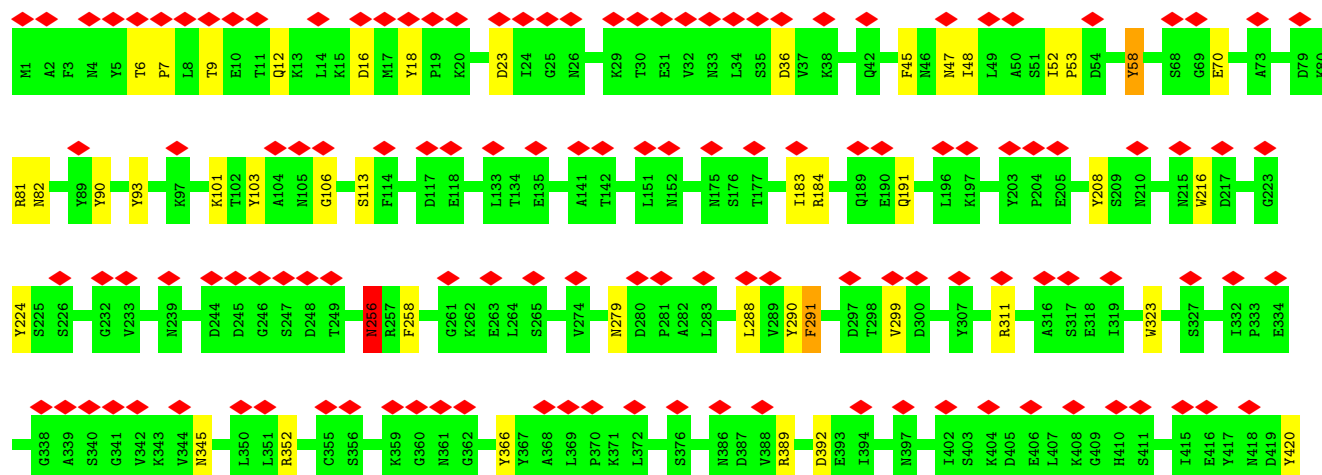
• Molecule 5: CBM-cenC domain-containing protein

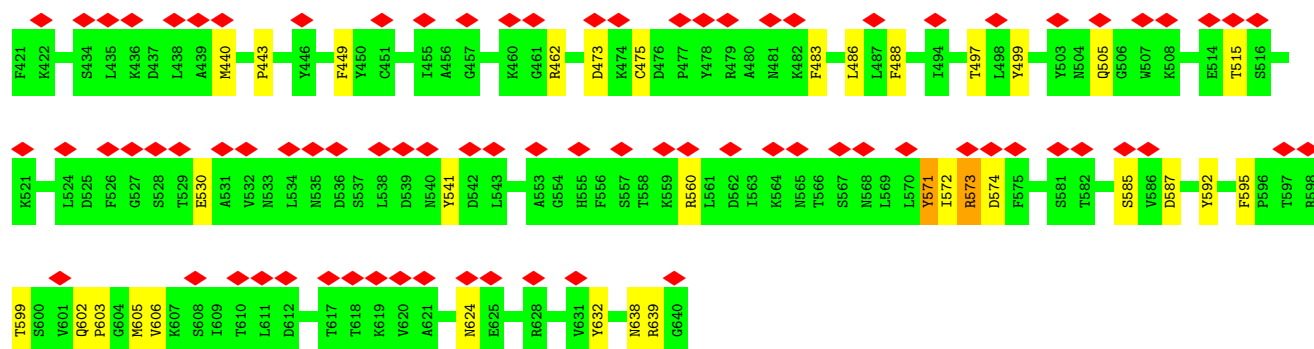
Chain AA: 33% 91% 8% .



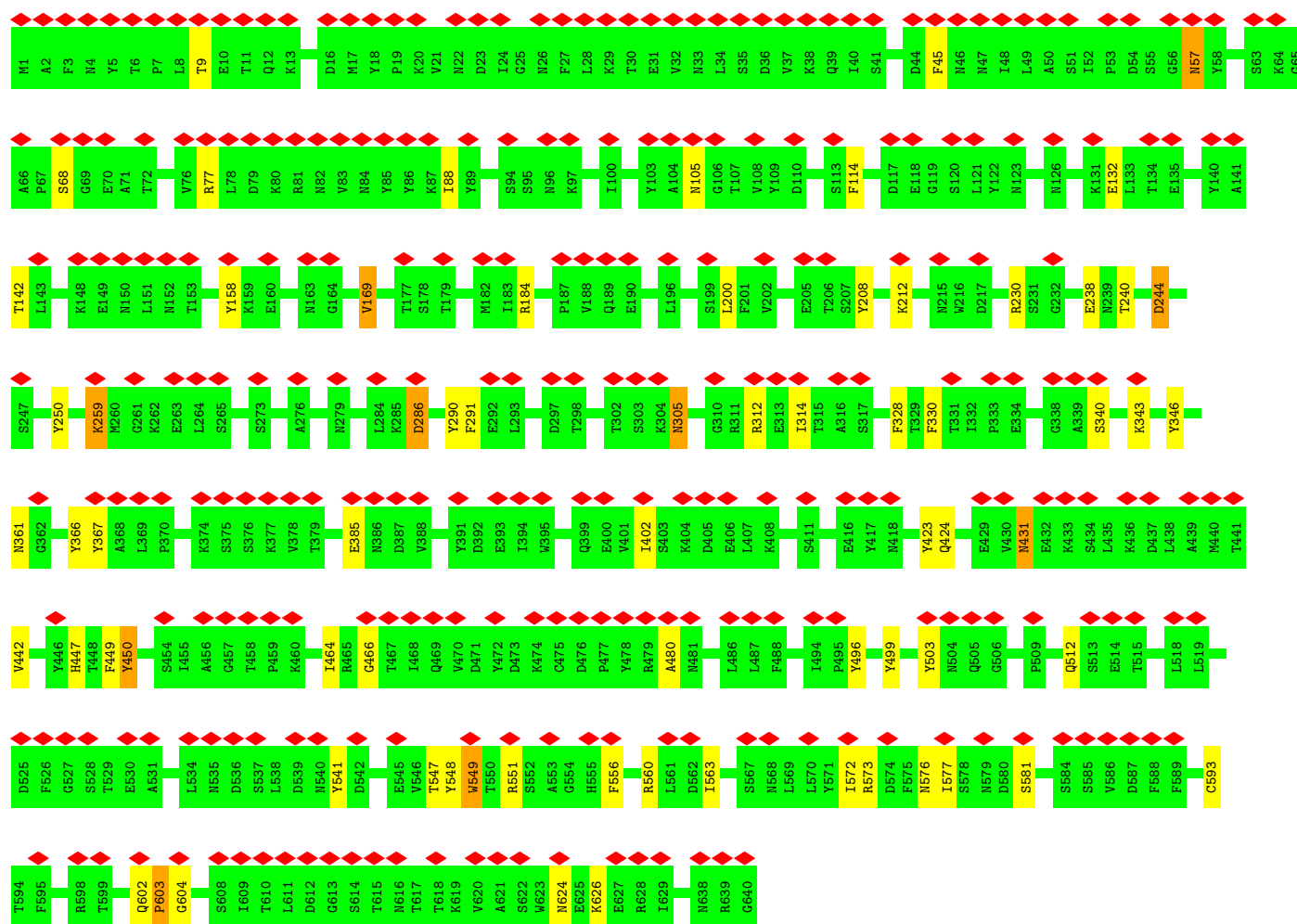
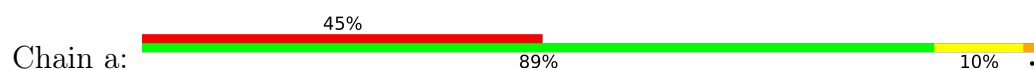
• Molecule 5: CBM-cenC domain-containing protein

Chain AB: 33% 88% 11% .

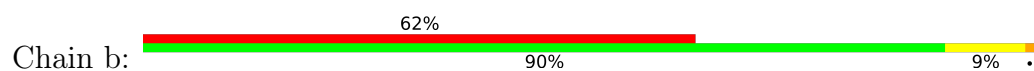


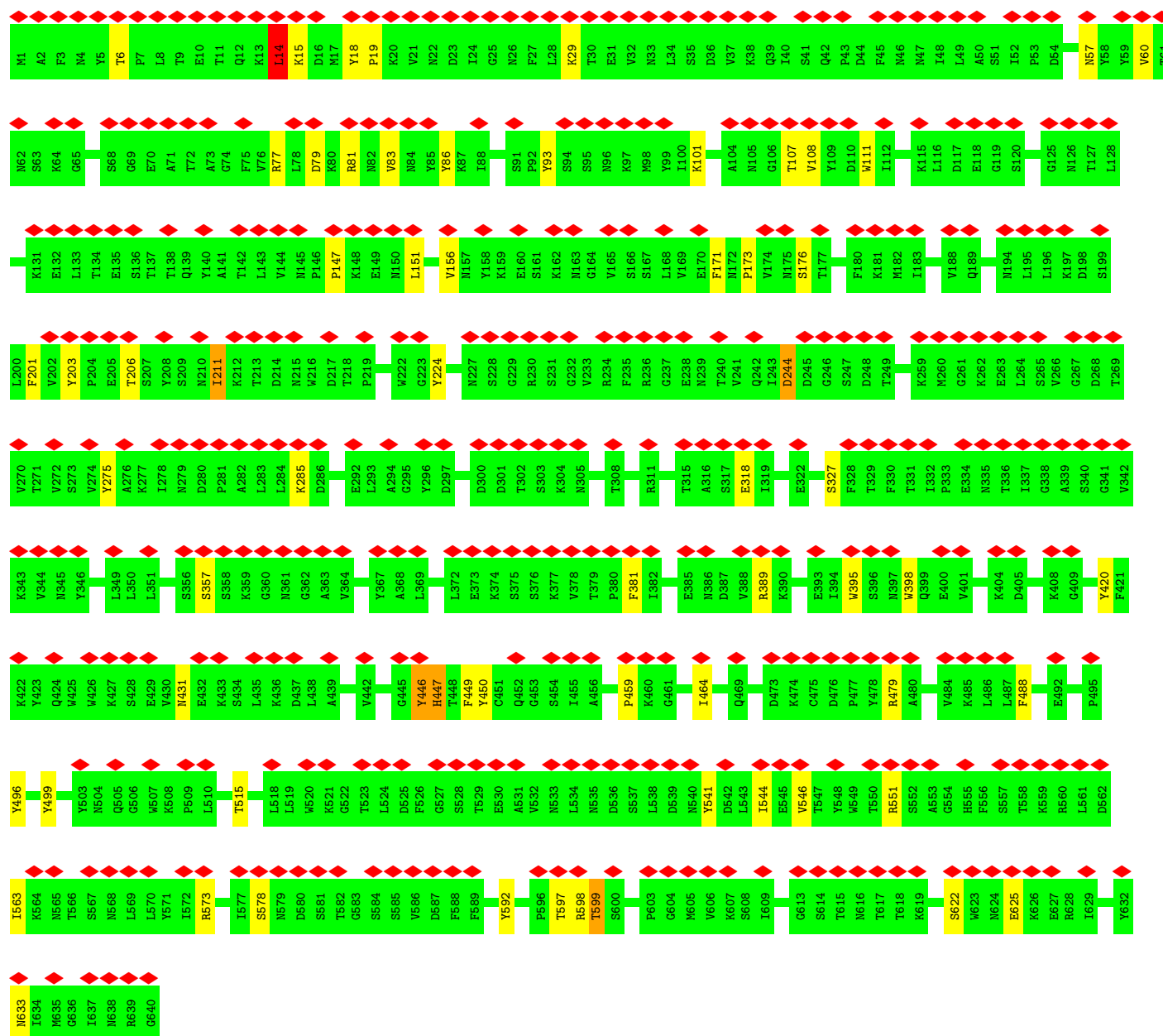


• Molecule 5: CBM-cenC domain-containing protein

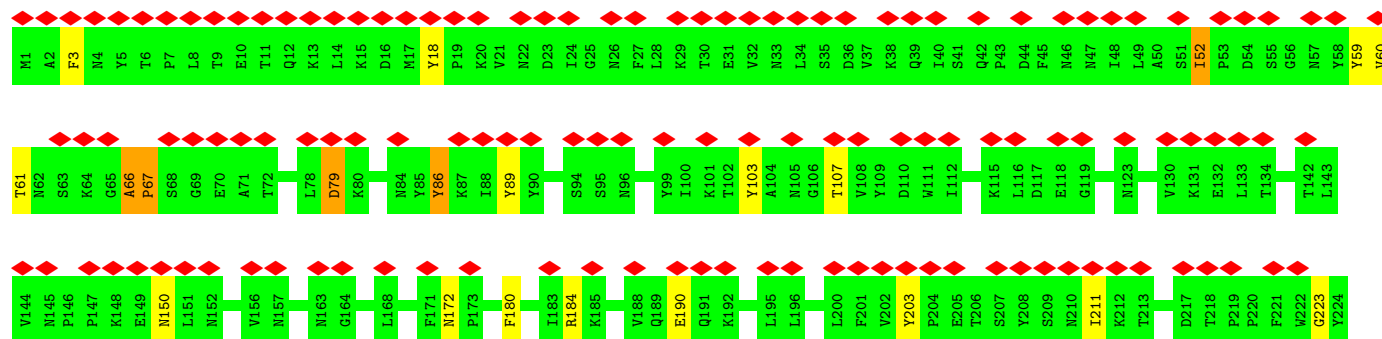
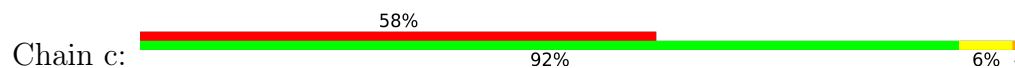


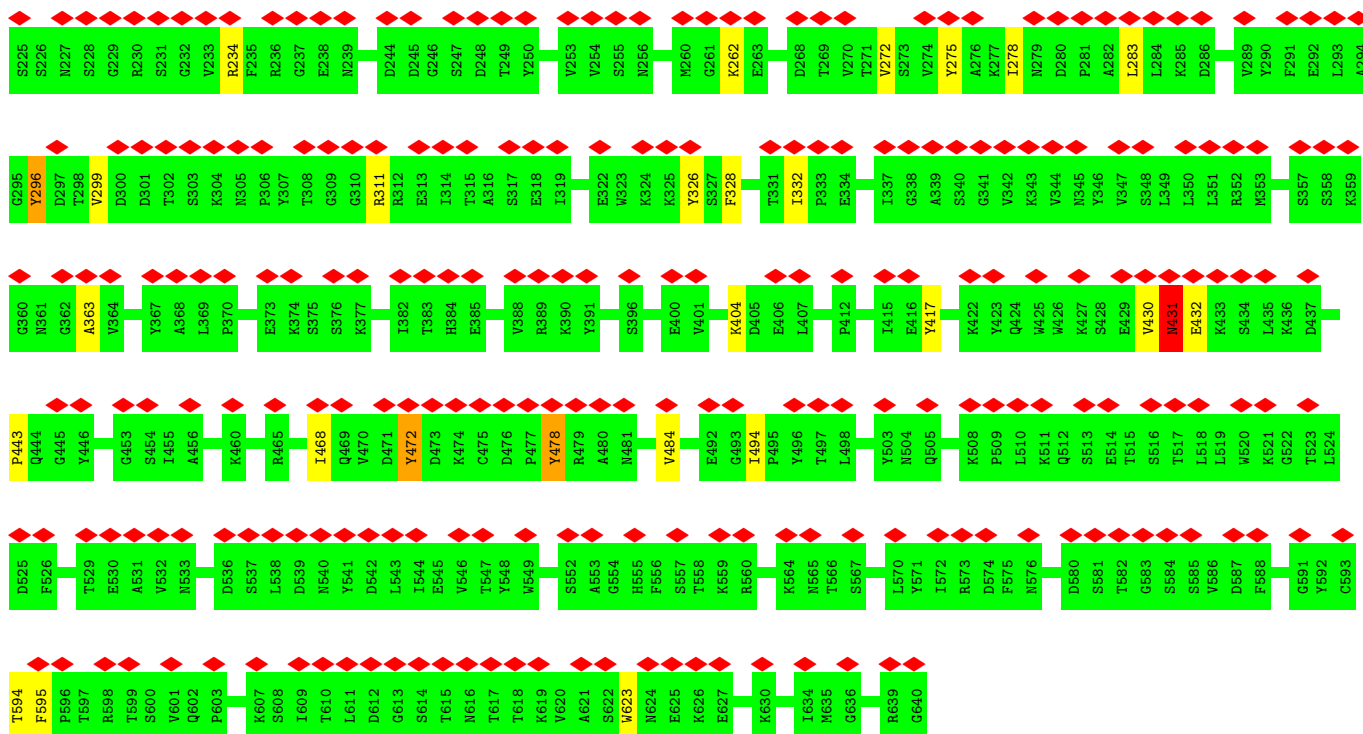
• Molecule 5: CBM-cenC domain-containing protein



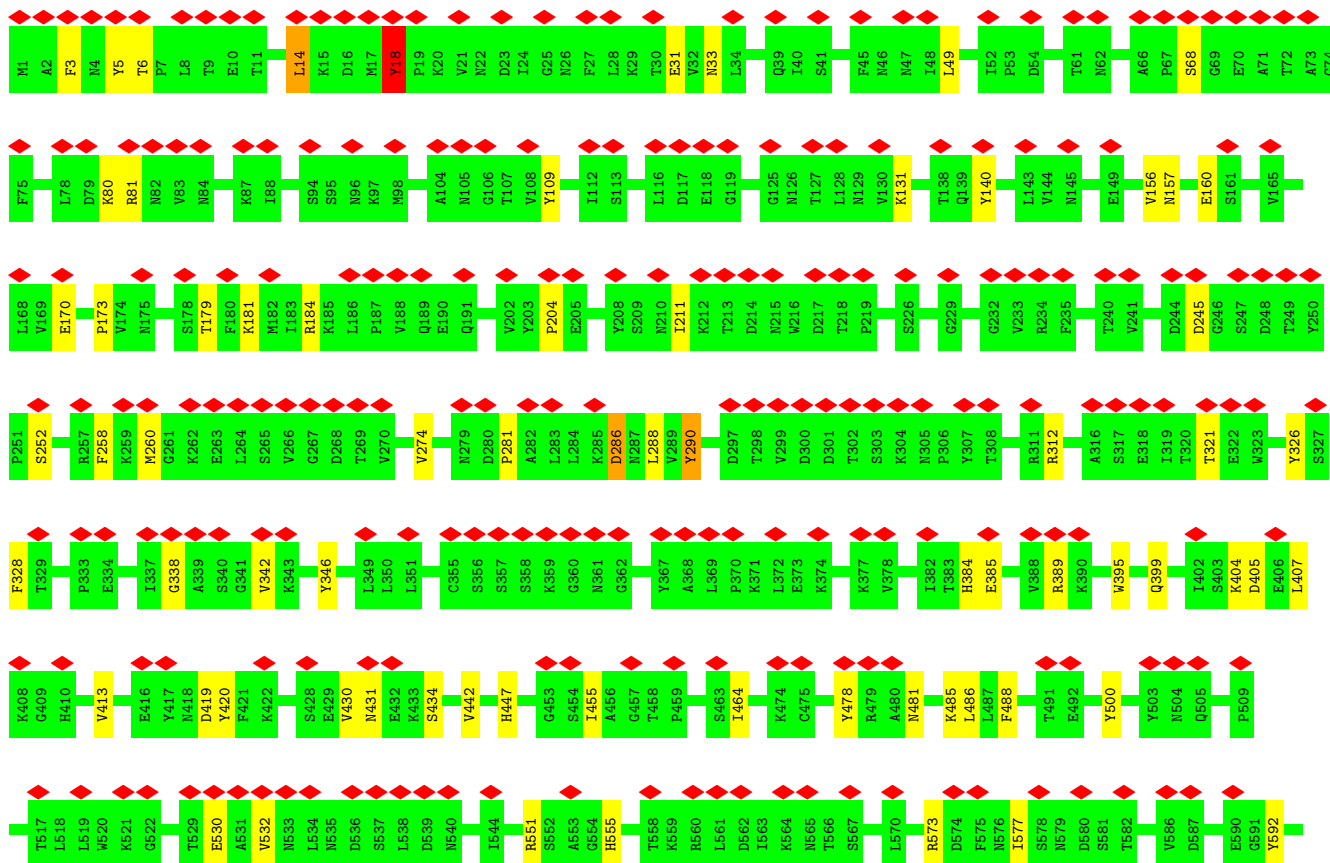
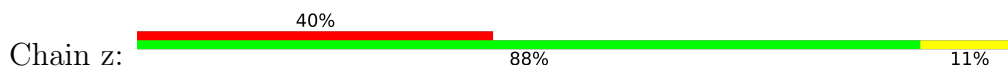


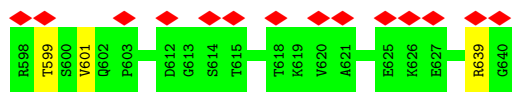
• Molecule 5: CBM-cenC domain-containing protein



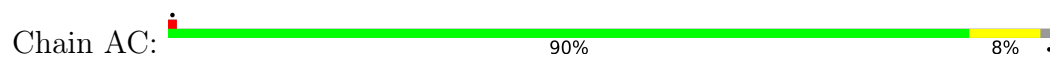


• Molecule 5: CBM-cenC domain-containing protein

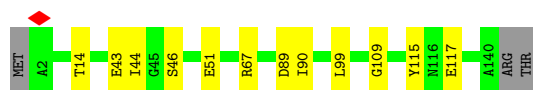




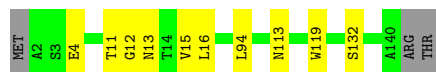
- Molecule 6: ORF50



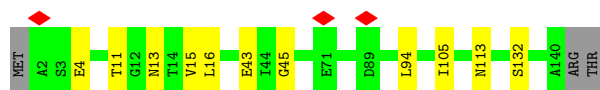
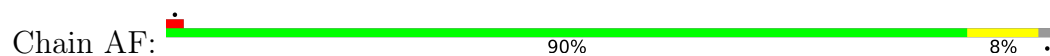
- Molecule 6: ORF50



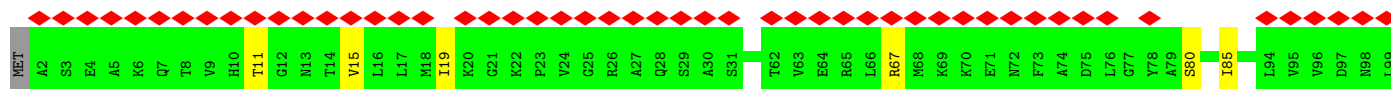
- Molecule 6: ORF50



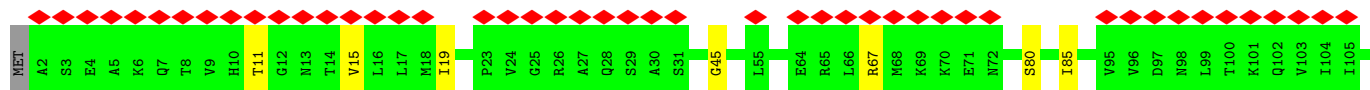
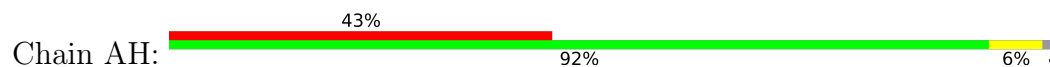
- Molecule 6: ORF50

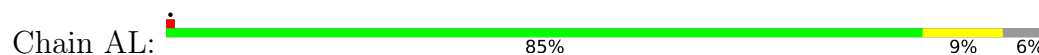


- Molecule 6: ORF50

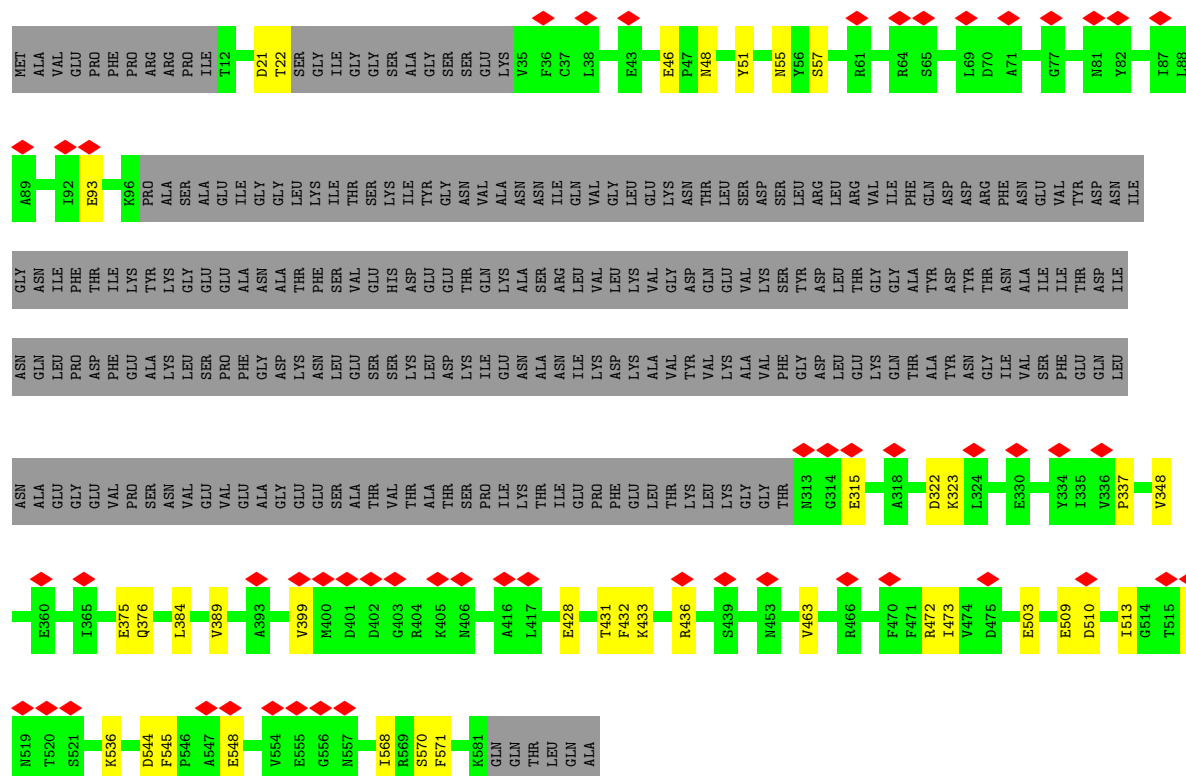


- Molecule 6: ORF50

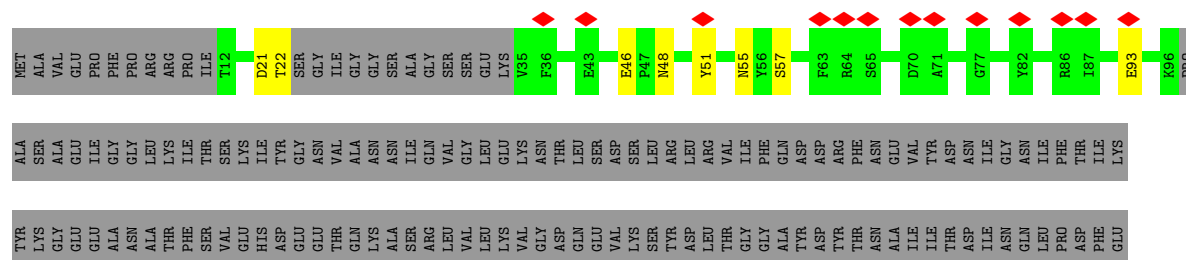


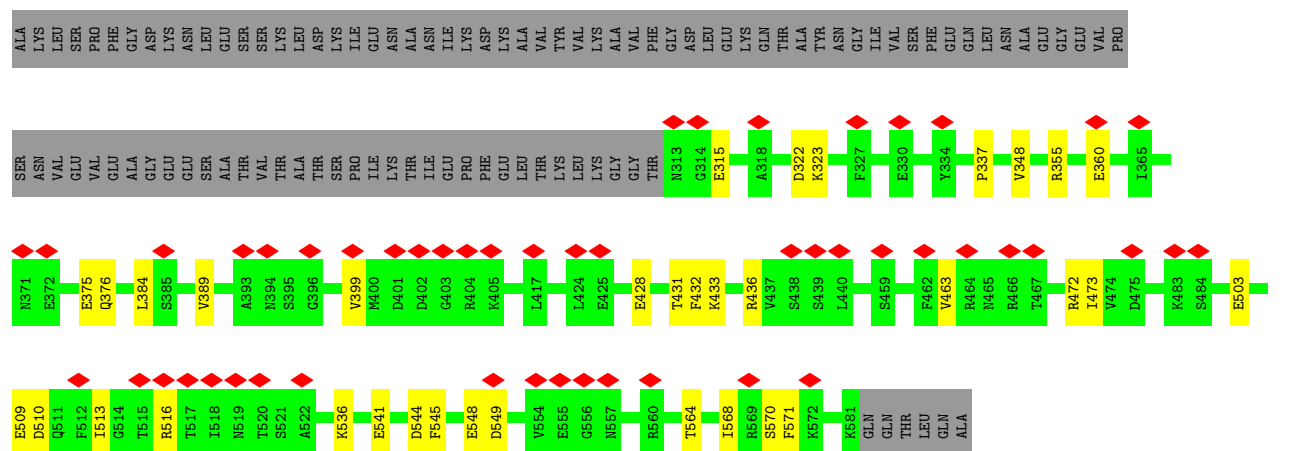


- Molecule 7: ORF49

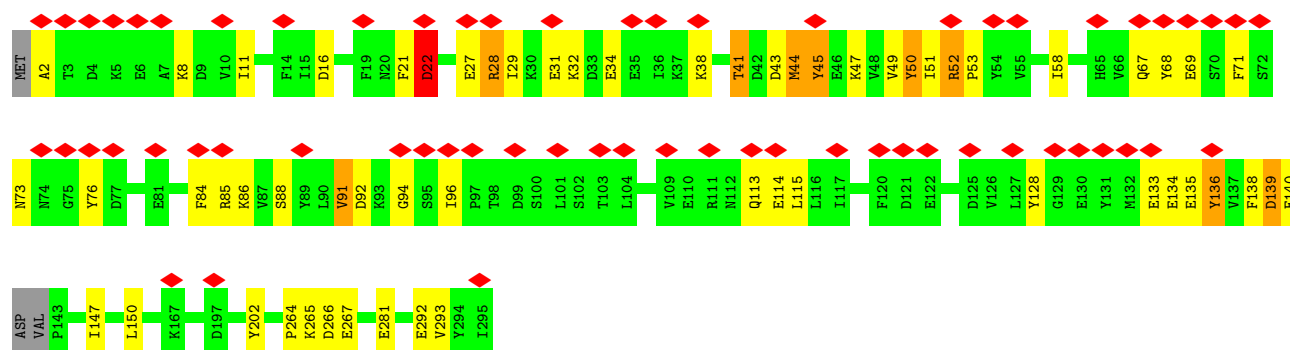
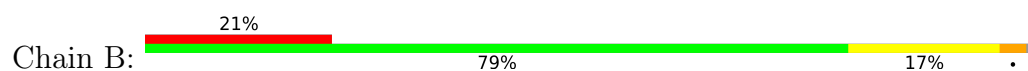


- Molecule 7: ORF49

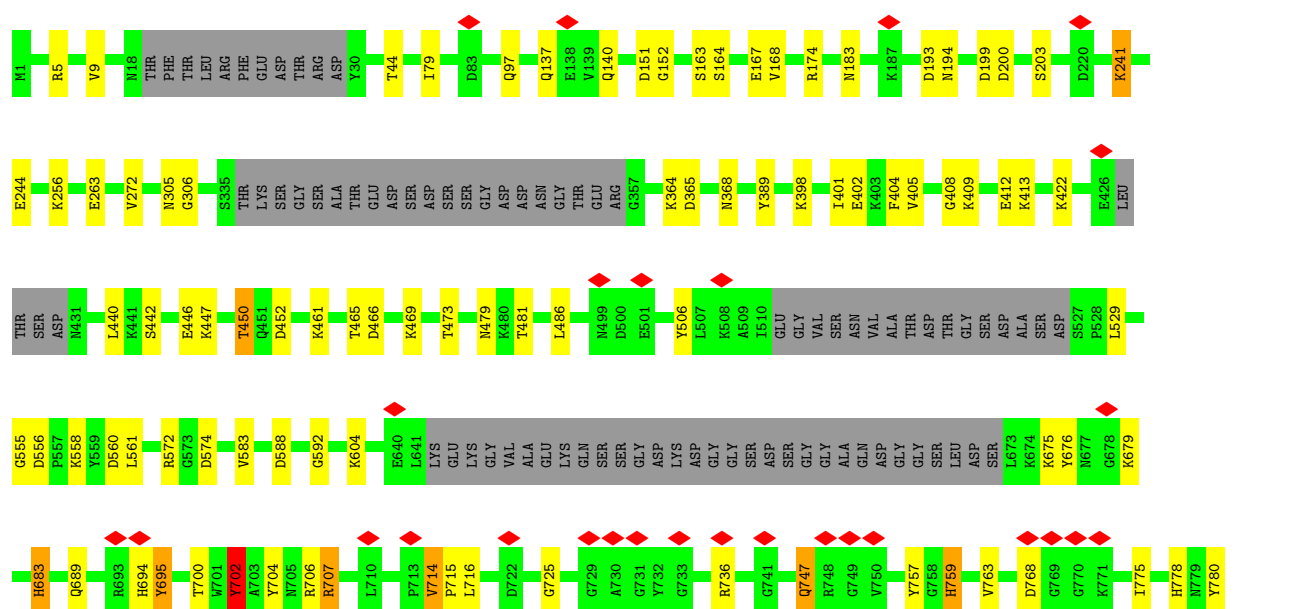
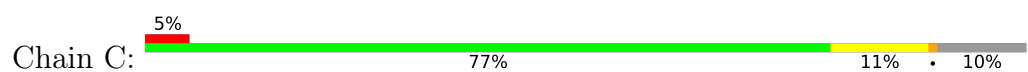


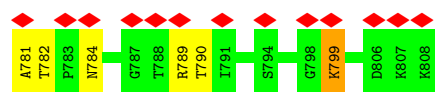


• Molecule 8: ORF57

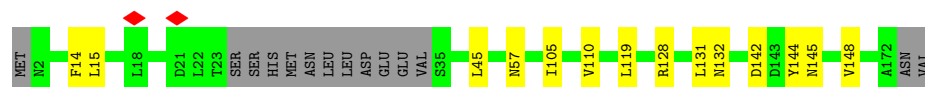
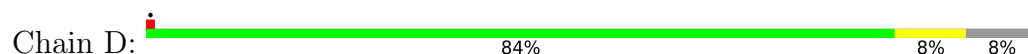


• Molecule 9: ORF56

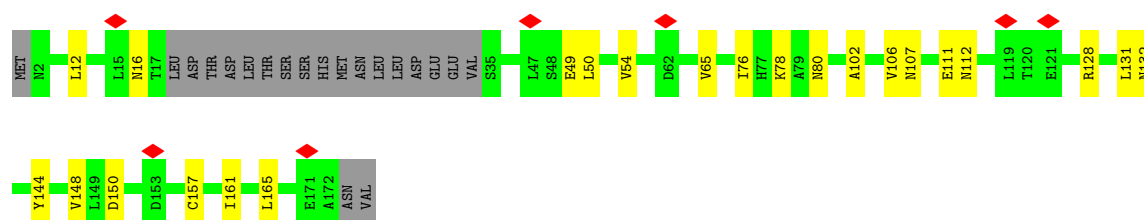
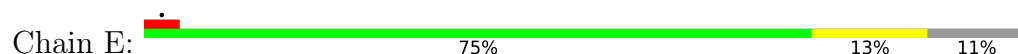




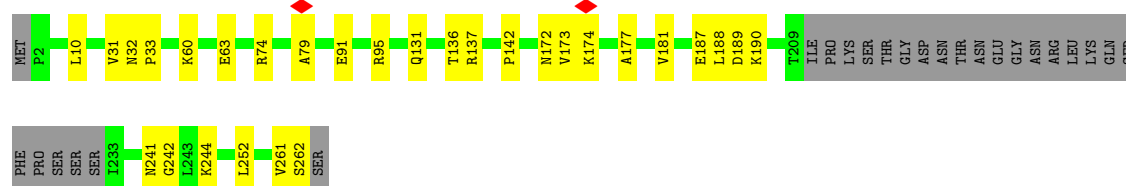
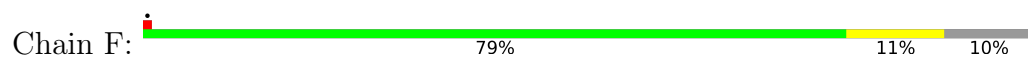
• Molecule 10: ORF60



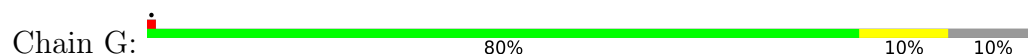
• Molecule 10: ORF60



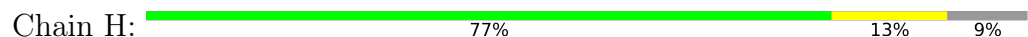
• Molecule 11: ORF59



• Molecule 11: ORF59



• Molecule 12: ORF61



GLU
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VAL
LEU
GLY
GLN
ASP
GLU
GLY
ILE
PHE
ALA
LEU
PHE
GLU

• Molecule 12: ORF61

Chain I:  74% 18% 9%

MET R2 Q9 H10 E11 Q15 Q19 E44 T45 D46 E47 E48 K49 M50 K51 D52 R55 L56 D73 V74 S75 V86 D95 L96 N97 H108 G109 T110 S111 D112 D124 L125 L126 D126 R141 H152 F163 M166 I174 E175 V178 S184 L193

I194 D195 W196 K197 I198 Q199 Q206 E210 V214 GLU GLU SER ILE ASN PHE VAL LEU GLY GLN ASP GLU GLY ILE PHE ALA LEU PHE GLU

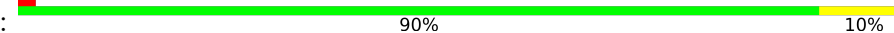
• Molecule 13: ORF62

Chain J:  90% 10%

K1 K16 T28 S31 R76 Q110 C133 K134 E135 D177 R180 T193 N194 V197 R198 I204 P205 D206 V207 V210 I238 L242 D253 V254 E261 V262 N263 I276 R289 D299 D315 V316 D320 V321 D324 N325 L326 D327

V332 I338 G341 E342 I343 L347 K348

• Molecule 13: ORF62

Chain K:  90% 10%

M1 L6 K16 D26 L36 V40 S41 L42 E45 E46 F47 I59 Q84 F85 T86 Q87 D90 A97 Q110 D117 E126 S154 R158 K179 R180 F181 F182 H183 V186 R191 T216 R226 L242 Q243 D244 V245 R246 P247

I250 D253 V254 N294 D299 D320 V321 N325 K348

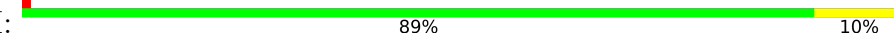
• Molecule 13: ORF62

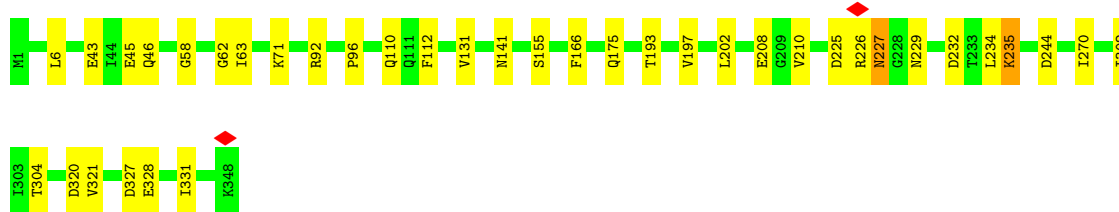
Chain L:  89% 11%

M1 K2 S11 K12 L13 I14 D15 S41 R72 R76 F85 P96 Q106 E107 Y108 L115 C133 R158 E176 R181 T193 V197 D225 R226 N229 K259 E260 E261 V268 R275 I276 G277 L284 L295 K296 T297 S298 D299

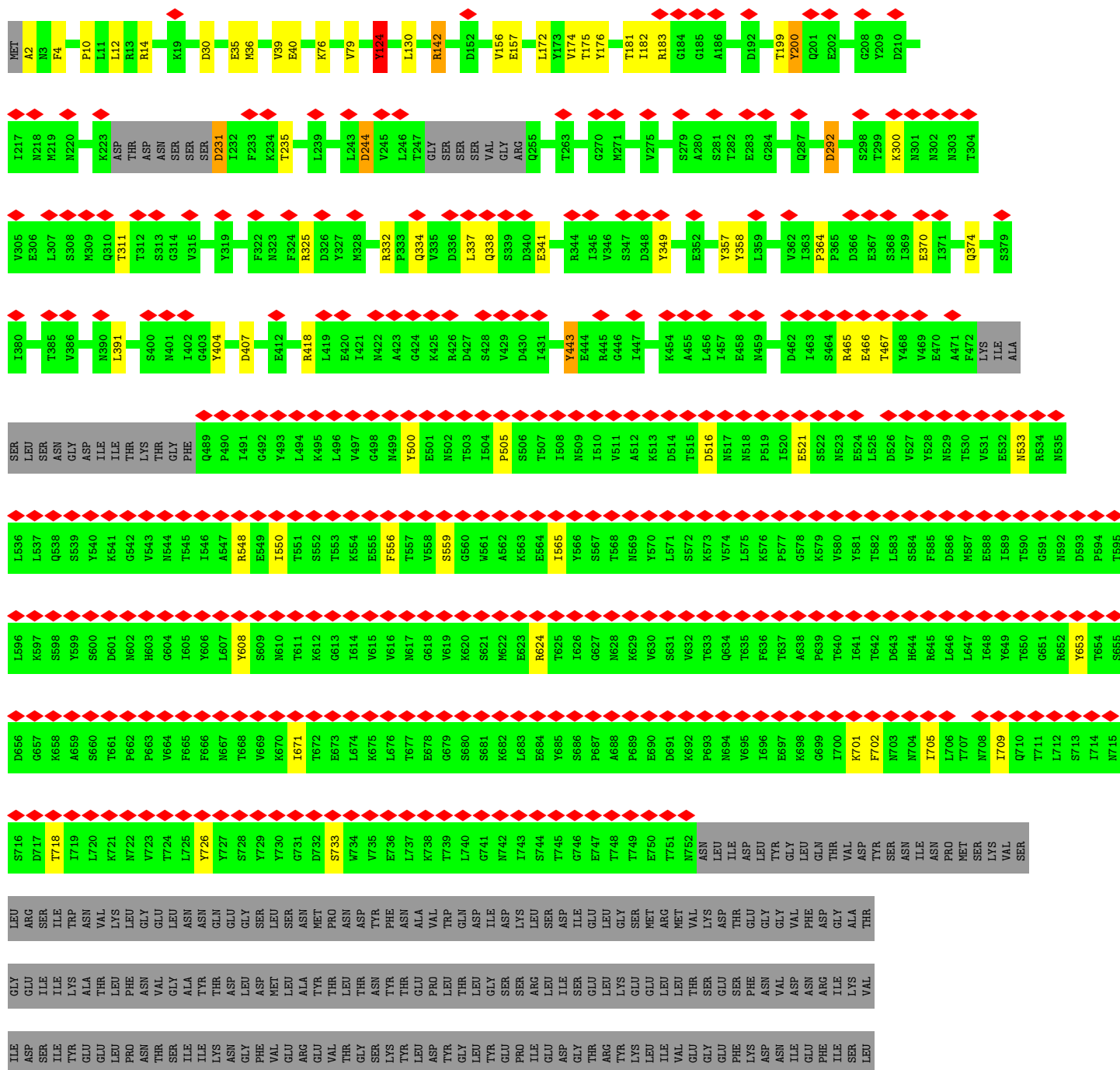
D315 V316 D320 V321 N325 Q335 I338 E342 I343 K344 V345 K348

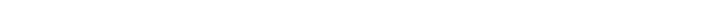
• Molecule 13: ORF62

Chain M:  89% 10%



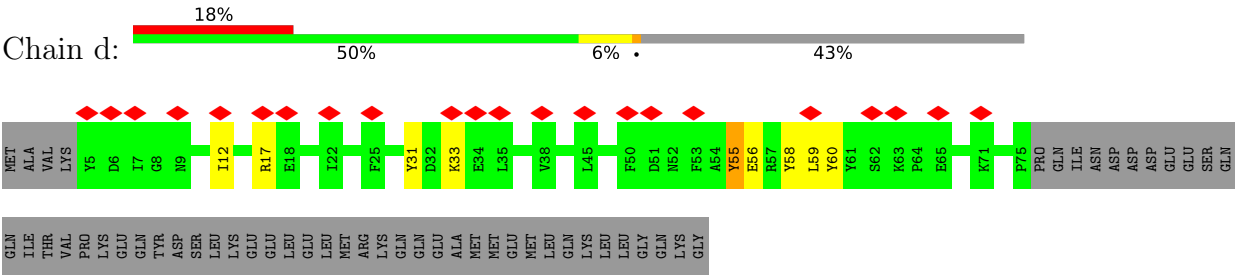
• Molecule 14: ORF63



Chain O:  31% 65% 6% 29%



● Molecule 15: ORF67



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	3586	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.106	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	1067.0079, 1067.0079, 1067.0079	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.6671999, 1.6671999, 1.6671999	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	0.78	0/3619	1.34	7/4913 (0.1%)
1	8	0.79	0/3619	1.35	11/4913 (0.2%)
1	9	0.80	0/3619	1.37	10/4913 (0.2%)
1	w	0.77	0/3619	1.34	13/4913 (0.3%)
1	x	0.77	0/3619	1.34	7/4913 (0.1%)
1	y	0.75	0/3619	1.33	7/4913 (0.1%)
2	1	0.80	0/1377	1.47	8/1872 (0.4%)
2	P	0.70	0/1292	1.29	1/1756 (0.1%)
2	Q	0.71	0/1303	1.27	5/1771 (0.3%)
2	R	0.74	0/1298	1.23	3/1764 (0.2%)
2	S	0.74	0/1377	1.32	5/1872 (0.3%)
2	T	0.74	0/1377	1.39	7/1872 (0.4%)
2	U	0.70	0/1377	1.41	8/1872 (0.4%)
2	V	0.74	0/1377	1.43	8/1872 (0.4%)
2	W	0.78	0/1377	1.46	11/1872 (0.6%)
2	X	0.80	0/1377	1.51	9/1872 (0.5%)
2	Y	0.75	0/1377	1.46	6/1872 (0.3%)
2	Z	0.75	0/1377	1.48	10/1872 (0.5%)
2	e	0.67	0/1306	1.15	2/1774 (0.1%)
2	f	0.65	0/1296	1.17	0/1760
2	g	0.65	0/1304	1.12	0/1771
2	h	0.67	0/1378	1.20	3/1872 (0.2%)
2	i	0.68	0/1224	1.26	2/1660 (0.1%)
2	j	0.73	0/1378	1.33	2/1872 (0.1%)
2	k	0.74	0/1378	1.38	6/1872 (0.3%)
2	l	0.77	0/1378	1.39	6/1872 (0.3%)
2	m	0.77	0/1378	1.37	6/1872 (0.3%)
2	n	0.76	0/1378	1.39	2/1872 (0.1%)
2	o	0.78	0/1378	1.36	4/1872 (0.2%)
2	p	0.79	0/1378	1.35	4/1872 (0.2%)
3	2	0.84	0/8526	1.46	36/11565 (0.3%)
3	3	0.84	0/8526	1.46	40/11565 (0.3%)
3	4	0.85	0/8526	1.47	43/11565 (0.4%)
3	5	0.89	0/8526	1.48	48/11565 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	6	0.90	0/8526	1.50	45/11565 (0.4%)
3	7	0.89	1/8526 (0.0%)	1.47	39/11565 (0.3%)
3	q	0.85	0/8526	1.45	37/11565 (0.3%)
3	r	0.83	1/8526 (0.0%)	1.42	38/11565 (0.3%)
3	s	0.85	0/8526	1.47	48/11565 (0.4%)
3	t	0.83	0/8526	1.42	35/11565 (0.3%)
3	u	0.82	0/8526	1.41	32/11565 (0.3%)
3	v	0.81	0/8526	1.41	38/11565 (0.3%)
4	A	0.13	0/2511	0.38	0/3394
5	AA	0.80	0/5253	1.39	25/7135 (0.4%)
5	AB	0.81	0/5253	1.44	30/7135 (0.4%)
5	a	0.84	0/5253	1.45	23/7135 (0.3%)
5	b	0.83	0/5253	1.42	17/7135 (0.2%)
5	c	0.83	0/5253	1.42	10/7135 (0.1%)
5	z	0.81	0/5253	1.39	22/7135 (0.3%)
6	AC	0.12	0/1107	0.33	0/1496
6	AD	0.11	0/1107	0.33	0/1496
6	AE	0.12	0/1107	0.33	0/1496
6	AF	0.12	0/1107	0.34	0/1496
6	AG	0.12	0/1107	0.33	0/1496
6	AH	0.12	0/1107	0.33	0/1496
7	AI	0.17	0/4355	0.44	2/5880 (0.0%)
7	AJ	0.11	0/4355	0.36	0/5880
7	AK	0.21	0/4335	0.45	0/5853
7	AL	0.20	0/4335	0.46	0/5853
7	AM	0.15	0/2712	0.40	0/3663
7	AN	0.15	0/2712	0.41	0/3663
8	B	0.62	0/2481	1.18	11/3349 (0.3%)
9	C	0.42	0/5985	0.75	6/8050 (0.1%)
10	D	0.12	0/1315	0.34	0/1788
10	E	0.16	0/1269	0.43	0/1724
11	F	0.12	0/1907	0.40	0/2565
11	G	0.12	0/1900	0.41	0/2555
12	H	0.12	0/1722	0.38	0/2331
12	I	0.12	0/1729	0.37	0/2341
13	J	0.15	0/2803	0.40	0/3794
13	K	0.17	0/2803	0.42	0/3794
13	L	0.31	0/2803	0.64	2/3794 (0.1%)
13	M	0.17	0/2803	0.43	0/3794
14	N	0.70	1/5967 (0.0%)	1.19	13/8098 (0.2%)
14	O	0.67	0/5967	1.11	7/8098 (0.1%)
15	d	0.82	0/613	1.41	0/830
All	All	0.72	3/262008 (0.0%)	1.25	820/355215 (0.2%)

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	5
1	8	0	4
1	9	0	3
1	w	0	3
1	x	0	4
1	y	0	2
2	1	0	3
2	P	0	1
2	Q	0	2
2	R	0	1
2	T	0	1
2	U	0	1
2	W	0	1
2	Y	0	1
2	Z	0	2
2	e	0	1
2	i	0	1
2	j	0	2
2	k	0	1
2	l	0	2
2	m	0	1
2	o	0	4
2	p	0	2
3	2	0	10
3	3	0	8
3	4	0	11
3	5	0	14
3	6	0	13
3	7	0	8
3	q	0	15
3	r	0	11
3	s	0	8
3	t	0	7
3	u	0	11
3	v	0	11
5	AA	0	5
5	AB	0	15
5	a	0	12
5	b	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	c	0	11
5	z	0	8
7	AI	0	1
8	B	0	6
9	C	0	8
13	L	0	1
14	N	0	13
14	O	0	8
15	d	0	2
All	All	0	272

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	r	271	ARG	CA-C	7.07	1.55	1.52
14	N	364	PRO	CA-C	6.17	1.55	1.51
3	7	424	GLU	CA-C	5.29	1.57	1.53

The worst 5 of 820 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	134	GLU	N-CA-C	9.13	121.93	108.60
3	s	26	ASN	CA-C-N	9.11	131.23	119.84
3	s	26	ASN	C-N-CA	9.11	131.23	119.84
3	u	381	ASN	CA-CB-CG	8.99	121.59	112.60
3	2	603	ASN	CA-CB-CG	8.90	121.50	112.60

There are no chirality outliers.

5 of 272 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	276	PHE	Sidechain
1	0	365	TYR	Sidechain
1	0	45	PHE	Sidechain
1	0	63	TYR	Sidechain
1	0	78	TYR	Sidechain

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	0	3548	0	3468	4	0
1	8	3548	0	3468	7	0
1	9	3548	0	3468	3	0
1	w	3548	0	3468	5	0
1	x	3548	0	3468	2	0
1	y	3548	0	3468	2	0
2	1	1349	0	1339	7	0
2	P	1266	0	1258	15	0
2	Q	1277	0	1274	4	0
2	R	1272	0	1264	8	0
2	S	1349	0	1339	5	0
2	T	1349	0	1339	7	0
2	U	1349	0	1339	6	0
2	V	1349	0	1339	5	0
2	W	1349	0	1339	6	0
2	X	1349	0	1339	7	0
2	Y	1349	0	1339	6	0
2	Z	1349	0	1339	8	0
2	e	1280	0	1275	11	0
2	f	1270	0	1263	4	0
2	g	1278	0	1274	0	0
2	h	1350	0	1339	3	0
2	i	1199	0	1195	4	0
2	j	1350	0	1339	2	0
2	k	1350	0	1339	2	0
2	l	1350	0	1339	3	0
2	m	1350	0	1339	4	0
2	n	1350	0	1339	5	0
2	o	1350	0	1339	6	0
2	p	1350	0	1339	1	0
3	2	8364	0	8206	25	0
3	3	8364	0	8206	20	0
3	4	8364	0	8206	19	0
3	5	8364	0	8206	14	0
3	6	8364	0	8206	19	0
3	7	8364	0	8206	24	0
3	q	8364	0	8206	14	0
3	r	8364	0	8206	23	0
3	s	8364	0	8206	19	0
3	t	8364	0	8206	12	0
3	u	8364	0	8206	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	v	8364	0	8206	18	0
4	A	2462	0	2382	17	0
5	AA	5127	0	4969	12	0
5	AB	5127	0	4969	5	0
5	a	5127	0	4969	7	0
5	b	5127	0	4969	15	0
5	c	5127	0	4969	8	0
5	z	5127	0	4969	14	0
6	AC	1091	0	1081	7	0
6	AD	1091	0	1079	26	0
6	AE	1091	0	1081	7	0
6	AF	1091	0	1081	8	0
6	AG	1091	0	1081	7	0
6	AH	1091	0	1081	6	0
7	AI	4284	0	4241	57	0
7	AJ	4284	0	4241	42	0
7	AK	4267	0	4220	44	0
7	AL	4267	0	4220	39	0
7	AM	2667	0	2631	24	0
7	AN	2667	0	2631	27	0
8	B	2424	0	2330	43	0
9	C	5852	0	5760	76	0
10	D	1294	0	1301	8	0
10	E	1248	0	1257	15	0
11	F	1878	0	1841	38	0
11	G	1871	0	1837	19	0
12	H	1694	0	1663	34	0
12	I	1701	0	1672	45	0
13	J	2760	0	2729	23	0
13	K	2760	0	2729	22	0
13	L	2760	0	2729	29	0
13	M	2760	0	2729	29	0
14	N	5845	0	5710	33	0
14	O	5845	0	5710	30	0
15	d	597	0	570	1	0
All	All	256934	0	252277	992	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 2.

The worst 5 of 992 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)
8:B:150:LEU:HD12	9:C:679:LYS:CE	1.36	1.52
8:B:150:LEU:HD12	9:C:679:LYS:NZ	1.09	1.40
8:B:150:LEU:CD1	9:C:679:LYS:HD2	1.62	1.28
8:B:150:LEU:CD1	9:C:679:LYS:CE	2.14	1.25
14:O:176:TYR:CE2	2:e:157:GLN:NE2	2.04	1.25

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	0	456/458 (100%)	412 (90%)	43 (9%)	1 (0%)	43	77
1	8	456/458 (100%)	419 (92%)	34 (8%)	3 (1%)	18	56
1	9	456/458 (100%)	419 (92%)	35 (8%)	2 (0%)	30	67
1	w	456/458 (100%)	419 (92%)	35 (8%)	2 (0%)	30	67
1	x	456/458 (100%)	416 (91%)	37 (8%)	3 (1%)	18	56
1	y	456/458 (100%)	421 (92%)	34 (8%)	1 (0%)	43	77
2	1	170/173 (98%)	149 (88%)	18 (11%)	3 (2%)	6	34
2	P	157/173 (91%)	151 (96%)	6 (4%)	0	100	100
2	Q	159/173 (92%)	152 (96%)	7 (4%)	0	100	100
2	R	158/173 (91%)	150 (95%)	8 (5%)	0	100	100
2	S	170/173 (98%)	154 (91%)	16 (9%)	0	100	100
2	T	170/173 (98%)	156 (92%)	12 (7%)	2 (1%)	10	43
2	U	170/173 (98%)	153 (90%)	14 (8%)	3 (2%)	6	34
2	V	170/173 (98%)	148 (87%)	17 (10%)	5 (3%)	3	23
2	W	170/173 (98%)	154 (91%)	14 (8%)	2 (1%)	10	43
2	X	170/173 (98%)	150 (88%)	16 (9%)	4 (2%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Y	170/173 (98%)	153 (90%)	15 (9%)	2 (1%)	10	43
2	Z	170/173 (98%)	149 (88%)	19 (11%)	2 (1%)	10	43
2	e	159/173 (92%)	155 (98%)	4 (2%)	0	100	100
2	f	158/173 (91%)	153 (97%)	4 (2%)	1 (1%)	21	59
2	g	159/173 (92%)	152 (96%)	7 (4%)	0	100	100
2	h	170/173 (98%)	161 (95%)	8 (5%)	1 (1%)	21	59
2	i	146/173 (84%)	138 (94%)	8 (6%)	0	100	100
2	j	170/173 (98%)	157 (92%)	11 (6%)	2 (1%)	10	43
2	k	170/173 (98%)	152 (89%)	16 (9%)	2 (1%)	10	43
2	l	170/173 (98%)	161 (95%)	8 (5%)	1 (1%)	21	59
2	m	170/173 (98%)	161 (95%)	9 (5%)	0	100	100
2	n	170/173 (98%)	162 (95%)	8 (5%)	0	100	100
2	o	170/173 (98%)	159 (94%)	10 (6%)	1 (1%)	21	59
2	p	170/173 (98%)	161 (95%)	7 (4%)	2 (1%)	10	43
3	2	1056/1152 (92%)	920 (87%)	113 (11%)	23 (2%)	5	29
3	3	1056/1152 (92%)	910 (86%)	118 (11%)	28 (3%)	4	25
3	4	1056/1152 (92%)	910 (86%)	126 (12%)	20 (2%)	6	31
3	5	1056/1152 (92%)	908 (86%)	131 (12%)	17 (2%)	7	37
3	6	1056/1152 (92%)	934 (88%)	107 (10%)	15 (1%)	9	40
3	7	1056/1152 (92%)	889 (84%)	152 (14%)	15 (1%)	9	40
3	q	1056/1152 (92%)	898 (85%)	136 (13%)	22 (2%)	5	29
3	r	1056/1152 (92%)	923 (87%)	111 (10%)	22 (2%)	5	29
3	s	1056/1152 (92%)	907 (86%)	123 (12%)	26 (2%)	4	26
3	t	1056/1152 (92%)	931 (88%)	107 (10%)	18 (2%)	7	36
3	u	1056/1152 (92%)	930 (88%)	109 (10%)	17 (2%)	7	37
3	v	1056/1152 (92%)	931 (88%)	112 (11%)	13 (1%)	10	43
4	A	307/848 (36%)	300 (98%)	7 (2%)	0	100	100
5	AA	638/640 (100%)	582 (91%)	53 (8%)	3 (0%)	24	63
5	AB	638/640 (100%)	574 (90%)	57 (9%)	7 (1%)	11	46
5	a	638/640 (100%)	564 (88%)	68 (11%)	6 (1%)	14	50
5	b	638/640 (100%)	574 (90%)	58 (9%)	6 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	c	638/640 (100%)	566 (89%)	66 (10%)	6 (1%)	14	50
5	z	638/640 (100%)	580 (91%)	49 (8%)	9 (1%)	9	40
6	AC	137/142 (96%)	137 (100%)	0	0	100	100
6	AD	137/142 (96%)	137 (100%)	0	0	100	100
6	AE	137/142 (96%)	136 (99%)	1 (1%)	0	100	100
6	AF	137/142 (96%)	136 (99%)	1 (1%)	0	100	100
6	AG	137/142 (96%)	136 (99%)	1 (1%)	0	100	100
6	AH	137/142 (96%)	136 (99%)	1 (1%)	0	100	100
7	AI	546/587 (93%)	534 (98%)	12 (2%)	0	100	100
7	AJ	546/587 (93%)	536 (98%)	10 (2%)	0	100	100
7	AK	545/587 (93%)	531 (97%)	14 (3%)	0	100	100
7	AL	545/587 (93%)	531 (97%)	14 (3%)	0	100	100
7	AM	336/587 (57%)	329 (98%)	7 (2%)	0	100	100
7	AN	336/587 (57%)	329 (98%)	7 (2%)	0	100	100
8	B	288/295 (98%)	252 (88%)	28 (10%)	8 (3%)	4	24
9	C	713/808 (88%)	685 (96%)	27 (4%)	1 (0%)	48	83
10	D	156/174 (90%)	154 (99%)	2 (1%)	0	100	100
10	E	150/174 (86%)	150 (100%)	0	0	100	100
11	F	234/263 (89%)	231 (99%)	3 (1%)	0	100	100
11	G	233/263 (89%)	232 (100%)	1 (0%)	0	100	100
12	H	210/234 (90%)	205 (98%)	5 (2%)	0	100	100
12	I	211/234 (90%)	207 (98%)	4 (2%)	0	100	100
13	J	346/348 (99%)	342 (99%)	4 (1%)	0	100	100
13	K	346/348 (99%)	342 (99%)	3 (1%)	1 (0%)	36	72
13	L	346/348 (99%)	338 (98%)	8 (2%)	0	100	100
13	M	346/348 (99%)	343 (99%)	3 (1%)	0	100	100
14	N	713/1019 (70%)	667 (94%)	44 (6%)	2 (0%)	36	72
14	O	713/1019 (70%)	672 (94%)	37 (5%)	4 (1%)	21	59
15	d	69/124 (56%)	60 (87%)	8 (12%)	1 (1%)	9	40
All	All	32279/35785 (90%)	29416 (91%)	2528 (8%)	335 (1%)	15	48

5 of 335 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	93	ALA
3	2	453	SER
3	2	590	ASN
3	2	997	LYS
3	3	356	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	405/405 (100%)	394 (97%)	11 (3%)	39	60
1	8	405/405 (100%)	390 (96%)	15 (4%)	30	51
1	9	405/405 (100%)	395 (98%)	10 (2%)	42	62
1	w	405/405 (100%)	389 (96%)	16 (4%)	28	49
1	x	405/405 (100%)	395 (98%)	10 (2%)	42	62
1	y	405/405 (100%)	391 (96%)	14 (4%)	32	53
2	1	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	P	142/153 (93%)	134 (94%)	8 (6%)	19	40
2	Q	143/153 (94%)	139 (97%)	4 (3%)	38	59
2	R	143/153 (94%)	142 (99%)	1 (1%)	76	81
2	S	152/153 (99%)	149 (98%)	3 (2%)	48	66
2	T	152/153 (99%)	138 (91%)	14 (9%)	8	27
2	U	152/153 (99%)	138 (91%)	14 (9%)	8	27
2	V	152/153 (99%)	138 (91%)	14 (9%)	8	27
2	W	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	X	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	Y	152/153 (99%)	140 (92%)	12 (8%)	11	31
2	Z	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	e	143/153 (94%)	140 (98%)	3 (2%)	47	65
2	f	142/153 (93%)	141 (99%)	1 (1%)	76	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	g	143/153 (94%)	143 (100%)	0	100	100
2	h	152/153 (99%)	150 (99%)	2 (1%)	61	73
2	i	134/153 (88%)	132 (98%)	2 (2%)	57	71
2	j	152/153 (99%)	146 (96%)	6 (4%)	28	49
2	k	152/153 (99%)	138 (91%)	14 (9%)	8	27
2	l	152/153 (99%)	143 (94%)	9 (6%)	18	39
2	m	152/153 (99%)	143 (94%)	9 (6%)	18	39
2	n	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	o	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	p	152/153 (99%)	141 (93%)	11 (7%)	13	34
3	2	934/1010 (92%)	879 (94%)	55 (6%)	18	39
3	3	934/1010 (92%)	874 (94%)	60 (6%)	16	37
3	4	934/1010 (92%)	868 (93%)	66 (7%)	13	35
3	5	934/1010 (92%)	864 (92%)	70 (8%)	12	33
3	6	934/1010 (92%)	864 (92%)	70 (8%)	12	33
3	7	934/1010 (92%)	881 (94%)	53 (6%)	18	40
3	q	934/1010 (92%)	876 (94%)	58 (6%)	16	38
3	r	934/1010 (92%)	873 (94%)	61 (6%)	15	37
3	s	934/1010 (92%)	879 (94%)	55 (6%)	18	39
3	t	934/1010 (92%)	869 (93%)	65 (7%)	14	35
3	u	934/1010 (92%)	875 (94%)	59 (6%)	16	37
3	v	934/1010 (92%)	887 (95%)	47 (5%)	22	42
4	A	278/758 (37%)	277 (100%)	1 (0%)	84	84
5	AA	577/577 (100%)	562 (97%)	15 (3%)	40	61
5	AB	577/577 (100%)	551 (96%)	26 (4%)	24	46
5	a	577/577 (100%)	546 (95%)	31 (5%)	20	41
5	b	577/577 (100%)	556 (96%)	21 (4%)	31	52
5	c	577/577 (100%)	558 (97%)	19 (3%)	33	55
5	z	577/577 (100%)	552 (96%)	25 (4%)	26	47
6	AC	119/122 (98%)	119 (100%)	0	100	100
6	AD	119/122 (98%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AE	119/122 (98%)	118 (99%)	1 (1%)	73	79
6	AF	119/122 (98%)	118 (99%)	1 (1%)	73	79
6	AG	119/122 (98%)	119 (100%)	0	100	100
6	AH	119/122 (98%)	119 (100%)	0	100	100
7	AI	466/495 (94%)	466 (100%)	0	100	100
7	AJ	466/495 (94%)	466 (100%)	0	100	100
7	AK	464/495 (94%)	463 (100%)	1 (0%)	87	86
7	AL	464/495 (94%)	463 (100%)	1 (0%)	87	86
7	AM	290/495 (59%)	289 (100%)	1 (0%)	86	85
7	AN	290/495 (59%)	289 (100%)	1 (0%)	86	85
8	B	268/271 (99%)	245 (91%)	23 (9%)	10	29
9	C	630/695 (91%)	612 (97%)	18 (3%)	37	58
10	D	150/164 (92%)	149 (99%)	1 (1%)	76	81
10	E	144/164 (88%)	144 (100%)	0	100	100
11	F	205/228 (90%)	204 (100%)	1 (0%)	81	83
11	G	204/228 (90%)	203 (100%)	1 (0%)	81	83
12	H	190/209 (91%)	190 (100%)	0	100	100
12	I	191/209 (91%)	189 (99%)	2 (1%)	68	77
13	J	311/311 (100%)	311 (100%)	0	100	100
13	K	311/311 (100%)	311 (100%)	0	100	100
13	L	311/311 (100%)	310 (100%)	1 (0%)	86	85
13	M	311/311 (100%)	308 (99%)	3 (1%)	68	77
14	N	658/928 (71%)	638 (97%)	20 (3%)	36	57
14	O	658/928 (71%)	645 (98%)	13 (2%)	48	66
15	d	63/112 (56%)	57 (90%)	6 (10%)	8	25
All	All	28711/31524 (91%)	27490 (96%)	1221 (4%)	27	47

5 of 1221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	r	1075	LYS
3	v	978	TRP
3	s	467	SER

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Mol	Chain	Res	Type
3	r	1014	ARG
3	t	1022	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 329 such sidechains are listed below:

Mol	Chain	Res	Type
15	d	37	GLN
3	t	37	ASN
2	j	7	ASN
3	q	590	ASN
3	u	480	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

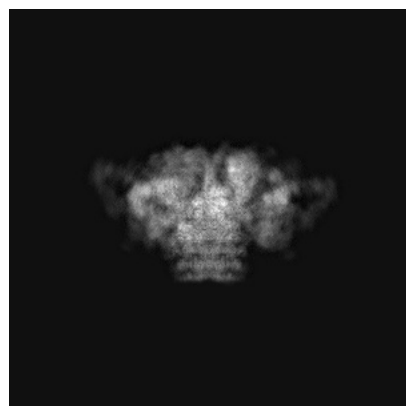
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55951. These allow visual inspection of the internal detail of the map and identification of artifacts.

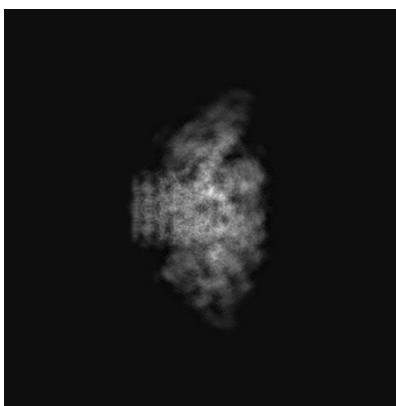
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

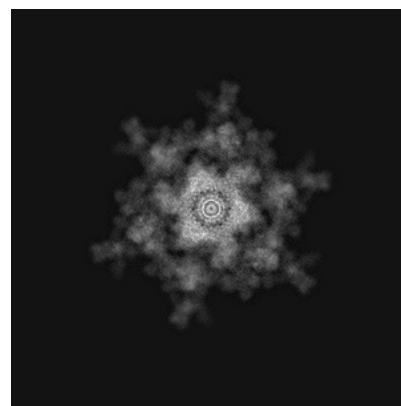
6.1.1 Primary map



X

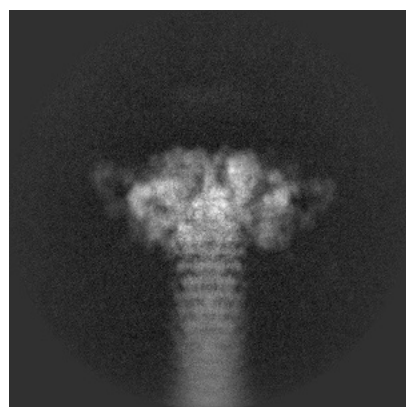


Y

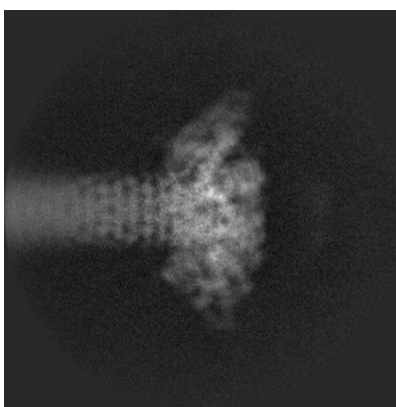


Z

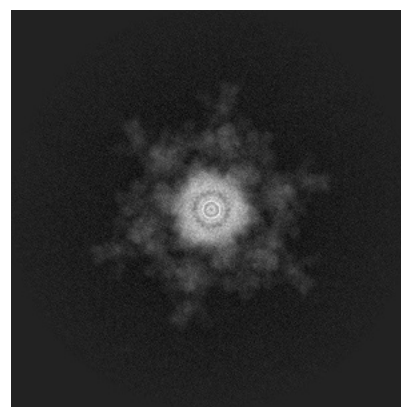
6.1.2 Raw map



X



Y

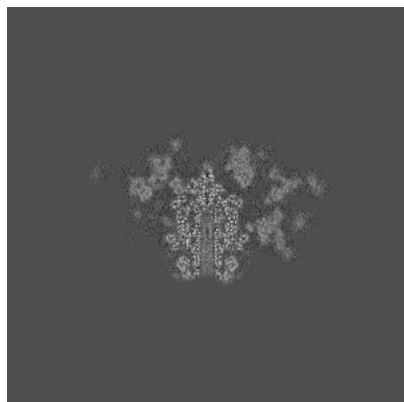


Z

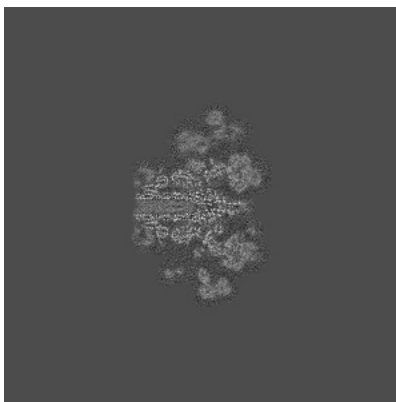
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

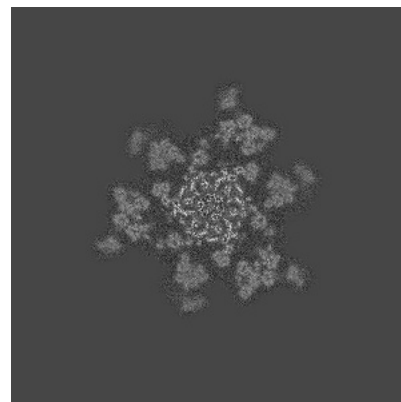
6.2.1 Primary map



X Index: 320

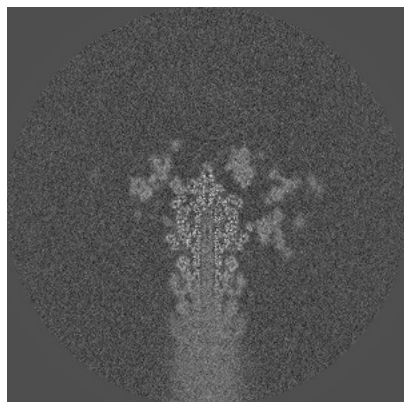


Y Index: 320

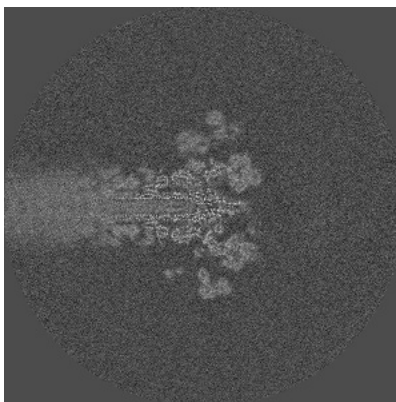


Z Index: 320

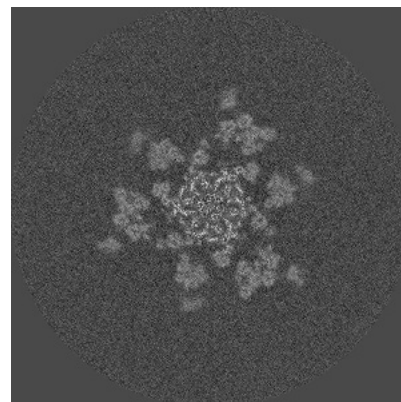
6.2.2 Raw map



X Index: 320



Y Index: 320

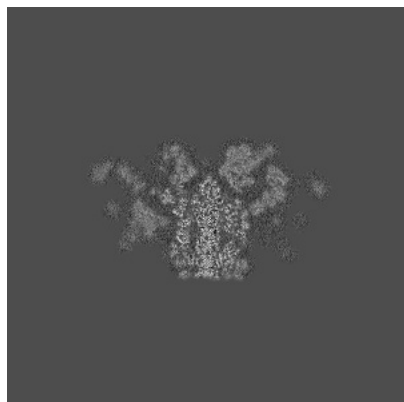


Z Index: 320

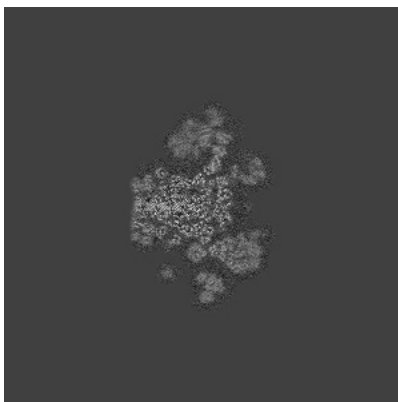
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

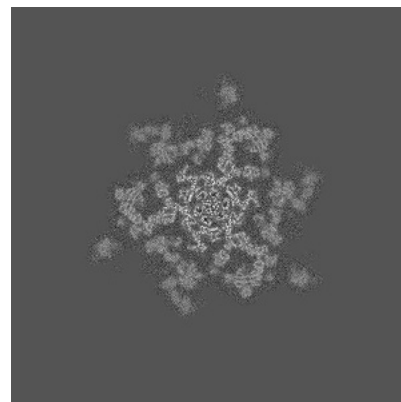
6.3.1 Primary map



X Index: 307

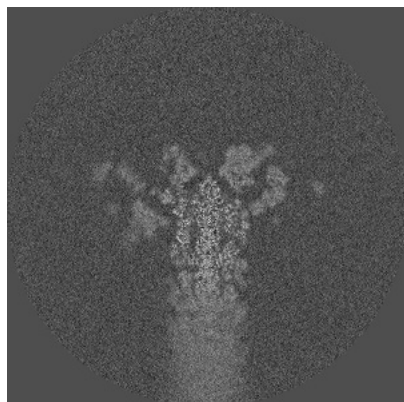


Y Index: 333

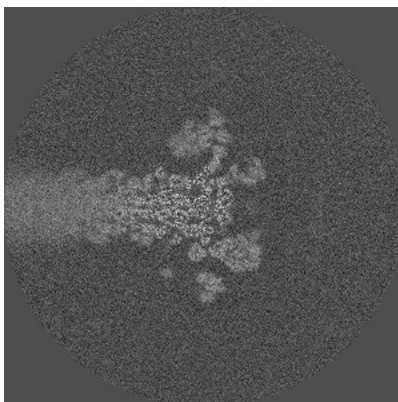


Z Index: 330

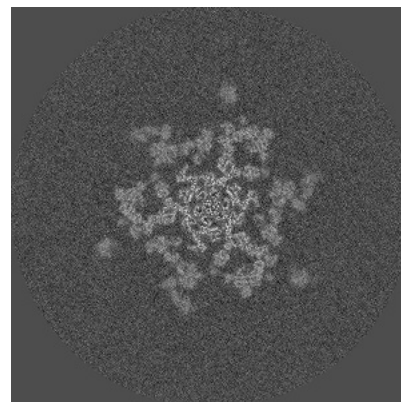
6.3.2 Raw map



X Index: 307



Y Index: 332

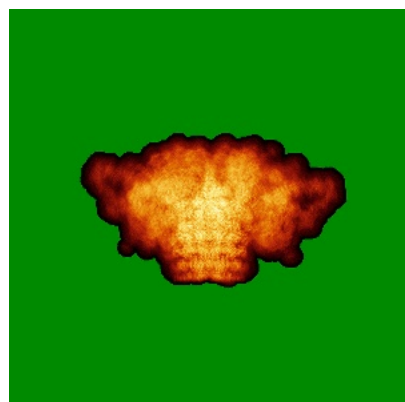


Z Index: 330

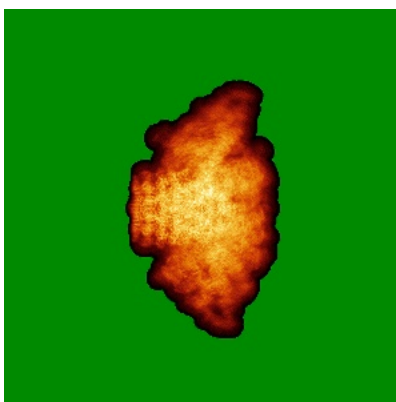
The images above show the largest variance slices of the map in three orthogonal directions.

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

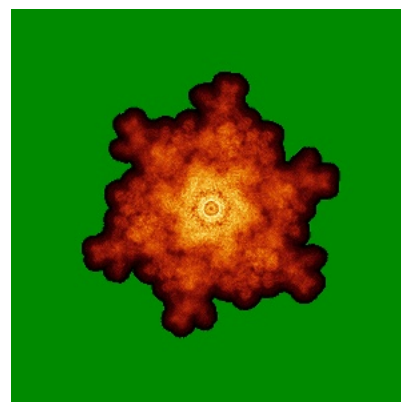
6.4.1 Primary map



X

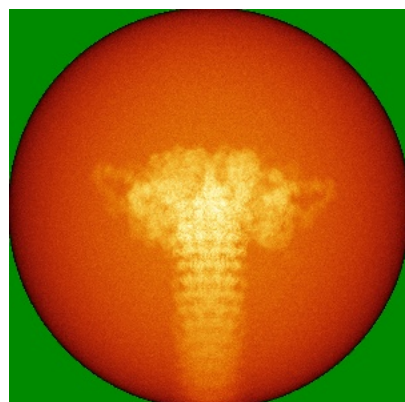


Y

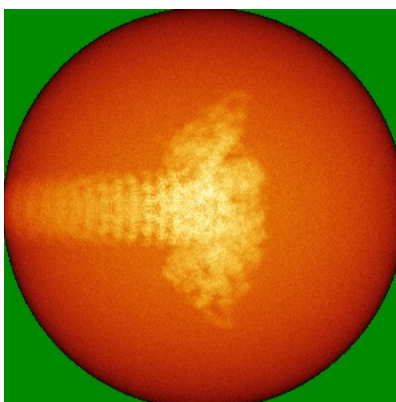


Z

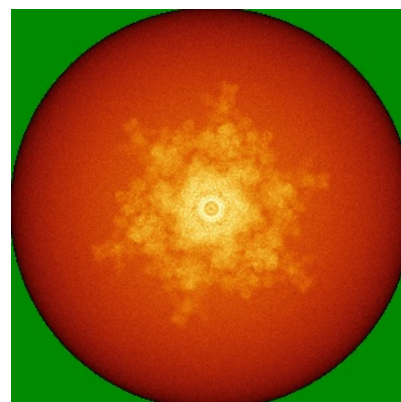
6.4.2 Raw map



X



Y

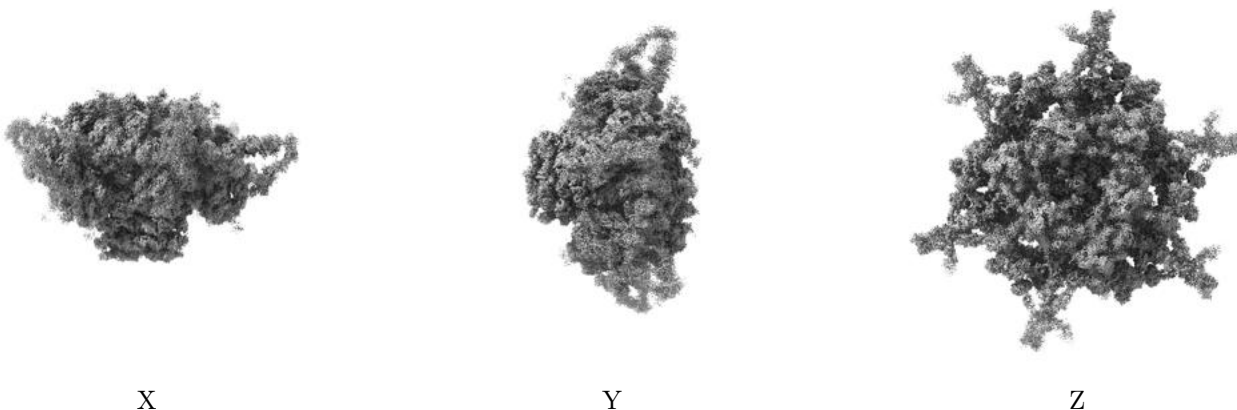


Z

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.

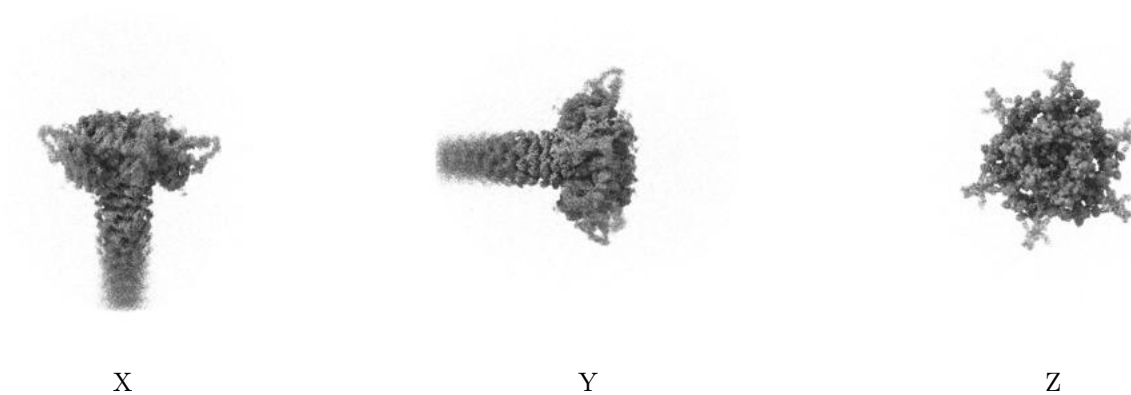
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

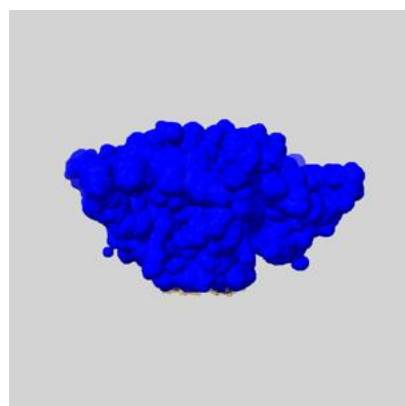
6.6 Mask visualisation [i](#)

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

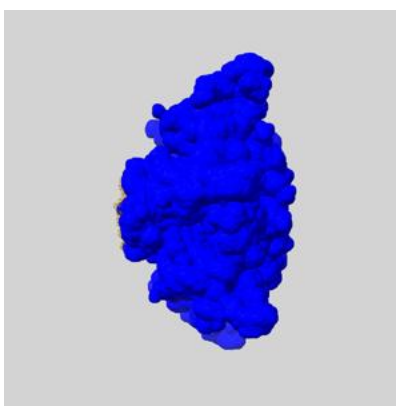
A mask typically either:

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

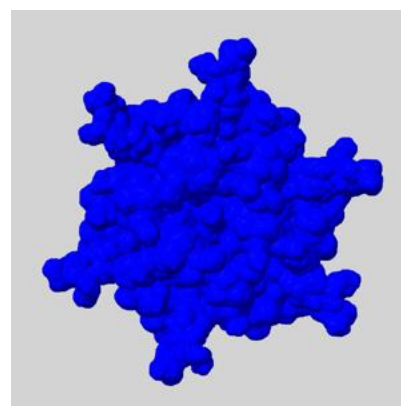
6.6.1 emd_55951_msk_1.map [i](#)



X



Y

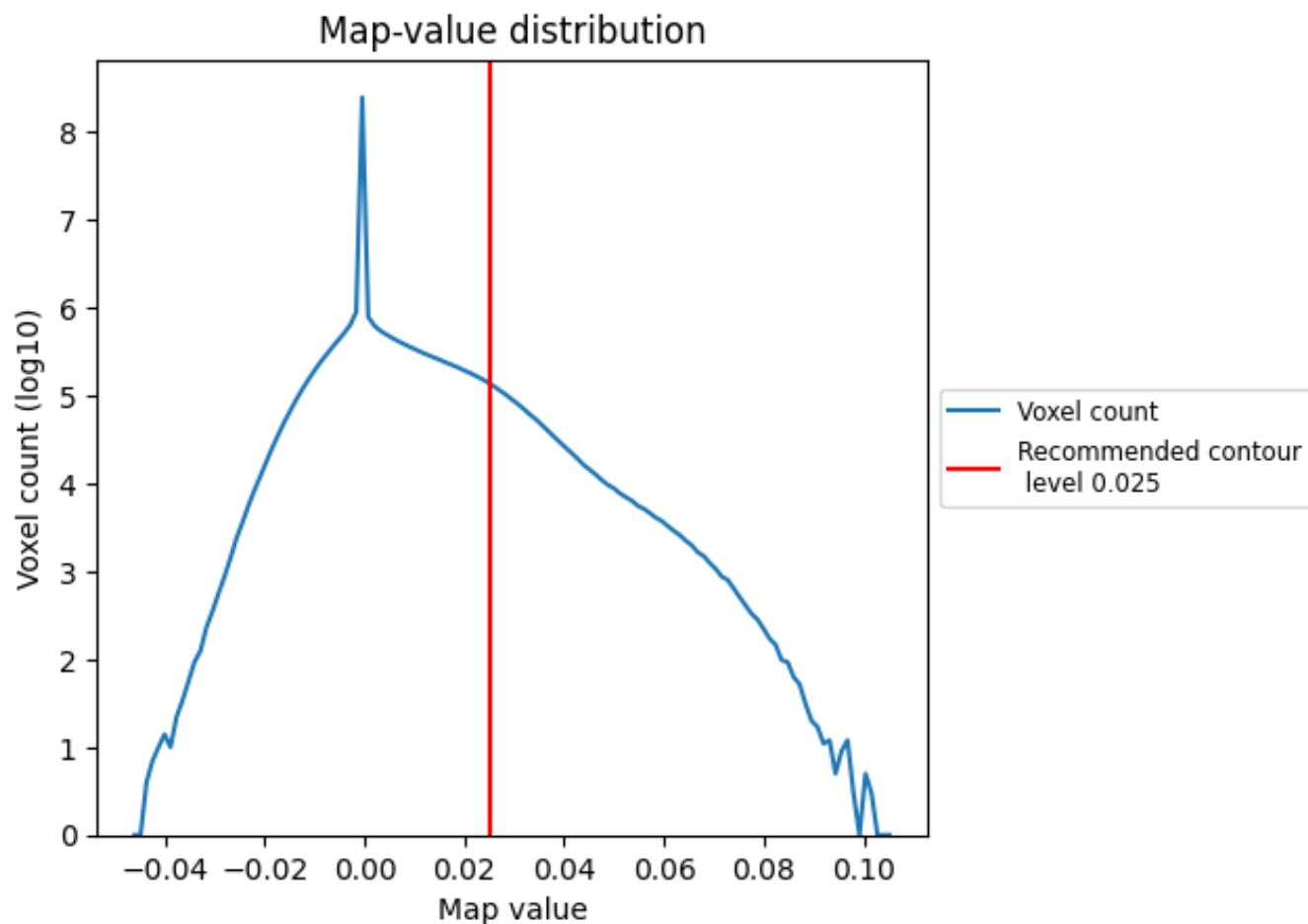


Z

7 Map analysis [i](#)

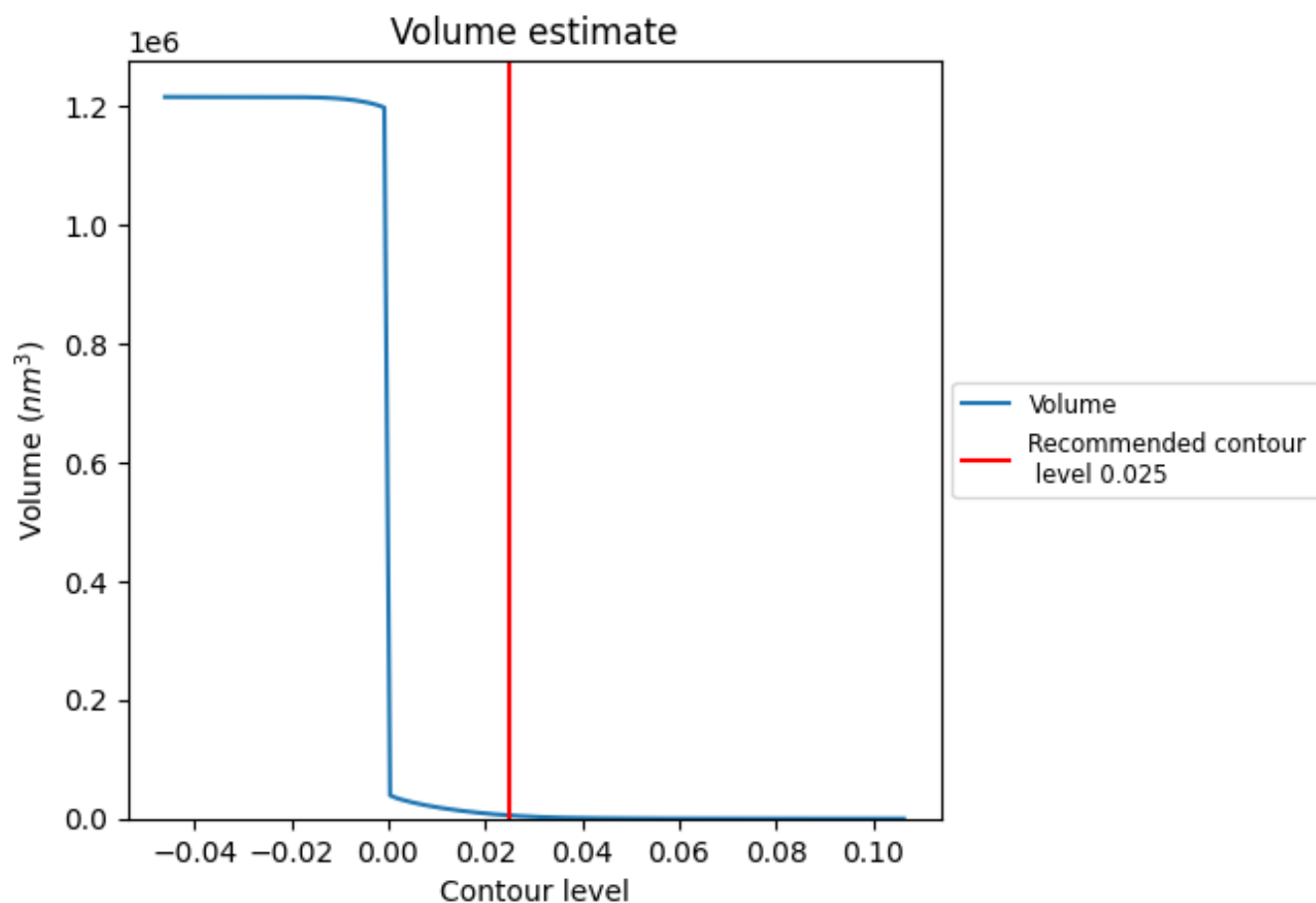
This section contains the results of statistical analysis of the map.

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.

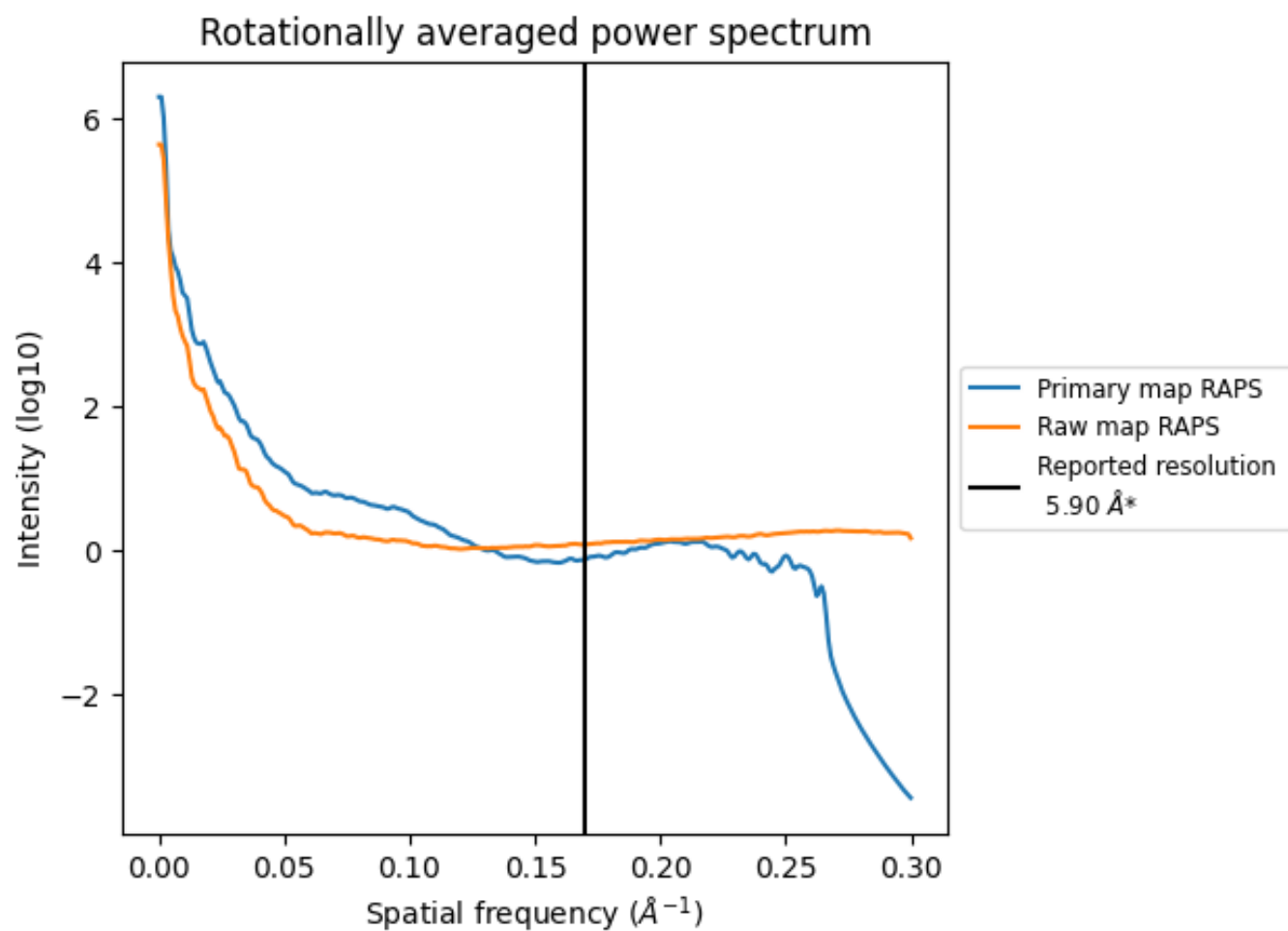
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5425 nm³; this corresponds to an approximate mass of 4901 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 ⓘ

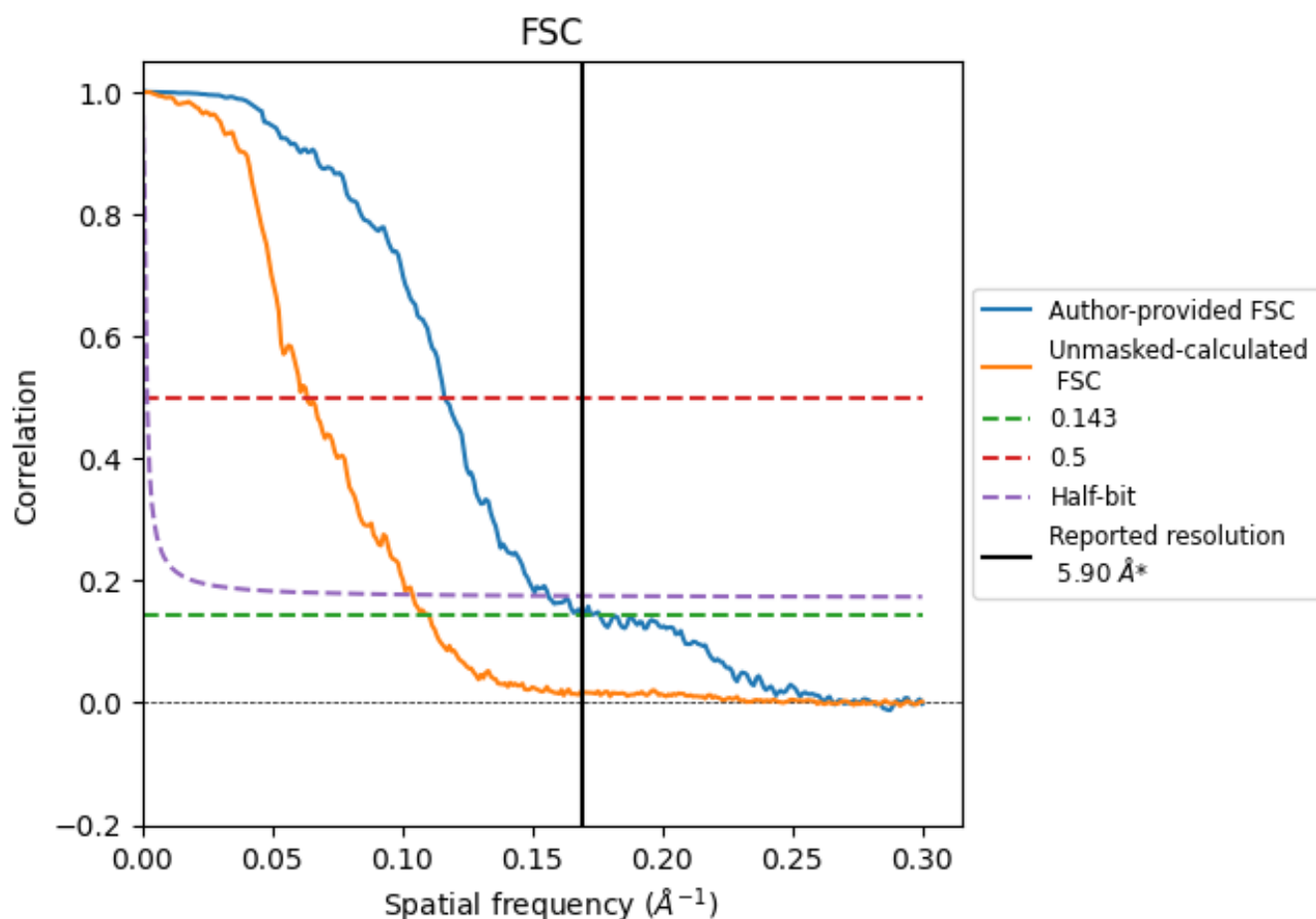


*Reported resolution corresponds to spatial frequency of 0.169 Å⁻¹

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 0.169 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.90	-	-
Author-provided FSC curve	5.90	8.61	6.40
Unmasked-calculated*	9.09	15.77	9.62

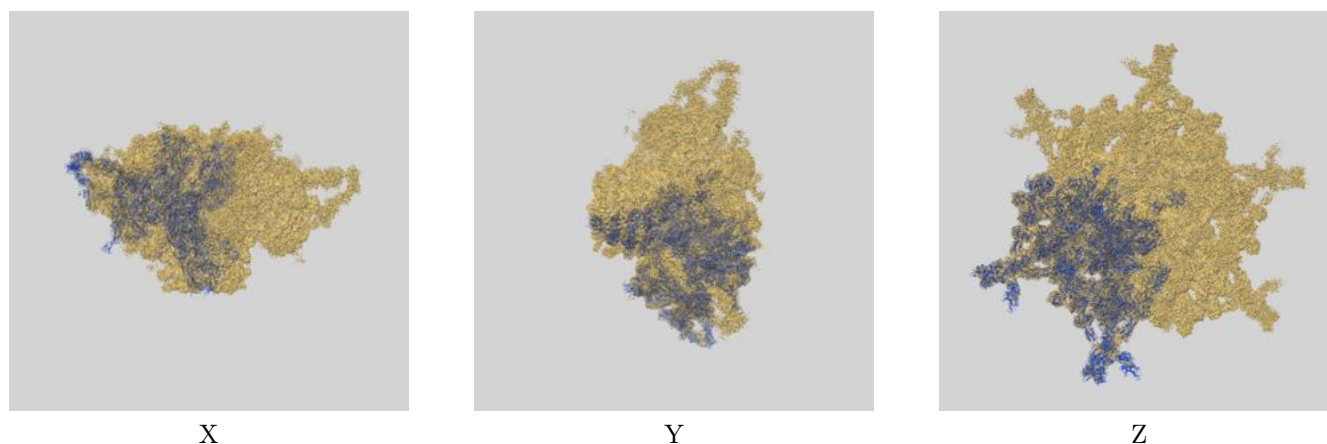
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.09 differs from the reported value 5.9 by more than 10 %

9 Map-model fit [i](#)

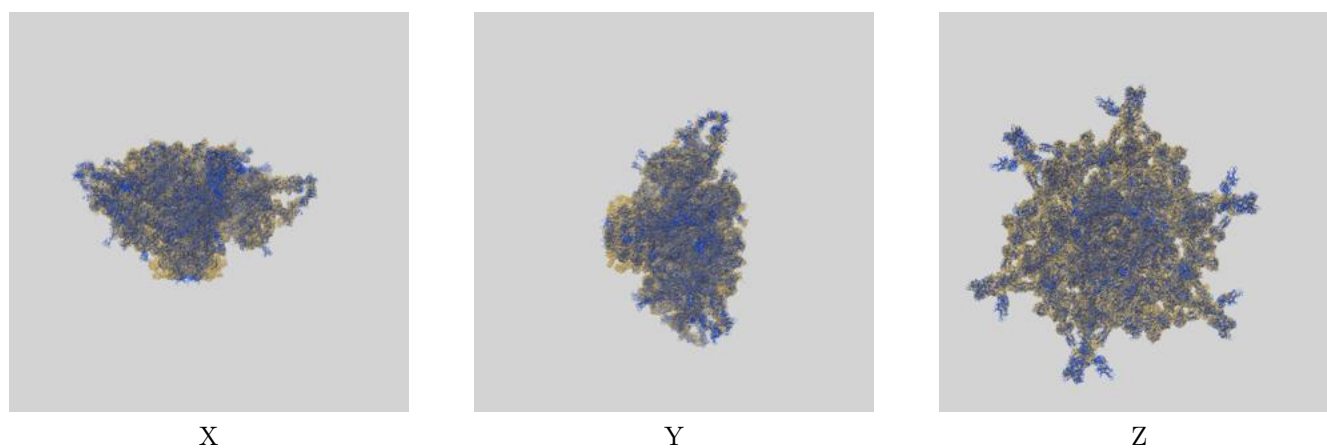
This section contains information regarding the fit between EMDB map EMD-55951 and PDB model 9TIC. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

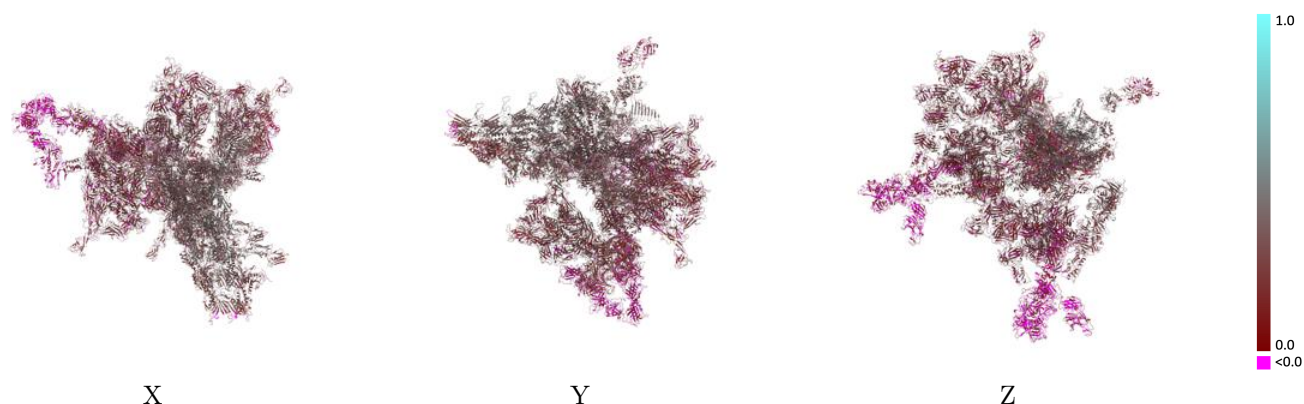


9.1.2 Map-model assembly overlay [i](#)



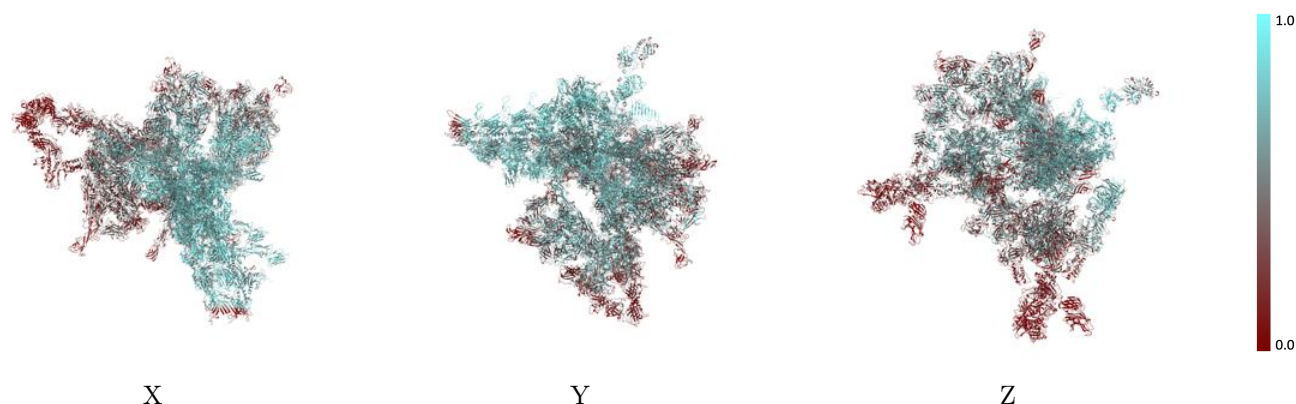
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



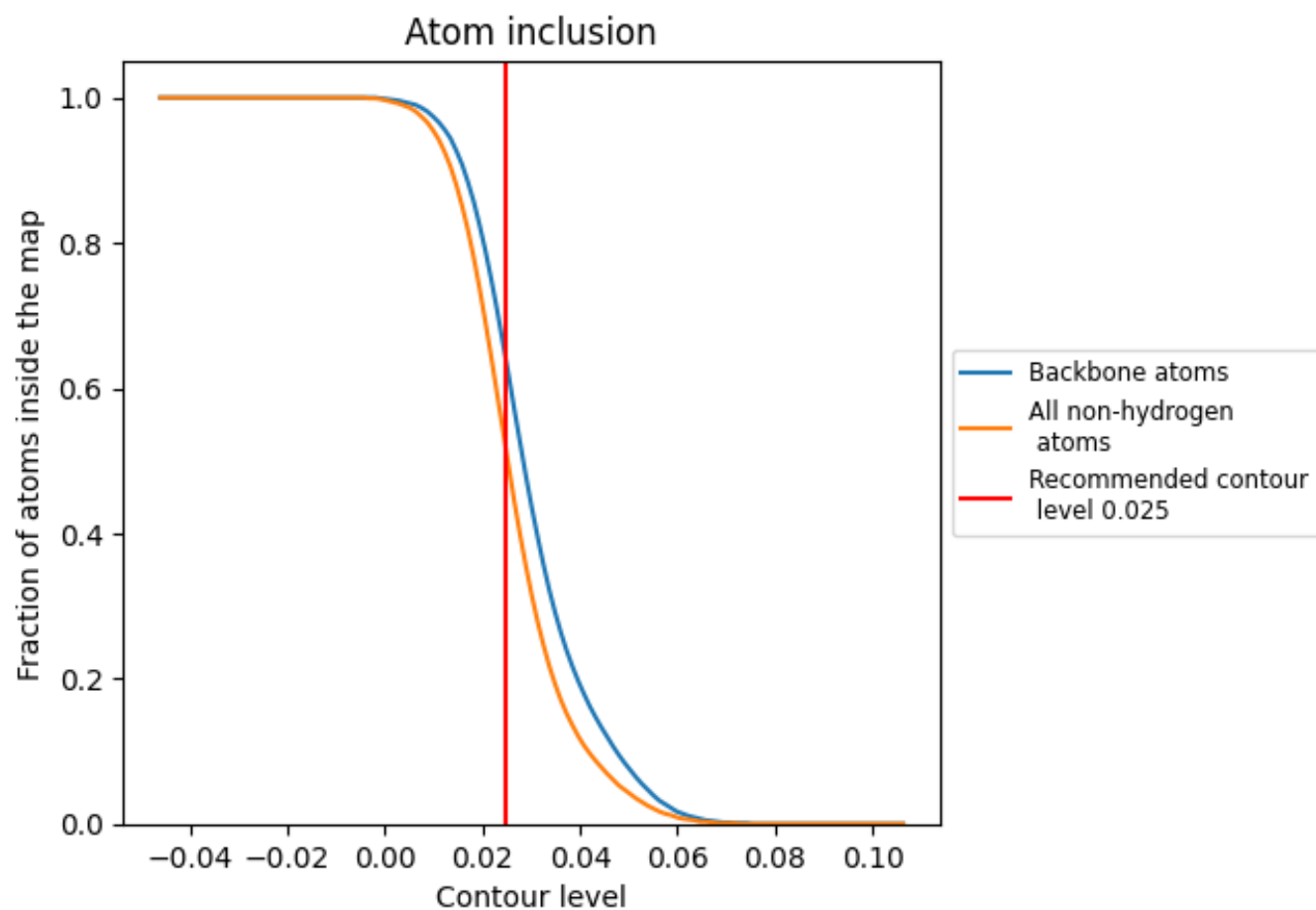
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 51% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5090	 0.2610
0	 0.5570	 0.2920
1	 0.0500	 0.0060
2	 0.5310	 0.2760
3	 0.5190	 0.2780
4	 0.5130	 0.2700
5	 0.3150	 0.2460
6	 0.3190	 0.2390
7	 0.2990	 0.2380
8	 0.5570	 0.2680
9	 0.5740	 0.2960
A	 0.7770	 0.3890
AA	 0.5150	 0.2590
AB	 0.5380	 0.2680
AC	 0.7680	 0.3970
AD	 0.7650	 0.4030
AE	 0.7580	 0.3830
AF	 0.7490	 0.3770
AG	 0.3760	 0.2410
AH	 0.4210	 0.2580
AI	 0.7540	 0.3540
AJ	 0.7510	 0.3580
AK	 0.7320	 0.3480
AL	 0.7370	 0.3420
AM	 0.6250	 0.2600
AN	 0.6200	 0.2590
B	 0.6120	 0.2620
C	 0.7180	 0.3380
D	 0.7400	 0.3590
E	 0.7340	 0.3550
F	 0.7700	 0.3970
G	 0.7710	 0.3900
H	 0.7520	 0.3700
I	 0.7600	 0.3710
J	 0.7550	 0.3680



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Chain	Atom inclusion	Q-score
K	 0.7540	 0.3680
L	 0.7440	 0.3510
M	 0.7620	 0.3520
N	 0.4010	 0.1610
O	 0.4640	 0.1870
P	 0.7080	 0.3200
Q	 0.5970	 0.2150
R	 0.4430	 0.1390
S	 0.3210	 0.0900
T	 0.1940	 0.0790
U	 0.1350	 0.0370
V	 0.0660	 0.0290
W	 0.0540	 0.0210
X	 0.0490	 0.0160
Y	 0.0400	 0.0130
Z	 0.0680	 0.0250
a	 0.4440	 0.2480
b	 0.3440	 0.2360
c	 0.3770	 0.2460
d	 0.4910	 0.2700
e	 0.7270	 0.3170
f	 0.6690	 0.2650
g	 0.6200	 0.2290
h	 0.4710	 0.1450
i	 0.4150	 0.1110
j	 0.2530	 0.0900
k	 0.1510	 0.0490
l	 0.0890	 0.0370
m	 0.1070	 0.0230
n	 0.1010	 0.0420
o	 0.1670	 0.0280
p	 0.1130	 0.0340
q	 0.5160	 0.2770
r	 0.5390	 0.2820
s	 0.5230	 0.2730
t	 0.5170	 0.2780
u	 0.5180	 0.2710
v	 0.5820	 0.2910
w	 0.5640	 0.3090
x	 0.5700	 0.3120
y	 0.5790	 0.3190
z	 0.4870	 0.2460