



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 11:46 PM UTC

PDB ID : 6Q1F / pdb_00006q1f
EMDB ID : EMD-20557
Title : Atomic structure of the Human Herpesvirus 6B Capsid and Capsid-Associated Tegument Complexes
Authors : Zhang, Y.B.; Liu, W.; Li, Z.H.; Kumar, V.; Alvarez-Cabrera, A.L.; Leibovitch, E.; Cui, Y.X.; Mei, Y.; Bi, G.Q.; Jacobson, S.; Zhou, Z.H.
Deposited on : 2019-08-03
Resolution : 9.00 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:

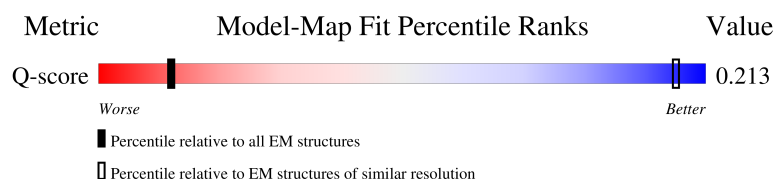
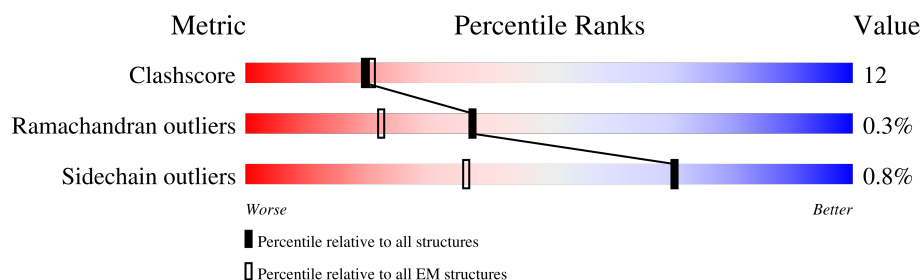
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

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 9.00 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	257 (8.50 - 9.50)

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	A	1345	39% 79% 20% .
1	B	1345	41% 78% 22%
1	C	1345	42% 80% 18% ..
1	D	1345	38% 79% 20% .

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Mol	Chain	Length	Quality of chain
1	E	1345	
1	F	1345	
1	G	1345	
1	H	1345	
1	I	1345	
1	q	1345	
1	r	1345	
1	s	1345	
1	t	1345	
1	u	1345	
1	v	1345	
1	w	1345	
2	e	858	
2	f	858	
2	g	858	
2	h	858	
2	i	858	
2	j	858	
2	k	858	
2	l	858	
2	m	858	
2	n	858	
2	o	858	
2	p	858	
3	1	89	

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Mol	Chain	Length	Quality of chain
3	2	89	
3	3	89	
3	4	89	
3	J	89	
3	K	89	
3	L	89	
3	M	89	
3	N	89	
3	O	89	
3	P	89	
3	Q	89	
3	R	89	
3	x	89	
3	y	89	
3	z	89	
4	5	299	
4	S	299	
4	T	299	
4	U	299	
4	V	299	
5	6	296	
5	7	296	
5	W	296	
5	X	296	
5	Y	296	

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Mol	Chain	Length	Quality of chain
5	Z	296	46% 74% 23%
5	a	296	48% 74% 23%
5	b	296	54% 75% 23%
5	c	296	46% 76% 22%
5	d	296	47% 69% 28%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 238552 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	B	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	C	1325	Total	C	N	O	S	0	0
			10552	6709	1792	1991	60		
1	D	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	E	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	F	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	G	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	H	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	I	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	q	1296	Total	C	N	O	S	0	0
			10313	6561	1751	1942	59		
1	r	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	s	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	t	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	u	1344	Total	C	N	O	S	0	0
			10690	6797	1814	2018	61		
1	v	1301	Total	C	N	O	S	0	0
			10331	6564	1759	1948	60		
1	w	1248	Total	C	N	O	S	0	0
			9933	6324	1691	1860	58		

- Molecule 2 is a protein called Large structural phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	e	269	Total	C	N	O	S	0	0
			2224	1417	376	426	5		
2	f	269	Total	C	N	O	S	0	0
			2224	1417	376	426	5		
2	g	269	Total	C	N	O	S	0	0
			2224	1417	376	426	5		
2	h	269	Total	C	N	O	S	0	0
			2224	1417	376	426	5		
2	i	269	Total	C	N	O	S	0	0
			2224	1417	376	426	5		
2	j	269	Total	C	N	O	S	0	0
			2224	1417	376	426	5		
2	k	269	Total	C	N	O	S	0	0
			2224	1417	376	426	5		
2	l	269	Total	C	N	O	S	0	0
			2224	1417	376	426	5		
2	m	269	Total	C	N	O	S	0	0
			2224	1417	376	426	5		
2	n	269	Total	C	N	O	S	0	0
			2224	1417	376	426	5		
2	o	269	Total	C	N	O	S	0	0
			2224	1417	376	426	5		
2	p	269	Total	C	N	O	S	0	0
			2224	1417	376	426	5		

- Molecule 3 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	K	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	L	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	M	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	N	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	O	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	P	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	Q	61	Total	C	N	O	S	0	0
			483	308	89	83	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	x	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	y	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	z	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	1	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	2	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	3	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	4	58	Total	C	N	O	S	0	0
			456	292	85	76	3		

- Molecule 4 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	251	Total	C	N	O	S	0	0
			2023	1306	327	376	14		
4	S	299	Total	C	N	O	S	0	0
			2398	1542	395	446	15		
4	T	299	Total	C	N	O	S	0	0
			2398	1542	395	446	15		
4	U	299	Total	C	N	O	S	0	0
			2398	1542	395	446	15		
4	V	299	Total	C	N	O	S	0	0
			2398	1542	395	446	15		

- Molecule 5 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	282	Total	C	N	O	S	0	0
			2226	1422	370	415	19		
5	W	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		
5	X	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		
5	Y	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		

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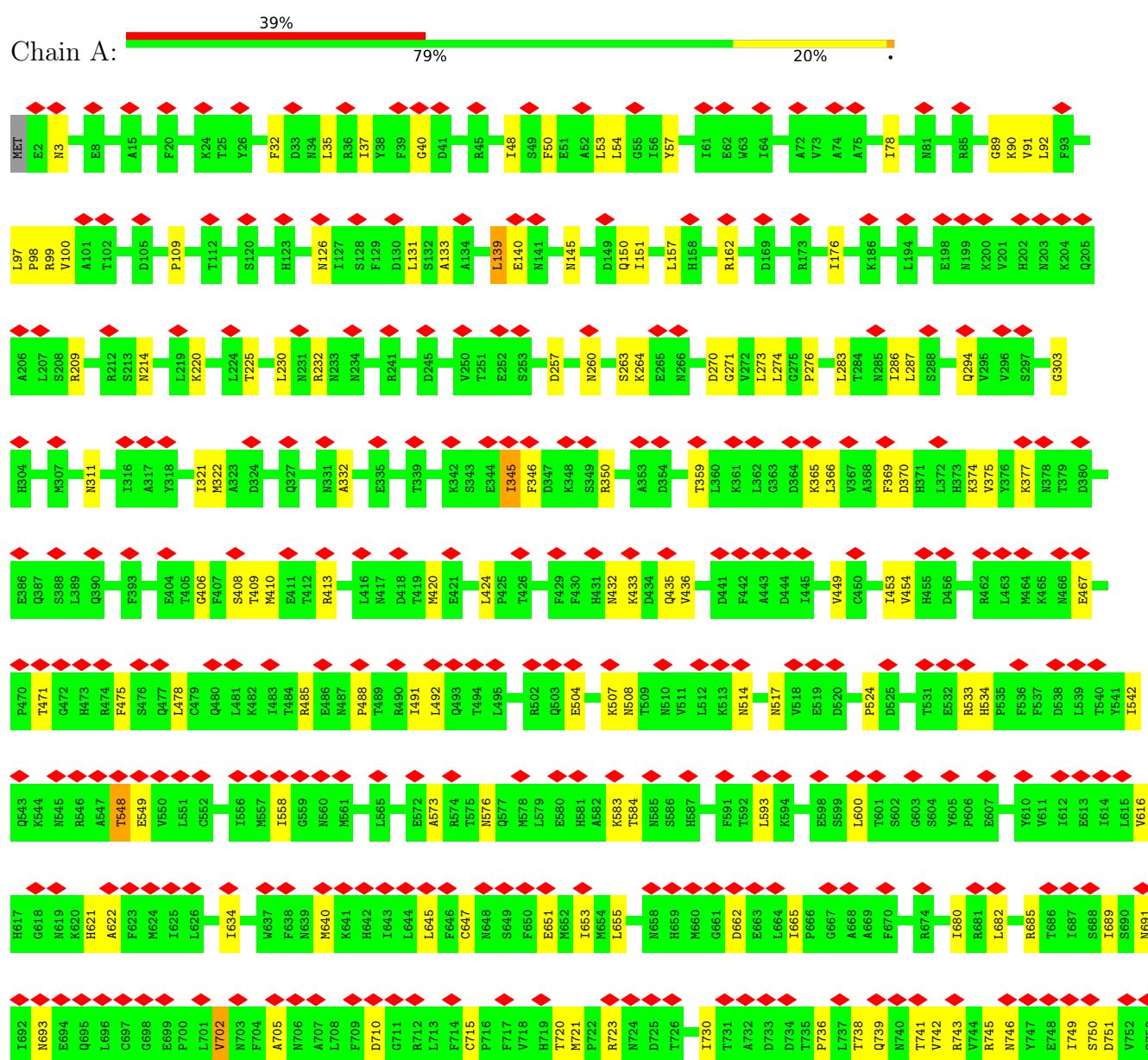
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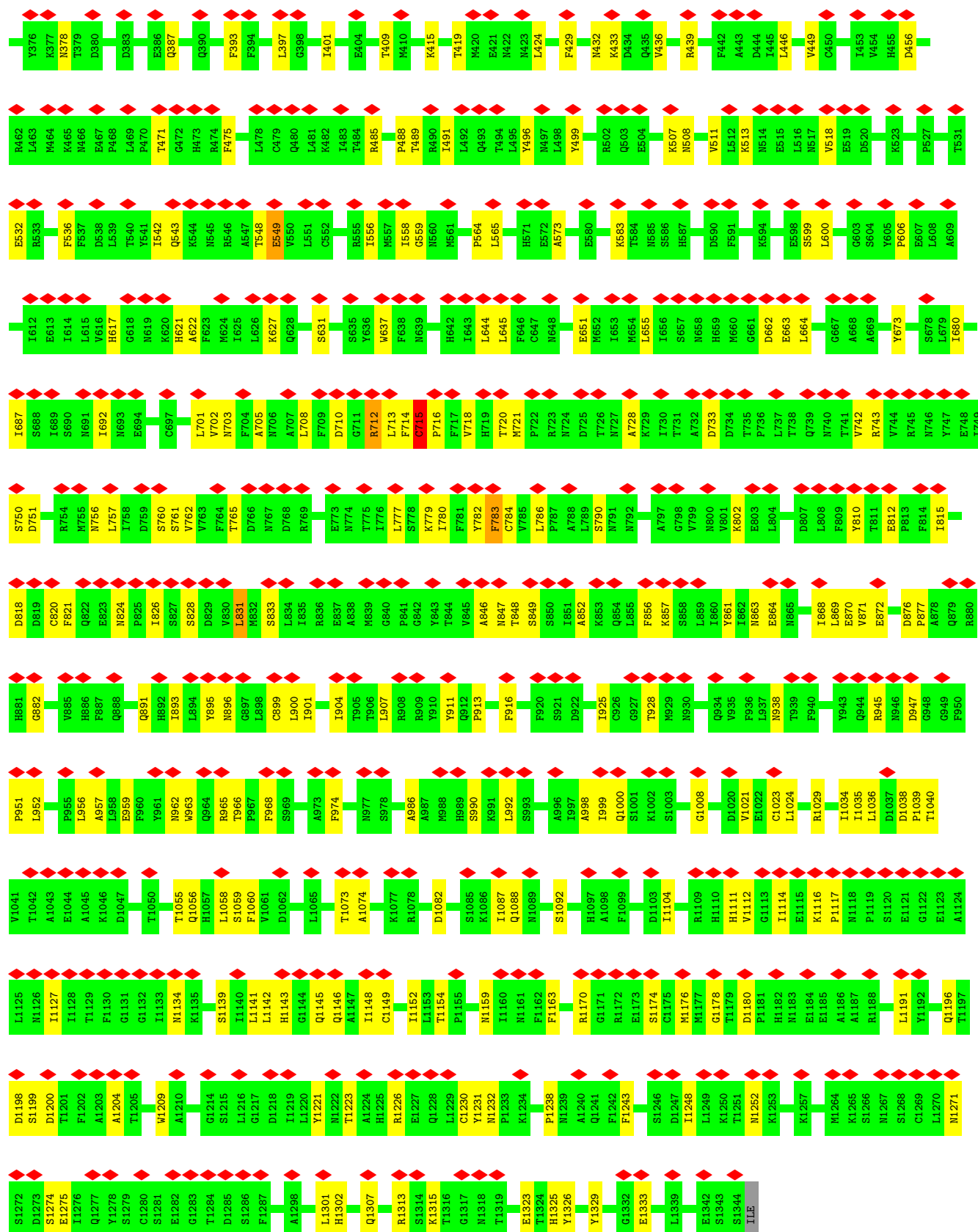
Mol	Chain	Residues	Atoms					AltConf	Trace
5	Z	296	Total 2337	C 1486	N 393	O 437	S 21	0	0
5	7	296	Total 2337	C 1486	N 393	O 437	S 21	0	0
5	a	295	Total 2329	C 1481	N 392	O 436	S 20	0	0
5	b	295	Total 2329	C 1481	N 392	O 436	S 20	0	0
5	c	295	Total 2329	C 1481	N 392	O 436	S 20	0	0
5	d	295	Total 2329	C 1481	N 392	O 436	S 20	0	0

3 Residue-property plots

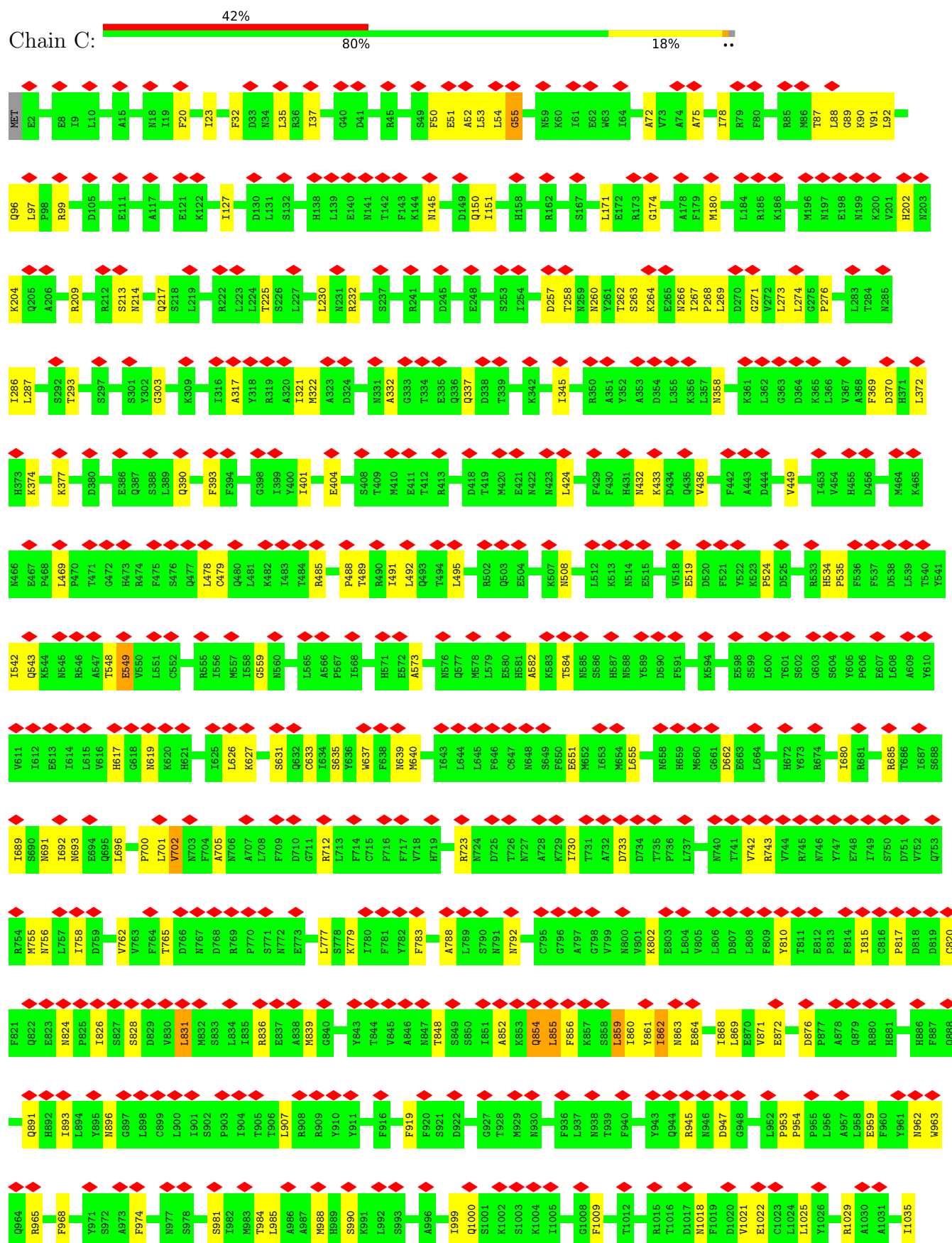
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

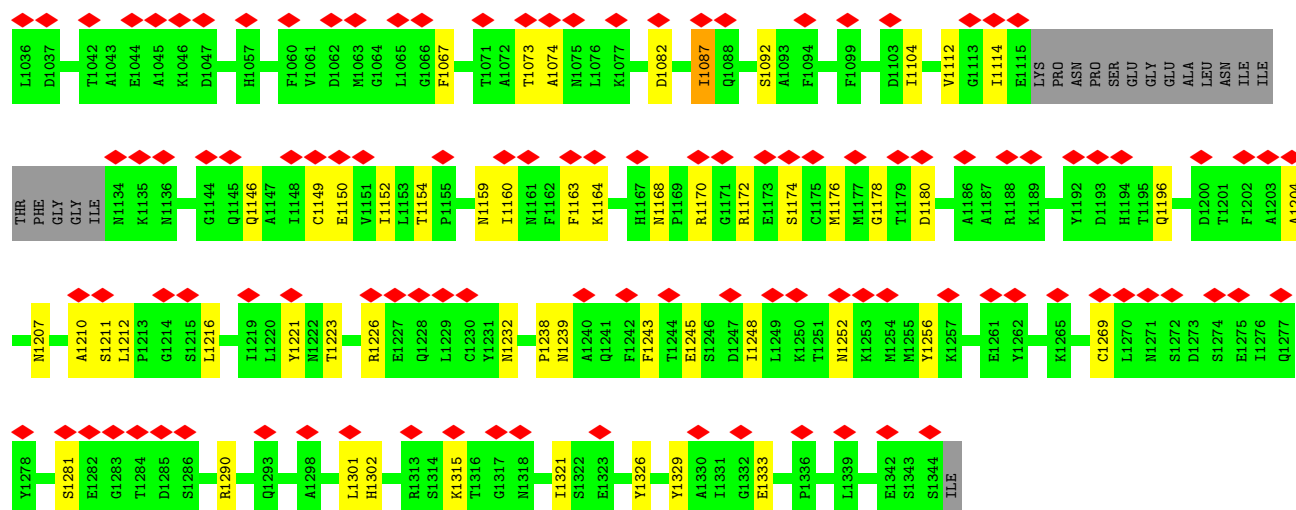
- Molecule 1: Major capsid protein



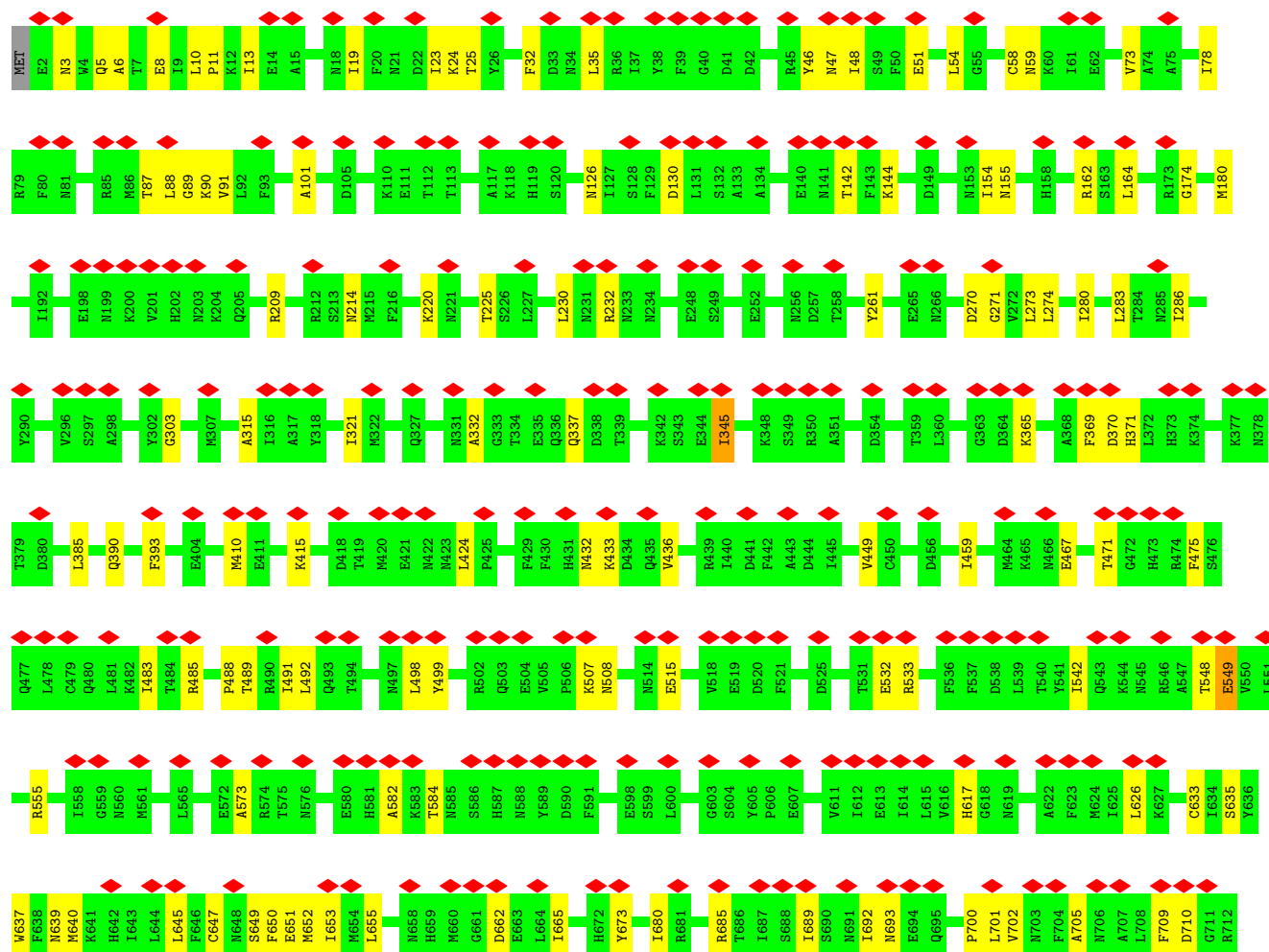
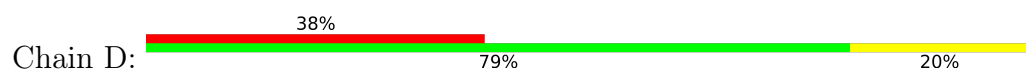


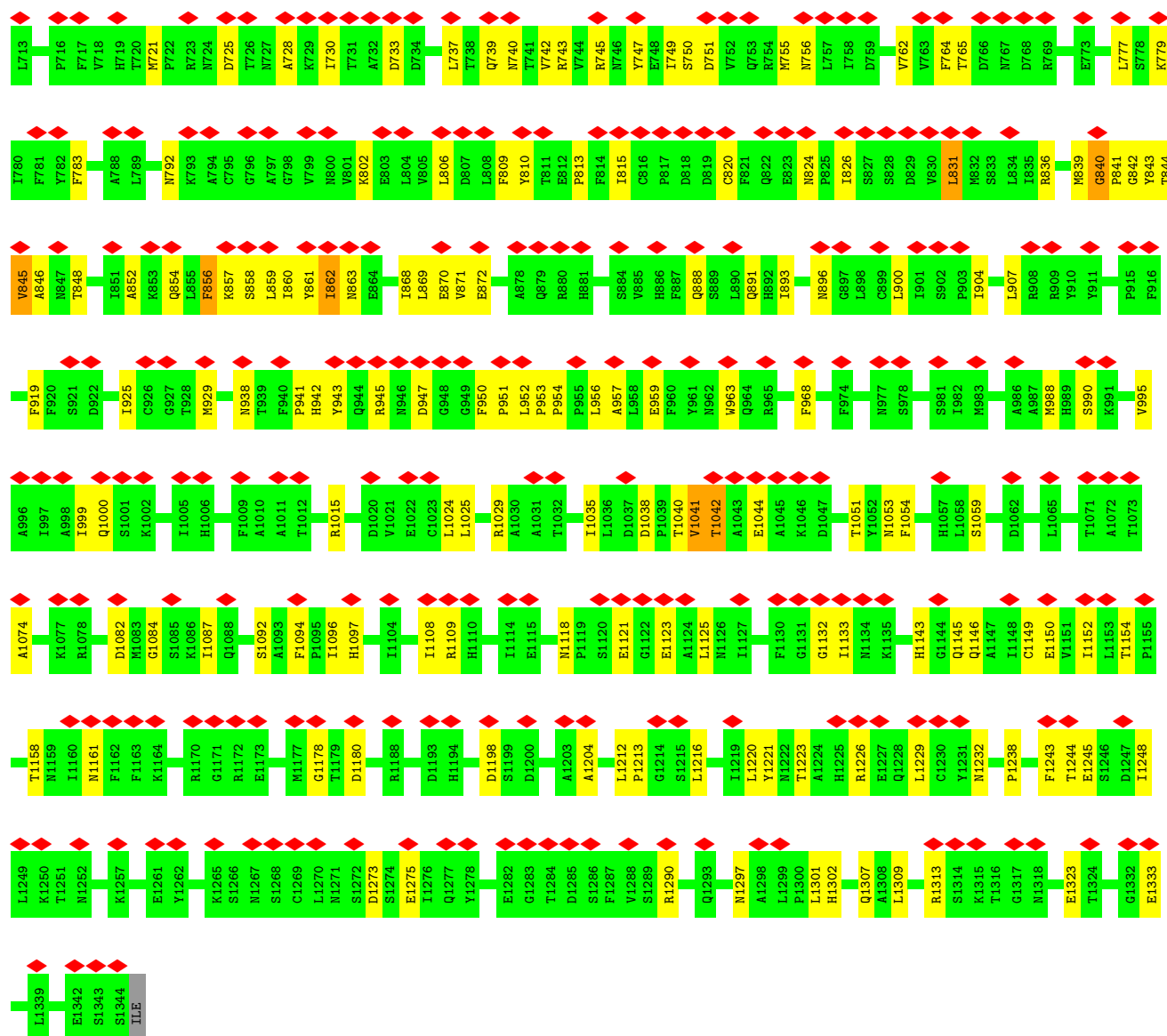
• Molecule 1: Major capsid protein



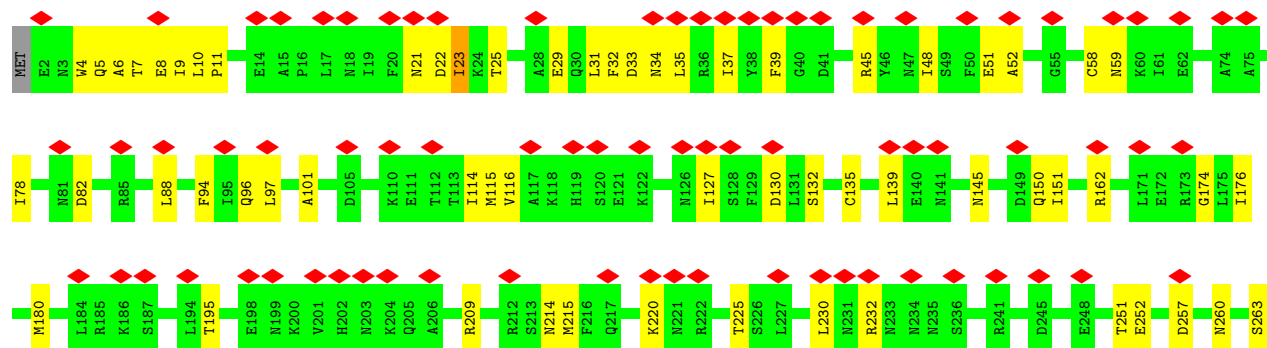
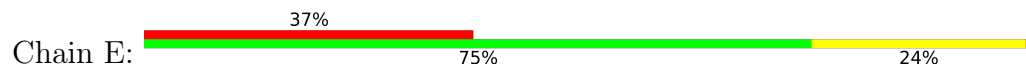


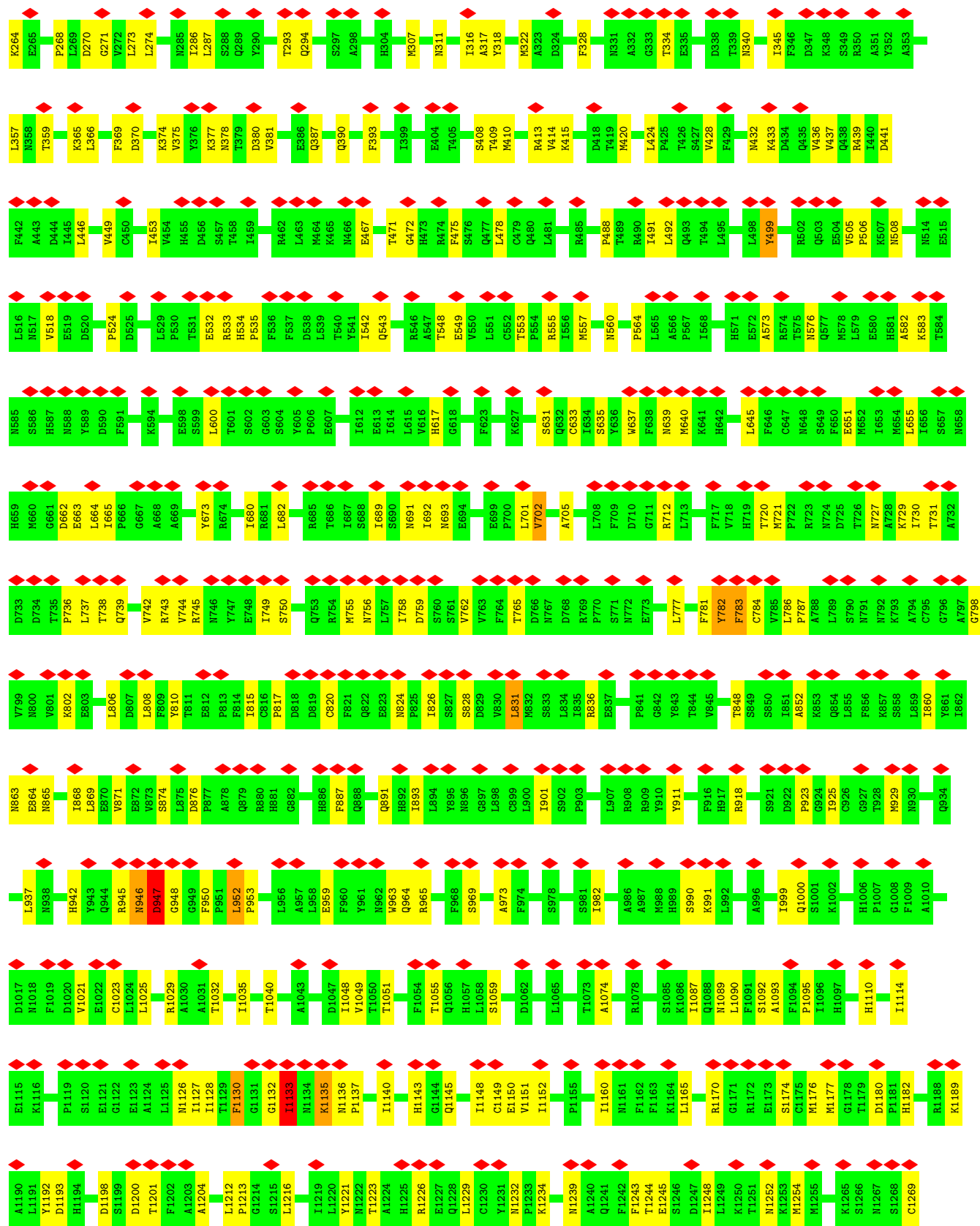
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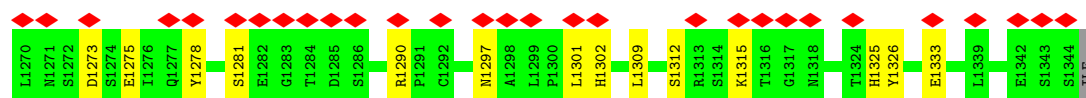




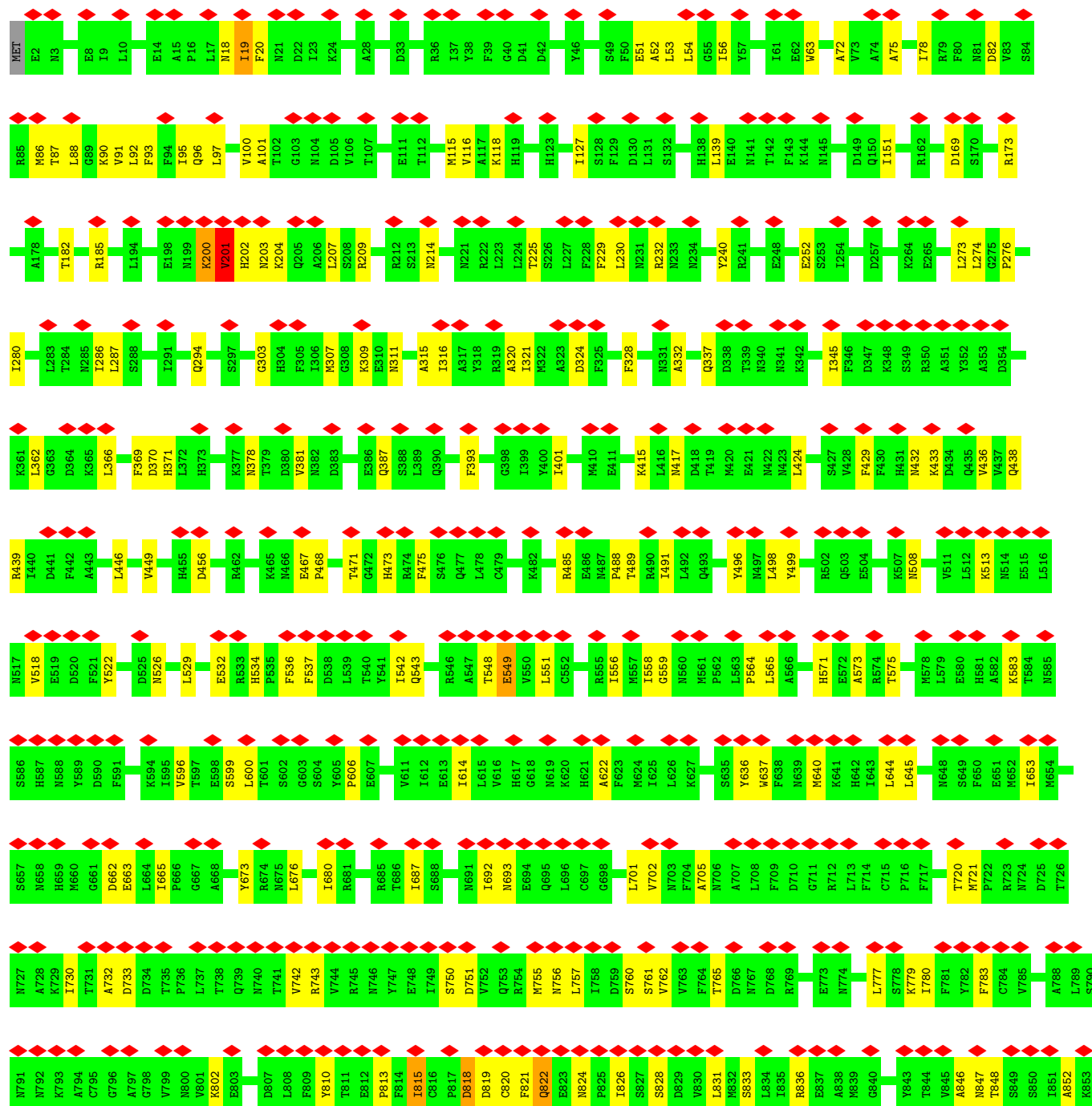
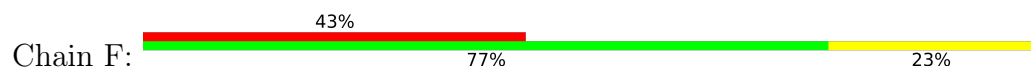
• Molecule 1: Major capsid protein

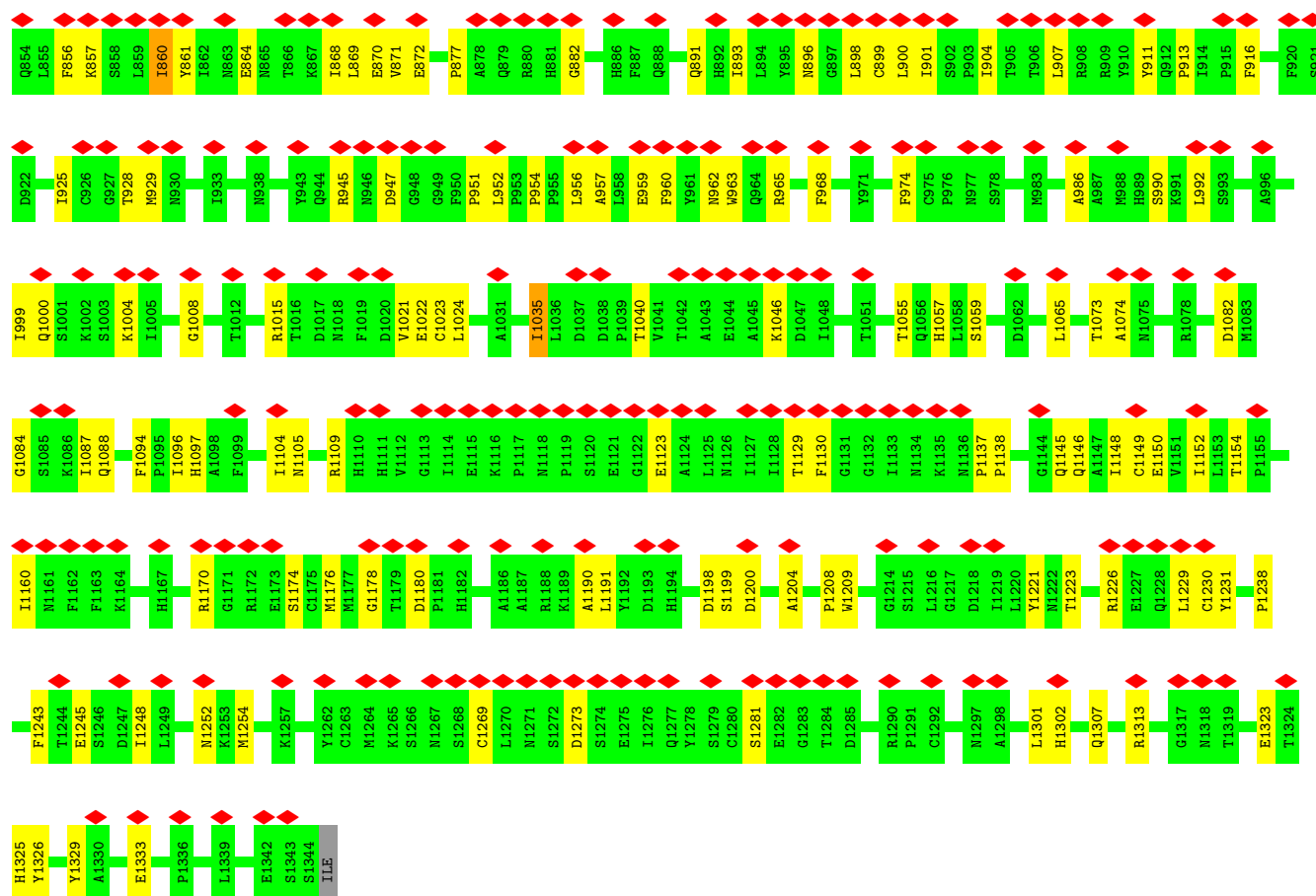




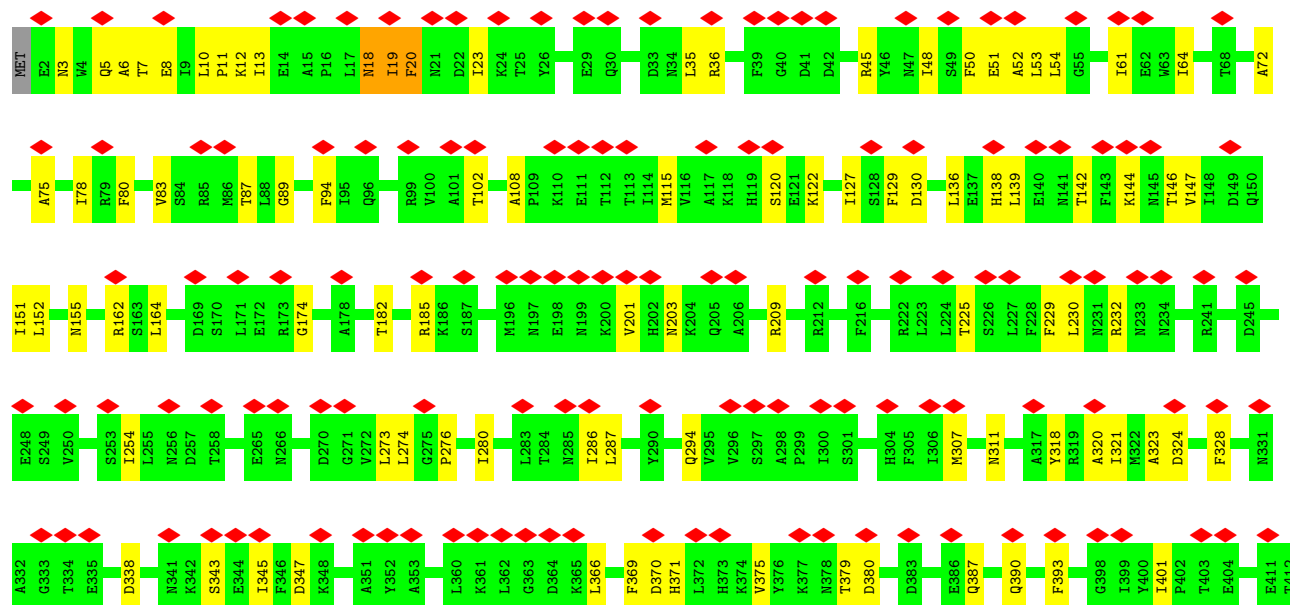
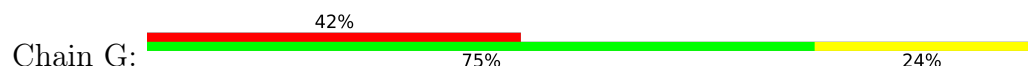


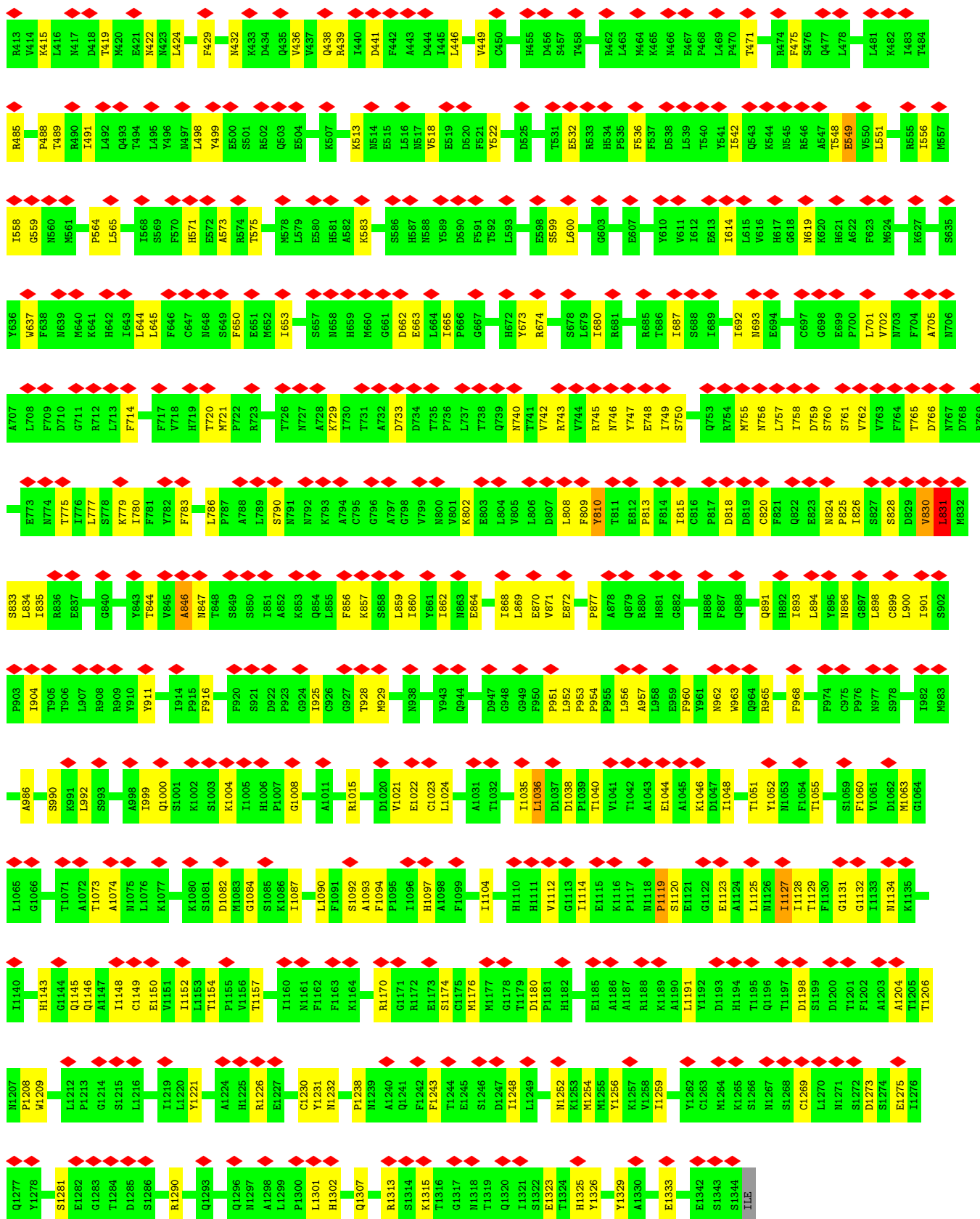
• Molecule 1: Major capsid protein





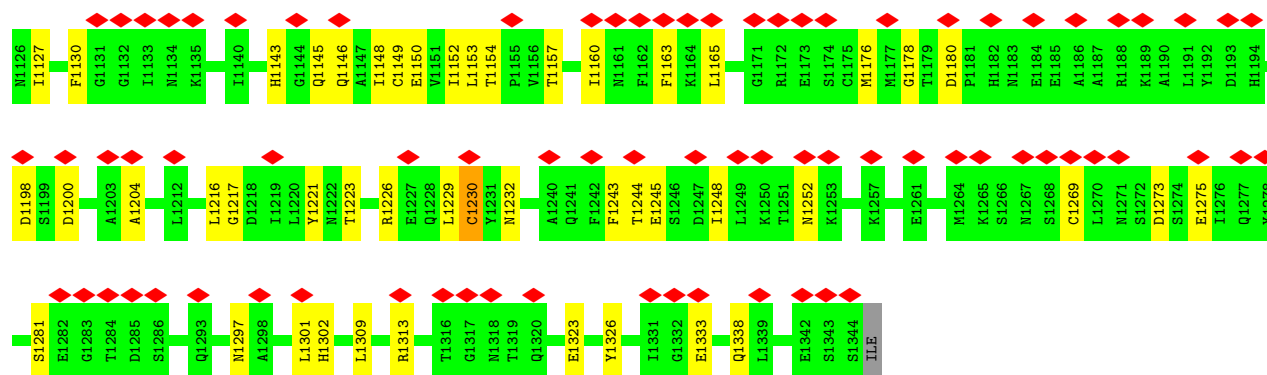
• Molecule 1: Major capsid protein



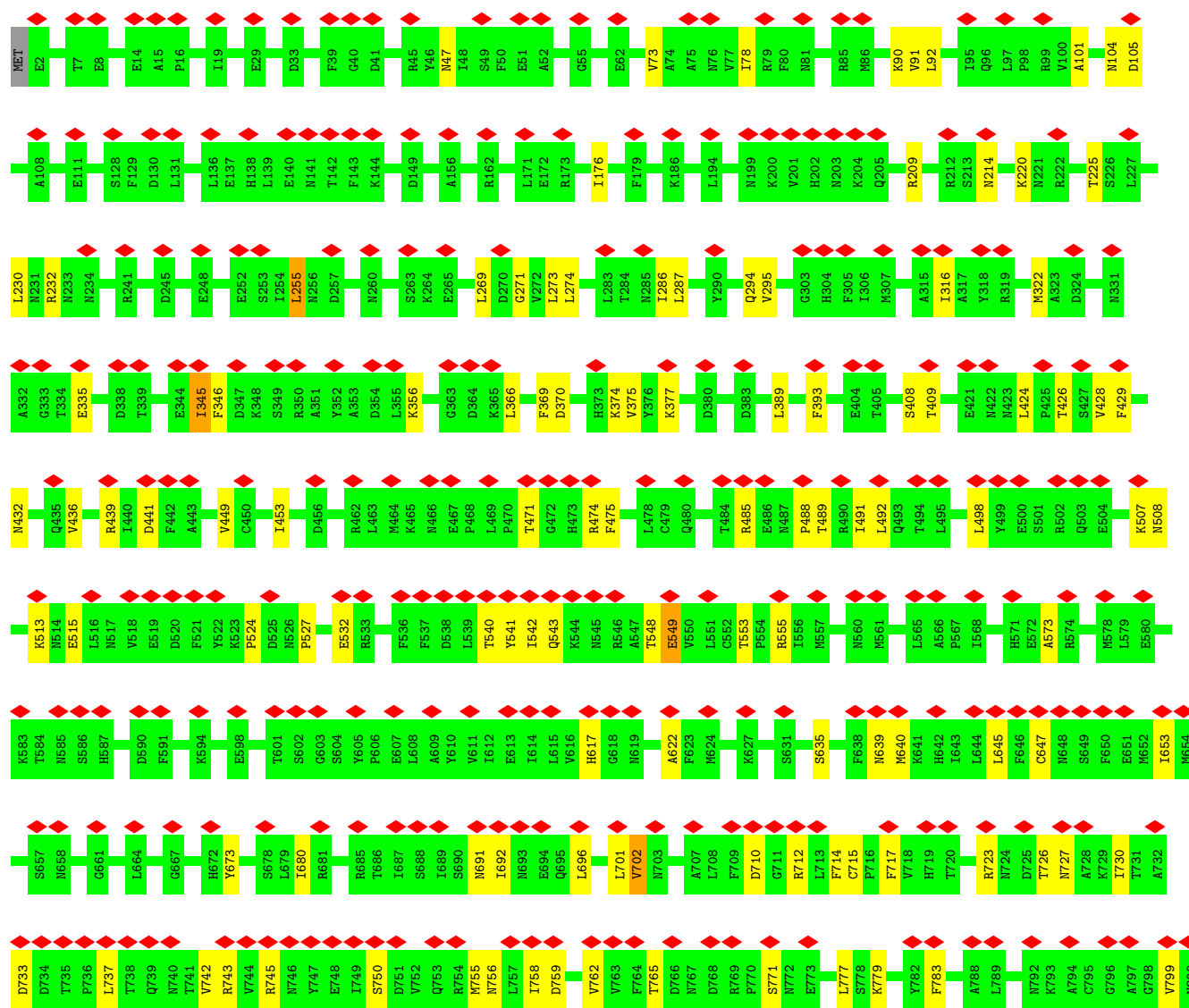
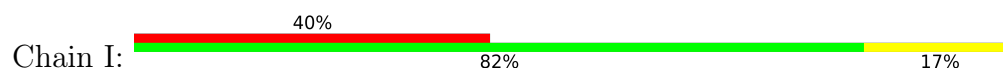


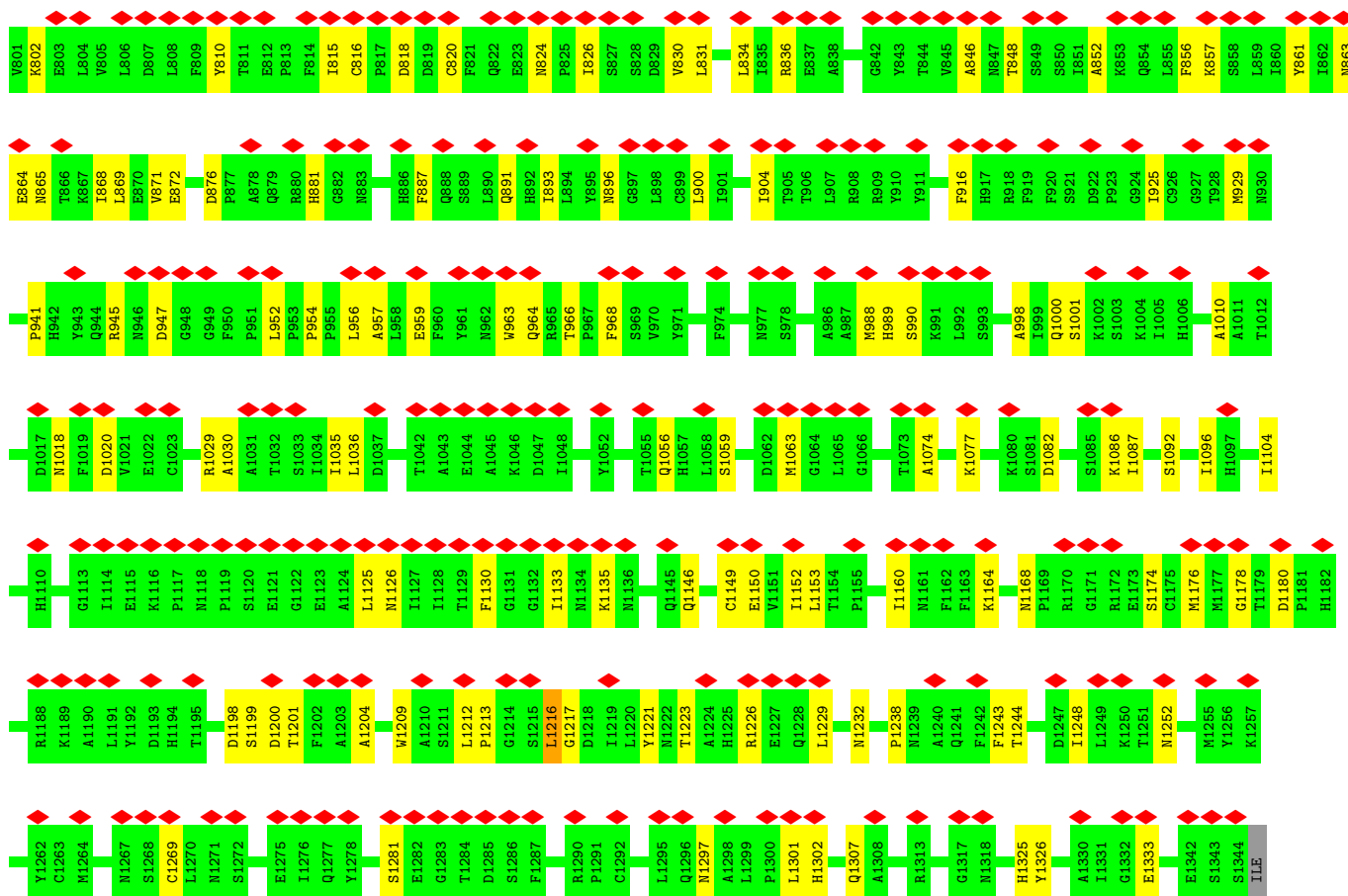
• Molecule 1: Major capsid protein



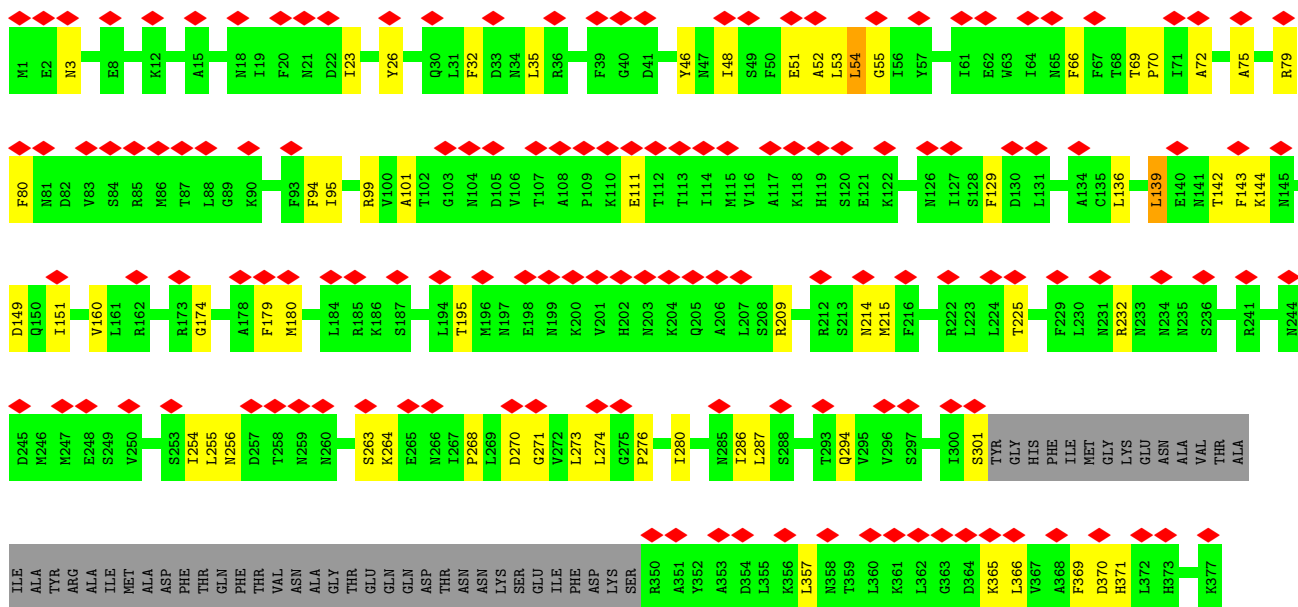
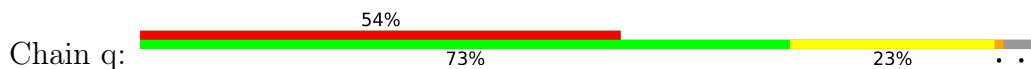


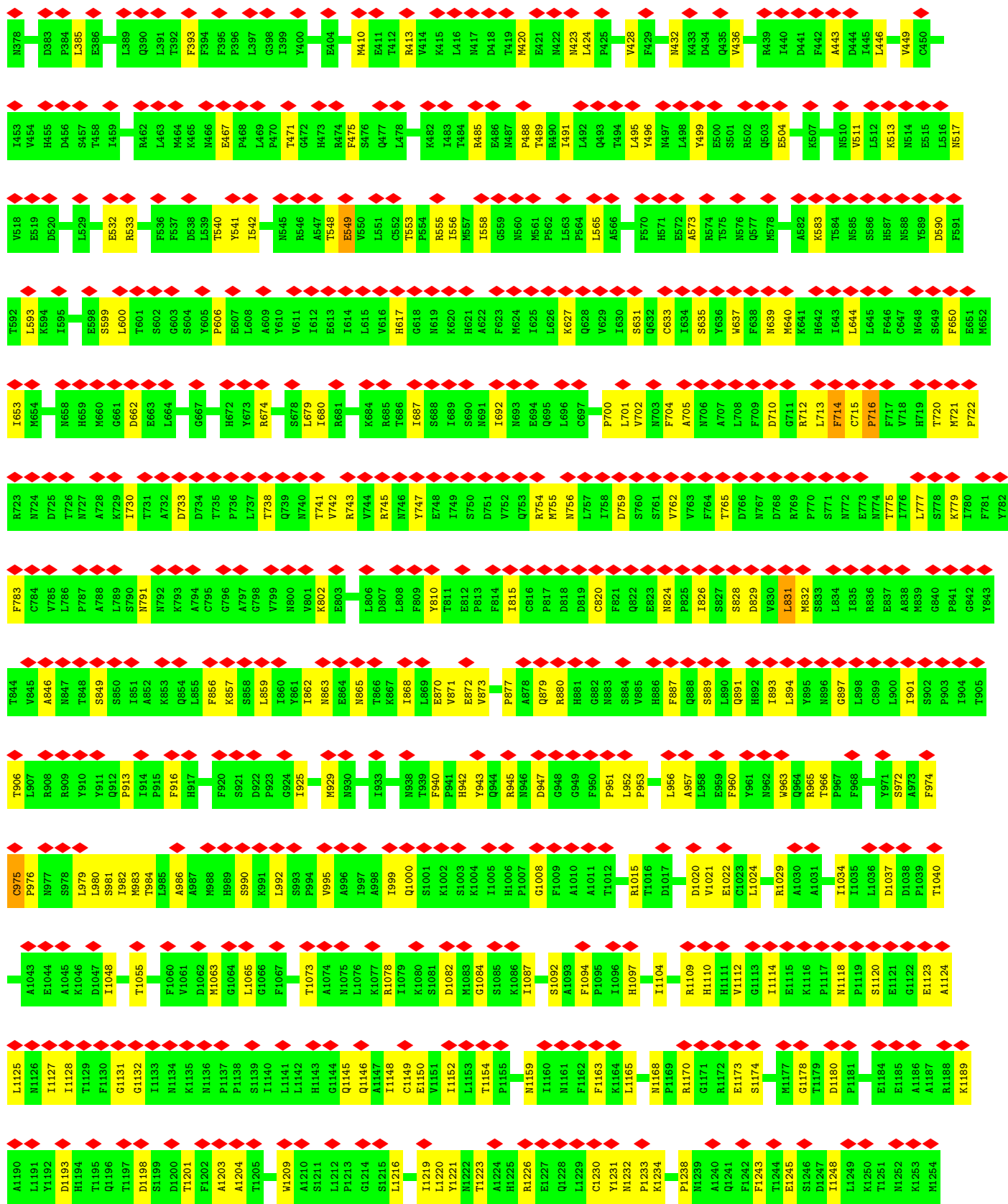
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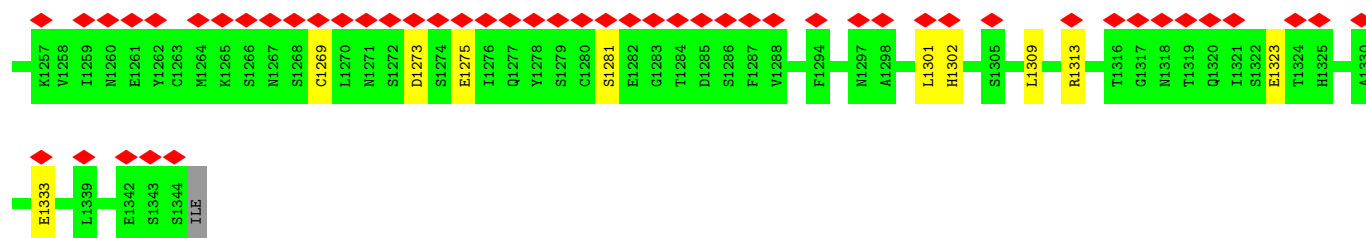




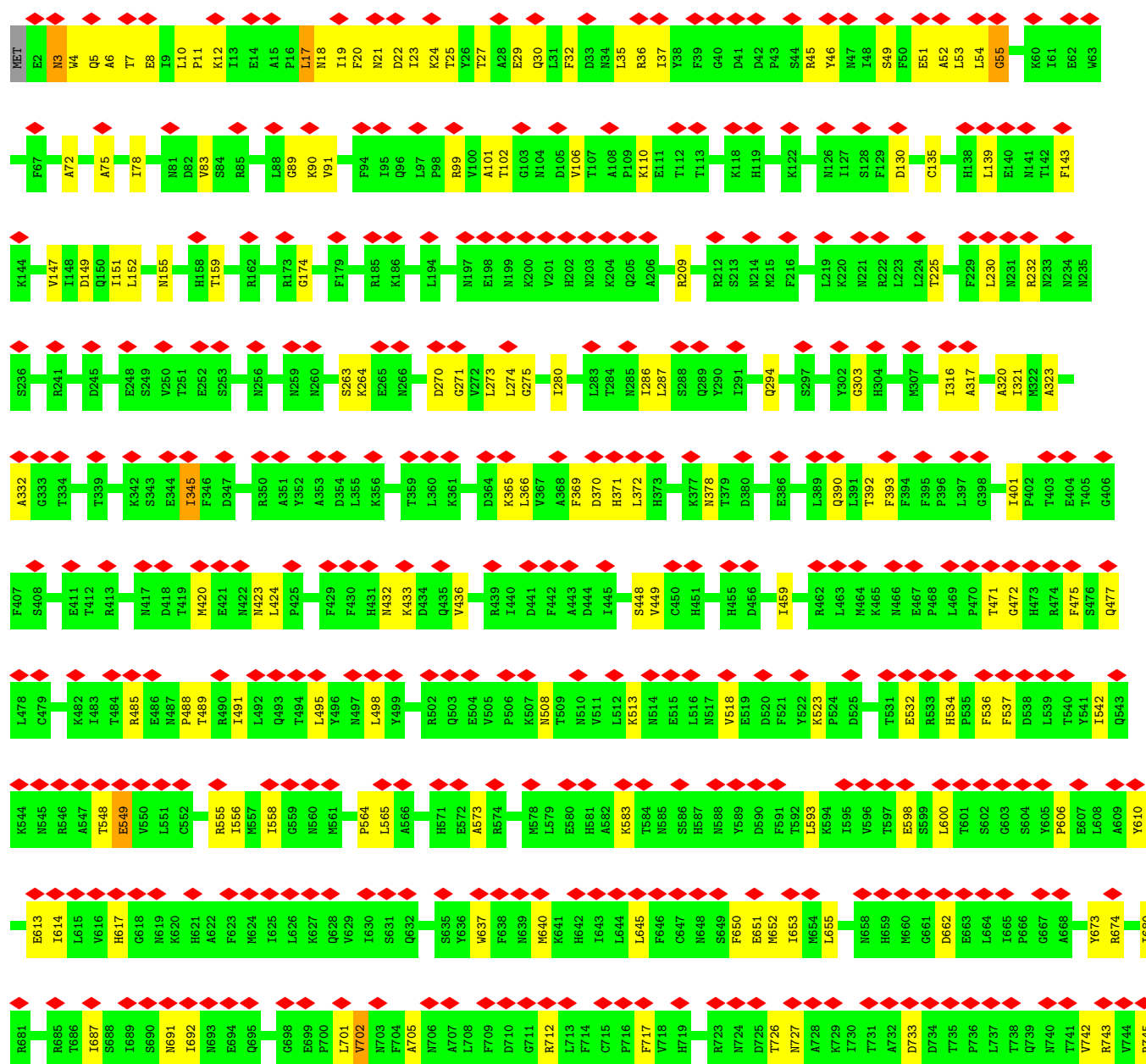
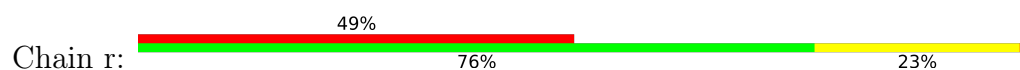
• Molecule 1: Major capsid protein

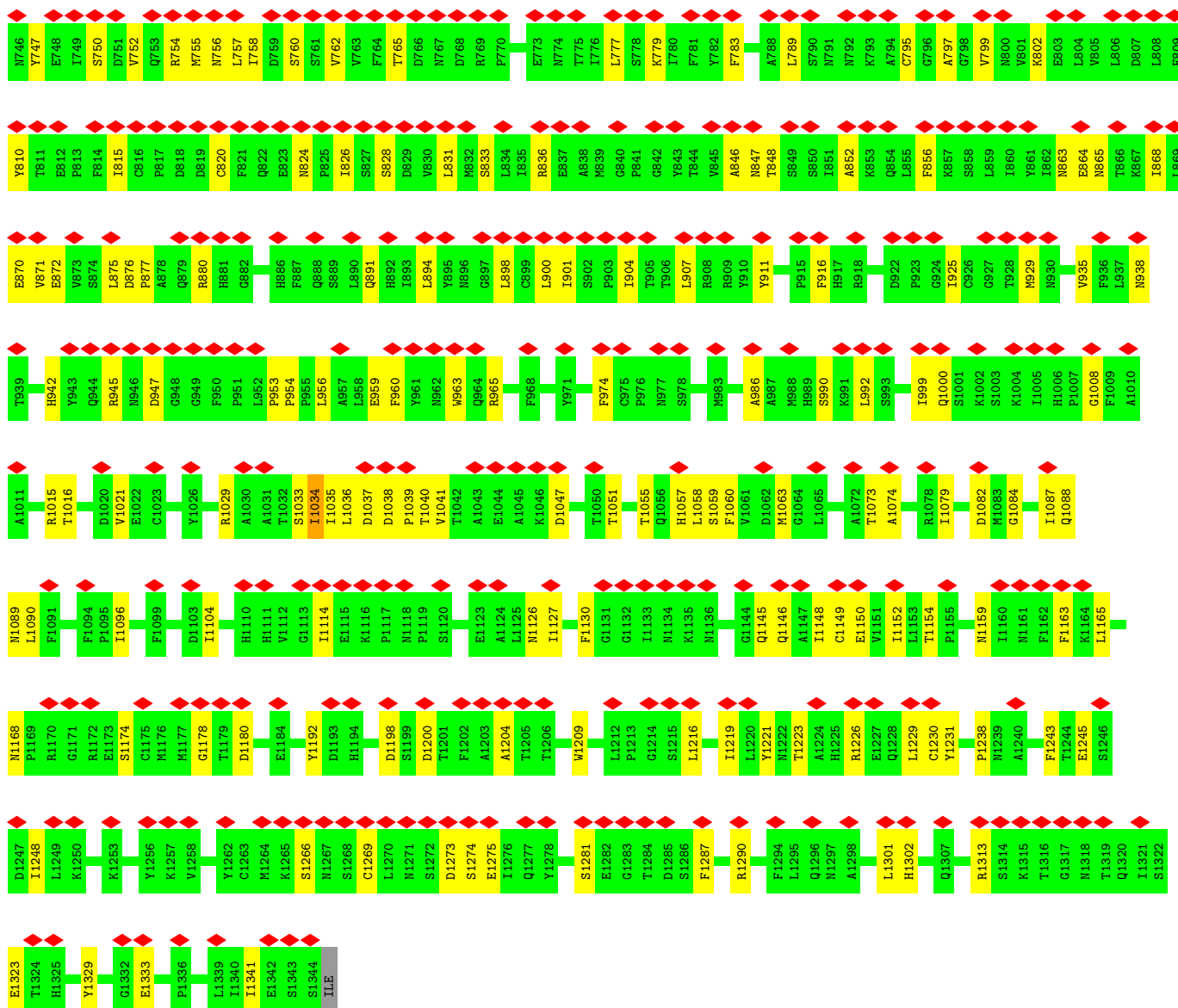




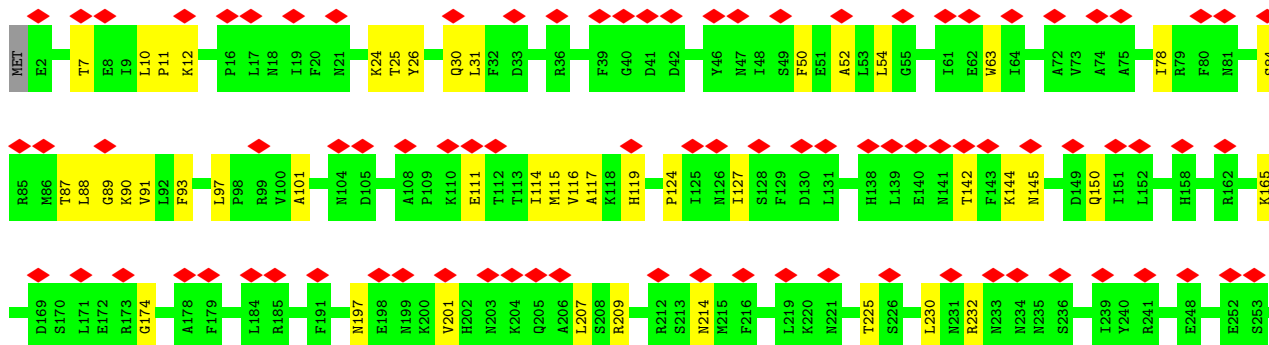
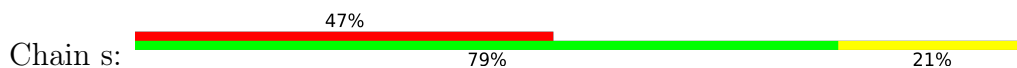


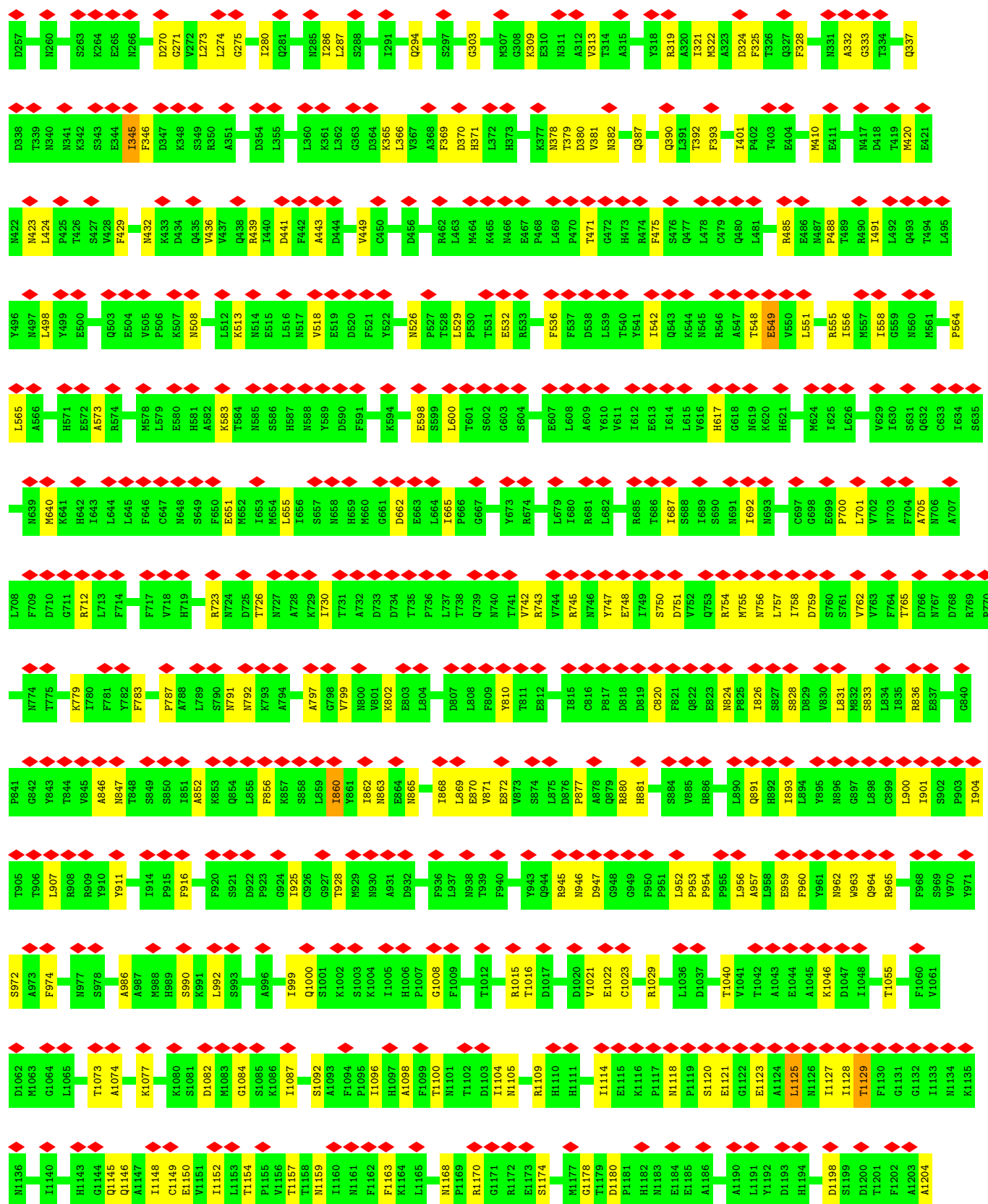
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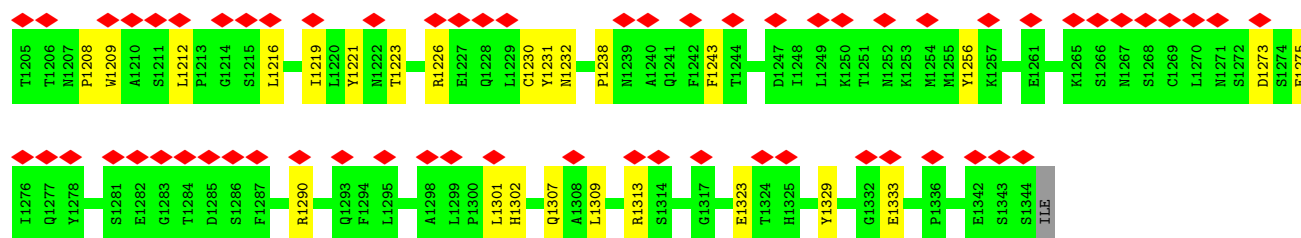




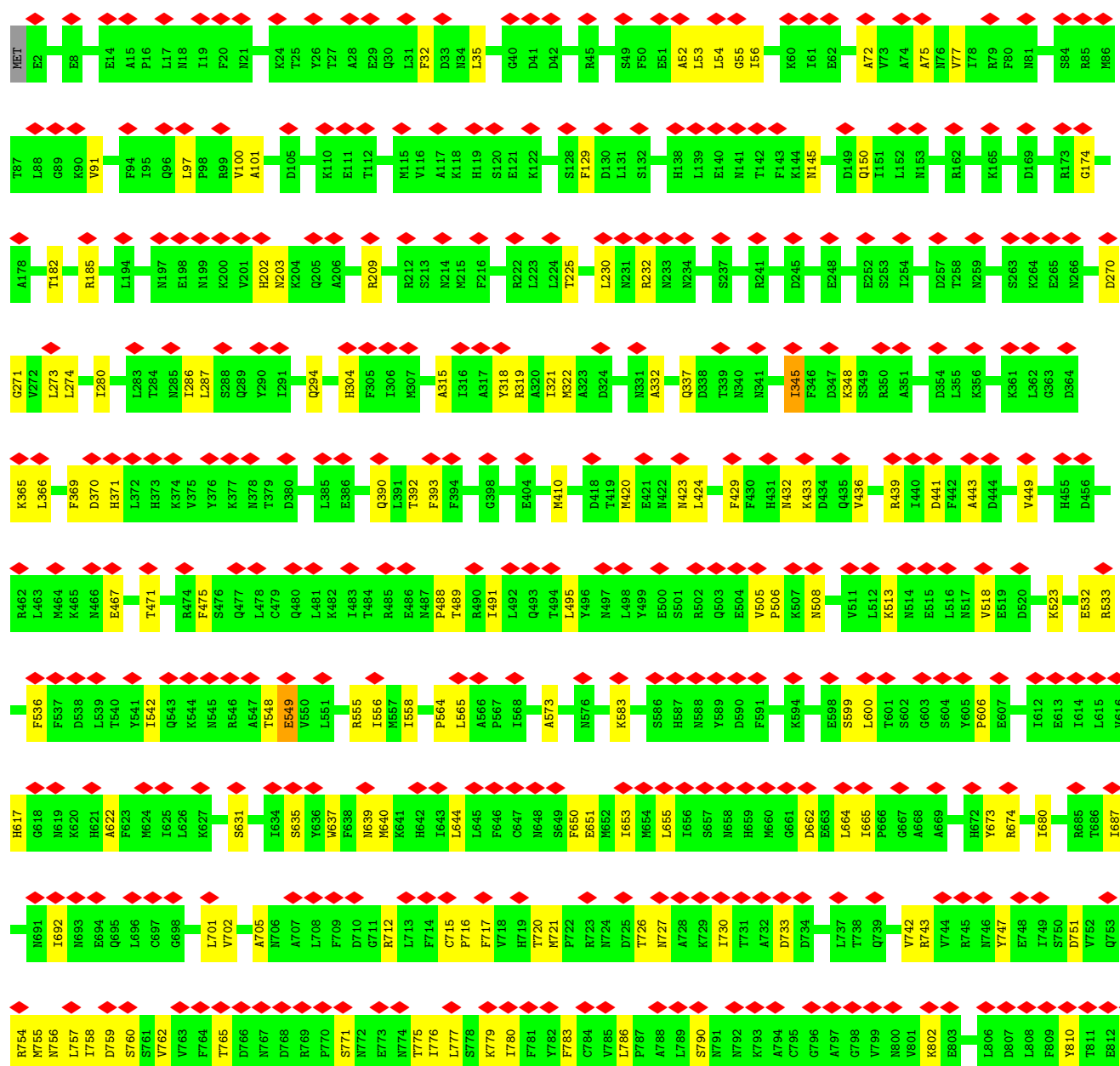
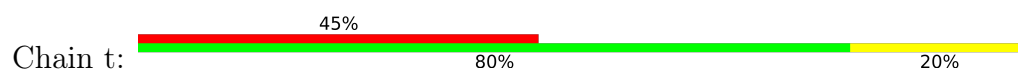
• Molecule 1: Major capsid protein

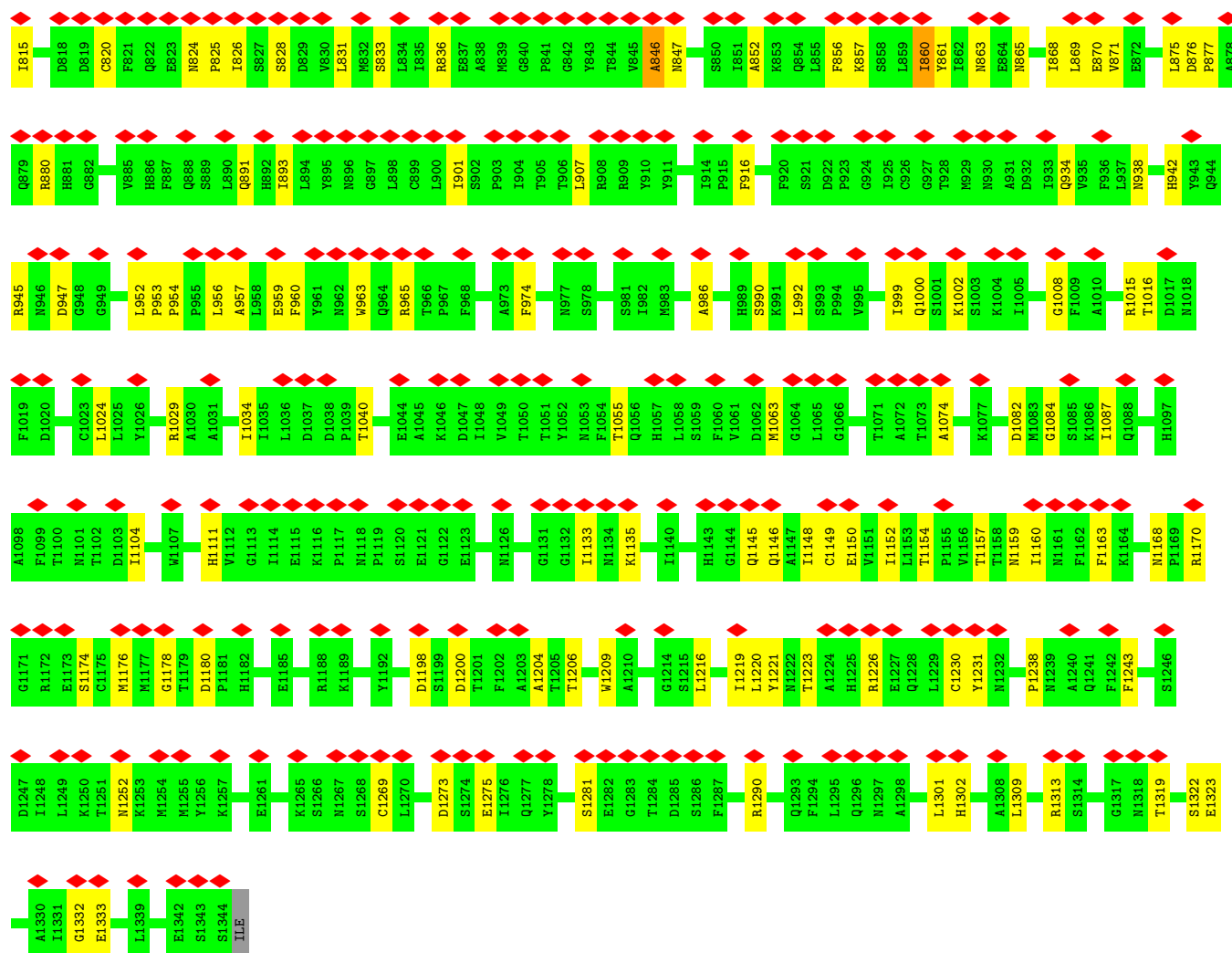




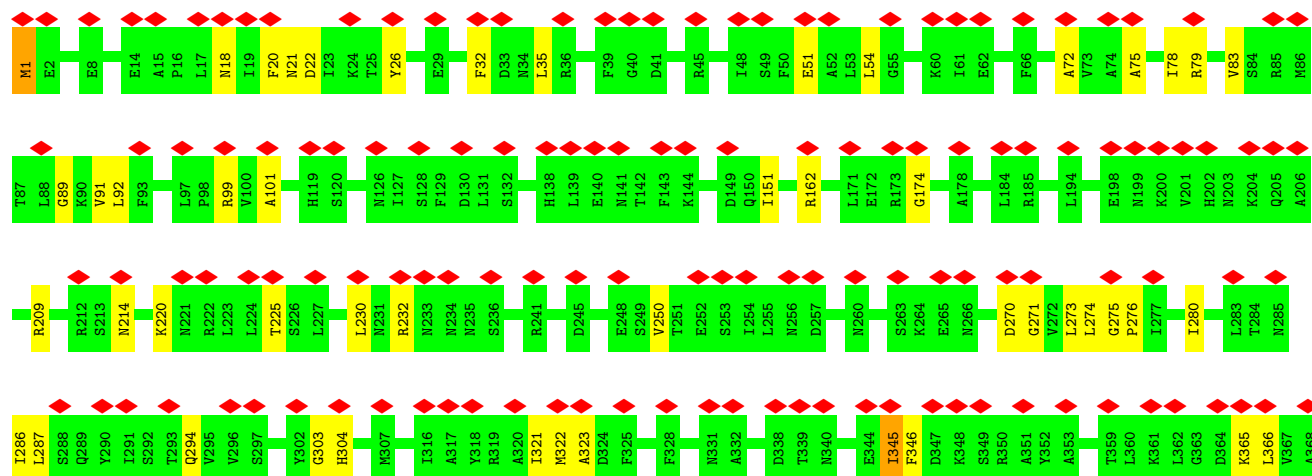
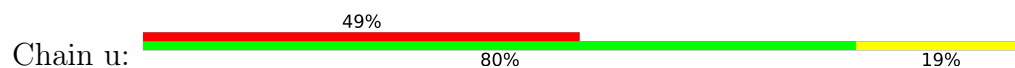


• Molecule 1: Major capsid protein

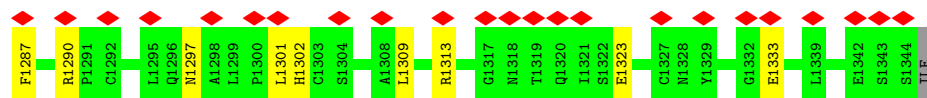




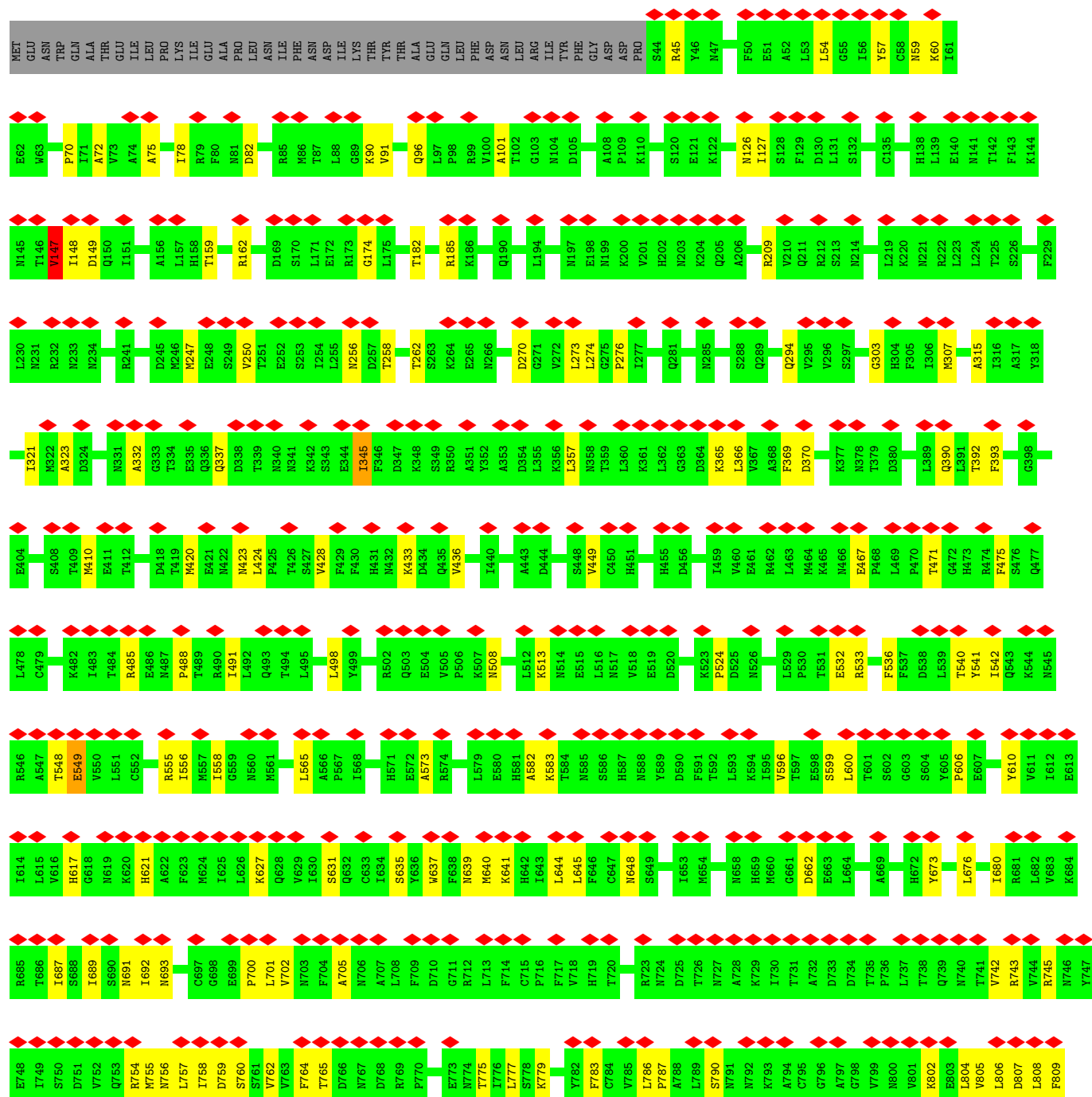
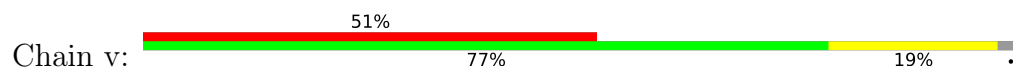
• Molecule 1: Major capsid protein

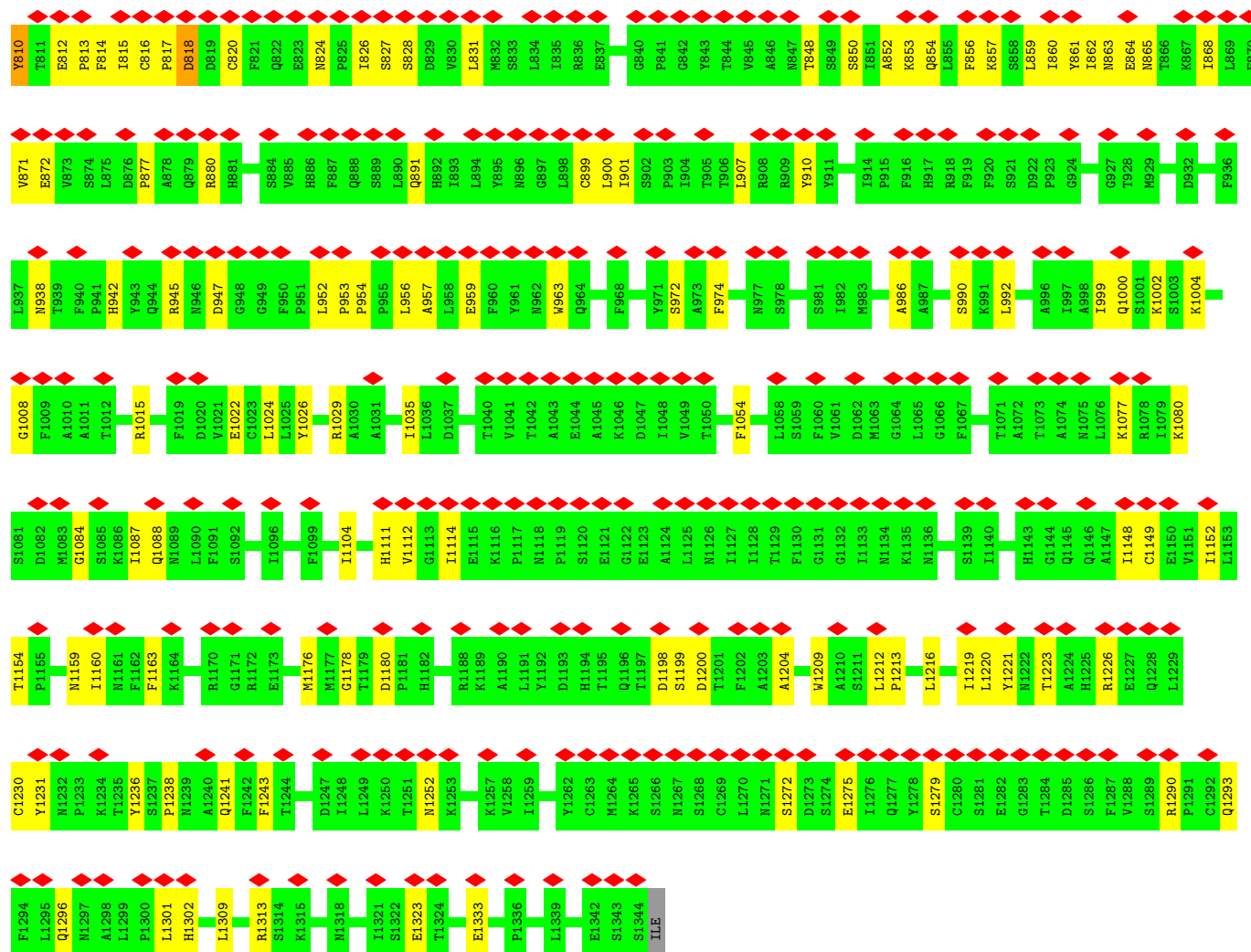


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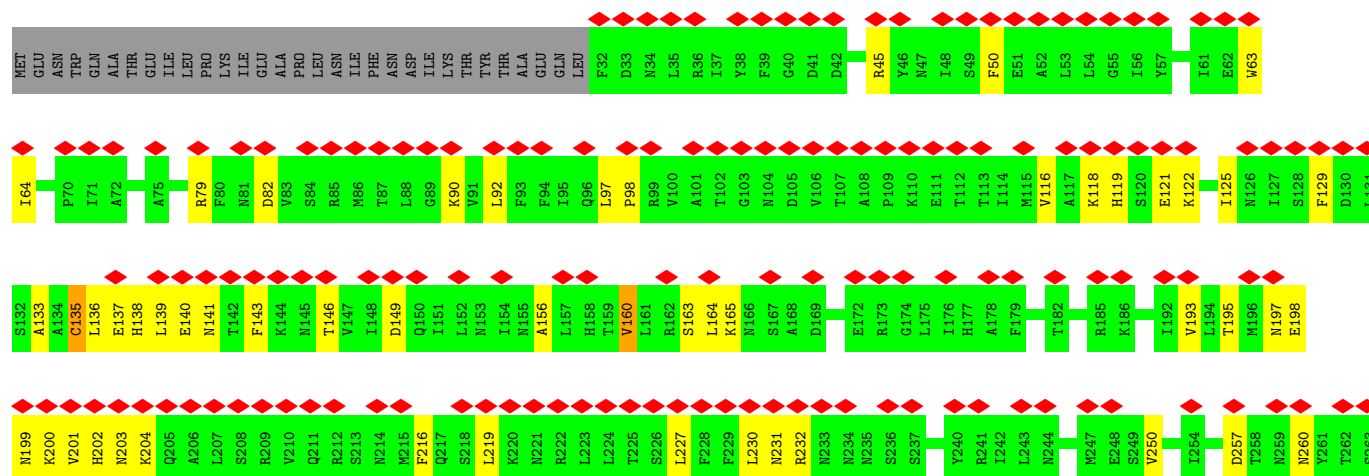
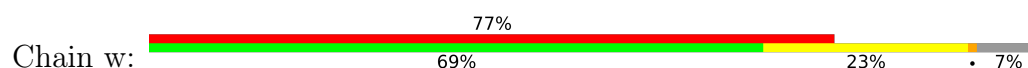


• Molecule 1: Major capsid protein

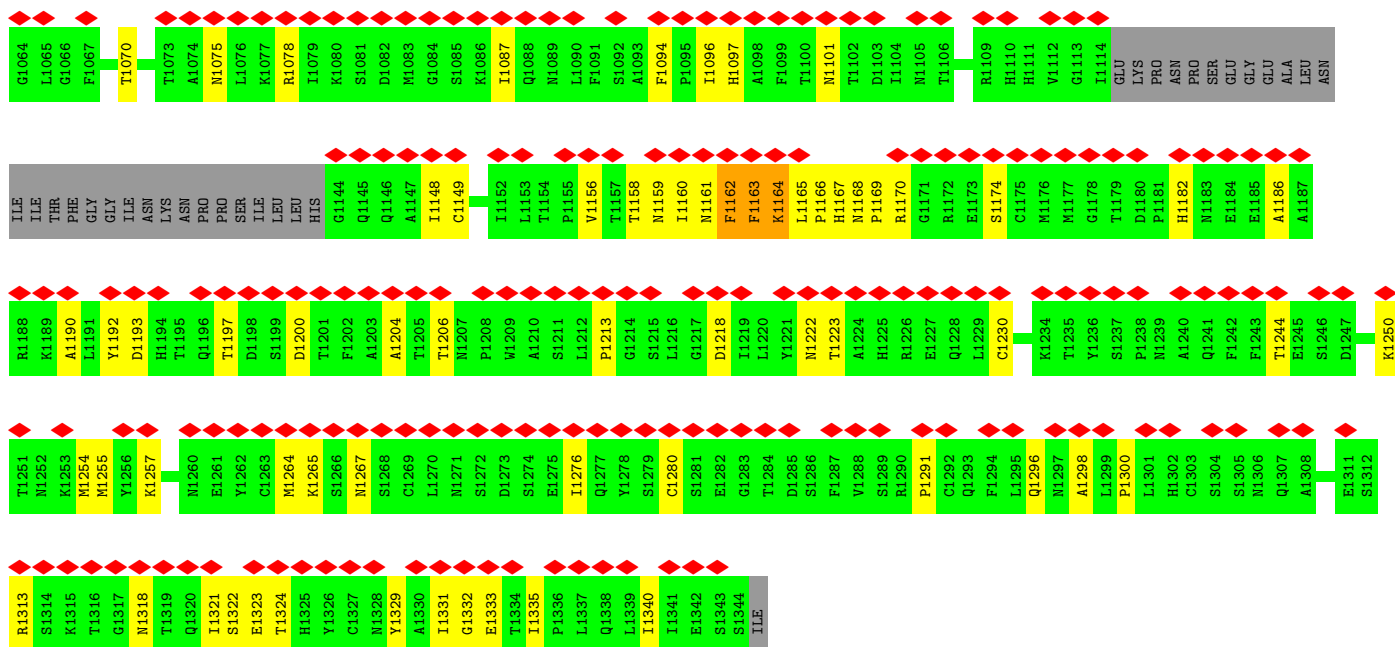




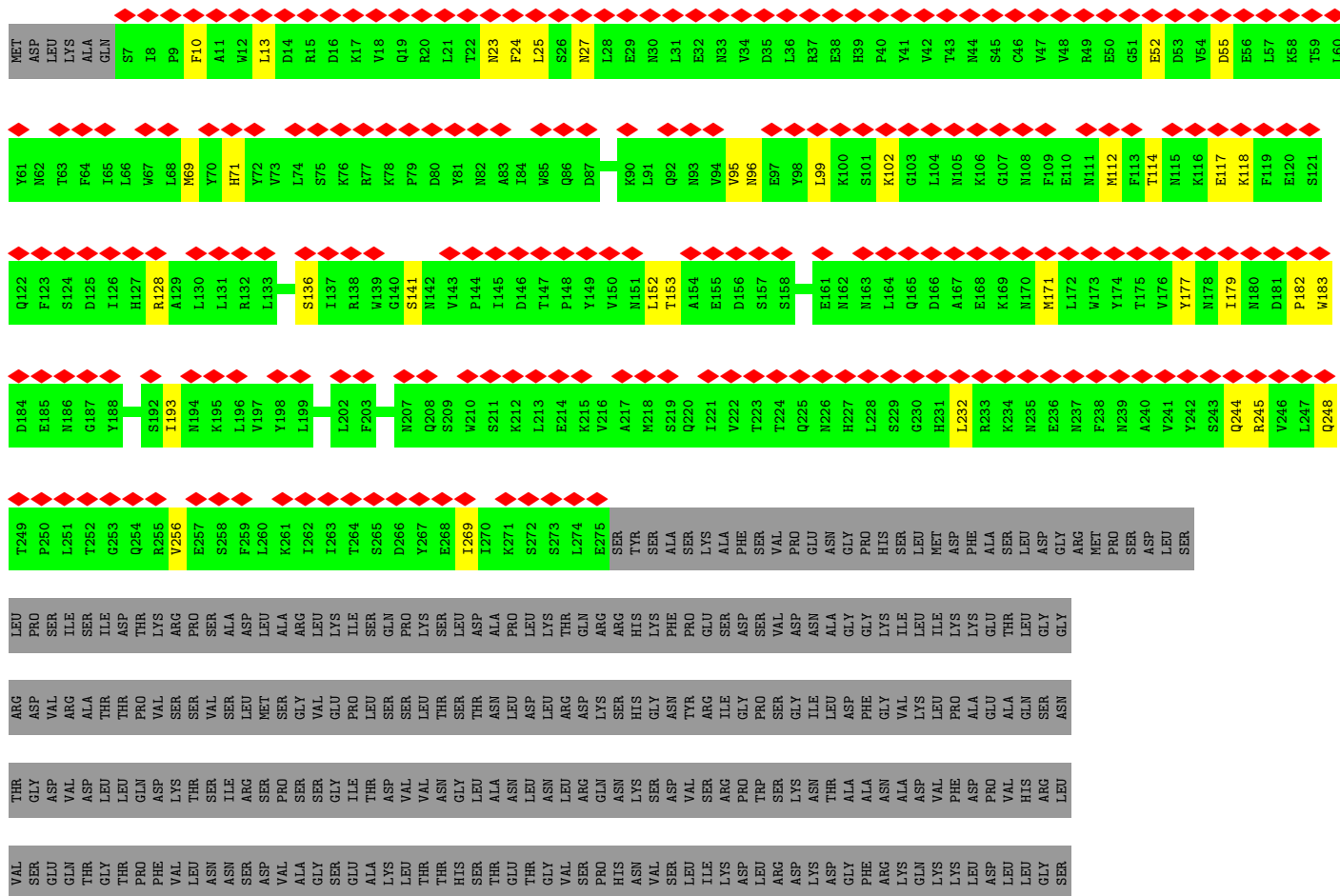
• Molecule 1: Major capsid protein



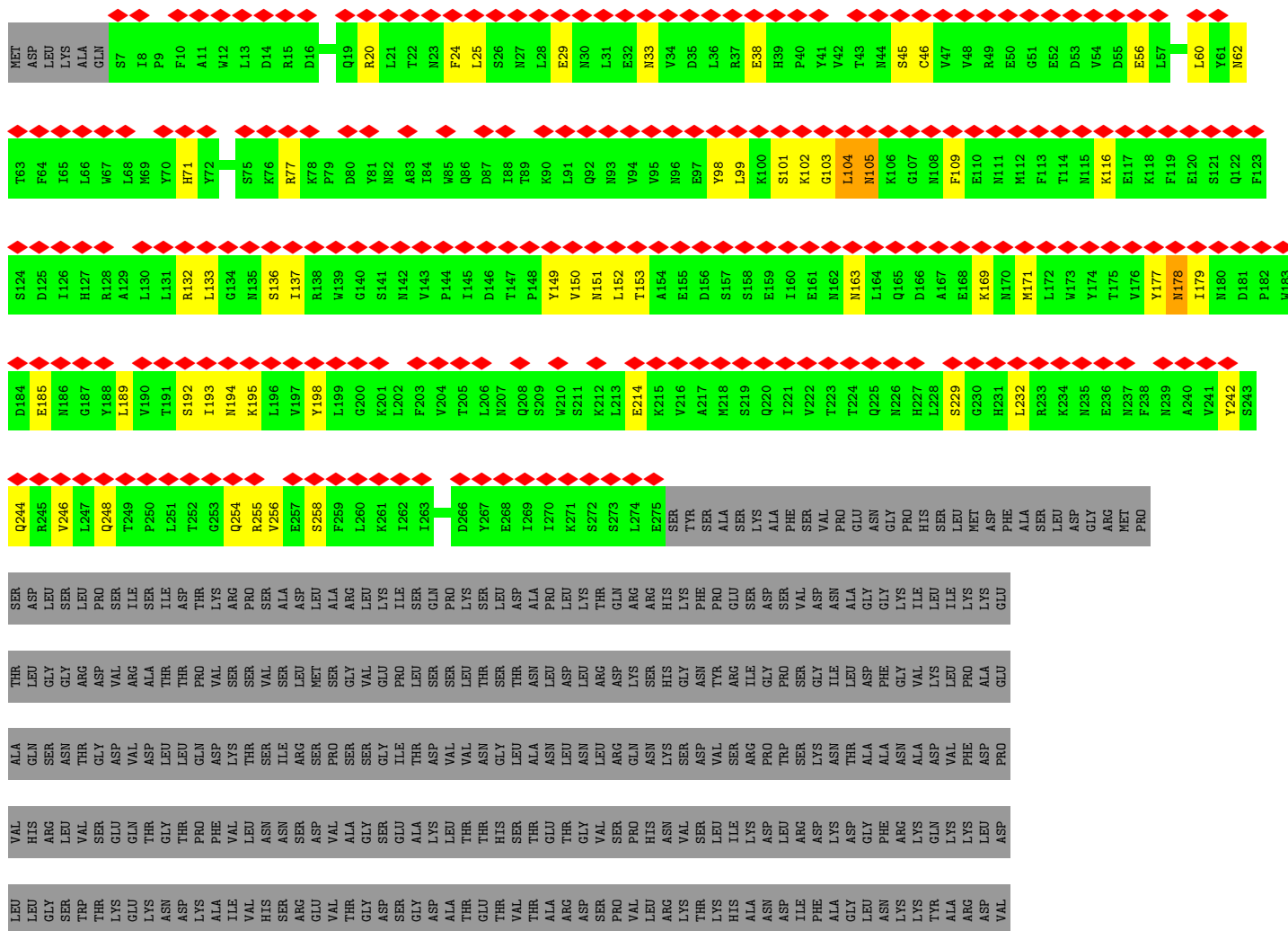
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• Molecule 2: Large structural phosphoprotein

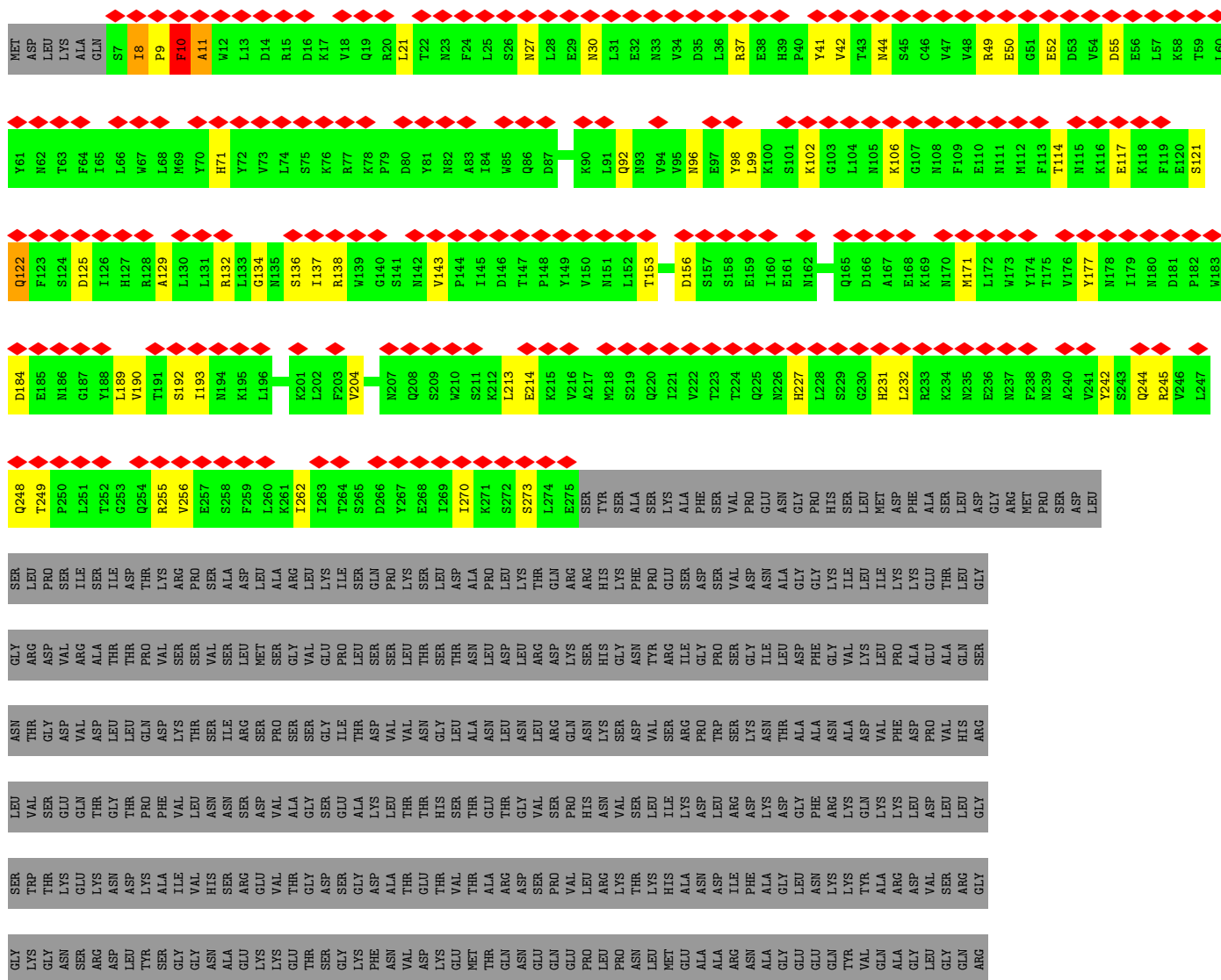


- Molecule 2: Large structural phosphoprotein



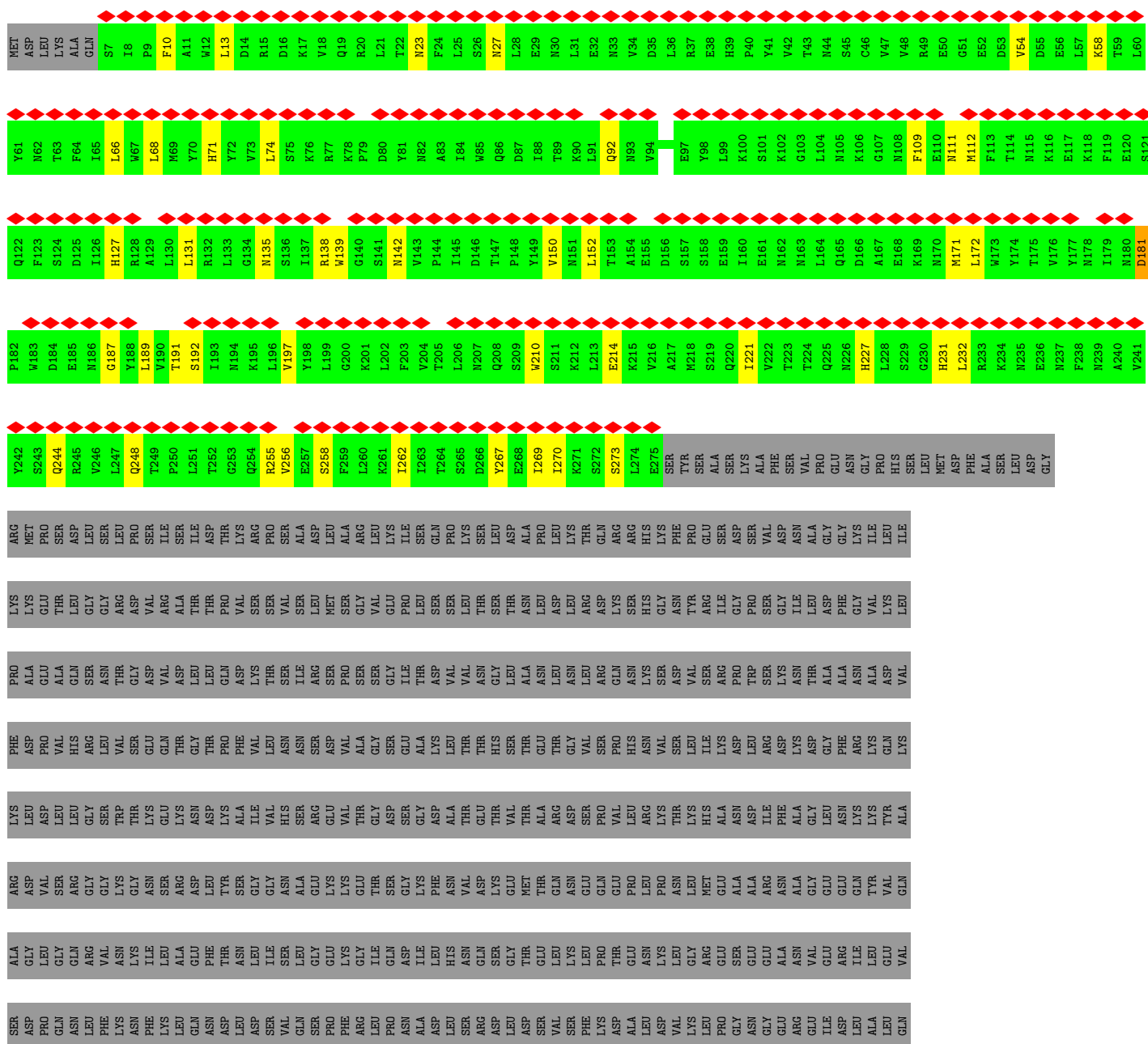
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- Molecule 2: Large structural phosphoprotein



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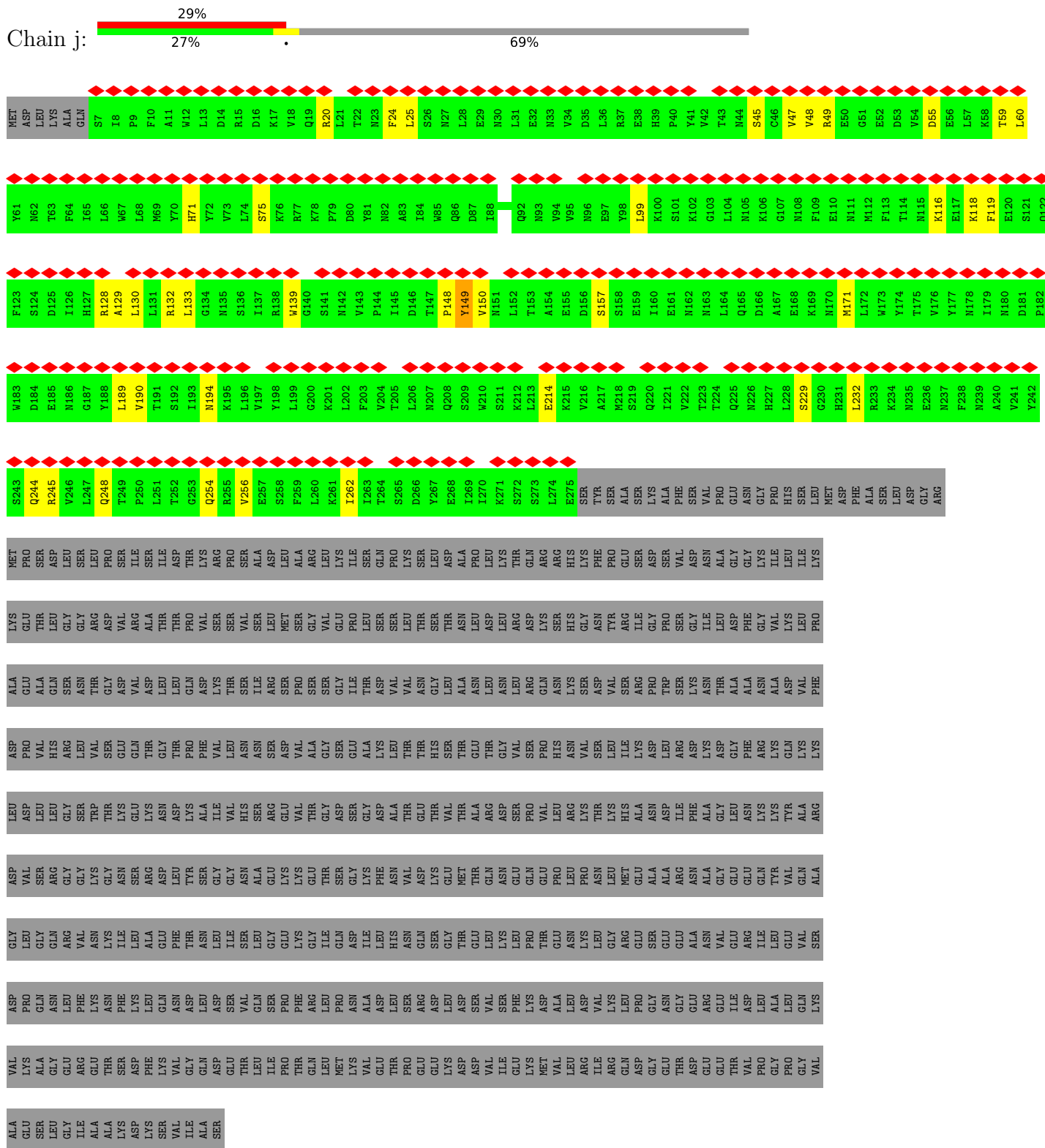
- Molecule 2: Large structural phosphoprotein



- Molecule 2: Large structural phosphoprotein

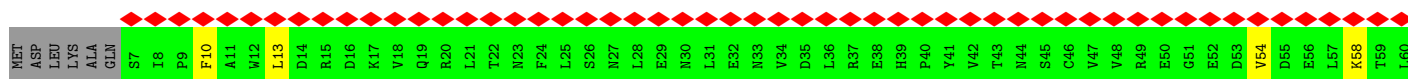
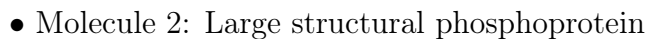
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Chain j:



Chain k:



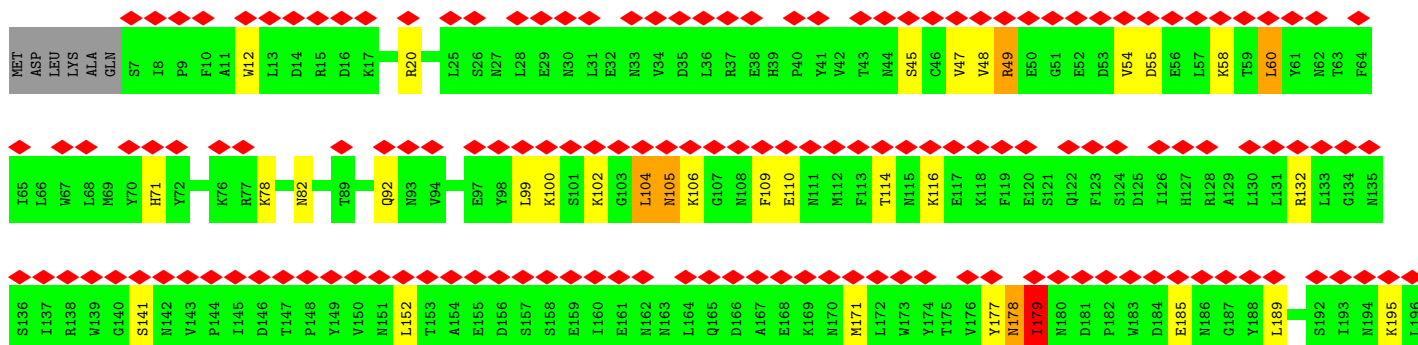
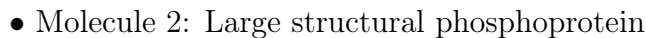


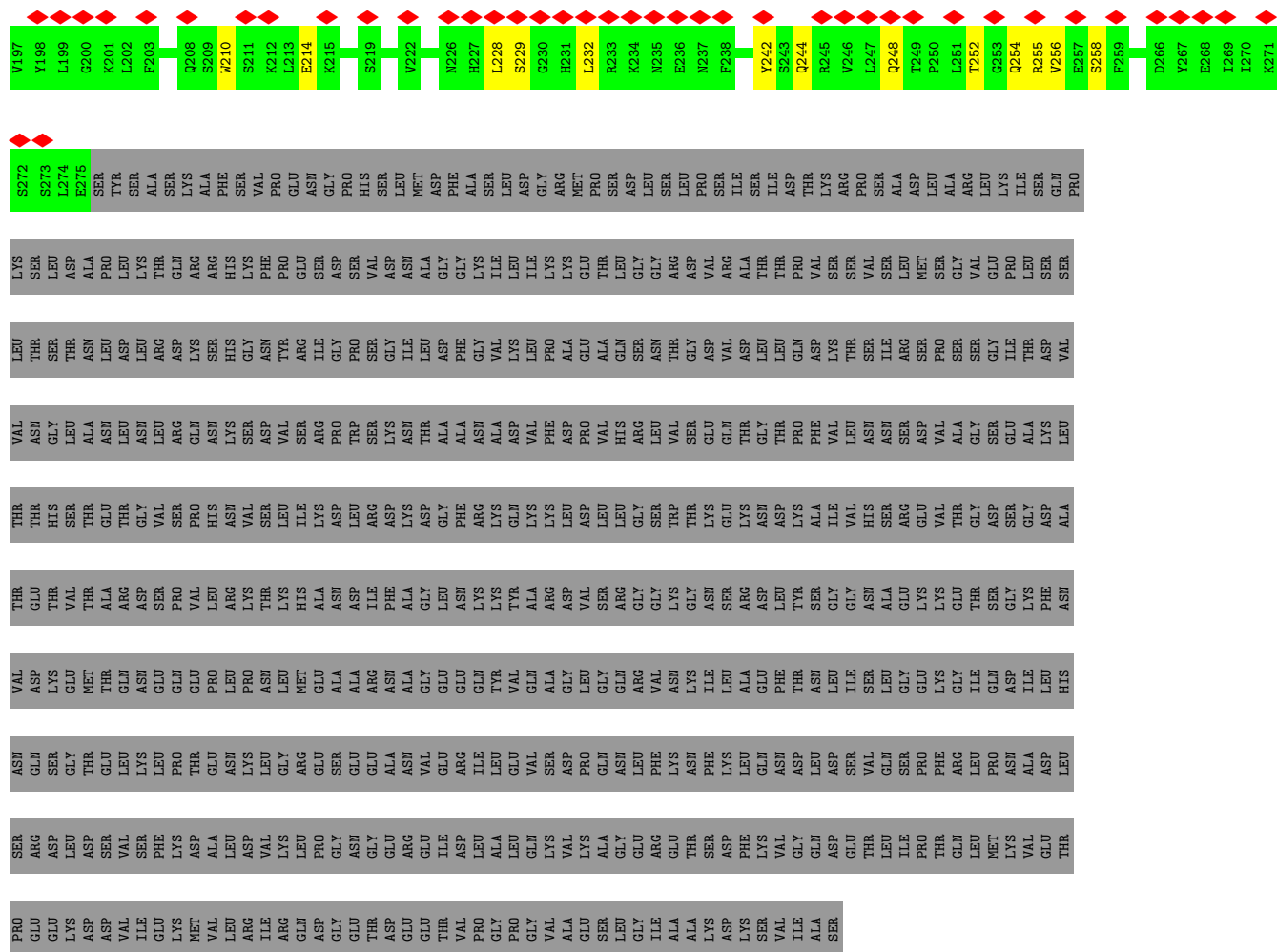
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● Molecule 2: Large structural phosphoprotein

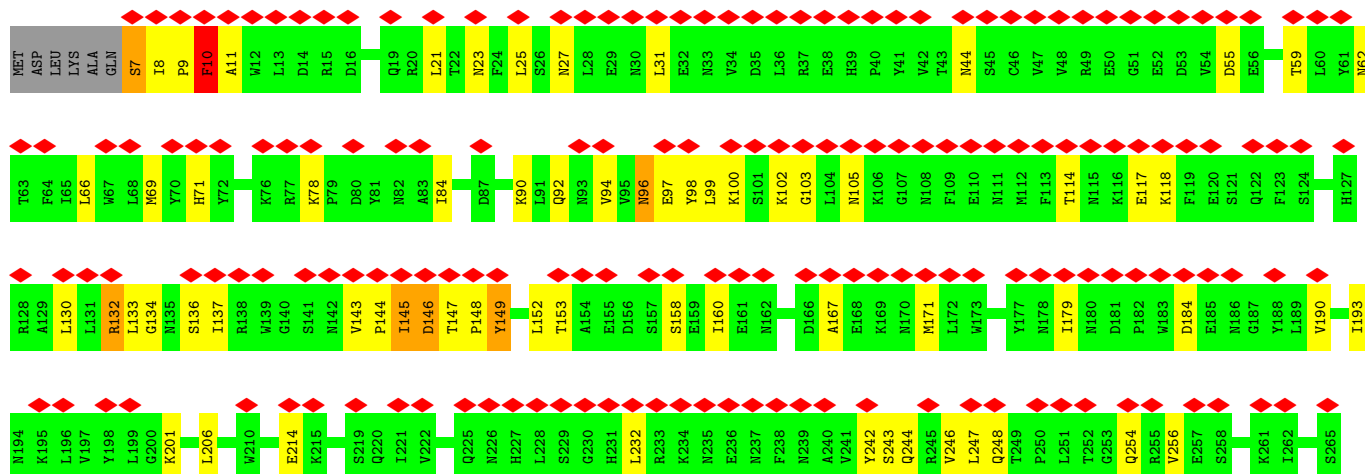


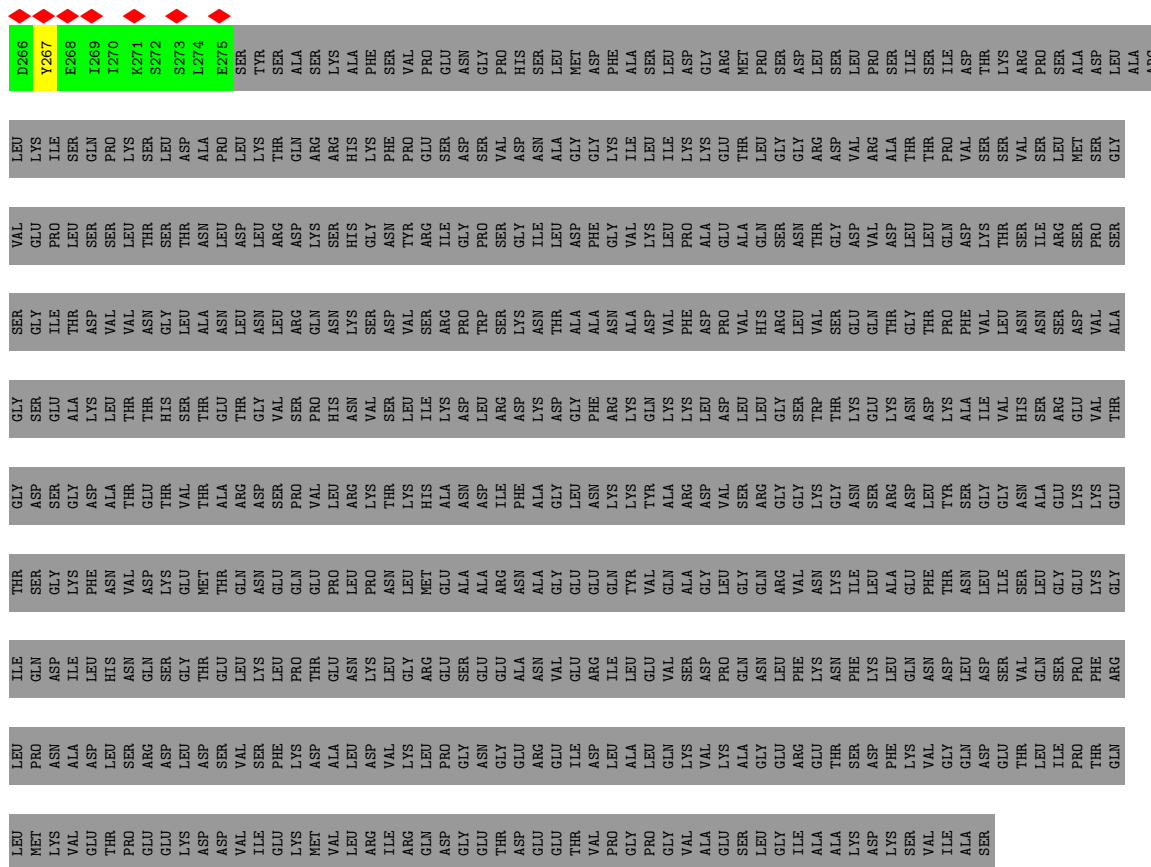
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V61	N62	T63	F64	I65	L66	W67	L68	M69	Y70	H71	Y72	S75	K76	R77	K78	P79	D80	Y81	N82	W85	Q86	D87	R90	L91	Q92	N93	V94	W95	N96	E97	Y98	L99	K100	S101	K102	G103	L104	M105	K106	G107	M108	F109	E110	N111	M112	F113	T114	N115	K116	E117	K118	F119	S120	S121	Q122	F123		



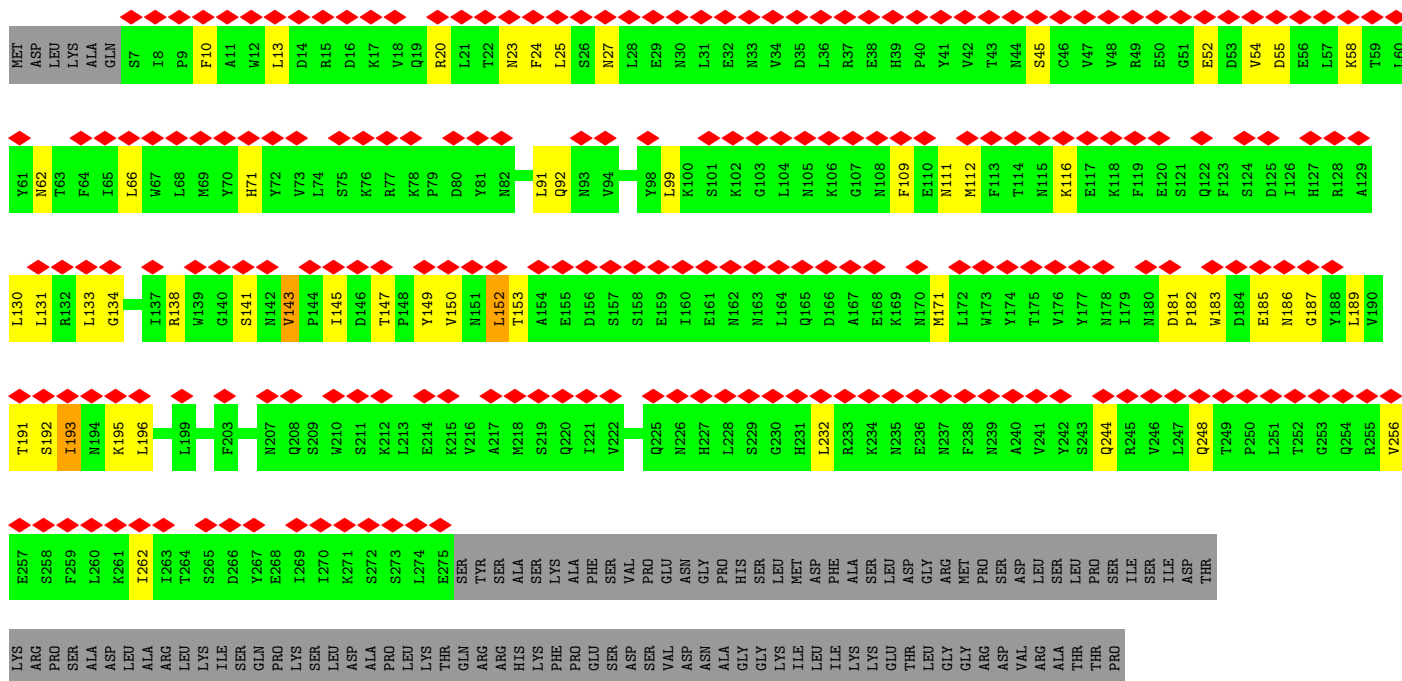


• Molecule 2: Large structural phosphoprotein



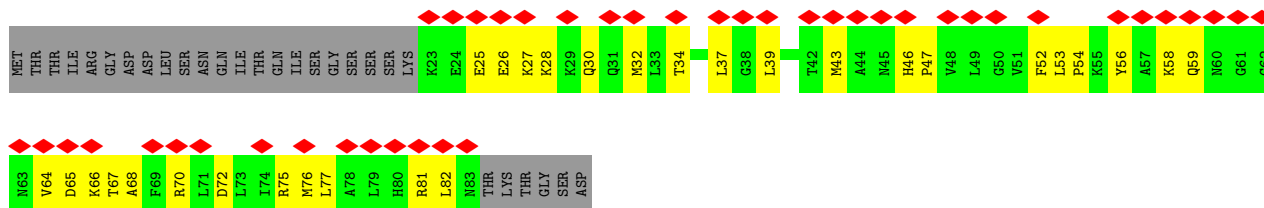


- Molecule 2: Large structural phosphoprotein

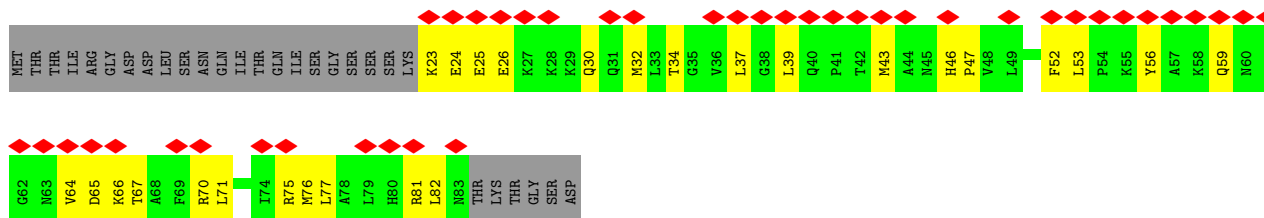


[illegible]

- Molecule 3: Small capsomere-interacting protein

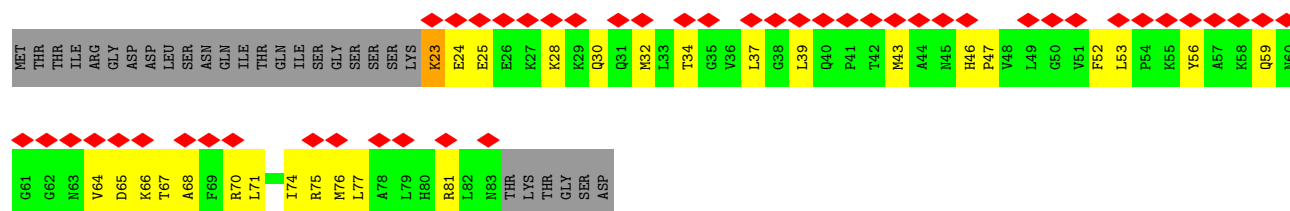


- Molecule 3: Small capsomere-interacting protein

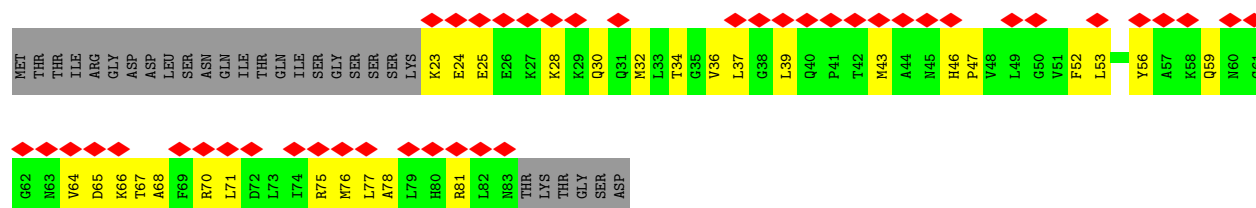


- Molecule 3: Small capsomere-interacting protein

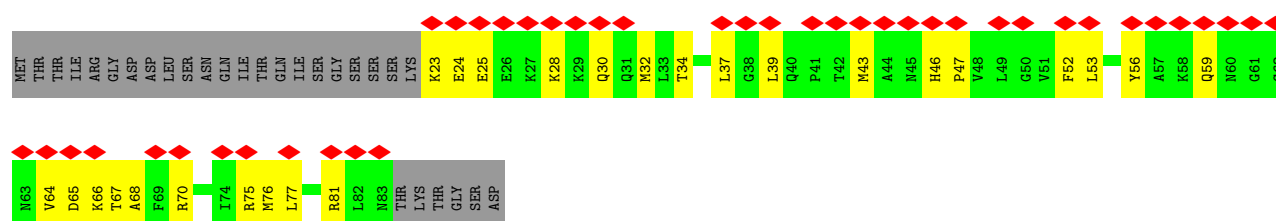




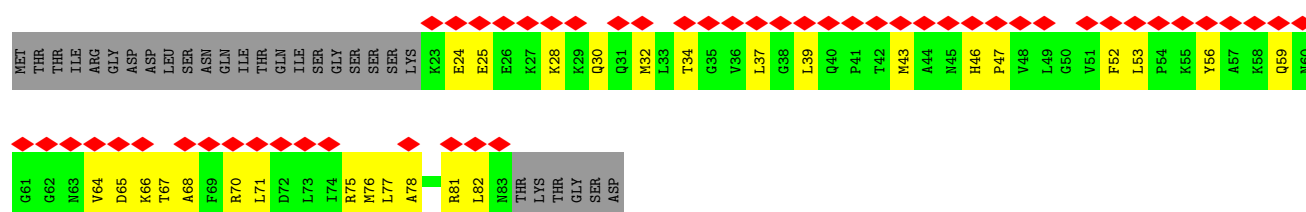
• Molecule 3: Small capsomere-interacting protein



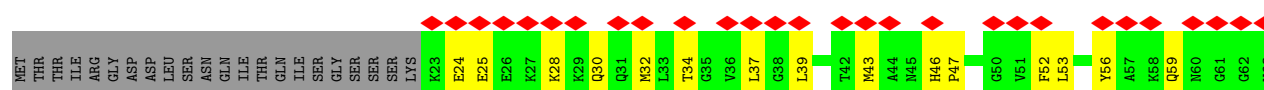
• Molecule 3: Small capsomere-interacting protein



• Molecule 3: Small capsomere-interacting protein

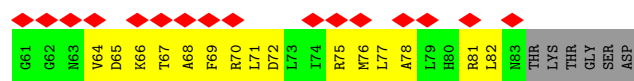


• Molecule 3: Small capsomere-interacting protein

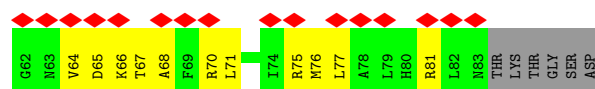
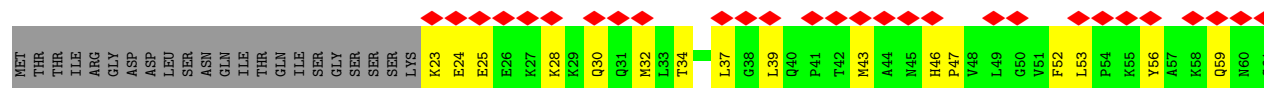




• Molecule 3: Small capsomere-interacting protein



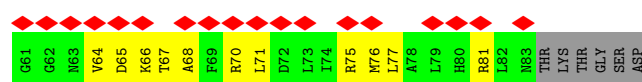
• Molecule 3: Small capsomere-interacting protein



• Molecule 3: Small capsomere-interacting protein



• Molecule 3: Small capsomere-interacting protein

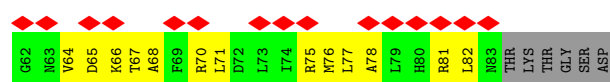


• Molecule 3: Small capsomere-interacting protein

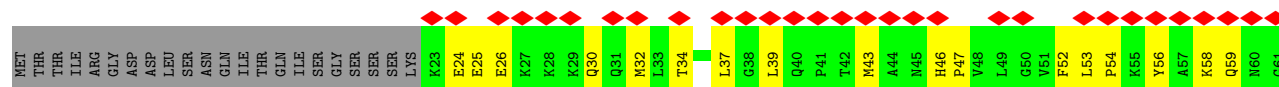




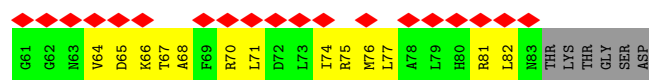
• Molecule 3: Small capsomere-interacting protein



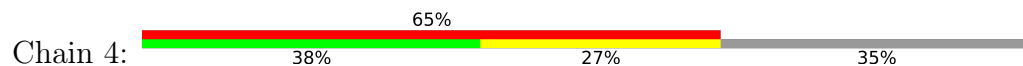
• Molecule 3: Small capsomere-interacting protein



• Molecule 3: Small capsomere-interacting protein

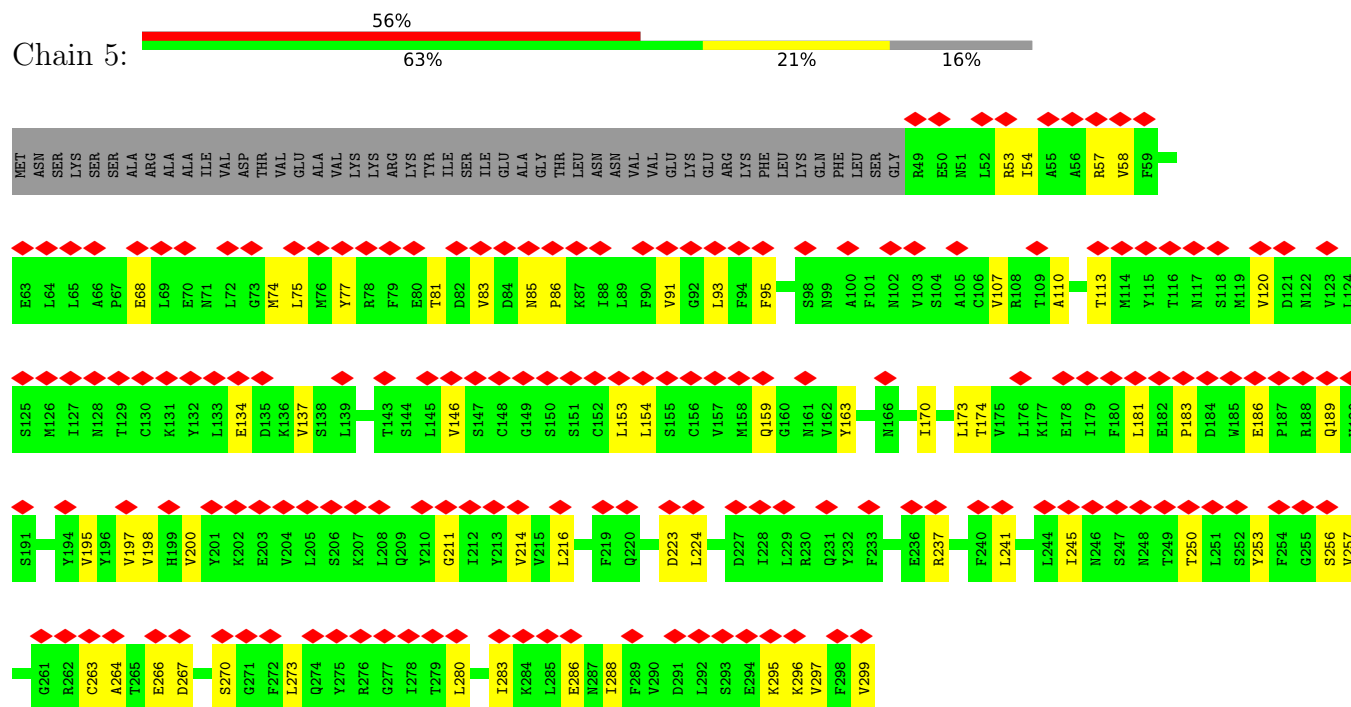


• Molecule 3: Small capsomere-interacting protein



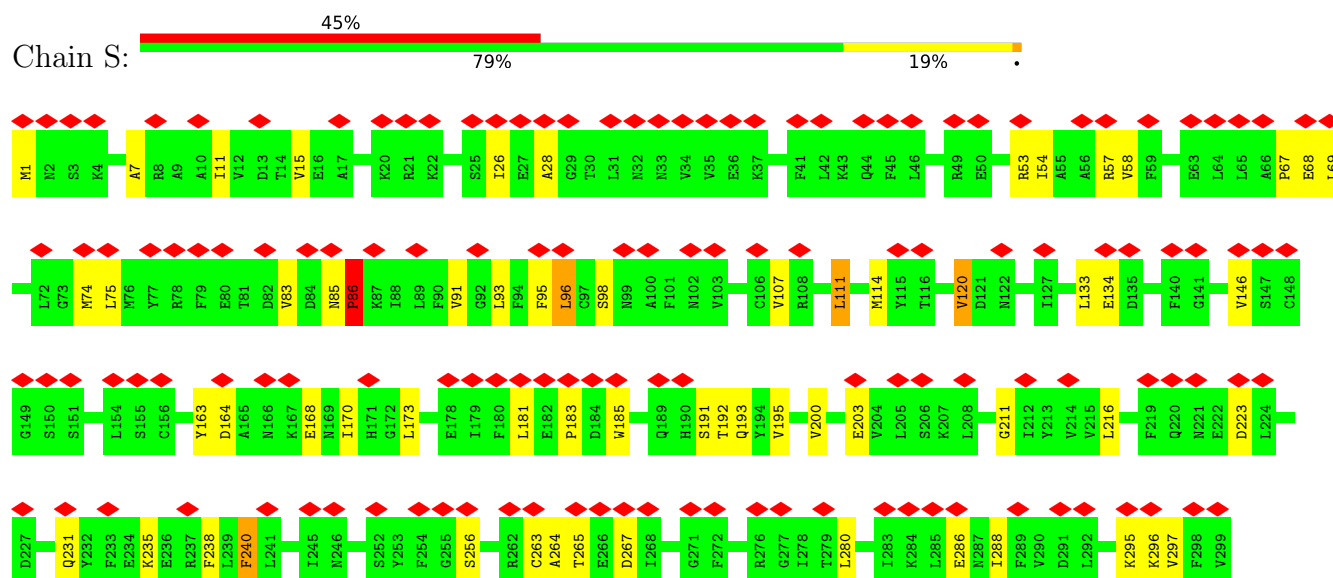
- Molecule 4: Triplex capsid protein 1

Chain 5:



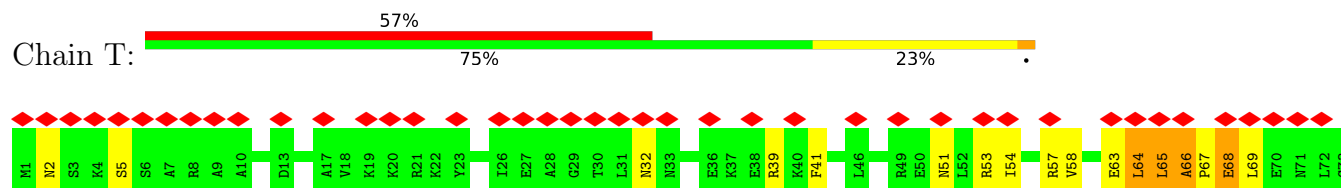
- Molecule 4: Triplex capsid protein 1

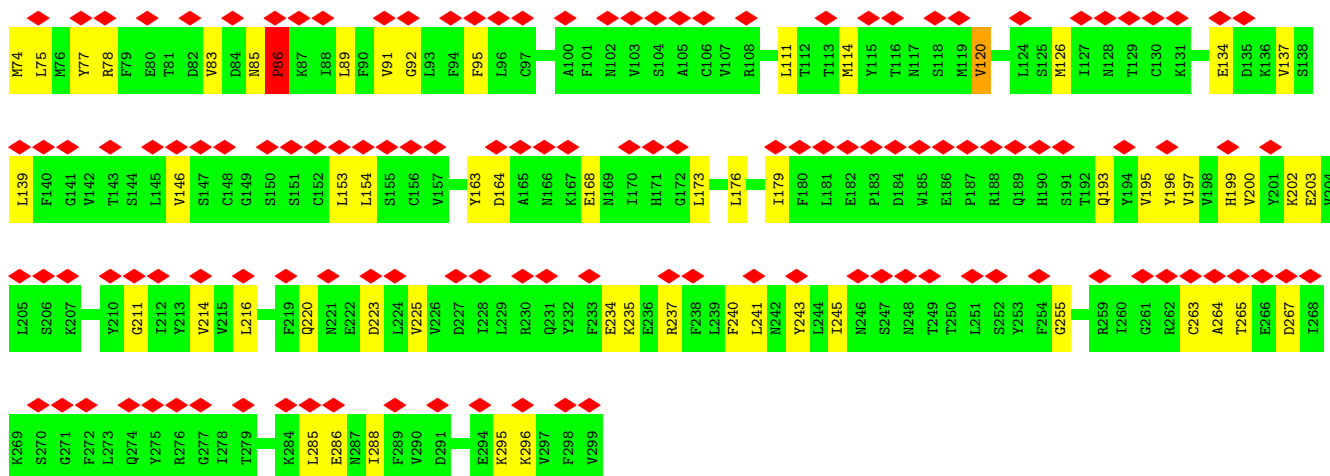
Chain S:



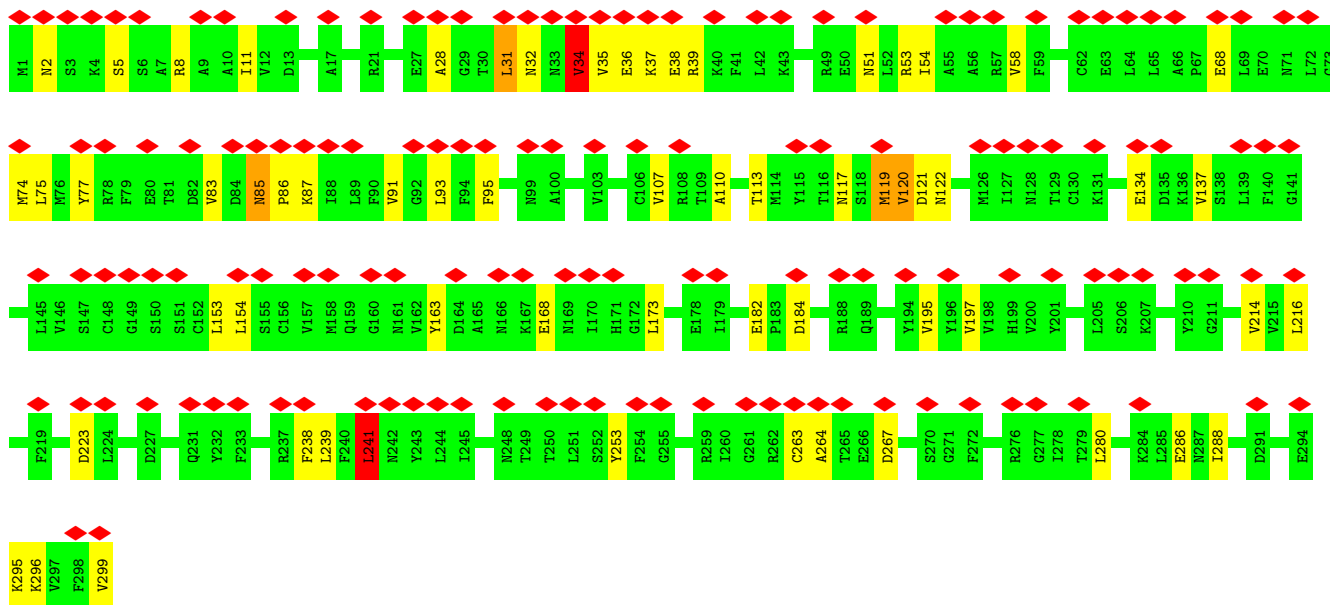
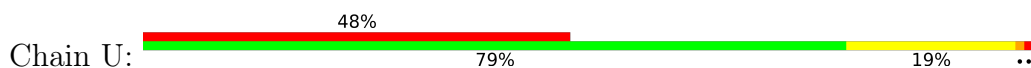
- Molecule 4: Triplex capsid protein 1

Chain T:

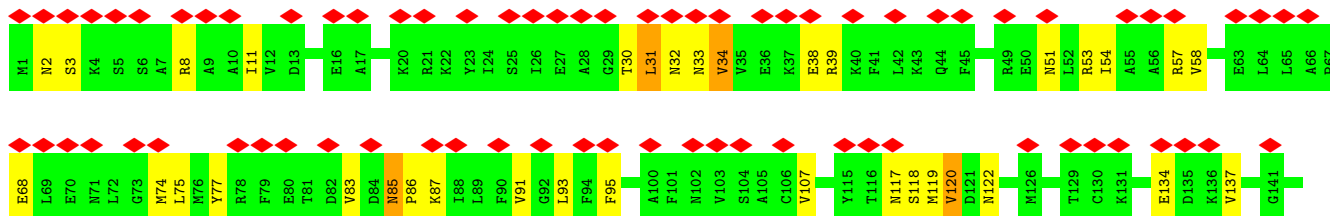
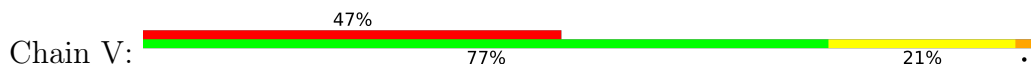


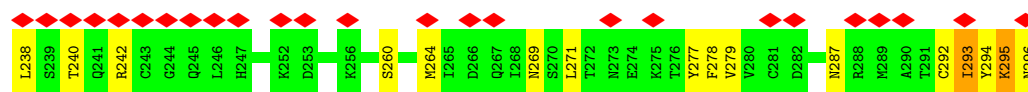


• Molecule 4: Triplex capsid protein 1

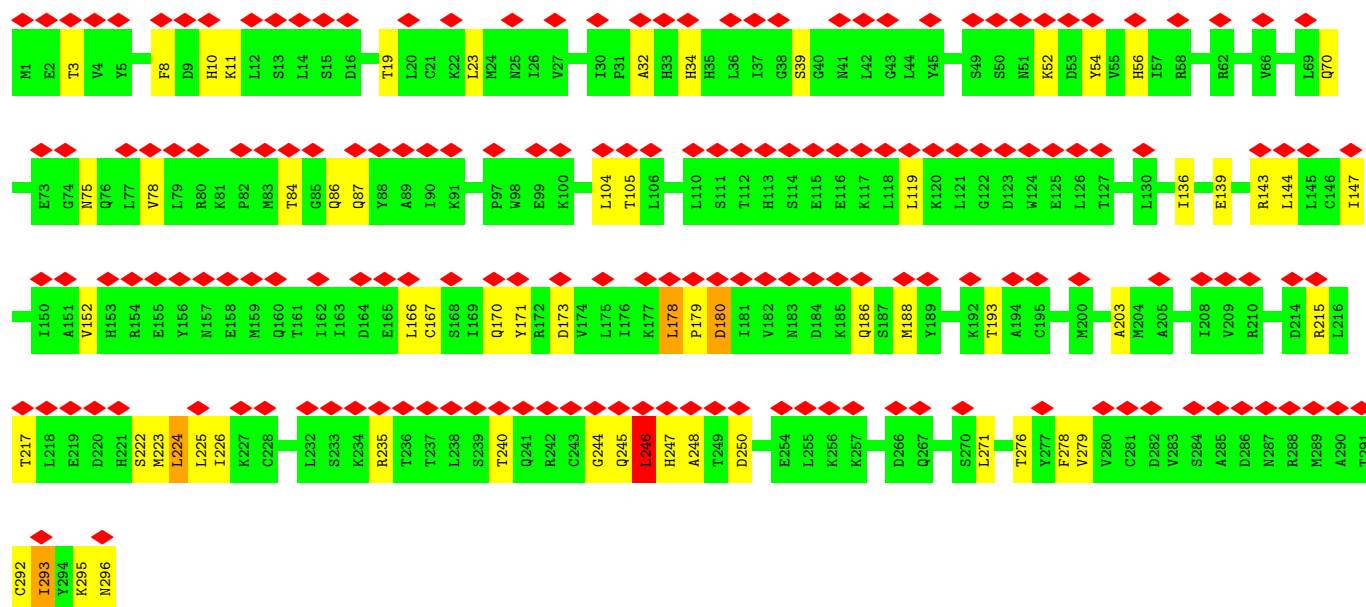
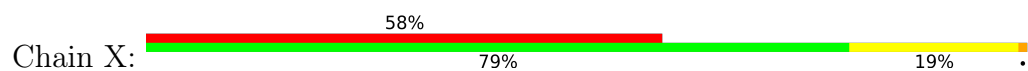


• Molecule 4: Triplex capsid protein 1

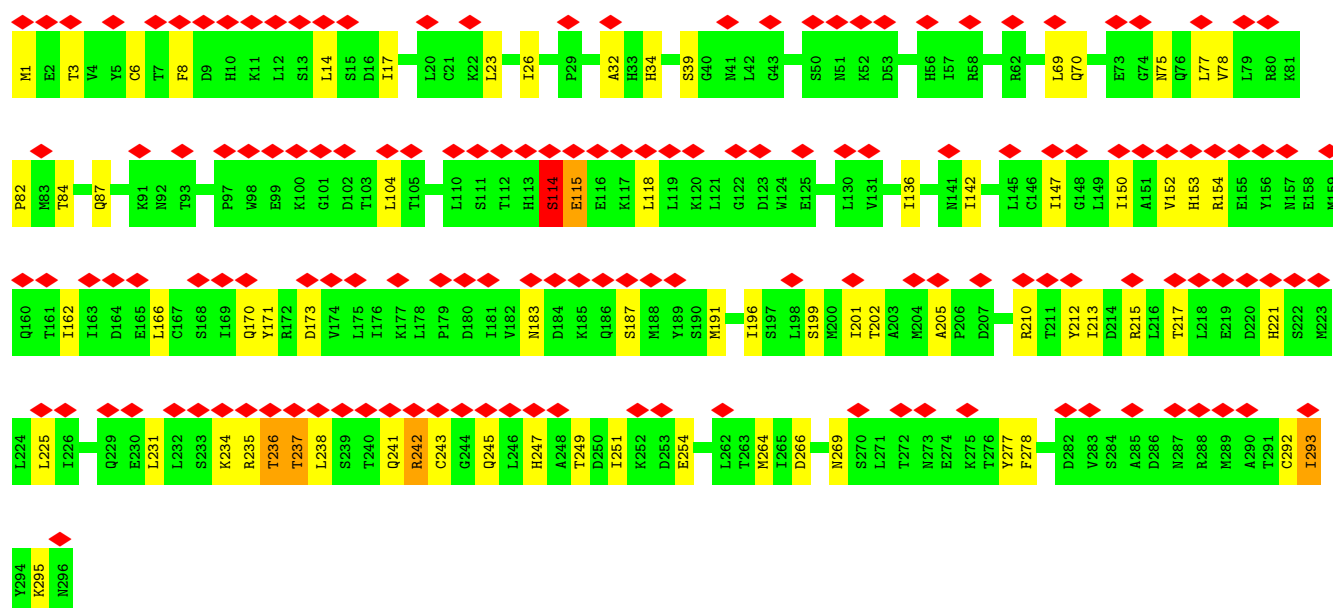
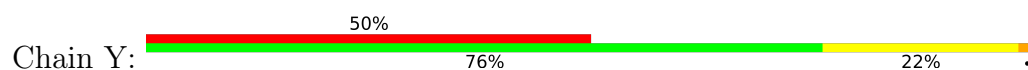




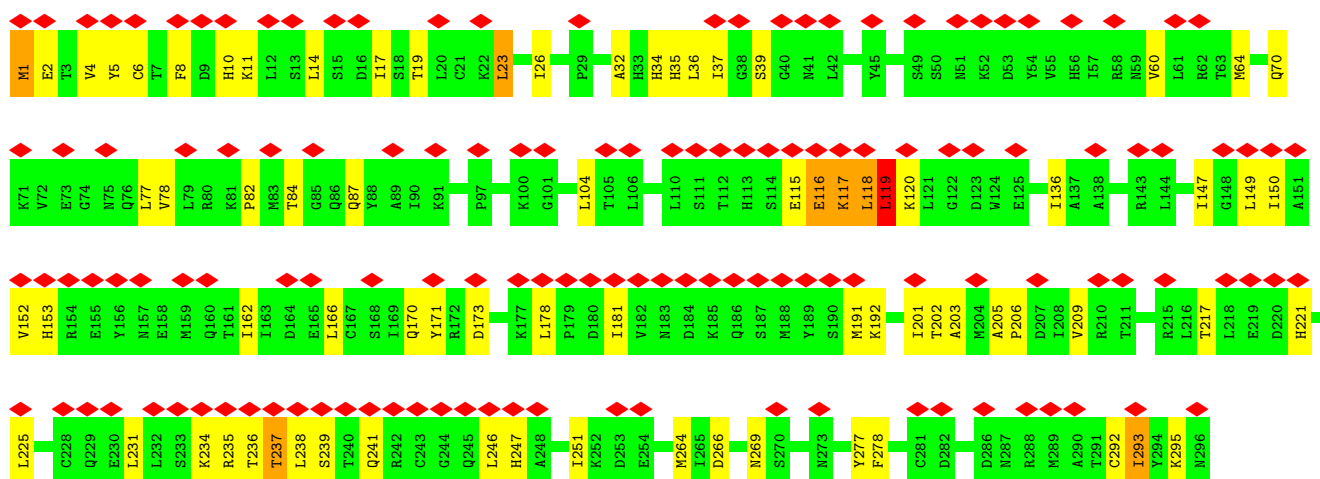
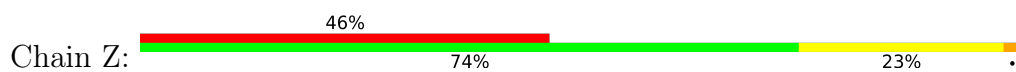
• Molecule 5: Triplex capsid protein 2



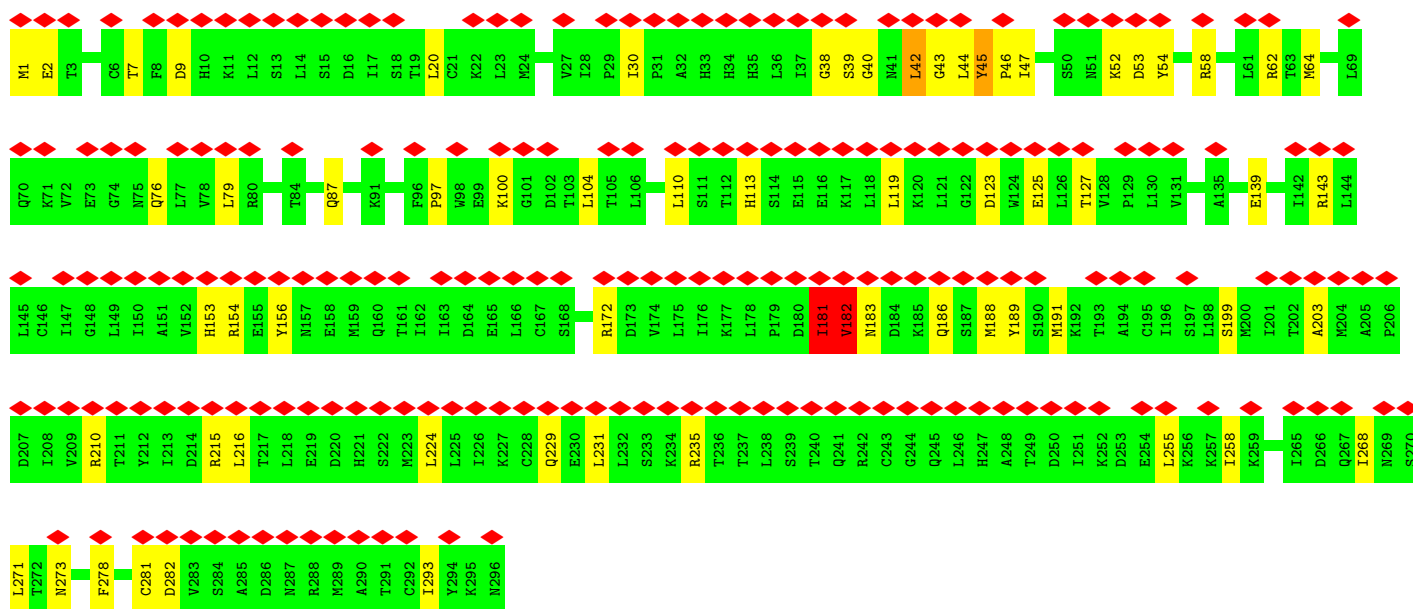
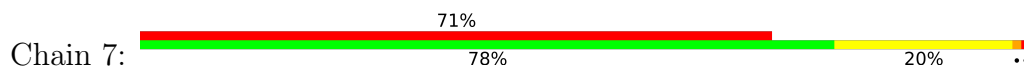
• Molecule 5: Triplex capsid protein 2



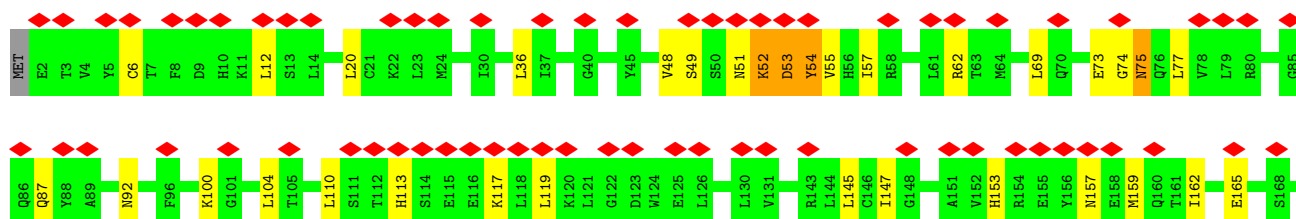
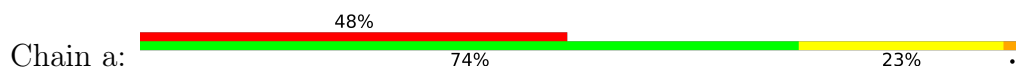
• Molecule 5: Triplex capsid protein 2

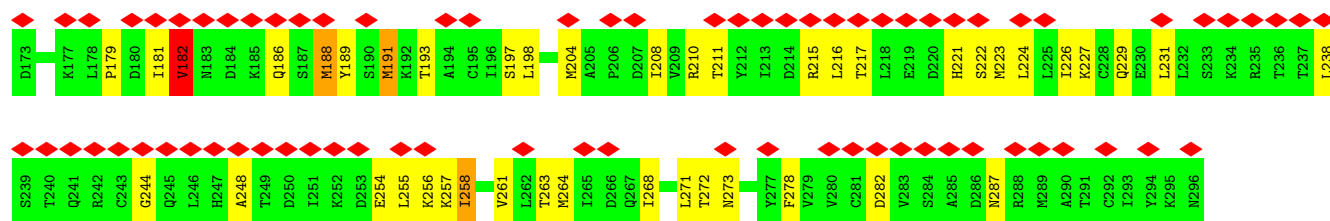


• Molecule 5: Triplex capsid protein 2

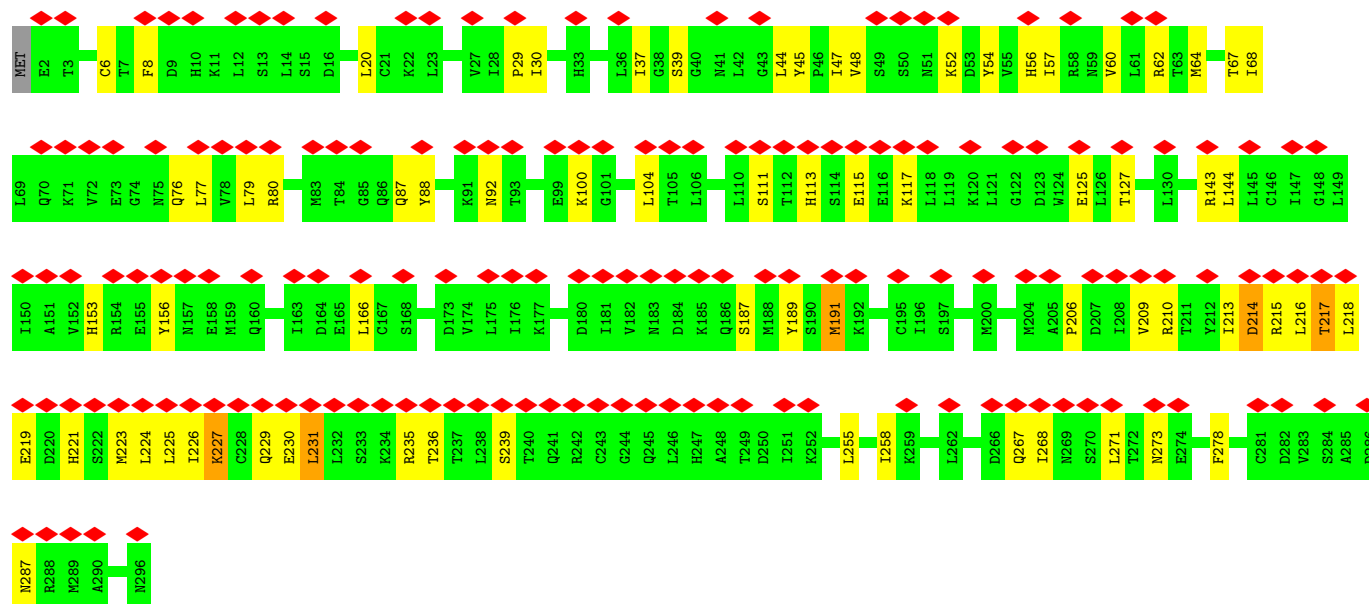
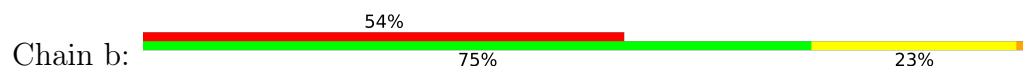


• Molecule 5: Triplex capsid protein 2

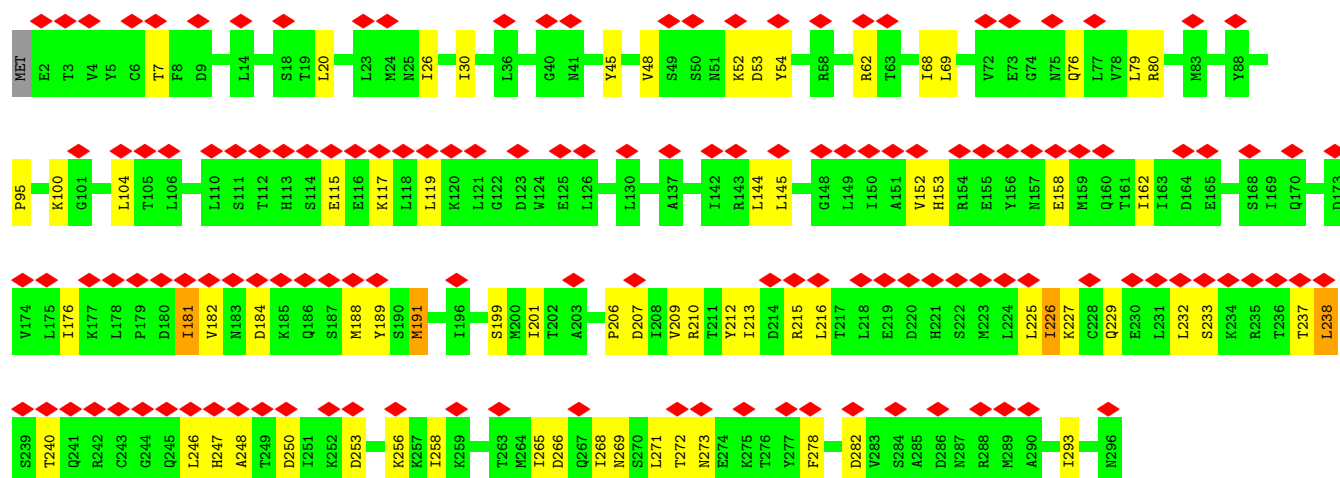
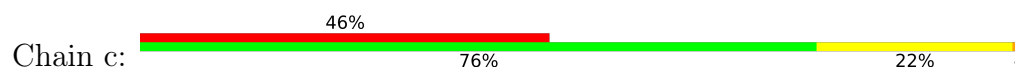




• Molecule 5: Triplex capsid protein 2



• Molecule 5: Triplex capsid protein 2



• Molecule 5: Triplex capsid protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	6443	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 ($e^-/\text{\AA}^2$)	23	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	64000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	1388.8, 1388.8, 1388.8	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.17, 2.17, 2.17	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.47	0/10927	0.74	10/14860 (0.1%)
1	B	0.40	0/10927	0.70	9/14860 (0.1%)
1	C	0.40	0/10793	0.66	5/14676 (0.0%)
1	D	0.41	0/10927	0.67	5/14860 (0.0%)
1	E	0.47	0/10927	0.71	10/14860 (0.1%)
1	F	0.36	0/10927	0.68	6/14860 (0.0%)
1	G	0.36	0/10927	0.70	6/14860 (0.0%)
1	H	0.46	0/10927	0.70	4/14860 (0.0%)
1	I	0.42	0/10927	0.67	5/14860 (0.0%)
1	q	0.36	0/10550	0.66	4/14349 (0.0%)
1	r	0.33	0/10927	0.64	2/14860 (0.0%)
1	s	0.34	0/10927	0.66	2/14860 (0.0%)
1	t	0.35	0/10927	0.63	2/14860 (0.0%)
1	u	0.33	0/10935	0.64	4/14870 (0.0%)
1	v	0.33	0/10566	0.63	2/14366 (0.0%)
1	w	0.34	0/10161	0.72	13/13814 (0.1%)
2	e	0.26	0/2272	0.59	0/3084
2	f	0.31	0/2272	0.66	0/3084
2	g	0.31	0/2272	0.77	4/3084 (0.1%)
2	h	0.26	0/2272	0.58	1/3084 (0.0%)
2	i	0.30	0/2272	0.68	2/3084 (0.1%)
2	j	0.28	0/2272	0.67	0/3084
2	k	0.29	0/2272	0.67	3/3084 (0.1%)
2	l	0.29	0/2272	0.65	3/3084 (0.1%)
2	m	0.33	0/2272	0.69	3/3084 (0.1%)
2	n	0.30	0/2272	0.73	3/3084 (0.1%)
2	o	0.38	0/2272	0.78	10/3084 (0.3%)
2	p	0.31	0/2272	0.70	5/3084 (0.2%)
3	1	0.20	0/490	0.48	0/656
3	2	0.21	0/490	0.49	0/656
3	3	0.21	0/490	0.49	0/656
3	4	0.21	0/463	0.49	0/621
3	J	0.21	0/490	0.52	0/656
3	K	0.21	0/490	0.49	0/656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	L	0.21	0/490	0.48	0/656
3	M	0.20	0/490	0.48	0/656
3	N	0.20	0/490	0.48	0/656
3	O	0.20	0/490	0.48	0/656
3	P	0.21	0/490	0.48	0/656
3	Q	0.20	0/490	0.48	0/656
3	R	0.20	0/490	0.48	0/656
3	x	0.20	0/490	0.48	0/656
3	y	0.21	0/490	0.48	0/656
3	z	0.21	0/490	0.48	0/656
4	5	0.32	0/2062	0.68	0/2793
4	S	0.41	0/2440	0.70	1/3297 (0.0%)
4	T	0.41	0/2440	0.81	4/3297 (0.1%)
4	U	0.34	0/2440	0.74	6/3297 (0.2%)
4	V	0.33	0/2440	0.69	2/3297 (0.1%)
5	6	0.34	0/2262	0.66	2/3069 (0.1%)
5	7	0.29	0/2374	0.75	10/3219 (0.3%)
5	W	0.39	0/2374	0.72	0/3219
5	X	0.36	0/2374	0.71	3/3219 (0.1%)
5	Y	0.36	0/2374	0.73	2/3219 (0.1%)
5	Z	0.39	0/2374	0.78	3/3219 (0.1%)
5	a	0.42	0/2366	0.83	10/3209 (0.3%)
5	b	0.43	0/2366	0.87	3/3209 (0.1%)
5	c	0.51	0/2366	0.83	3/3209 (0.1%)
5	d	0.41	0/2366	0.87	10/3209 (0.3%)
All	All	0.37	0/243697	0.68	182/330985 (0.1%)

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
2	o	0	1

There are no bond length outliers.

The worst 5 of 182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	g	8	ILE	CA-C-N	14.37	135.00	119.05
2	g	8	ILE	C-N-CA	14.37	135.00	119.05
5	b	226	ILE	N-CA-C	12.78	122.55	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	154	ALA	N-CA-C	10.27	125.51	111.54
1	w	563	LEU	CA-C-N	9.30	131.46	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	o	7	SER	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10682	0	10575	252	0
1	B	10682	0	10575	263	0
1	C	10552	0	10444	234	0
1	D	10682	0	10575	272	0
1	E	10682	0	10574	370	0
1	F	10682	0	10574	394	0
1	G	10682	0	10575	402	0
1	H	10682	0	10574	287	0
1	I	10682	0	10575	197	0
1	q	10313	0	10230	279	0
1	r	10682	0	10575	378	0
1	s	10682	0	10574	372	0
1	t	10682	0	10575	238	0
1	u	10690	0	10587	258	0
1	v	10331	0	10242	229	0
1	w	9933	0	9844	358	0
2	e	2224	0	2186	39	0
2	f	2224	0	2186	79	0
2	g	2224	0	2186	87	0
2	h	2224	0	2186	39	0
2	i	2224	0	2186	61	0
2	j	2224	0	2186	33	0
2	k	2224	0	2186	48	0
2	l	2224	0	2186	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	m	2224	0	2186	61	0
2	n	2224	0	2186	63	0
2	o	2224	0	2186	93	0
2	p	2224	0	2186	43	0
3	1	483	0	513	58	0
3	2	483	0	513	57	0
3	3	483	0	513	53	0
3	4	456	0	488	94	0
3	J	483	0	513	61	0
3	K	483	0	513	36	0
3	L	483	0	513	38	0
3	M	483	0	513	55	0
3	N	483	0	513	54	0
3	O	483	0	513	45	0
3	P	483	0	513	48	0
3	Q	483	0	513	68	0
3	R	483	0	513	53	0
3	x	483	0	513	44	0
3	y	483	0	513	53	0
3	z	483	0	513	55	0
4	5	2023	0	2034	42	0
4	S	2398	0	2438	116	0
4	T	2398	0	2438	81	0
4	U	2398	0	2438	65	0
4	V	2398	0	2438	101	0
5	6	2226	0	2318	47	0
5	7	2337	0	2437	64	0
5	W	2337	0	2436	120	0
5	X	2337	0	2437	110	0
5	Y	2337	0	2437	78	0
5	Z	2337	0	2437	67	0
5	a	2329	0	2425	116	0
5	b	2329	0	2419	152	0
5	c	2329	0	2425	83	0
5	d	2329	0	2425	90	0
All	All	238552	0	238065	5944	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 12.

The worst 5 of 5944 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:q:810:TYR:CE1	3:x:37:LEU:HD12	1.22	1.71
5:X:188:MET:SD	5:b:218:LEU:HD21	1.25	1.70
1:F:1130:PHE:CE1	5:b:52:LYS:HG3	1.33	1.61
1:I:810:TYR:CE2	3:R:37:LEU:HD12	1.33	1.59
1:s:1123:GLU:CB	5:a:264:MET:HE1	1.34	1.58

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1341/1345 (100%)	1238 (92%)	102 (8%)	1 (0%)	48	83
1	B	1341/1345 (100%)	1251 (93%)	87 (6%)	3 (0%)	43	78
1	C	1321/1345 (98%)	1239 (94%)	80 (6%)	2 (0%)	43	78
1	D	1341/1345 (100%)	1248 (93%)	89 (7%)	4 (0%)	36	72
1	E	1341/1345 (100%)	1243 (93%)	94 (7%)	4 (0%)	36	72
1	F	1341/1345 (100%)	1243 (93%)	96 (7%)	2 (0%)	48	83
1	G	1341/1345 (100%)	1253 (93%)	83 (6%)	5 (0%)	30	67
1	H	1341/1345 (100%)	1253 (93%)	84 (6%)	4 (0%)	36	72
1	I	1341/1345 (100%)	1242 (93%)	98 (7%)	1 (0%)	48	83
1	q	1292/1345 (96%)	1190 (92%)	99 (8%)	3 (0%)	43	78
1	r	1341/1345 (100%)	1235 (92%)	103 (8%)	3 (0%)	43	78
1	s	1341/1345 (100%)	1246 (93%)	93 (7%)	2 (0%)	48	83
1	t	1341/1345 (100%)	1240 (92%)	98 (7%)	3 (0%)	43	78
1	u	1342/1345 (100%)	1234 (92%)	106 (8%)	2 (0%)	48	83
1	v	1299/1345 (97%)	1204 (93%)	89 (7%)	6 (0%)	24	63
1	w	1240/1345 (92%)	1141 (92%)	98 (8%)	1 (0%)	48	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	e	267/858 (31%)	254 (95%)	13 (5%)	0	100	100
2	f	267/858 (31%)	248 (93%)	16 (6%)	3 (1%)	11	46
2	g	267/858 (31%)	255 (96%)	9 (3%)	3 (1%)	11	46
2	h	267/858 (31%)	248 (93%)	19 (7%)	0	100	100
2	i	267/858 (31%)	245 (92%)	17 (6%)	5 (2%)	6	32
2	j	267/858 (31%)	249 (93%)	16 (6%)	2 (1%)	18	56
2	k	267/858 (31%)	249 (93%)	17 (6%)	1 (0%)	30	67
2	l	267/858 (31%)	247 (92%)	19 (7%)	1 (0%)	30	67
2	m	267/858 (31%)	248 (93%)	18 (7%)	1 (0%)	30	67
2	n	267/858 (31%)	244 (91%)	18 (7%)	5 (2%)	6	32
2	o	267/858 (31%)	247 (92%)	16 (6%)	4 (2%)	8	40
2	p	267/858 (31%)	249 (93%)	18 (7%)	0	100	100
3	1	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	2	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	3	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	4	56/89 (63%)	49 (88%)	7 (12%)	0	100	100
3	J	59/89 (66%)	51 (86%)	7 (12%)	1 (2%)	7	36
3	K	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	L	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	M	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	N	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	O	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	P	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	Q	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	R	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	x	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	y	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	z	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
4	5	249/299 (83%)	226 (91%)	23 (9%)	0	100	100
4	S	297/299 (99%)	269 (91%)	27 (9%)	1 (0%)	36	72
4	T	297/299 (99%)	275 (93%)	21 (7%)	1 (0%)	36	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	U	297/299 (99%)	267 (90%)	29 (10%)	1 (0%)	36	72
4	V	297/299 (99%)	268 (90%)	27 (9%)	2 (1%)	18	56
5	6	278/296 (94%)	260 (94%)	18 (6%)	0	100	100
5	7	294/296 (99%)	259 (88%)	32 (11%)	3 (1%)	12	49
5	W	294/296 (99%)	277 (94%)	17 (6%)	0	100	100
5	X	294/296 (99%)	273 (93%)	20 (7%)	1 (0%)	36	72
5	Y	294/296 (99%)	269 (92%)	22 (8%)	3 (1%)	12	49
5	Z	294/296 (99%)	274 (93%)	19 (6%)	1 (0%)	36	72
5	a	293/296 (99%)	262 (89%)	28 (10%)	3 (1%)	12	49
5	b	293/296 (99%)	268 (92%)	24 (8%)	1 (0%)	36	72
5	c	293/296 (99%)	259 (88%)	33 (11%)	1 (0%)	36	72
5	d	293/296 (99%)	258 (88%)	30 (10%)	5 (2%)	7	36
All	All	29747/37695 (79%)	27475 (92%)	2177 (7%)	95 (0%)	37	72

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	55	GLY
1	F	19	ILE
1	G	810	TYR
1	H	21	ASN
1	H	818	ASP

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	A	1218/1220 (100%)	1205 (99%)	13 (1%)	65	76
1	B	1218/1220 (100%)	1210 (99%)	8 (1%)	76	81
1	C	1204/1220 (99%)	1195 (99%)	9 (1%)	76	81
1	D	1218/1220 (100%)	1209 (99%)	9 (1%)	76	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	1218/1220 (100%)	1207 (99%)	11 (1%)	70	79
1	F	1218/1220 (100%)	1209 (99%)	9 (1%)	76	81
1	G	1218/1220 (100%)	1207 (99%)	11 (1%)	70	79
1	H	1218/1220 (100%)	1204 (99%)	14 (1%)	65	76
1	I	1218/1220 (100%)	1209 (99%)	9 (1%)	76	81
1	q	1180/1220 (97%)	1175 (100%)	5 (0%)	84	84
1	r	1218/1220 (100%)	1212 (100%)	6 (0%)	81	83
1	s	1218/1220 (100%)	1213 (100%)	5 (0%)	84	84
1	t	1218/1220 (100%)	1215 (100%)	3 (0%)	87	87
1	u	1219/1220 (100%)	1214 (100%)	5 (0%)	84	84
1	v	1180/1220 (97%)	1175 (100%)	5 (0%)	84	84
1	w	1133/1220 (93%)	1127 (100%)	6 (0%)	81	83
2	e	253/761 (33%)	252 (100%)	1 (0%)	84	84
2	f	253/761 (33%)	253 (100%)	0	100	100
2	g	253/761 (33%)	252 (100%)	1 (0%)	84	84
2	h	253/761 (33%)	252 (100%)	1 (0%)	84	84
2	i	253/761 (33%)	249 (98%)	4 (2%)	55	70
2	j	253/761 (33%)	252 (100%)	1 (0%)	84	84
2	k	253/761 (33%)	251 (99%)	2 (1%)	73	80
2	l	253/761 (33%)	253 (100%)	0	100	100
2	m	253/761 (33%)	252 (100%)	1 (0%)	84	84
2	n	253/761 (33%)	250 (99%)	3 (1%)	63	75
2	o	253/761 (33%)	249 (98%)	4 (2%)	55	70
2	p	253/761 (33%)	251 (99%)	2 (1%)	73	80
3	1	52/77 (68%)	52 (100%)	0	100	100
3	2	52/77 (68%)	52 (100%)	0	100	100
3	3	52/77 (68%)	52 (100%)	0	100	100
3	4	49/77 (64%)	49 (100%)	0	100	100
3	J	52/77 (68%)	52 (100%)	0	100	100
3	K	52/77 (68%)	52 (100%)	0	100	100
3	L	52/77 (68%)	51 (98%)	1 (2%)	50	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	52/77 (68%)	52 (100%)	0	100	100
3	N	52/77 (68%)	52 (100%)	0	100	100
3	O	52/77 (68%)	52 (100%)	0	100	100
3	P	52/77 (68%)	52 (100%)	0	100	100
3	Q	52/77 (68%)	52 (100%)	0	100	100
3	R	52/77 (68%)	52 (100%)	0	100	100
3	x	52/77 (68%)	52 (100%)	0	100	100
3	y	52/77 (68%)	52 (100%)	0	100	100
3	z	52/77 (68%)	52 (100%)	0	100	100
4	5	232/273 (85%)	231 (100%)	1 (0%)	84	84
4	S	273/273 (100%)	268 (98%)	5 (2%)	51	68
4	T	273/273 (100%)	270 (99%)	3 (1%)	65	76
4	U	273/273 (100%)	266 (97%)	7 (3%)	40	62
4	V	273/273 (100%)	268 (98%)	5 (2%)	51	68
5	6	261/274 (95%)	259 (99%)	2 (1%)	73	80
5	7	274/274 (100%)	272 (99%)	2 (1%)	76	81
5	W	274/274 (100%)	268 (98%)	6 (2%)	45	64
5	X	274/274 (100%)	269 (98%)	5 (2%)	51	68
5	Y	274/274 (100%)	272 (99%)	2 (1%)	76	81
5	Z	274/274 (100%)	266 (97%)	8 (3%)	37	58
5	a	273/274 (100%)	269 (98%)	4 (2%)	57	72
5	b	273/274 (100%)	268 (98%)	5 (2%)	51	68
5	c	273/274 (100%)	267 (98%)	6 (2%)	45	64
5	d	273/274 (100%)	268 (98%)	5 (2%)	51	68
All	All	27226/33989 (80%)	27011 (99%)	215 (1%)	70	80

5 of 215 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	u	860	ILE
2	o	31	LEU
5	b	214	ASP
1	v	428	VAL
2	h	66	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 722 such sidechains are listed below:

Mol	Chain	Res	Type
1	v	1325	HIS
2	o	39	HIS
1	w	587	HIS
1	v	1241	GLN
2	h	237	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.

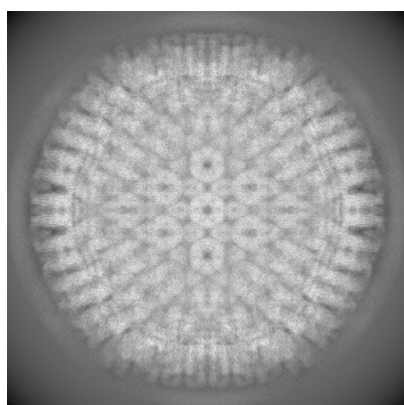
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20557. These allow visual inspection of the internal detail of the map and identification of artifacts.

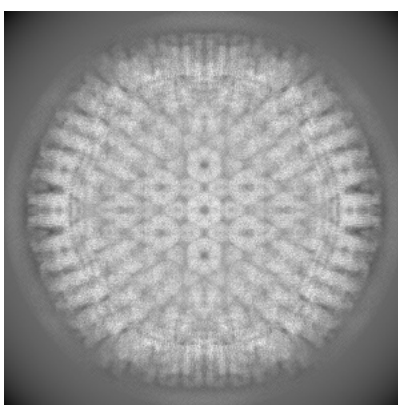
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

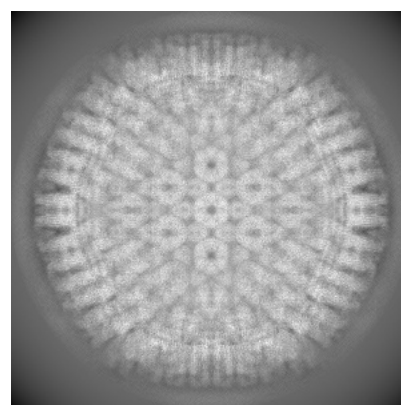
6.1.1 Primary map



X



Y

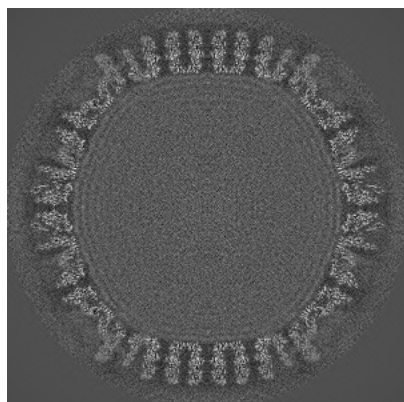


Z

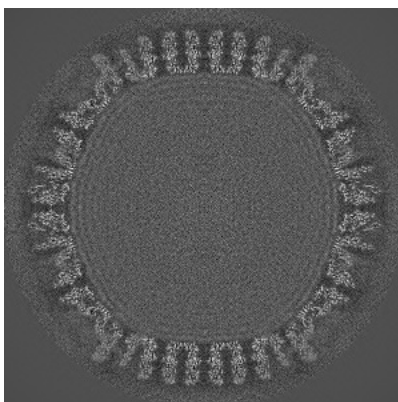
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

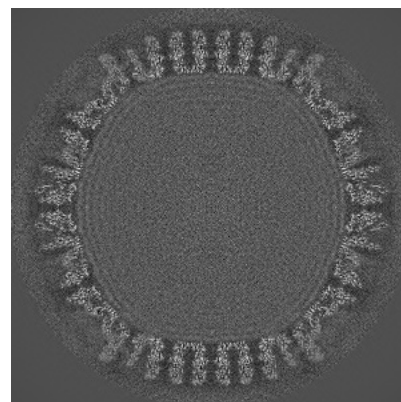
6.2.1 Primary map



X Index: 320



Y Index: 320

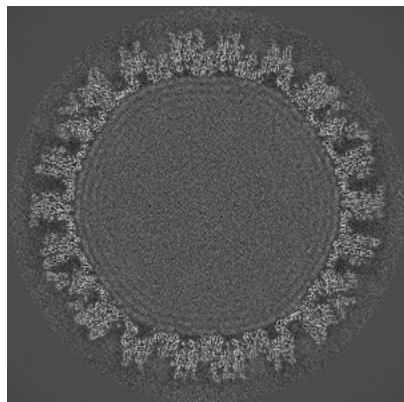


Z Index: 320

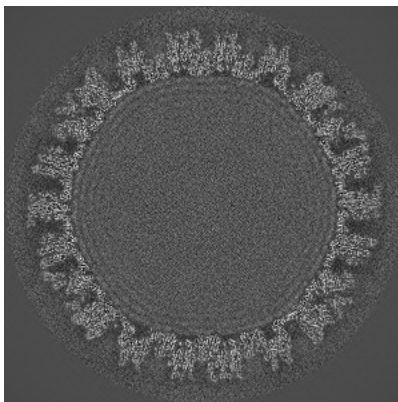
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

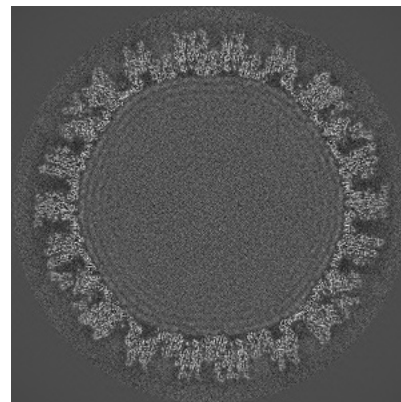
6.3.1 Primary map



X Index: 266



Y Index: 266

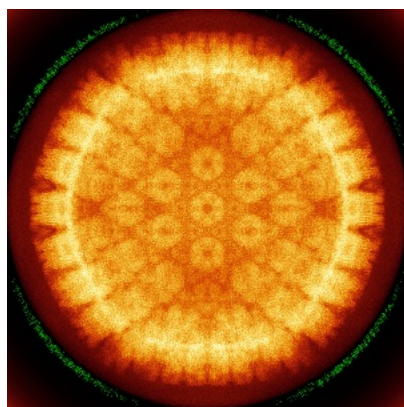


Z Index: 266

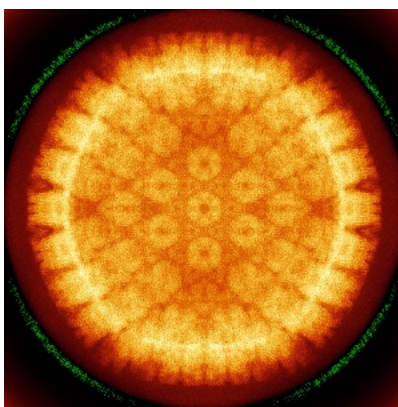
The images above show the largest variance slices of the map in three orthogonal directions.

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

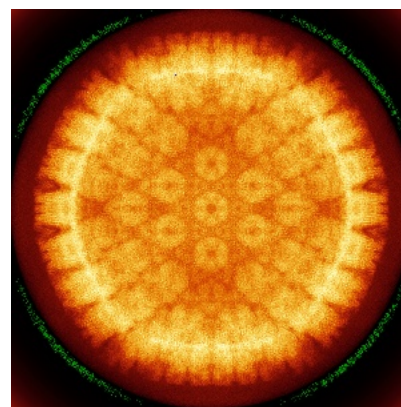
6.4.1 Primary map



X



Y

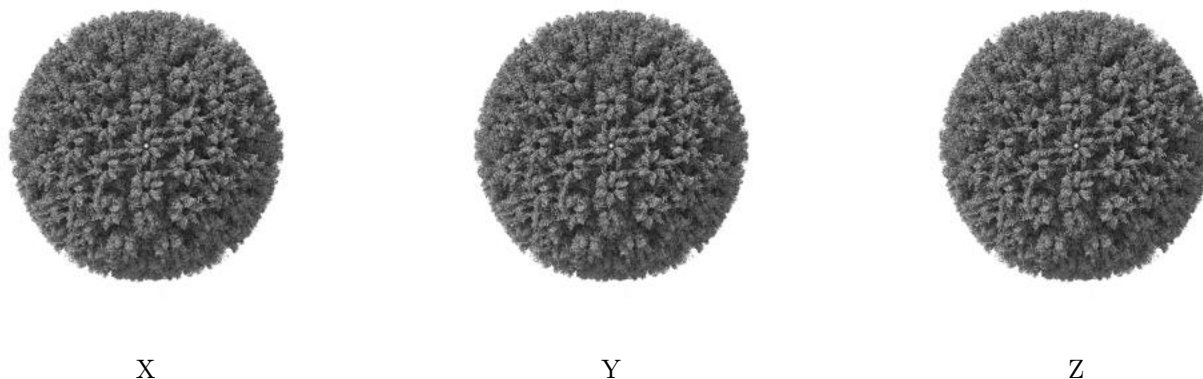


Z

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 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

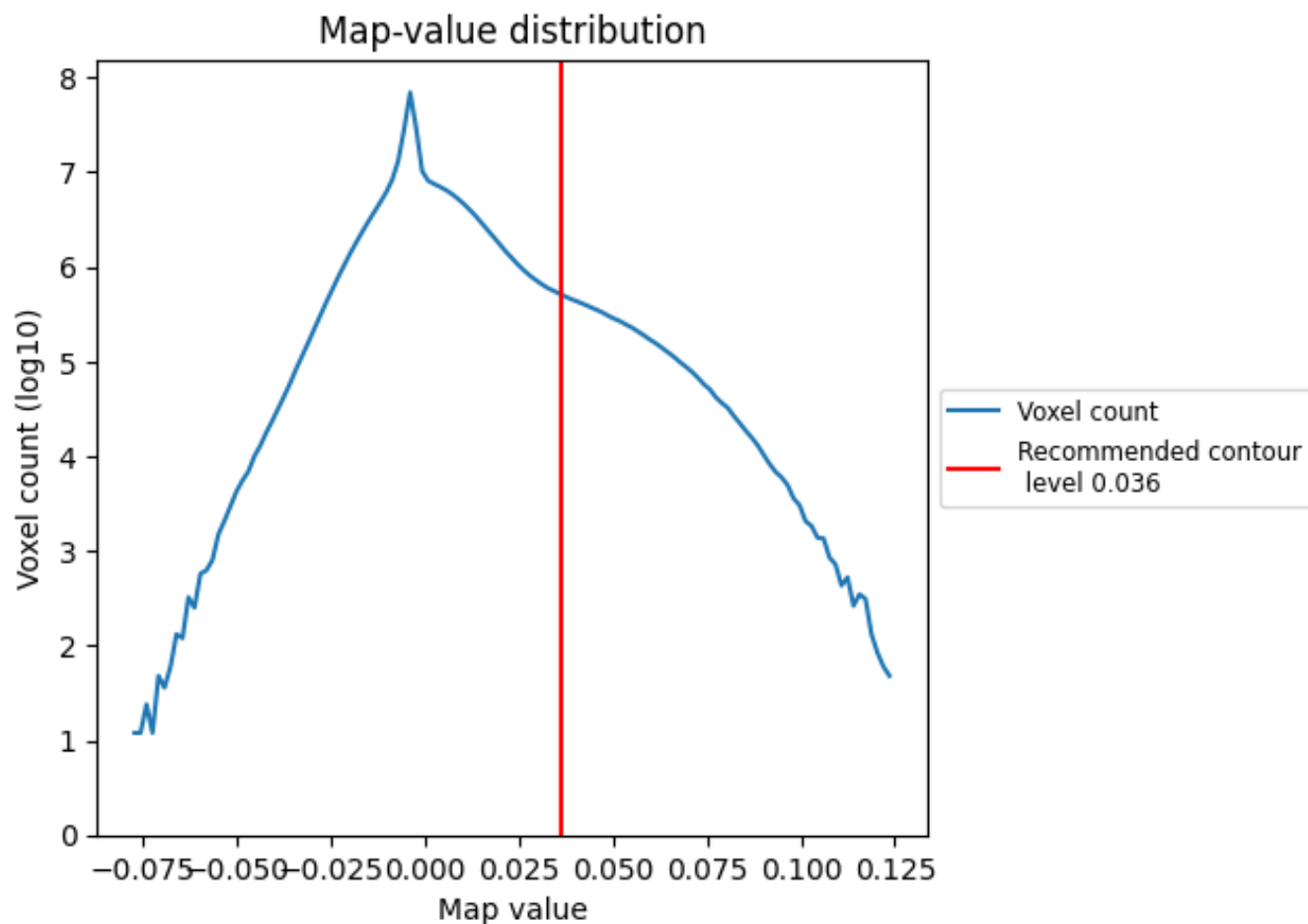
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

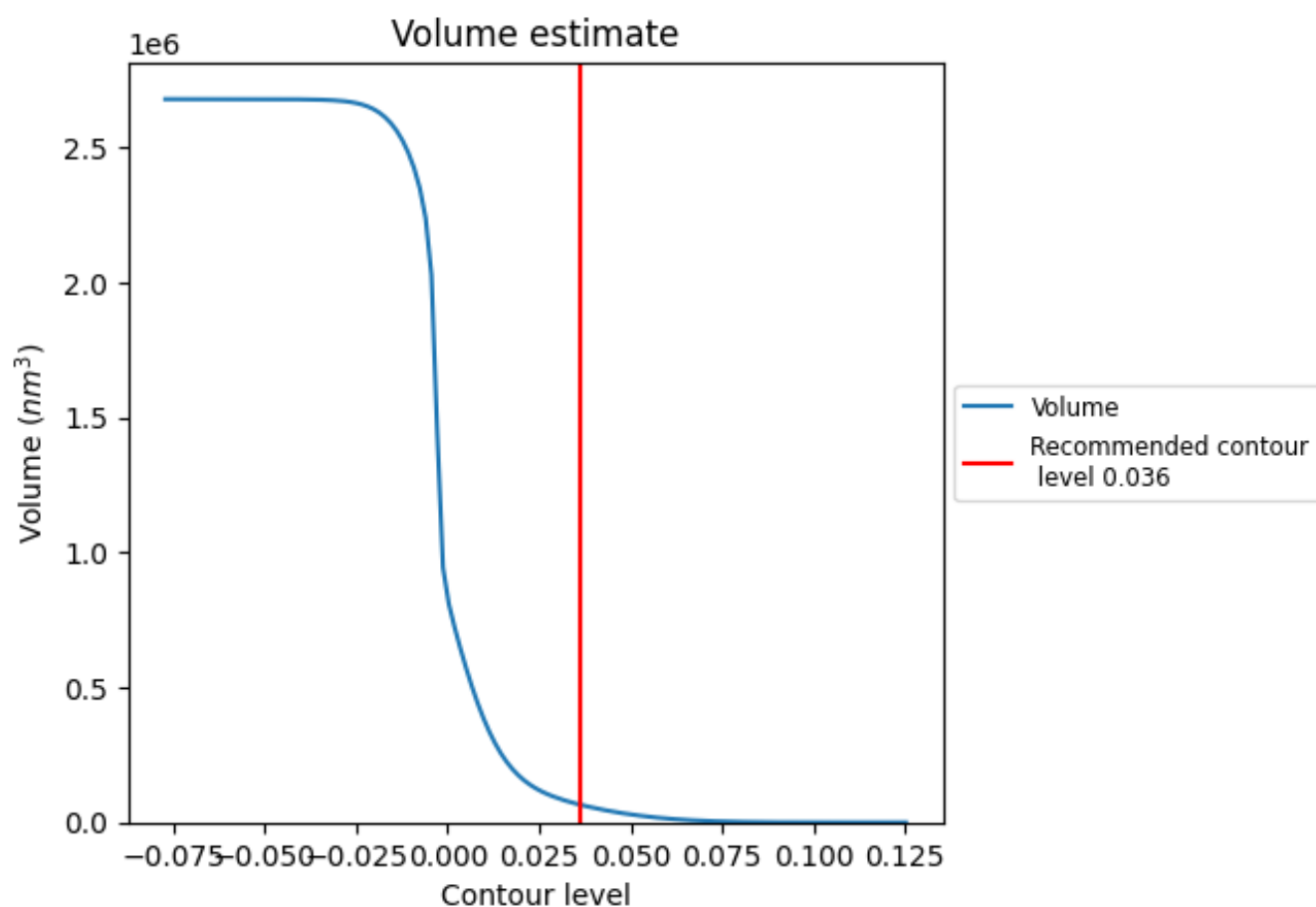
This section contains the results of statistical analysis of the map.

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.

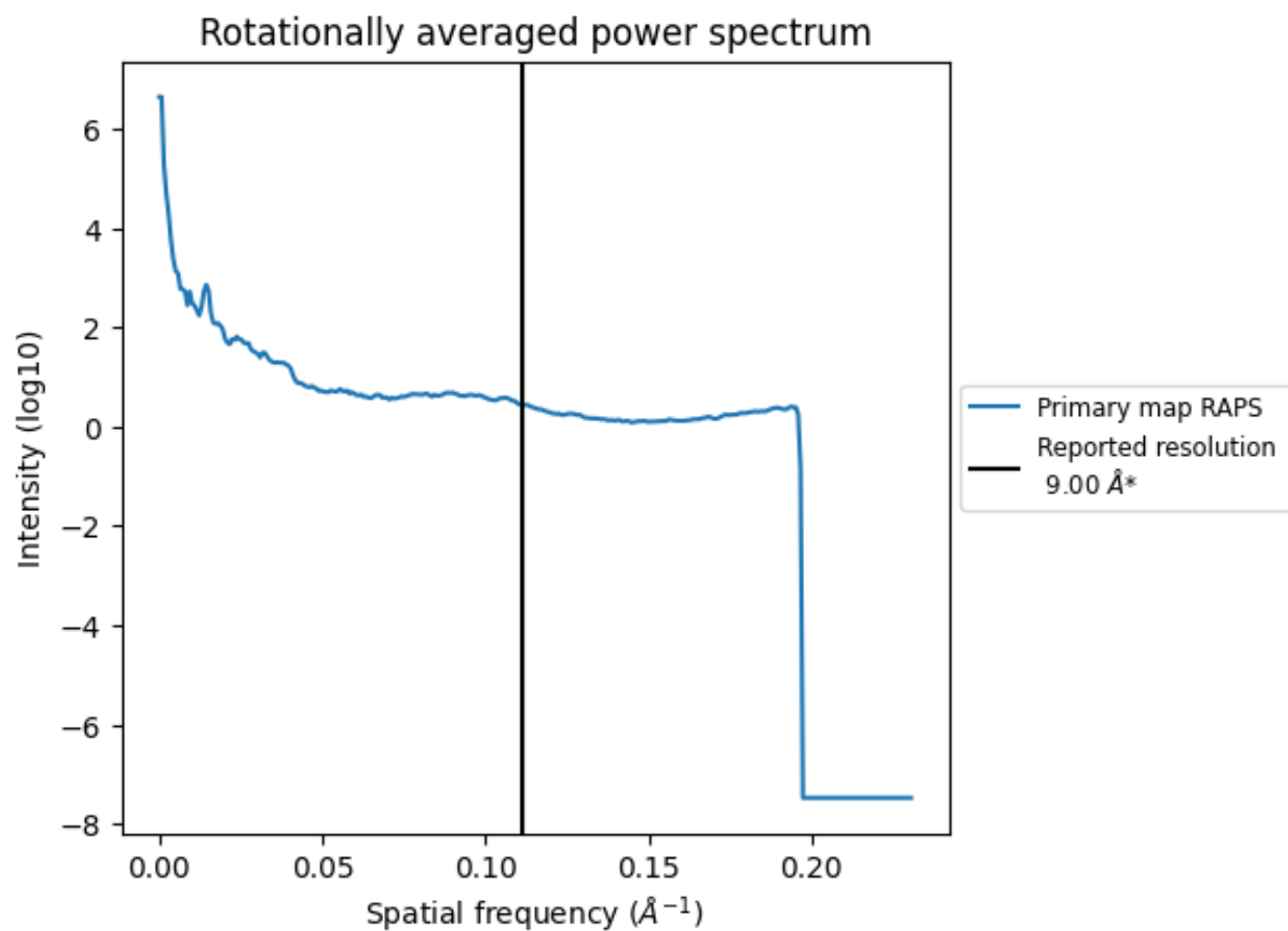
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66298 nm³; this corresponds to an approximate mass of 59889 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 0.111 Å⁻¹

8 Fourier-Shell correlation

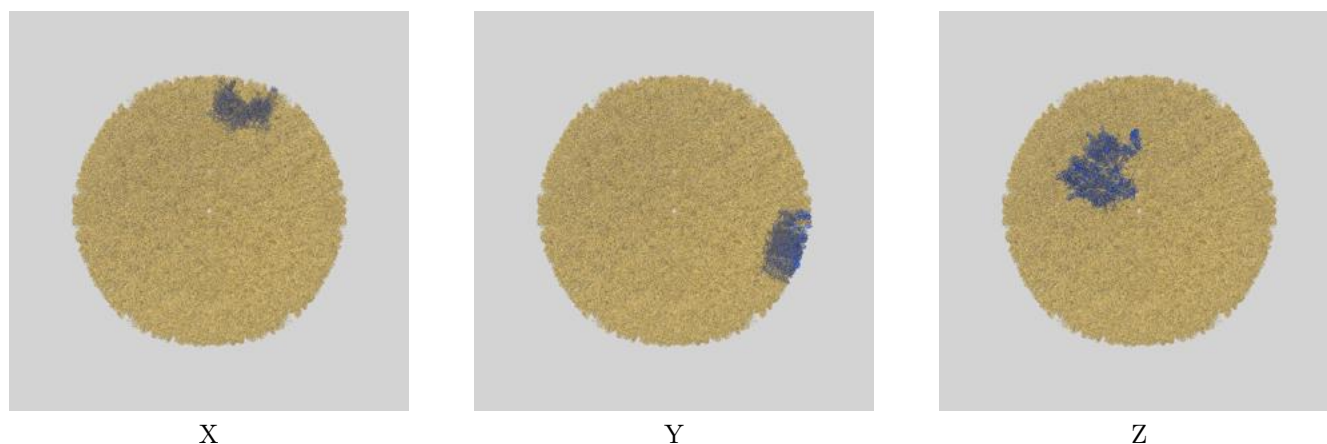
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

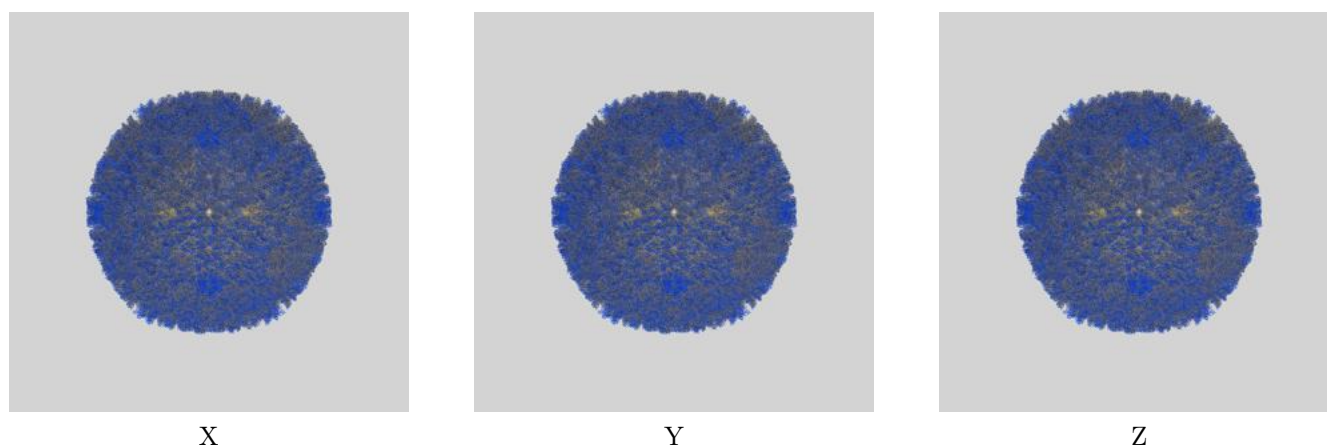
This section contains information regarding the fit between EMDB map EMD-20557 and PDB model 6Q1F. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

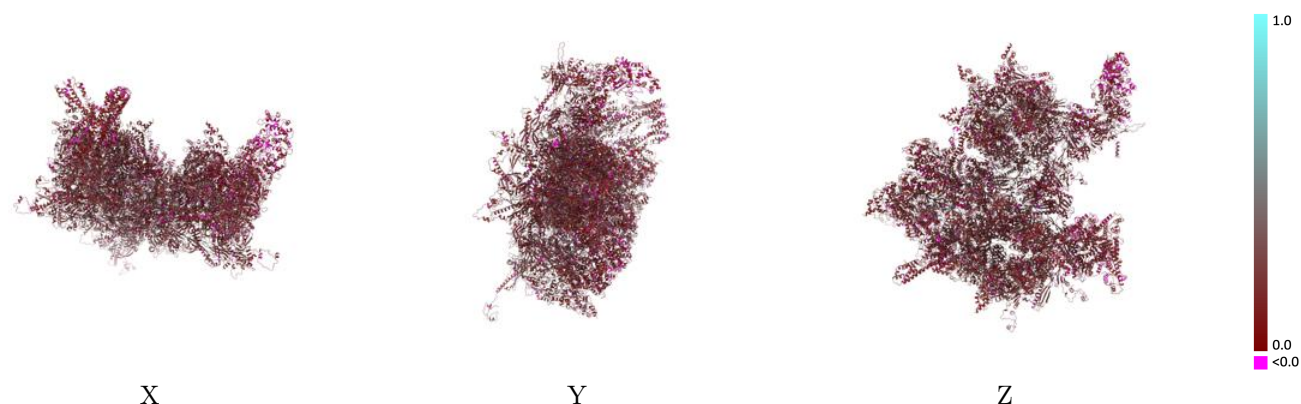


9.1.2 Map-model assembly overlay [i](#)



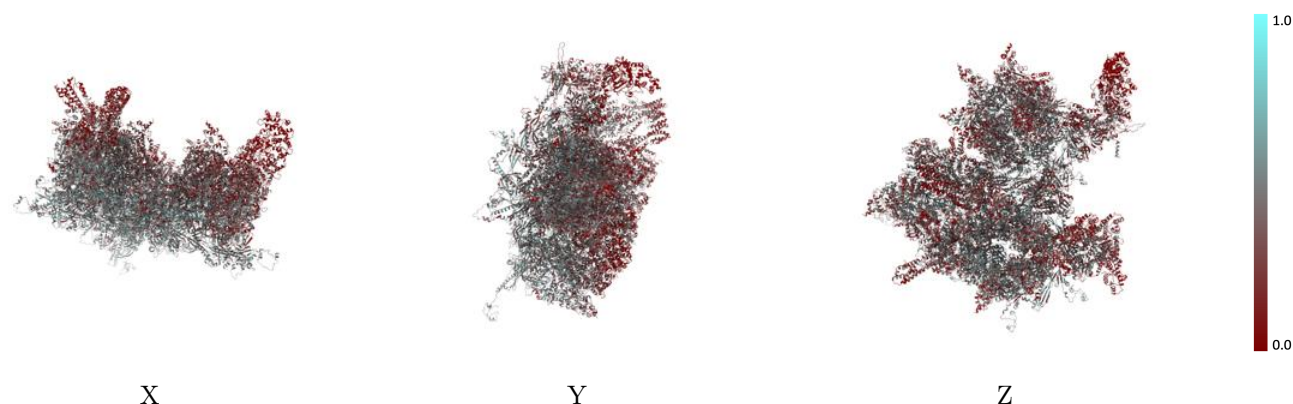
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



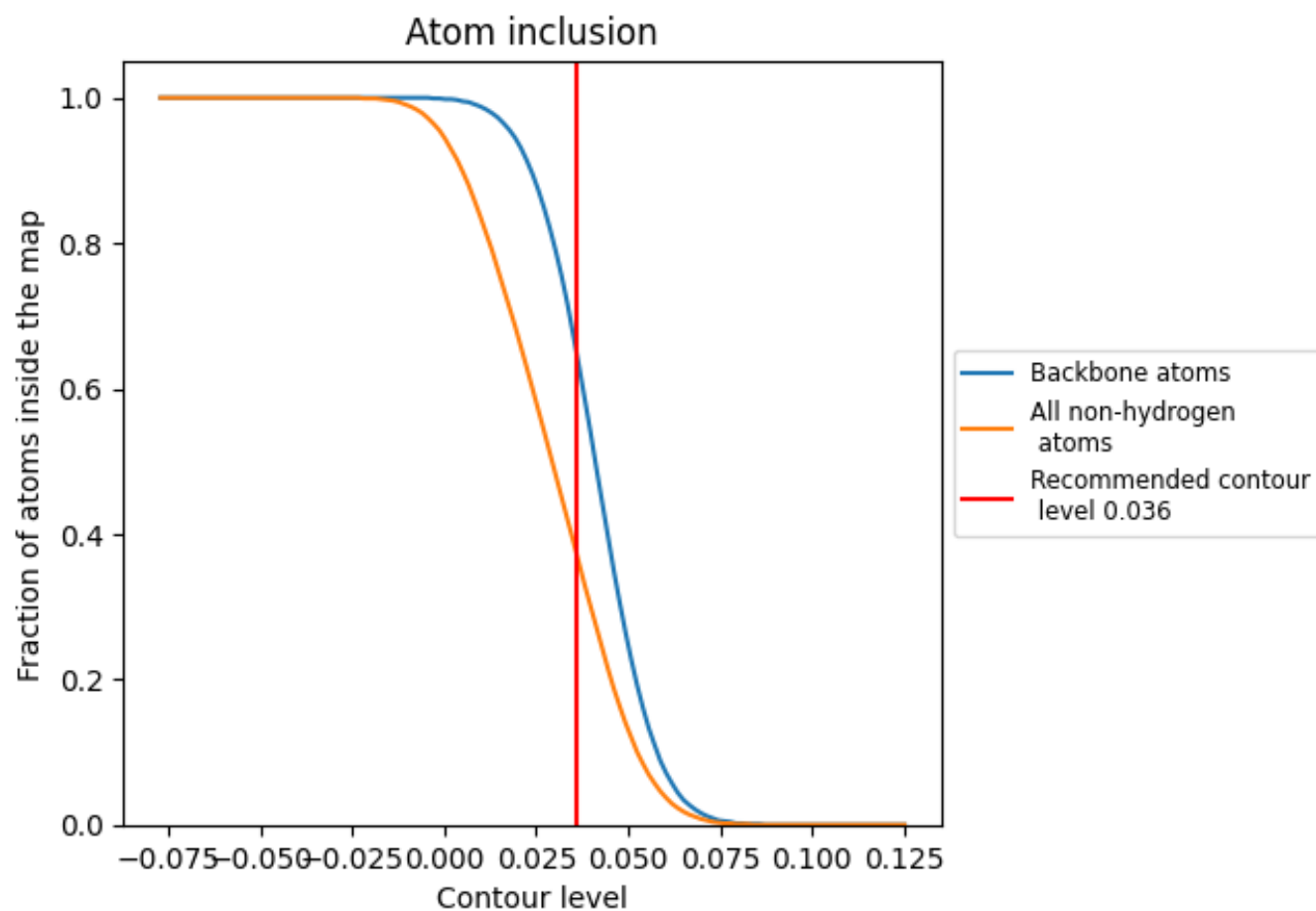
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.036).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 37% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3730	 0.2130
1	 0.3130	 0.1980
2	 0.2630	 0.1960
3	 0.1550	 0.1720
4	 0.0020	 0.1250
5	 0.3020	 0.2000
6	 0.2610	 0.1820
7	 0.2510	 0.1770
A	 0.4450	 0.2310
B	 0.4320	 0.2250
C	 0.4360	 0.2330
D	 0.4520	 0.2340
E	 0.4520	 0.2330
F	 0.4260	 0.2240
G	 0.4410	 0.2260
H	 0.4620	 0.2370
I	 0.4430	 0.2290
J	 0.2860	 0.1930
K	 0.2750	 0.2050
L	 0.2460	 0.2050
M	 0.2900	 0.1910
N	 0.2610	 0.2000
O	 0.2160	 0.2160
P	 0.2900	 0.1820
Q	 0.2480	 0.1880
R	 0.2790	 0.1850
S	 0.4240	 0.2310
T	 0.3590	 0.2160
U	 0.4060	 0.2300
V	 0.4190	 0.2280
W	 0.3780	 0.2090
X	 0.3300	 0.2030
Y	 0.3680	 0.2050
Z	 0.3840	 0.2100
a	 0.3800	 0.2150



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Chain	Atom inclusion	Q-score
b	 0.3540	 0.2050
c	 0.3910	 0.2110
d	 0.3850	 0.2110
e	 0.1900	 0.1650
f	 0.1630	 0.1710
g	 0.2110	 0.1730
h	 0.1070	 0.1560
i	 0.1960	 0.1750
j	 0.1240	 0.1680
k	 0.2250	 0.1540
l	 0.1050	 0.1590
m	 0.2480	 0.1690
n	 0.2660	 0.1640
o	 0.2990	 0.1730
p	 0.2170	 0.1740
q	 0.3610	 0.2130
r	 0.4000	 0.2230
s	 0.4050	 0.2190
t	 0.4220	 0.2250
u	 0.4020	 0.2170
v	 0.3810	 0.2120
w	 0.1810	 0.1650
x	 0.1410	 0.1800
y	 0.1680	 0.1790
z	 0.2250	 0.1960