



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 10:45 PM UTC

PDB ID : 6W19 / pdb_00006w19
EMDB ID : EMD-21504
Title : Structures of Capsid and Capsid-Associated Tegument Complex inside the Epstein-Barr Virus
Authors : Liu, W.; Cui, Y.X.; Wang, C.Y.; Li, Z.H.; Gong, D.Y.; Dai, X.H.; Bi, G.Q.; Sun, R.; Zhou, Z.H.
Deposited on : 2020-03-03
Resolution : 5.50 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

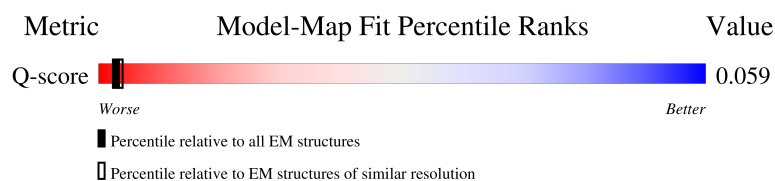
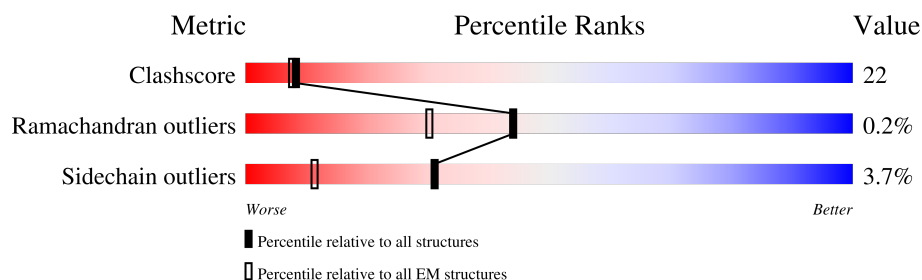
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.50 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	520 (5.00 - 6.00)

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	1381	24% 68% 30% .
1	B	1381	22% 67% 29% ..
1	C	1381	21% 69% 28% ..
1	D	1381	23% 68% 30% .

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Mol	Chain	Length	Quality of chain
1	E	1381	
1	F	1381	
1	G	1381	
1	H	1381	
1	I	1381	
1	J	1381	
1	K	1381	
1	L	1381	
1	M	1381	
1	N	1381	
1	O	1381	
1	P	1381	
2	Q	176	
2	R	176	
2	S	176	
2	T	176	
2	U	176	
2	V	176	
2	W	176	
2	X	176	
2	Y	176	
2	Z	176	
2	a	176	
2	b	176	
2	c	176	

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Mol	Chain	Length	Quality of chain
2	d	176	
2	e	176	
2	u	176	
3	l	364	
3	f	364	
3	g	364	
3	h	364	
3	i	364	
3	j	364	
4	2	301	
4	3	301	
4	k	301	
4	l	301	
4	m	301	
4	n	301	
4	o	301	
4	p	301	
4	q	301	
4	r	301	
4	s	301	
4	t	301	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 225047 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	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	B	1364	Total	C	N	O	S	0	0
			10701	6788	1859	1993	61		
1	C	1363	Total	C	N	O	S	0	0
			10690	6782	1855	1992	61		
1	D	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	E	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	F	1362	Total	C	N	O	S	0	0
			10683	6777	1854	1991	61		
1	G	1381	Total	C	N	O	S	0	0
			10831	6868	1884	2017	62		
1	H	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	I	1364	Total	C	N	O	S	0	0
			10702	6787	1860	1994	61		
1	J	1348	Total	C	N	O	S	0	0
			10601	6730	1844	1966	61		
1	K	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	L	1365	Total	C	N	O	S	0	0
			10705	6790	1860	1994	61		
1	M	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	N	1362	Total	C	N	O	S	0	0
			10683	6777	1854	1991	61		
1	O	1335	Total	C	N	O	S	0	0
			10473	6647	1819	1947	60		
1	P	1292	Total	C	N	O	S	0	0
			10173	6466	1764	1884	59		

- Molecule 2 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	R	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	S	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	T	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	U	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	V	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	W	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	X	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	Y	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	Z	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	a	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	b	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	c	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	d	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	e	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
2	u	63	Total	C	N	O	S	0	0
			528	339	90	98	1		

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	f	315	Total	C	N	O	S	0	0
			2474	1586	436	444	8		
3	g	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		
3	h	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		
3	i	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	j	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		
3	1	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		

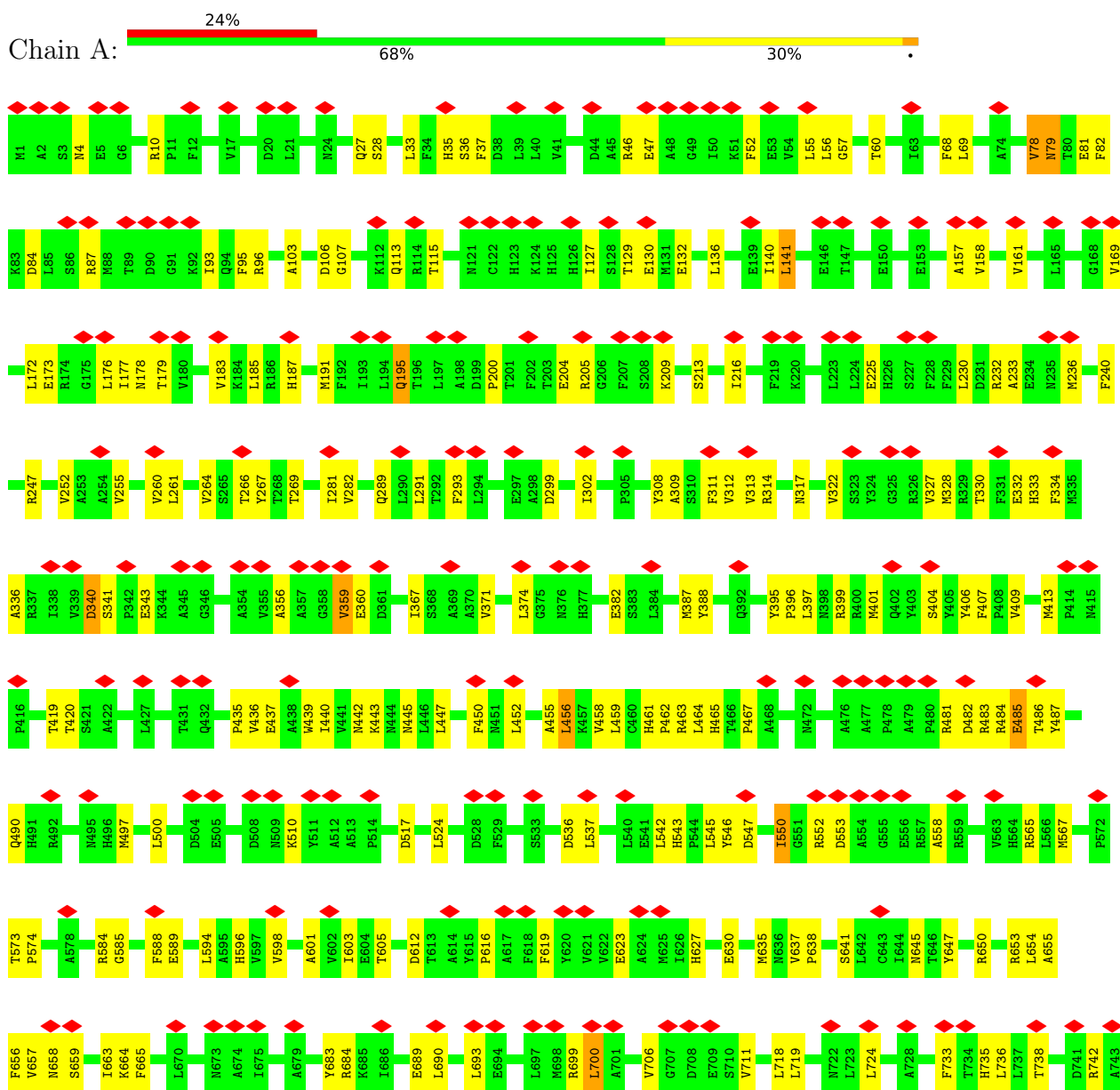
- Molecule 4 is a protein called Triplex capsid protein 2.

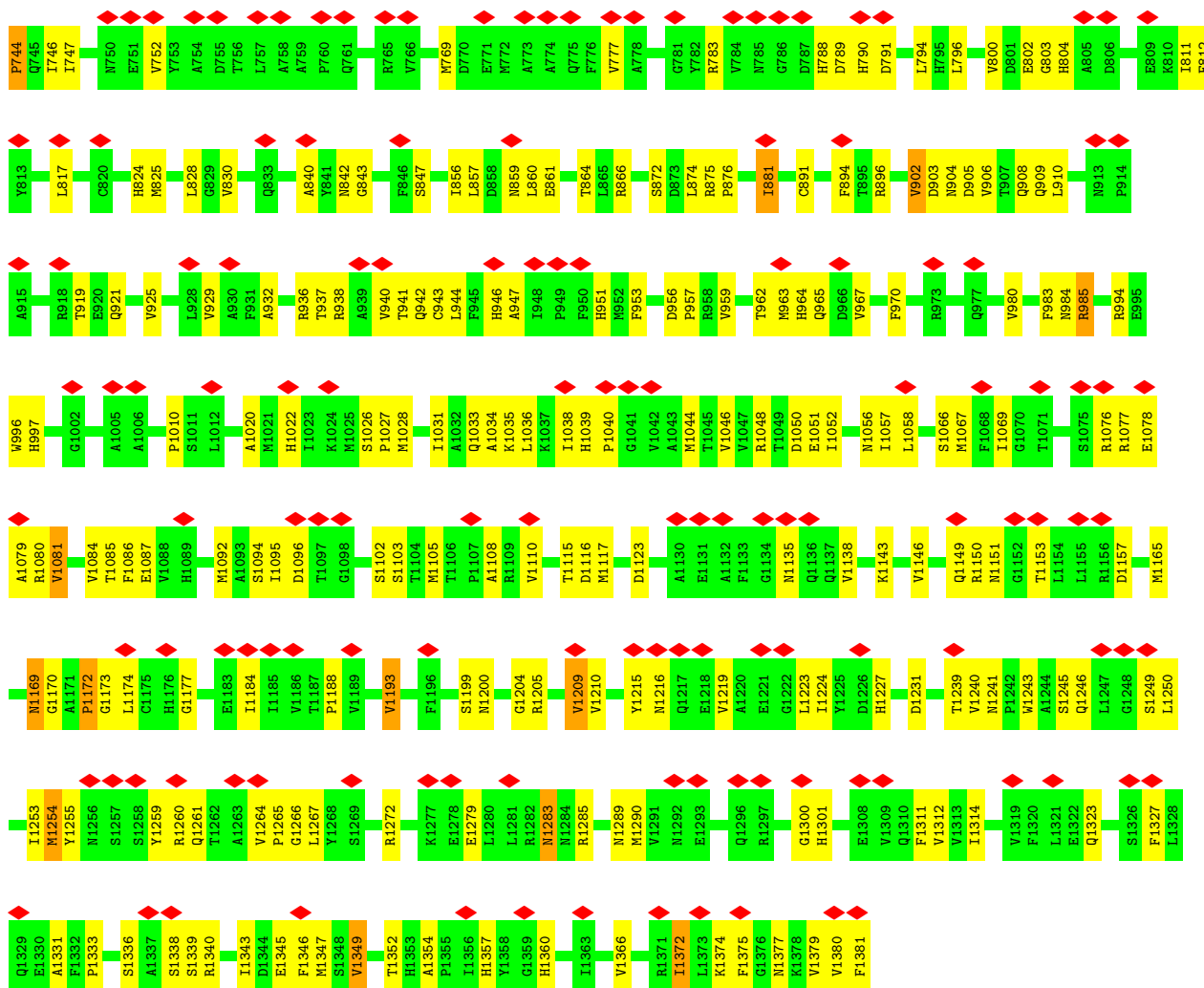
Mol	Chain	Residues	Atoms					AltConf	Trace
4	k	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	l	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	m	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	n	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	o	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	2	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	p	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	q	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	r	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	s	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	t	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
4	3	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		

3 Residue-property plots

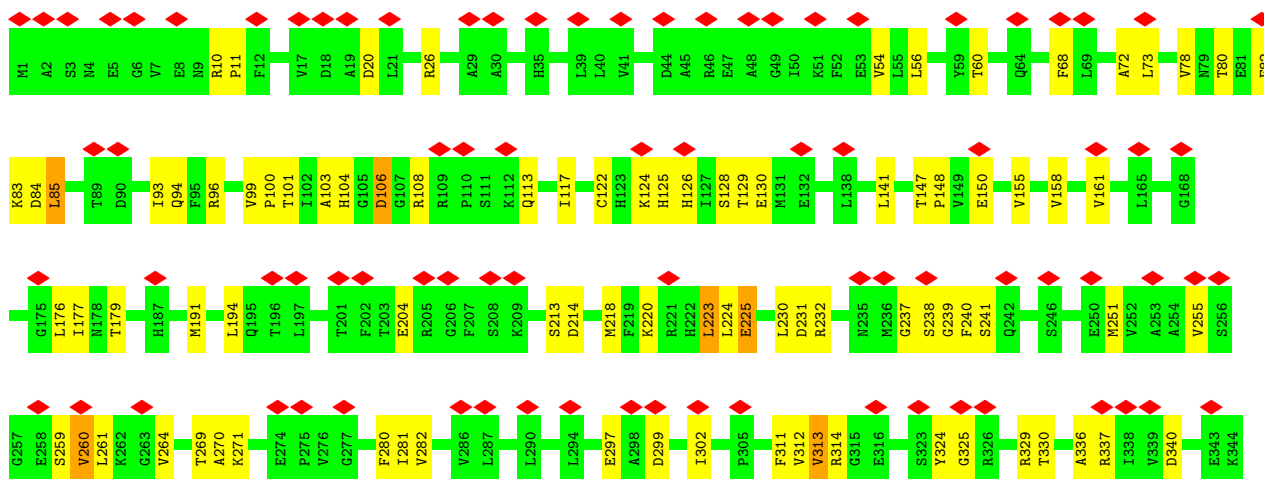
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

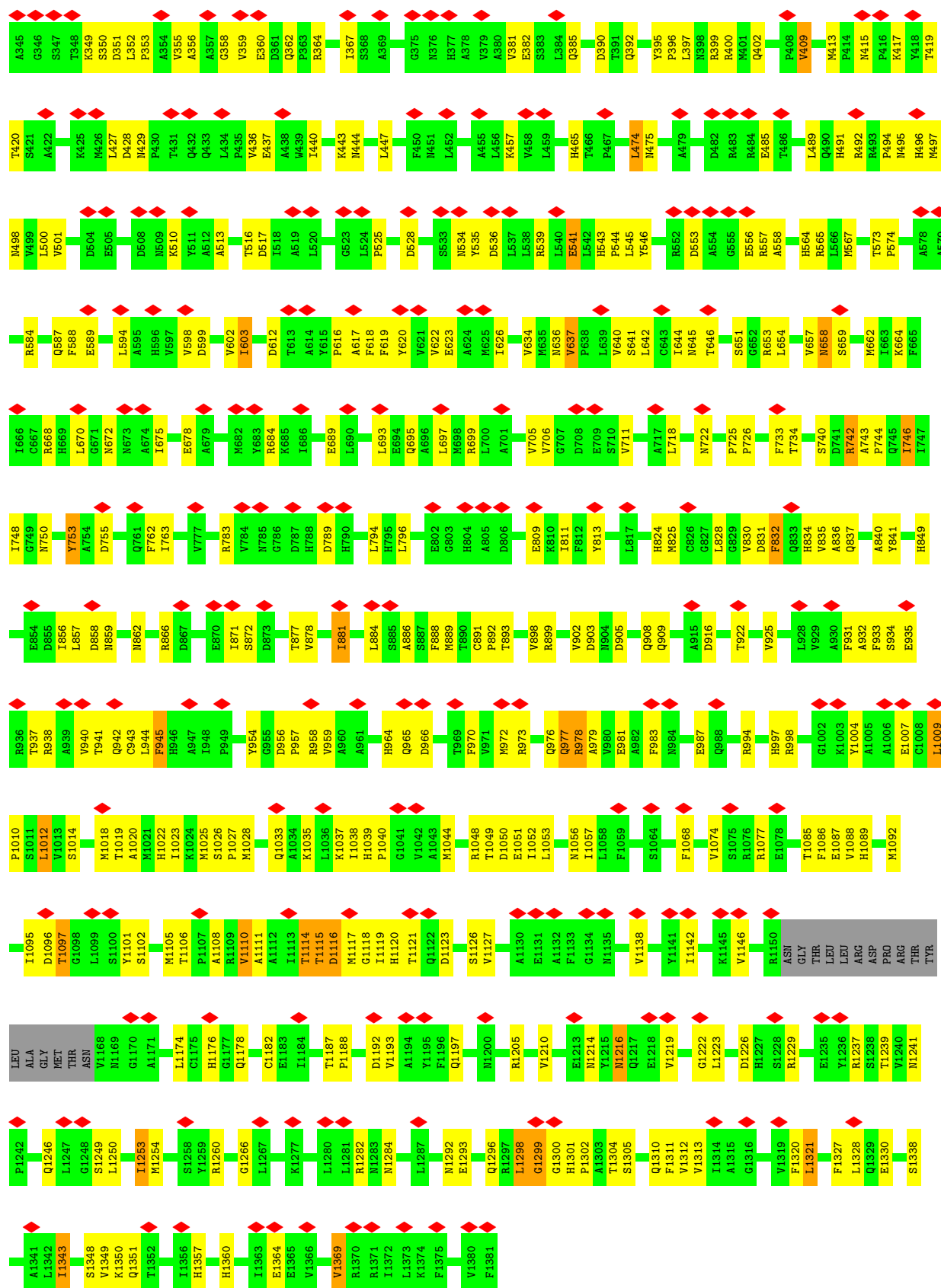
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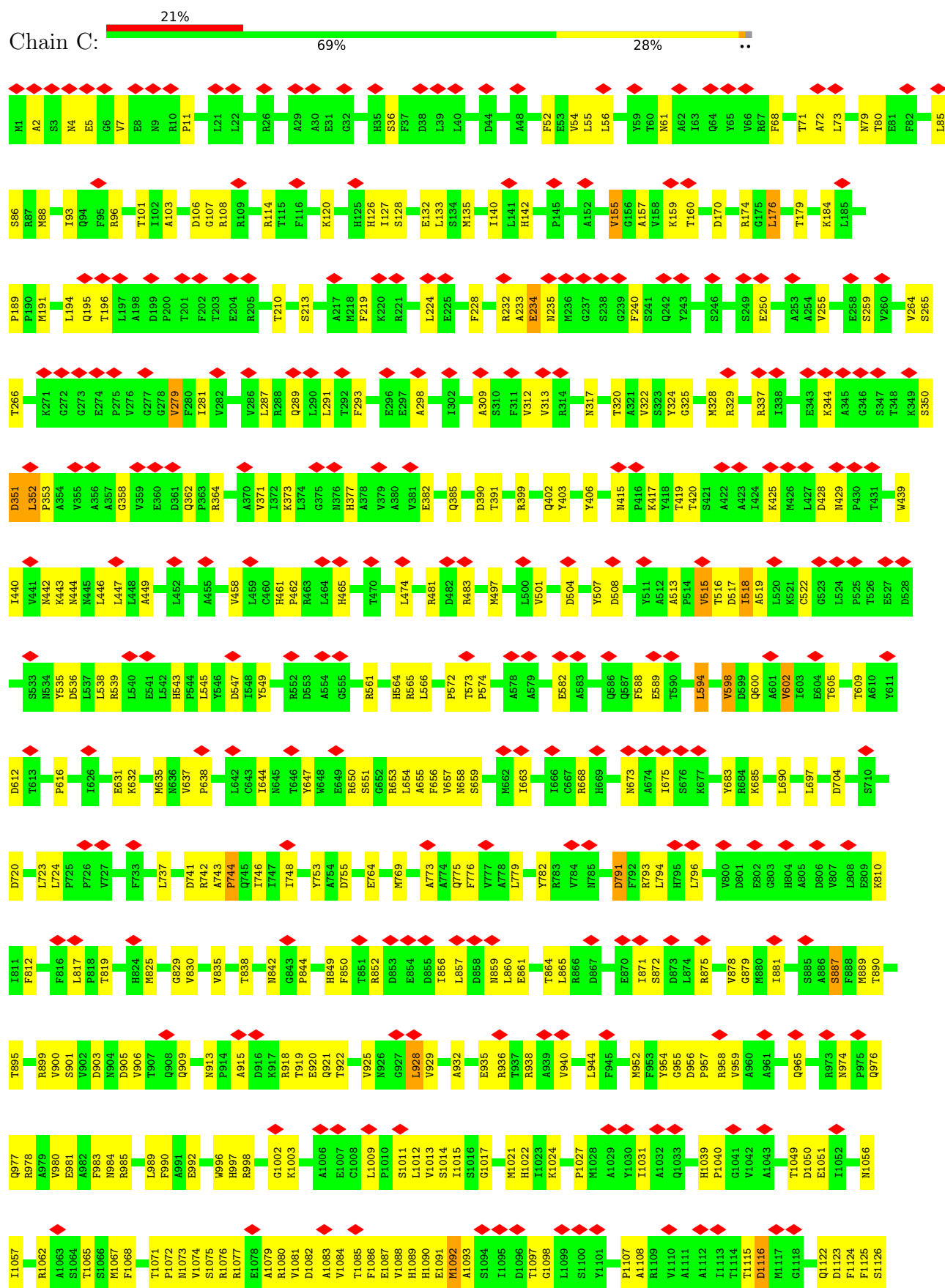


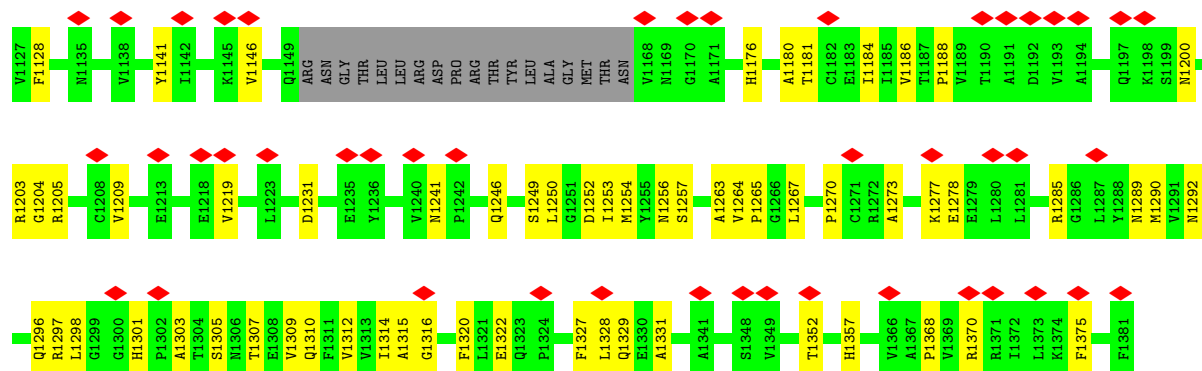
• Molecule 1: Major capsid protein





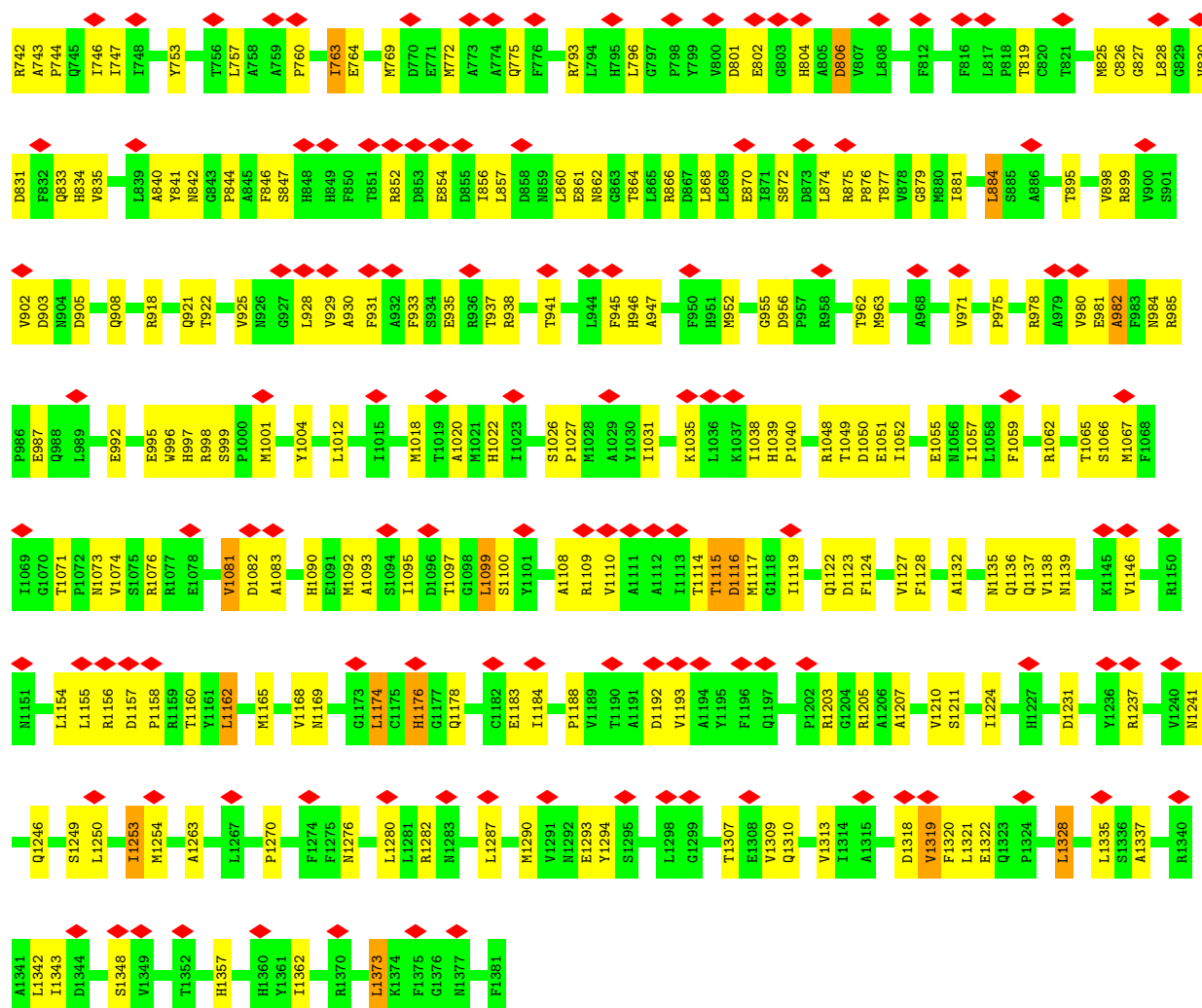
- Molecule 1: Major capsid protein



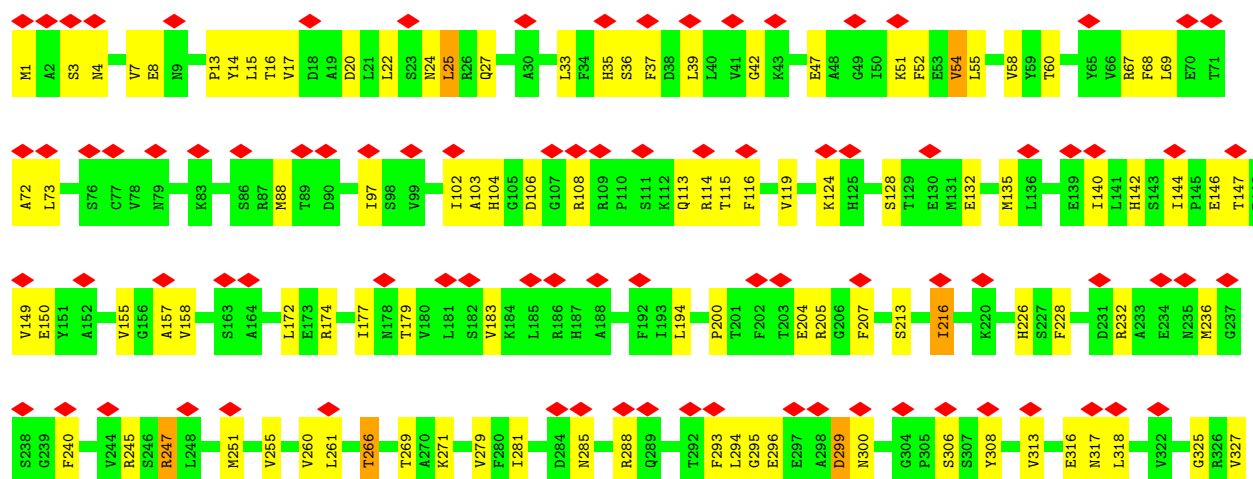


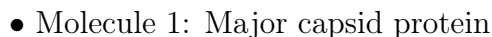
• Molecule 1: Major capsid protein

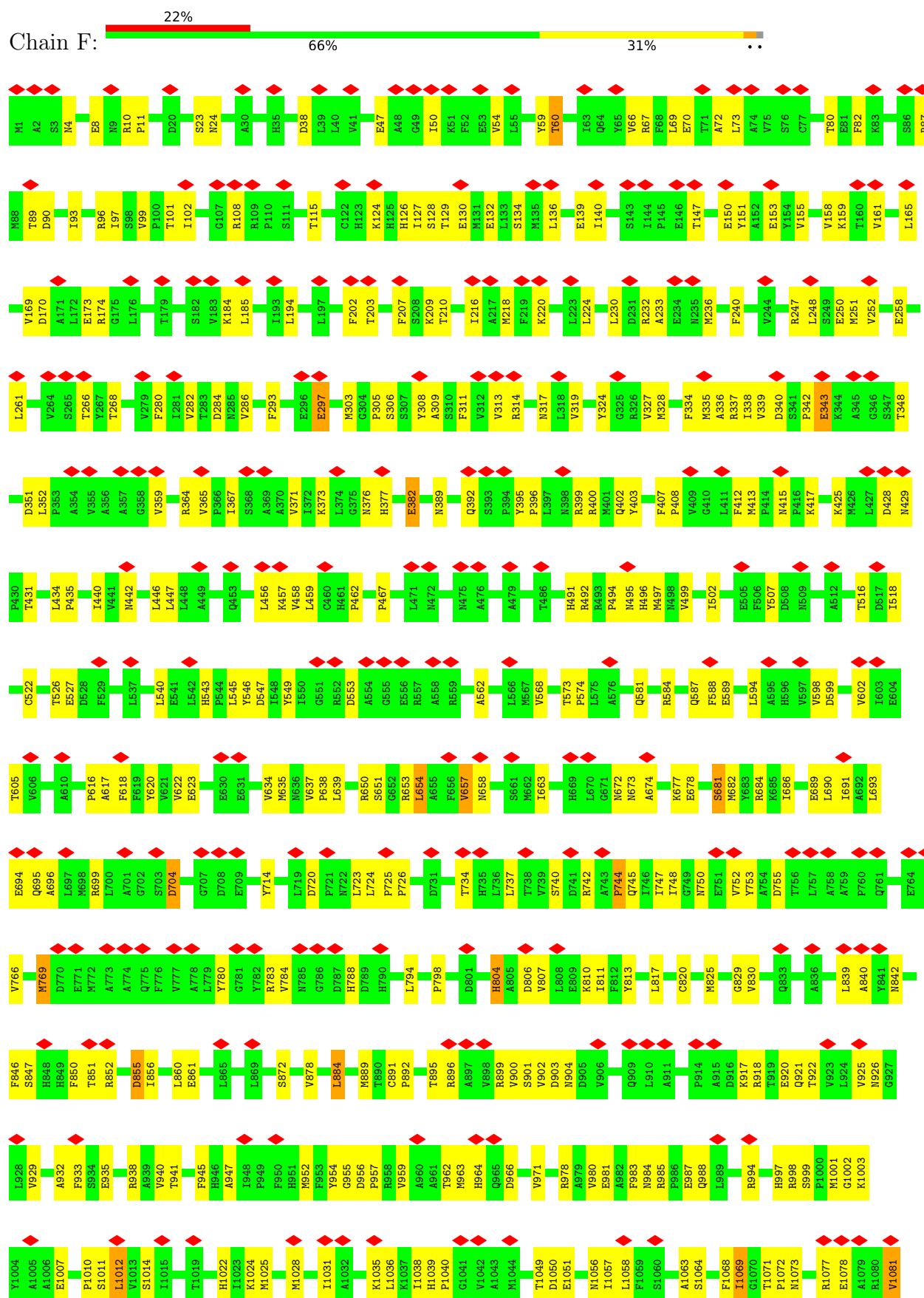


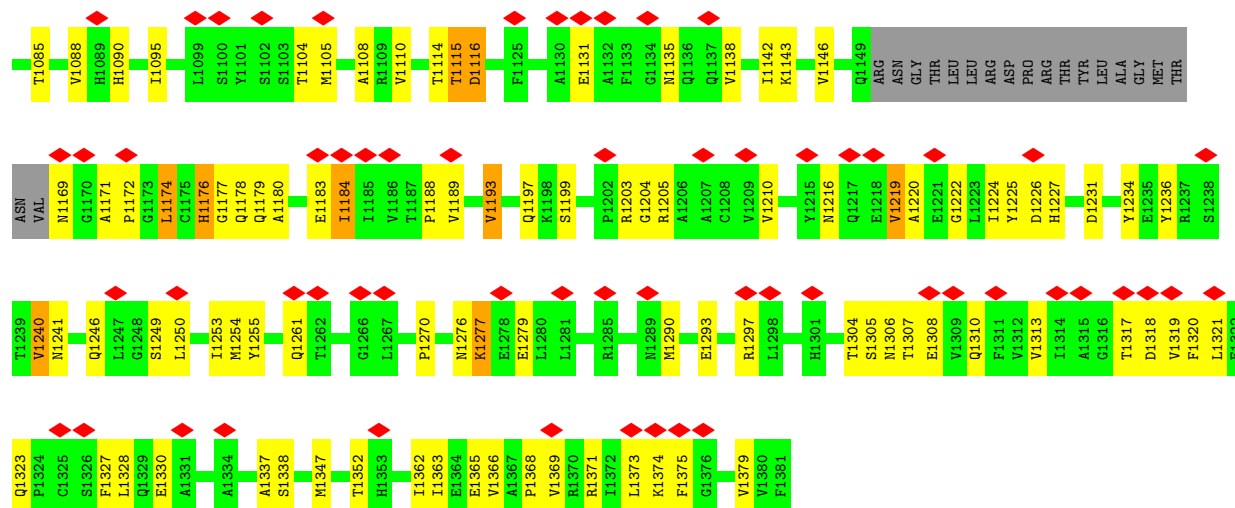


• Molecule 1: Major capsid protein

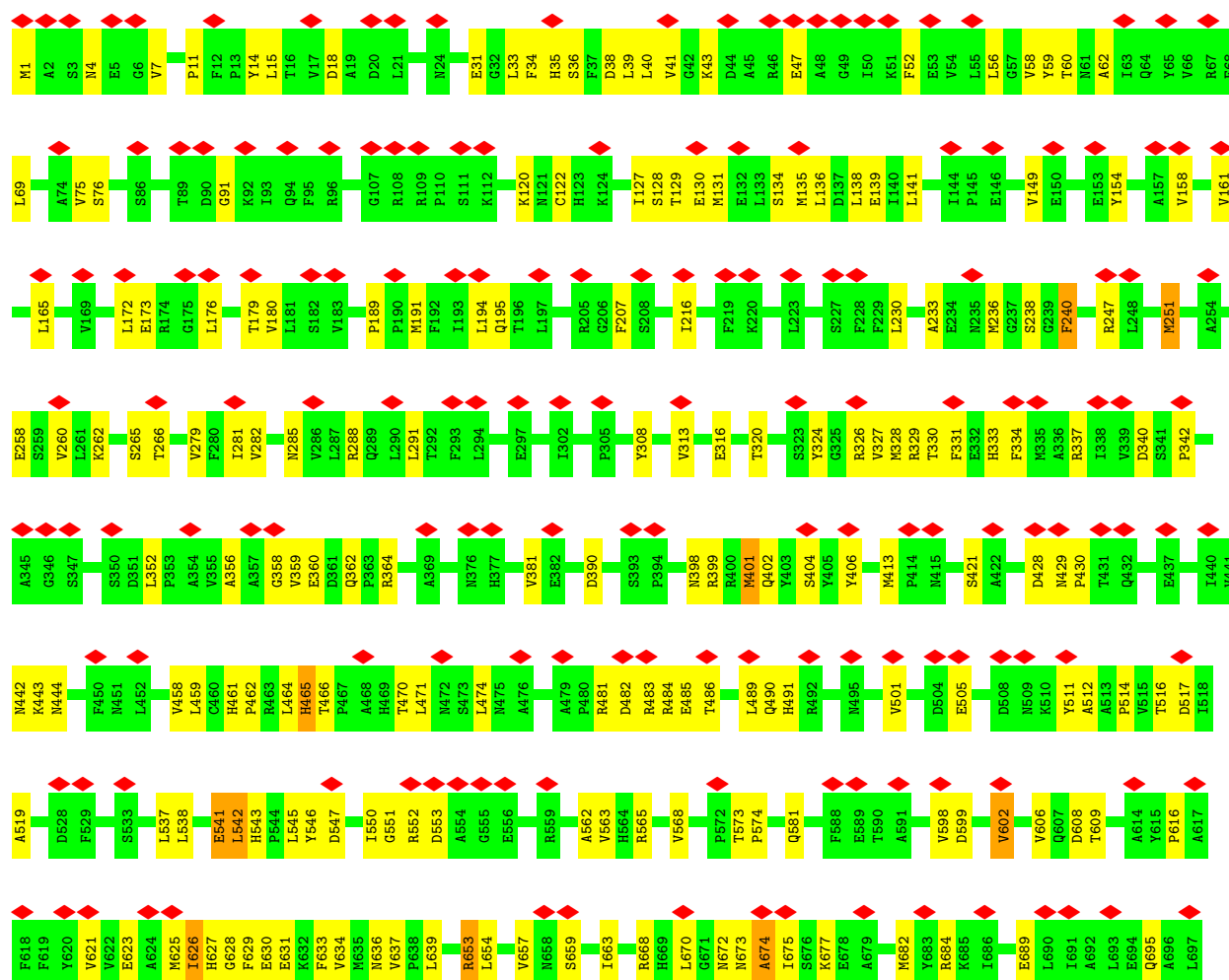
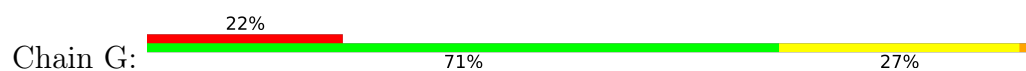


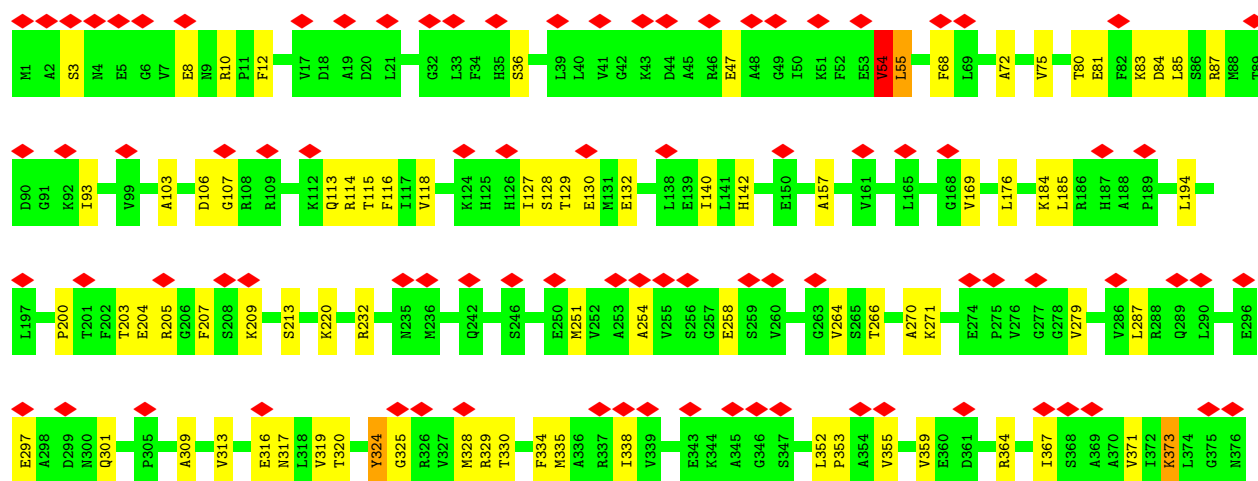


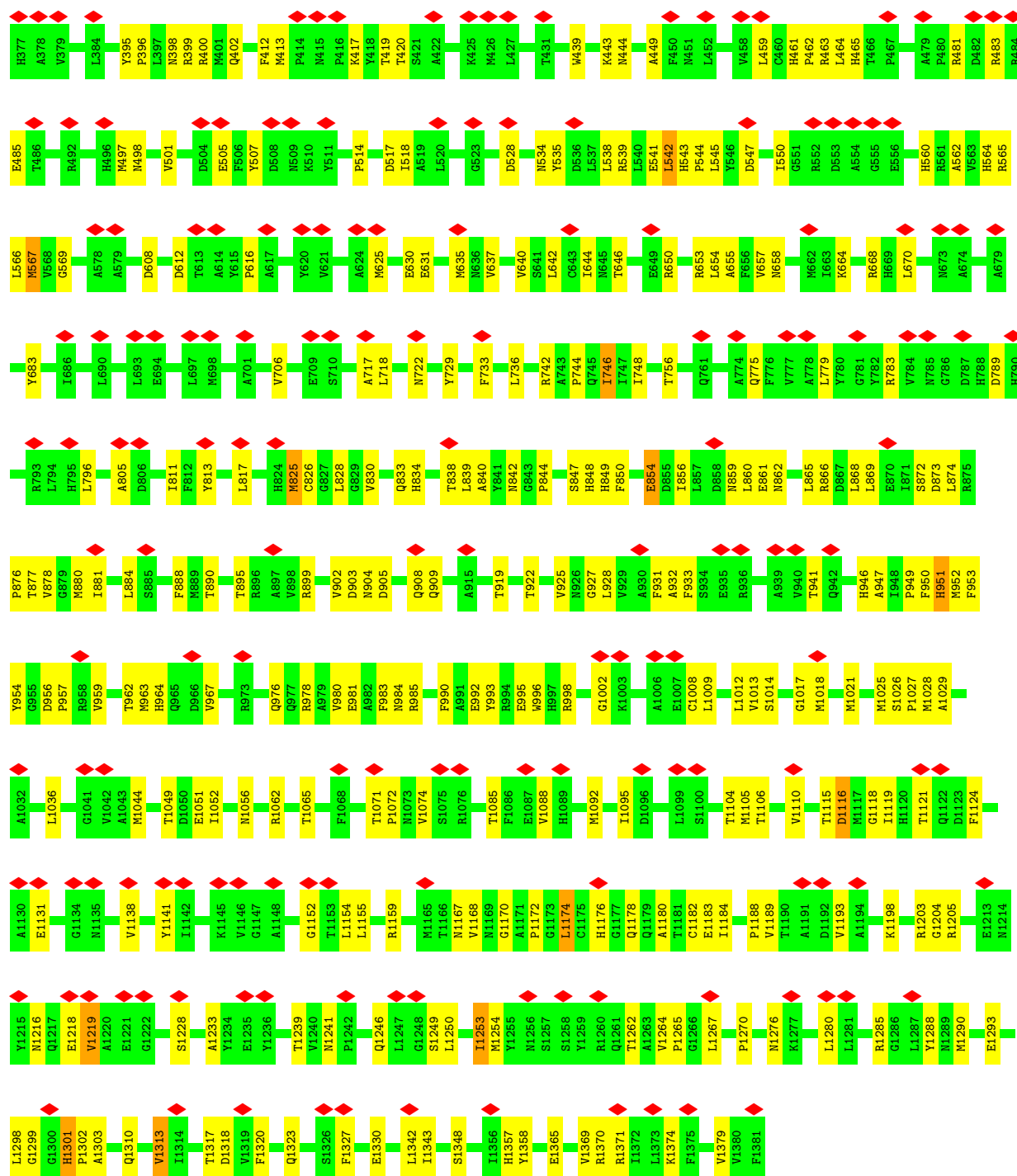




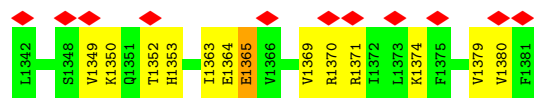
• Molecule 1: Major capsid protein



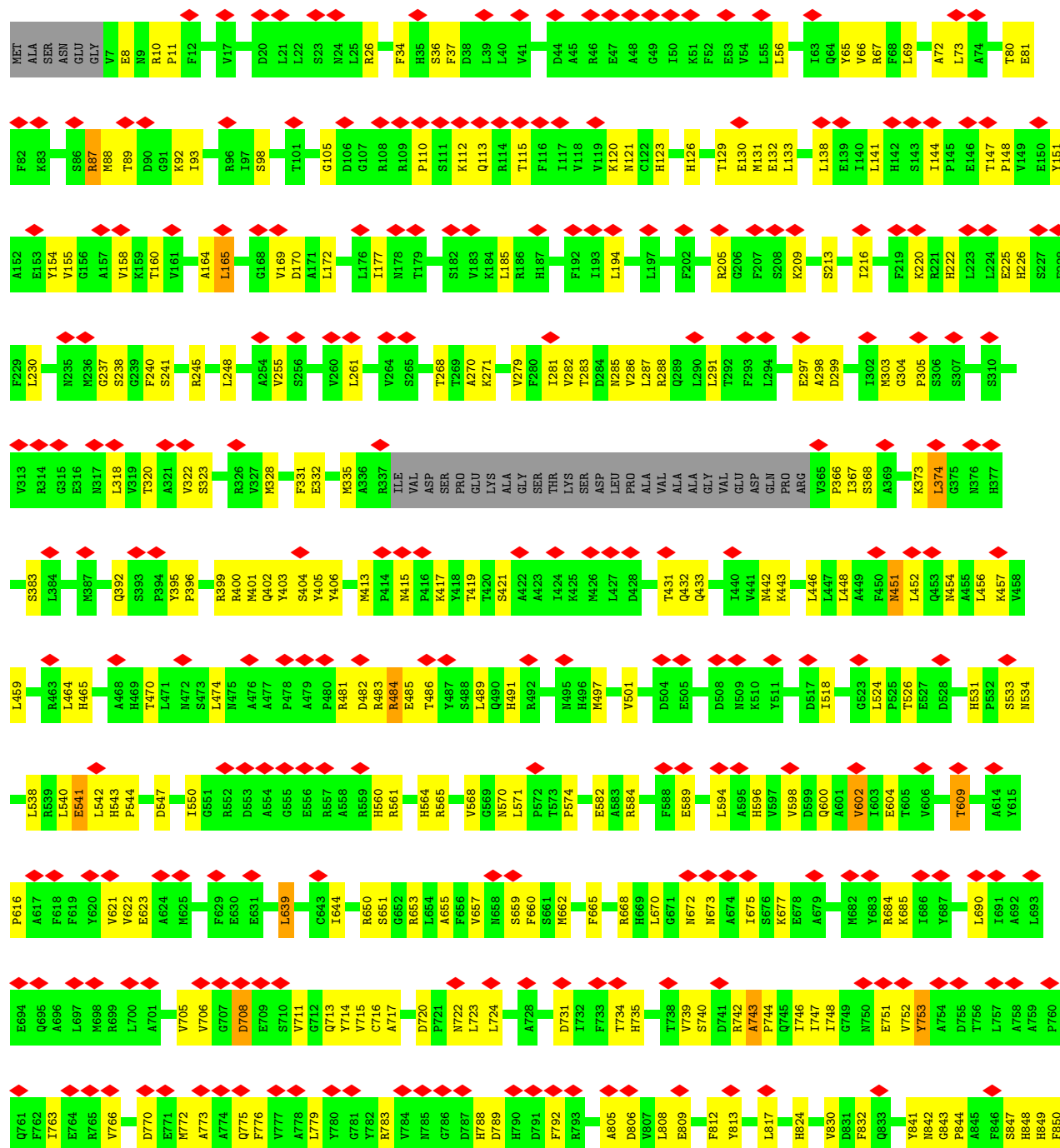


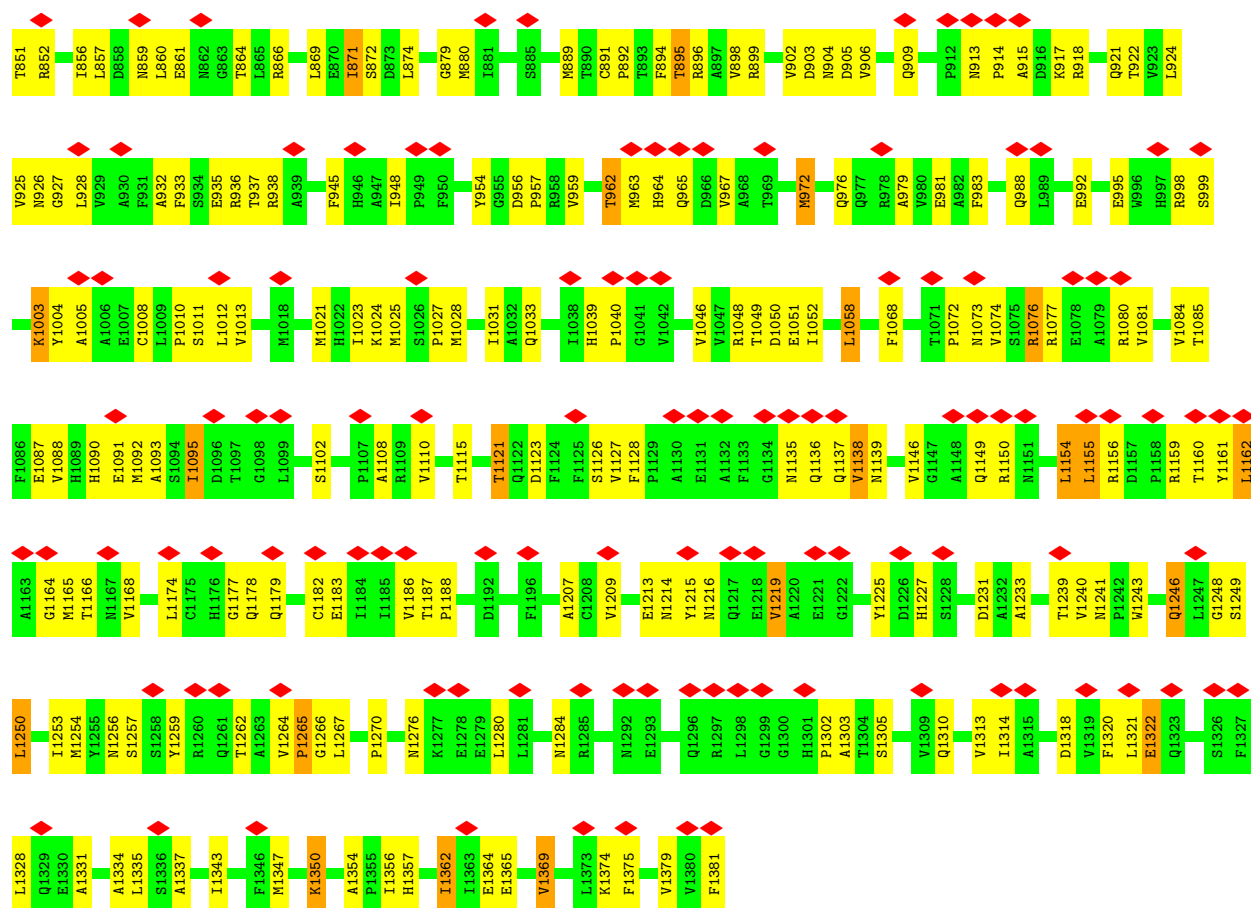




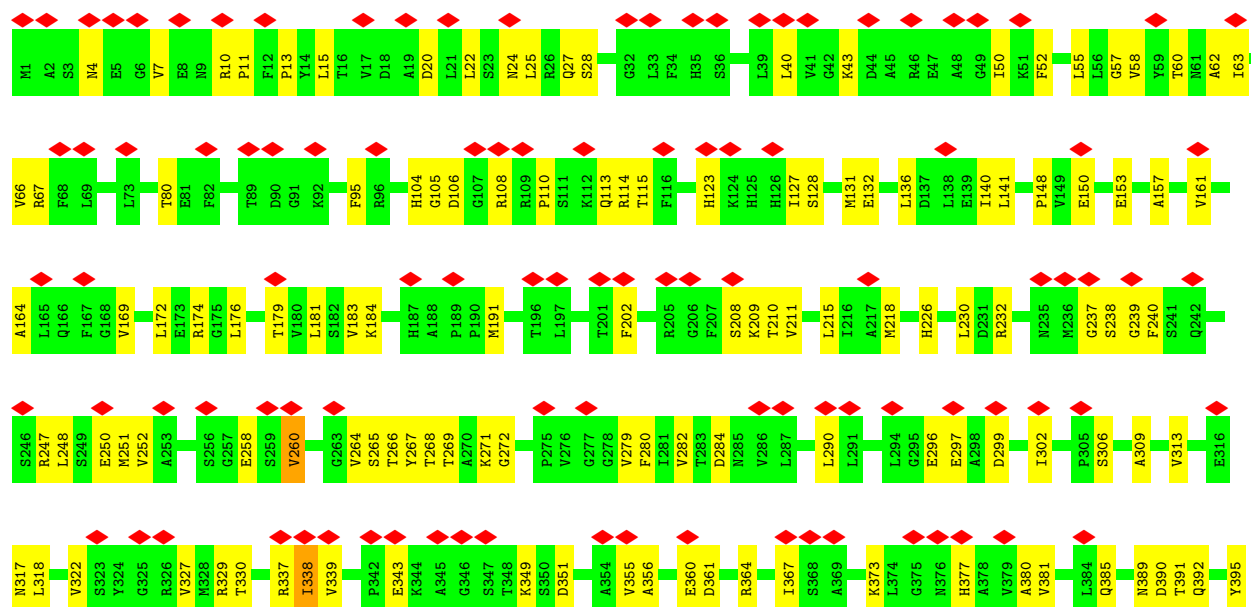


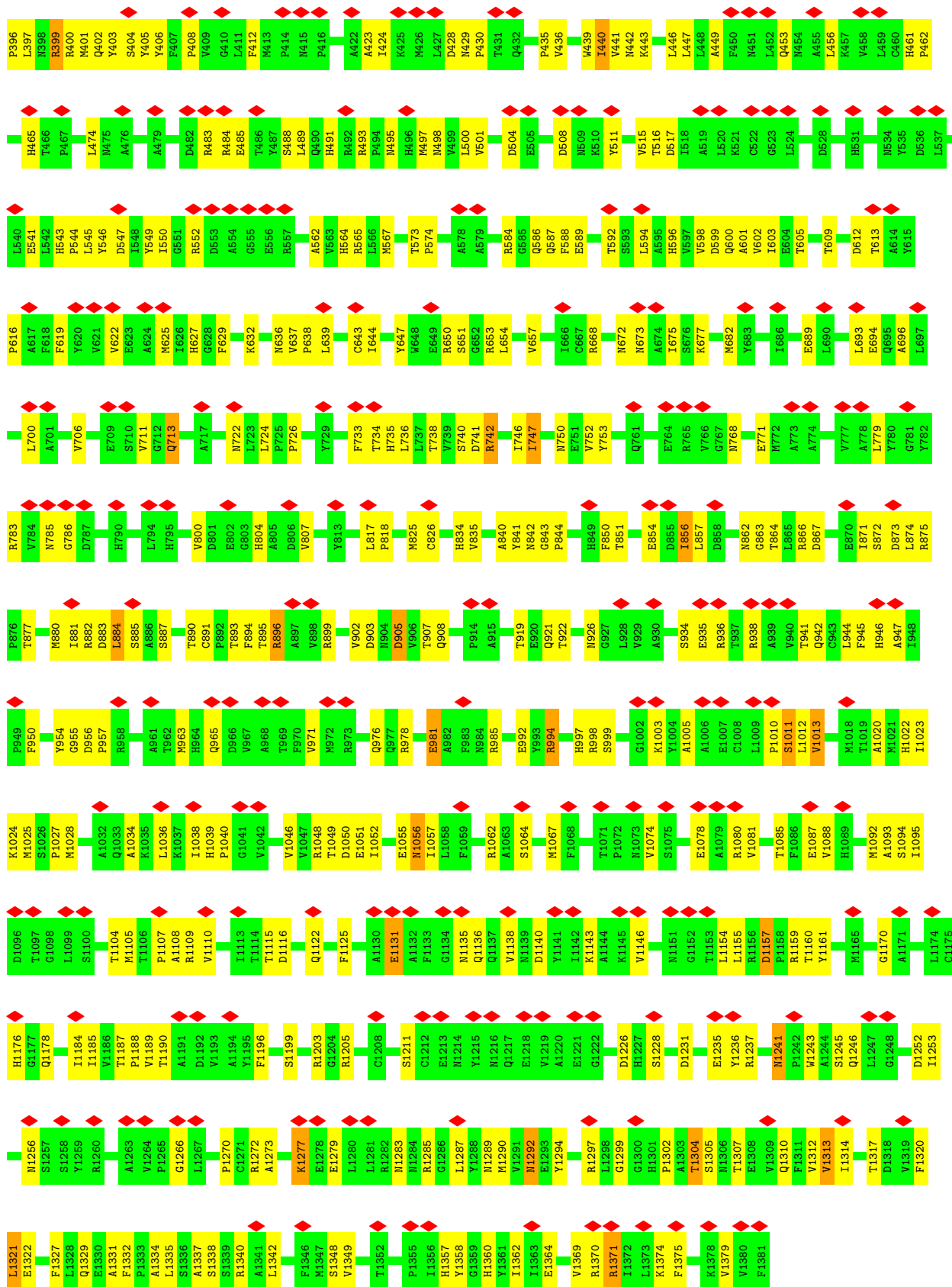
• Molecule 1: Major capsid protein



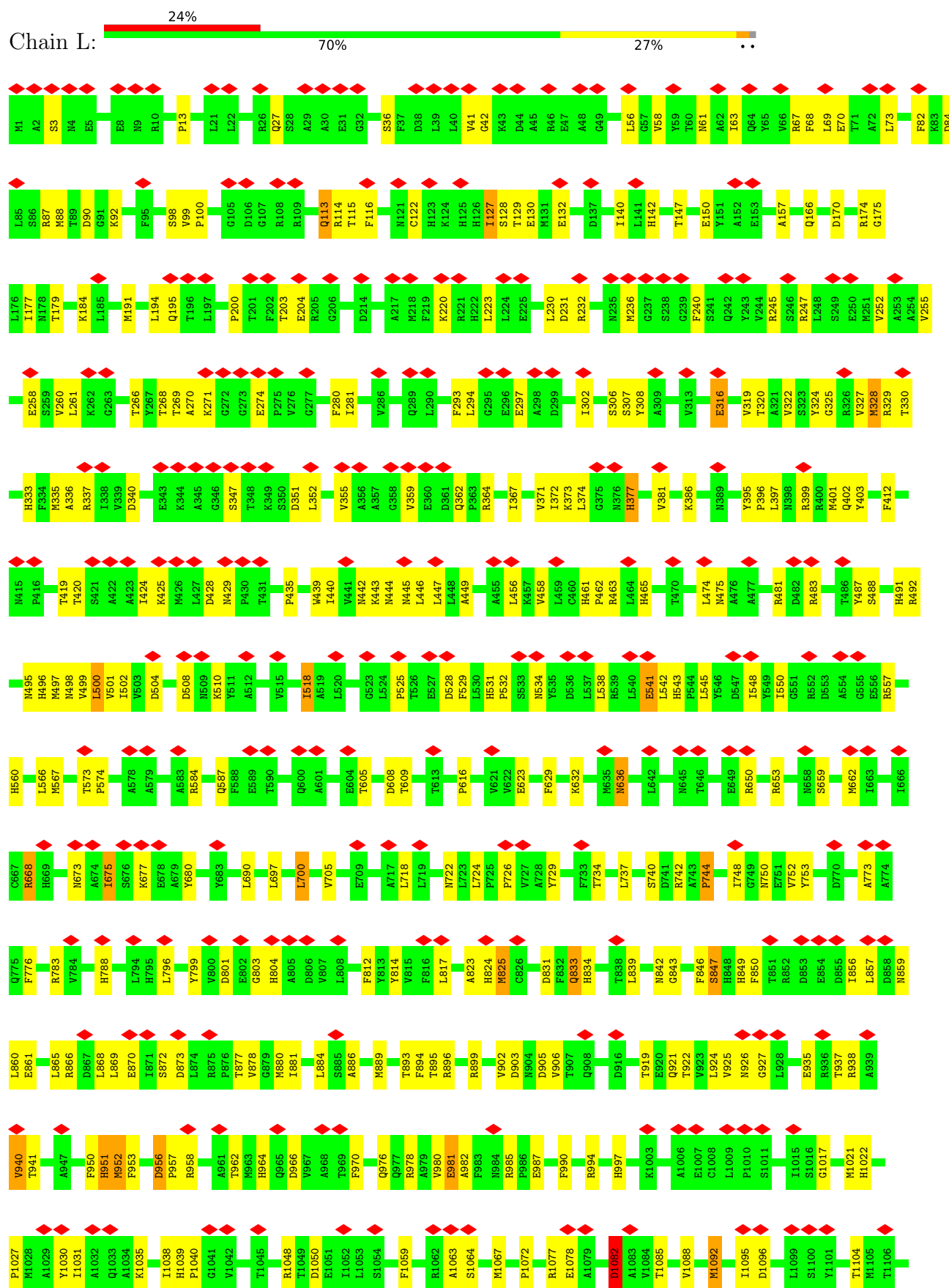


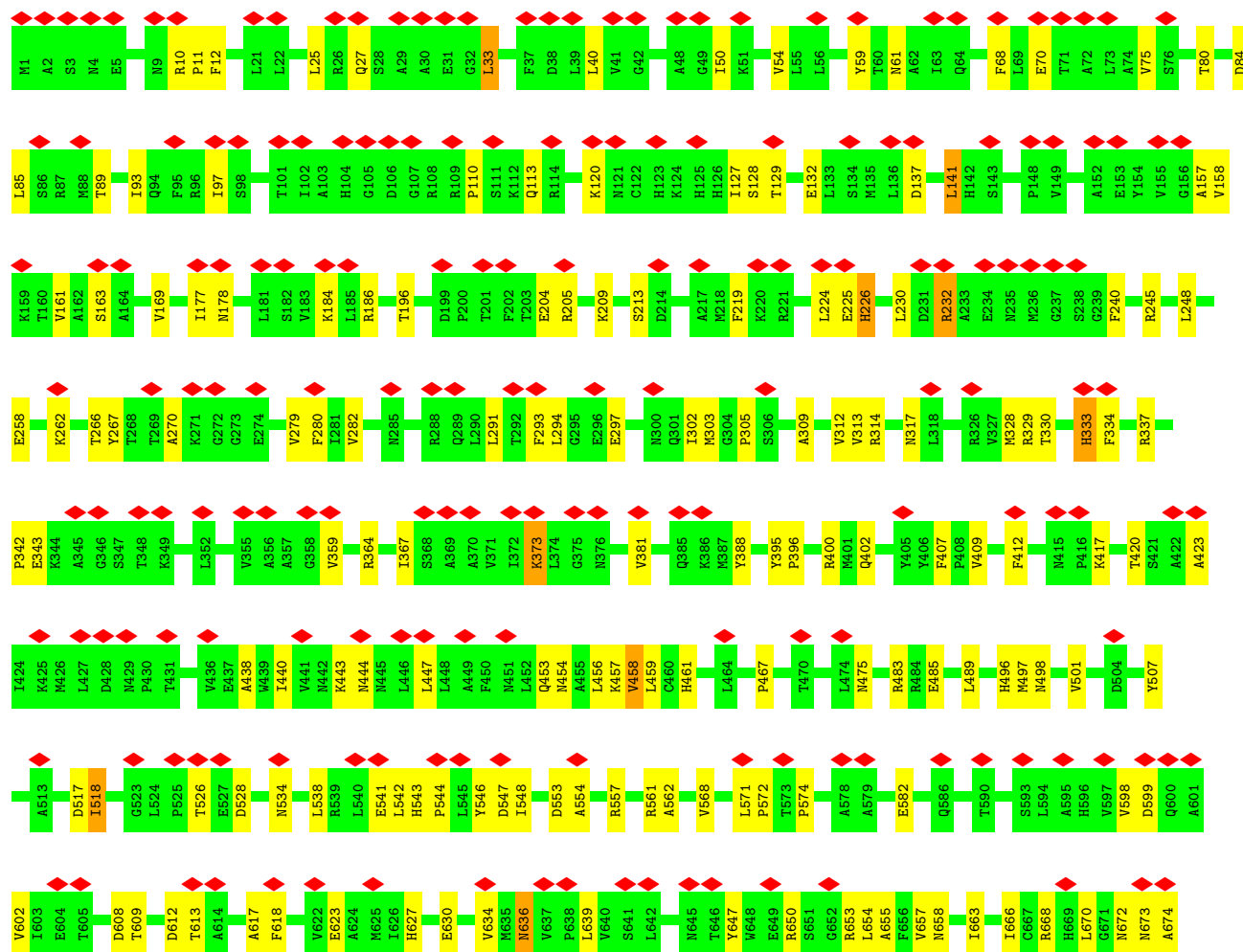
• Molecule 1: Major capsid protein

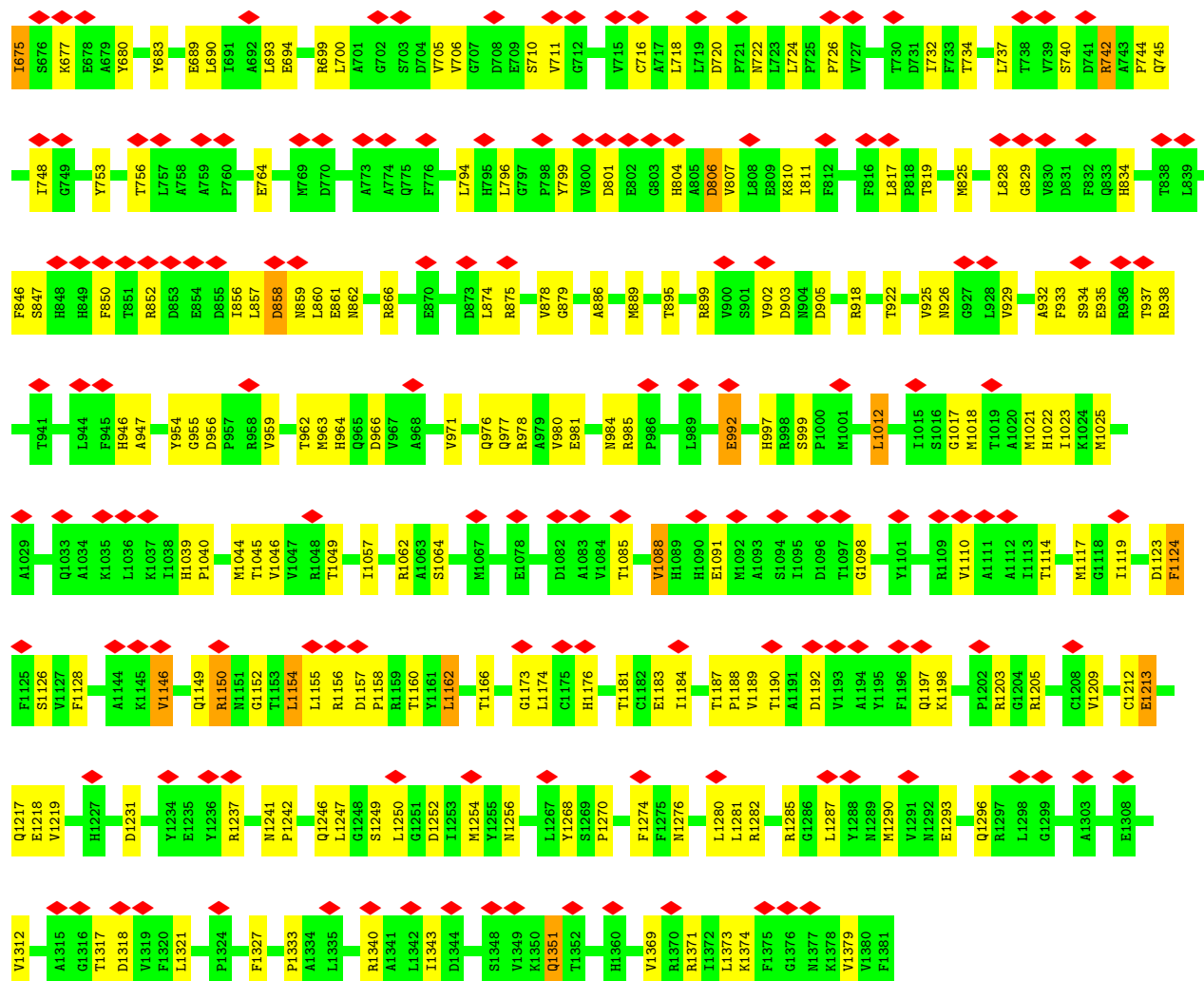




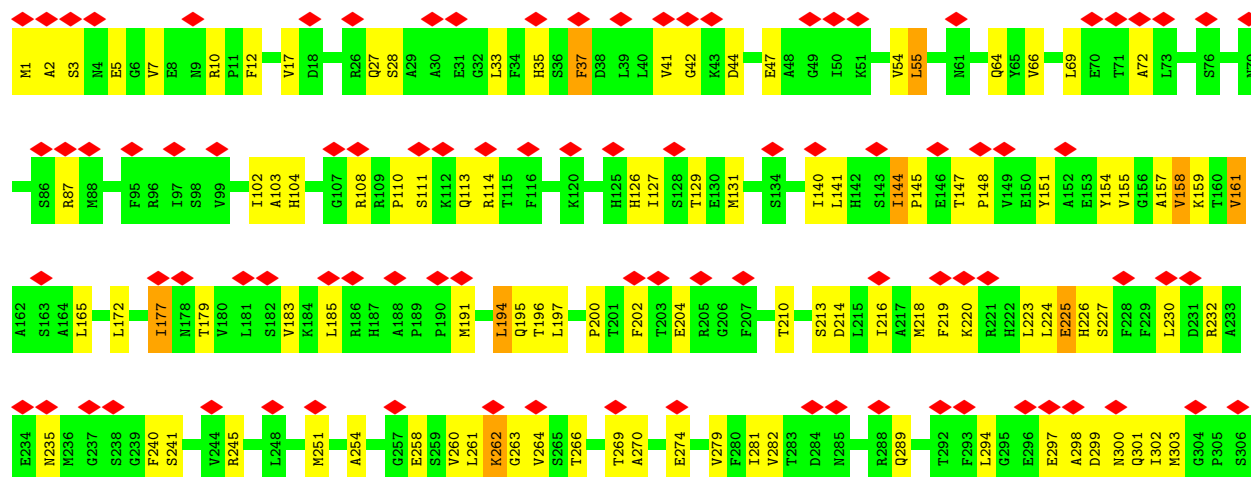
- Molecule 1: Major capsid protein



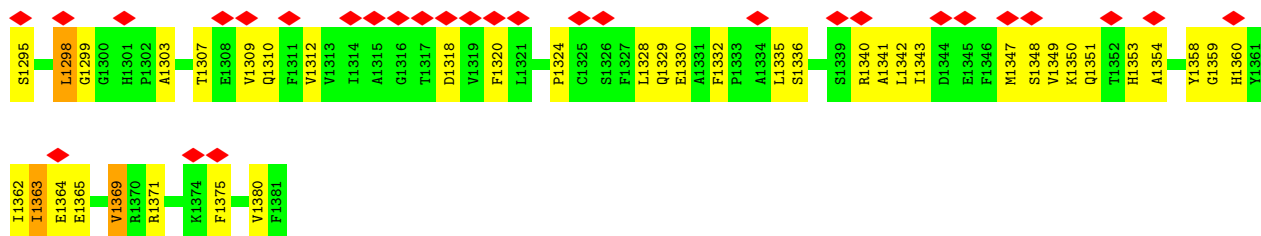




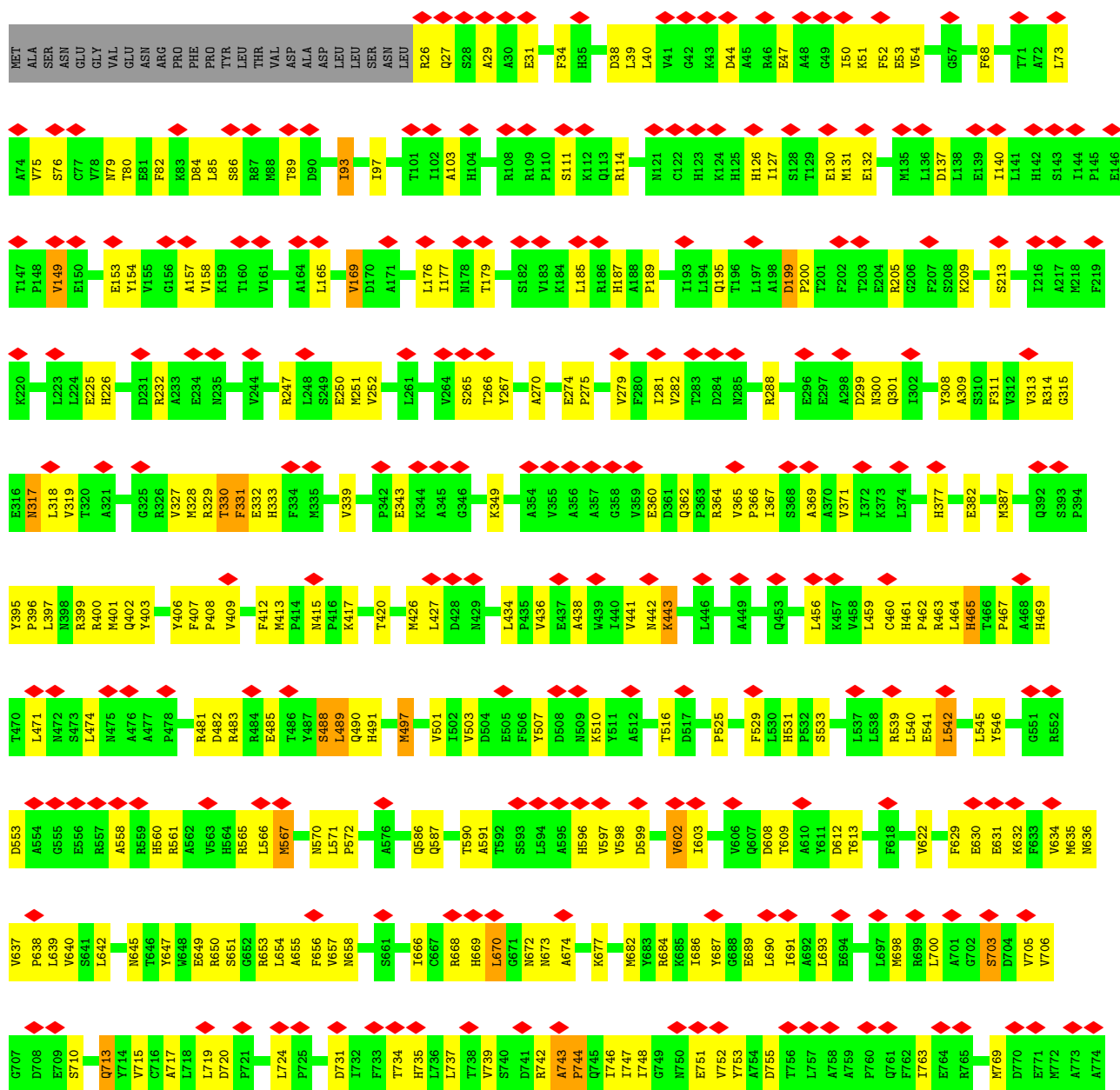
- Molecule 1: Major capsid protein

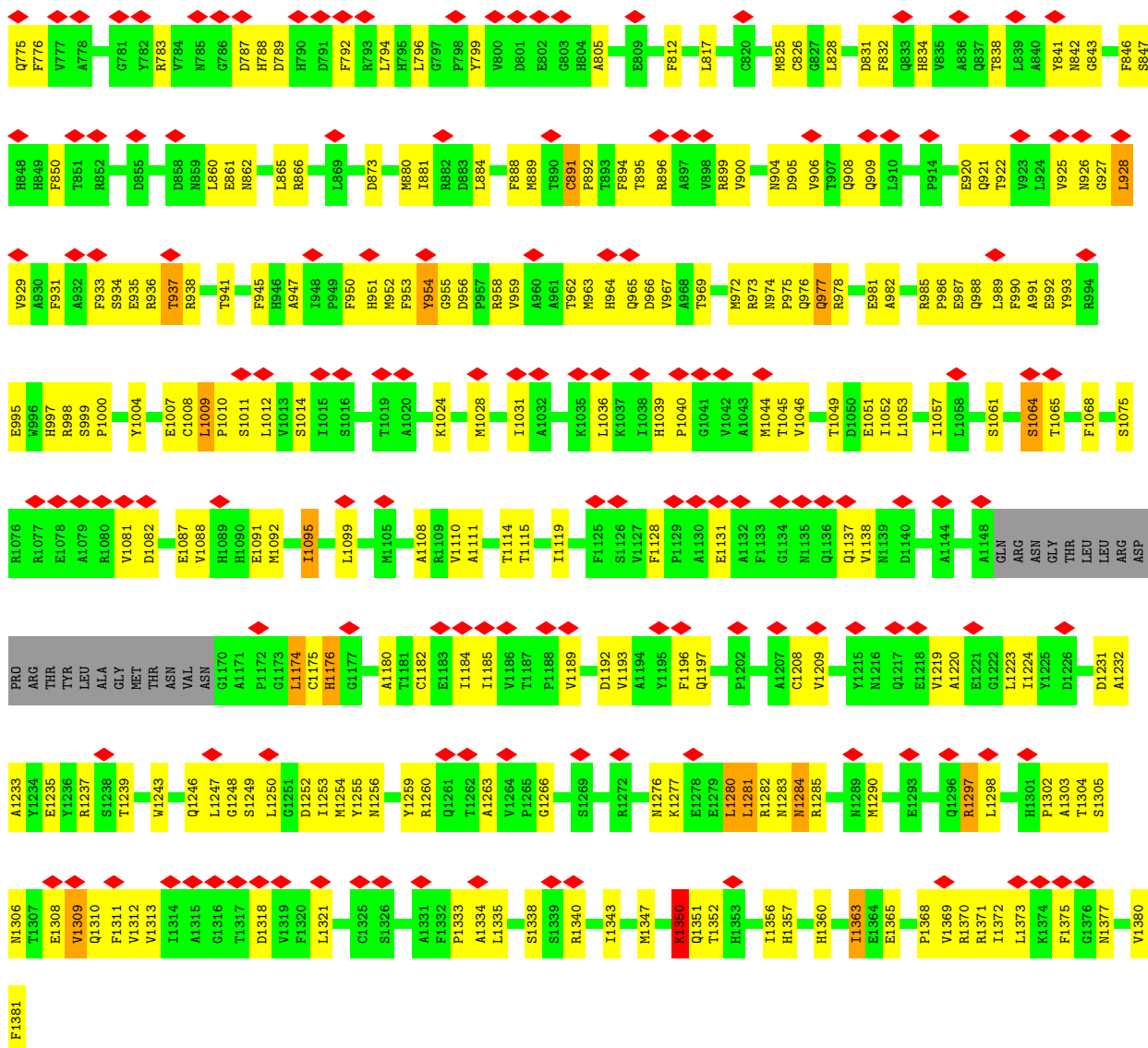


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K1143	A1144	S1211	K1145		A1148	Q1149	ARG	ASN	GLY	THR	LEU	LEU	ARG	ASP	PRO	ARG	THR	TYR	LEU	ALA	GLY	MET	THR	ASN	VAL	N1169	G1170	P1172	G1173	L1174	C1175	H1176	G1177	Q1178	Q1179	C1182	E1183	I1184	I1185	V1186	T1187	P1188	V1189	T1190	A1191	D1192	V1193	F1196	Q1197	P1202	G1203	G1204	R1205	A1206	A1207			
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L757	A758	A759	P760	F762	I763	E764	R765	W768	W769	D770	E771	A773	A774	W775	F776	V777	A778	R783	W784	N785	H788	R793	P798	W799	D801	E802	G803	H804	A805	L806	V807	L808	E809	F812	Y813		L817	C820	T821	M825		S887	F888	M889		T895	R896	A897	V898	R899	V900	S901	V902	D903	N904	P905	V906	
A836	L839	A840	Y841	R842	R843	P844	A845	S847	H848	H849	F850	T851	R852	D853	E854	D855	T856	L857	D858	N859	L860	E861	N862		L865	R866	D867	L868	L869	E870	R875	P876	T877	W878	G879	H880	L881		L884	S887	F888	M889		T895	R896	A897	V898	R899	V900	S901	V902	D903	N904	P905	V906			
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T907	Q908	N913	P914		T919	G943	R944	A945	S947	H948	H949	F950	T951	R952	D953	E954	D955	T956	L957	D958	N959	L960	E961	N962		Q942	Q943	F945	H946	A947	P950	N951	F952	F953	Y954	G955	G956	H957	L958	V959		M963	H964	Q965	D966		F970		V980	E981	A982	F983	N984	R985	P986	I1036	E987	Q988
L989	F990	A991	E992		E995	W996	H997	R998	S999	P1000	M1001	G1002	K1003	Y1004	E1007	C1008	L1009	P1010	S1011	L1012	V1013	S1014	I1015	G1016	S1017	M1018	T1019	A1020	M1021	H1022	I1023	K1024	M1025	S1026	P1027	M1028	A1029	Y1030	I1031	A1032	Q1033	A1034	K1035	L1036	H1039	P1040	A1043	M1044	T1045	V1046	N1047	R1048	T1049	P1050	E1051	I1052		
M1056	I1057	L1058			S1064	T1065	S1066	M1067		R1077		D1082	T1085	F1086	E1087		E1091	M1092	I1095	D1096	T1097	G1098	L1099	S1103	T1104	M1105	T1106	R1109	V1110	A1111	A1112	I1113	T1114	T1115	D1116	M1117	G1118	I1119	H1120	D1123	F1124	F1125	S1126	P1129	A1130		F1133	G1134	N1135	Q1136	Q1137	D1140						
K1143	A1144	S1211	K1145		A1148	Q1149	ARG	ASN	GLY	THR	LEU	LEU	ARG	ASP	PRO	ARG	THR	TYR	LEU	ALA	GLY	MET	THR	ASN	VAL	N1169	G1170	P1172	G1173	L1174	C1175	H1176	G1177	Q1178	Q1179	C1182	E1183	I1184	I1185	V1186	T1187	P1188	V1189	T1190	A1191	D1192	V1193	F1196	Q1197	P1202	G1203	G1204	R1205	A1206	A1207			

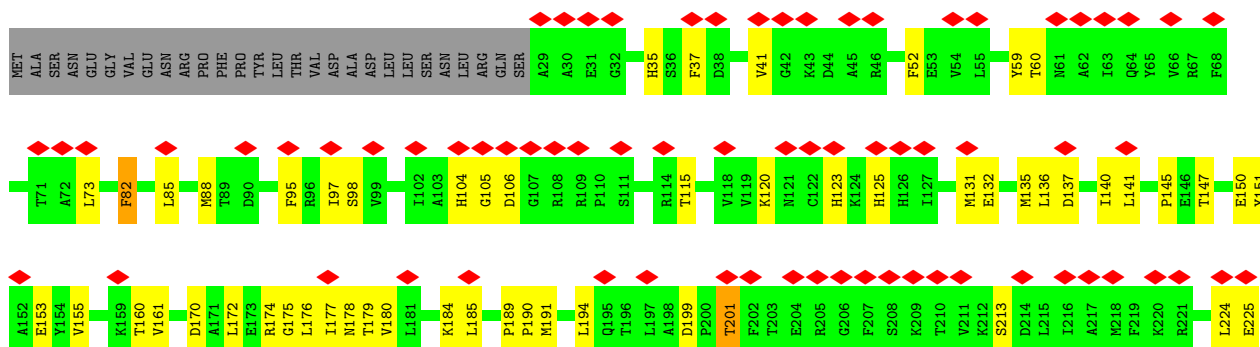


• Molecule 1: Major capsid protein

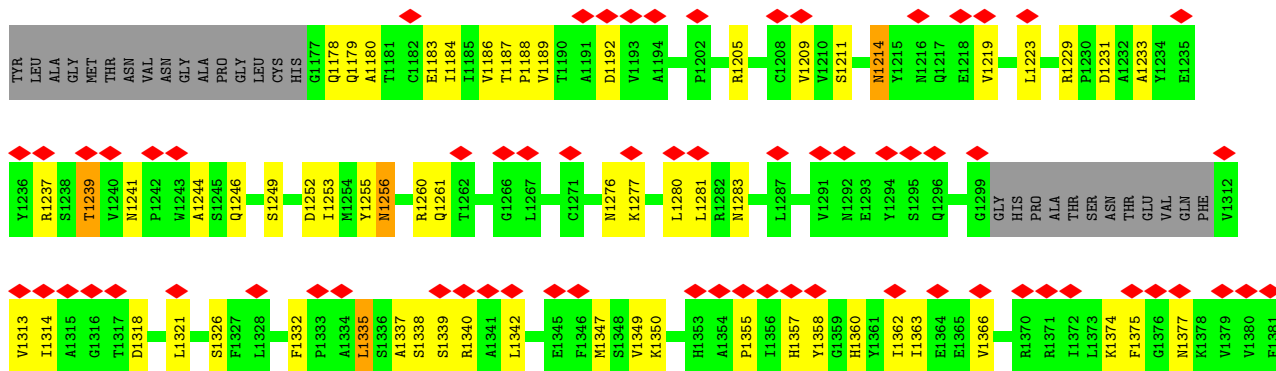




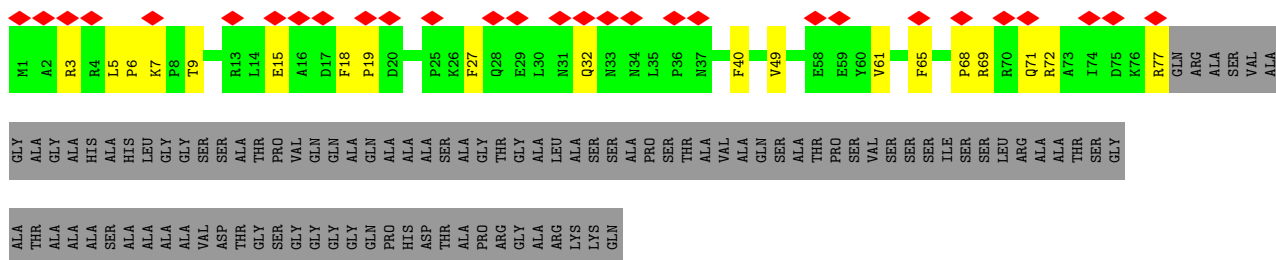
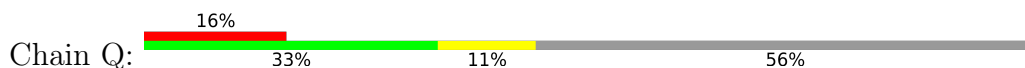
• Molecule 1: Major capsid protein



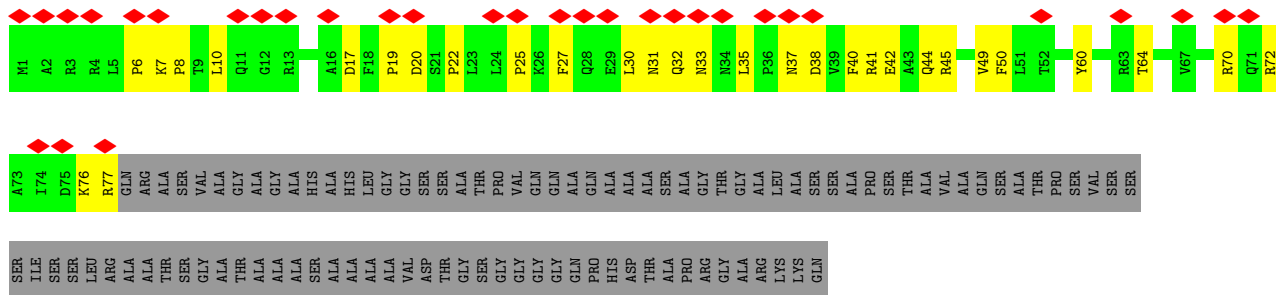




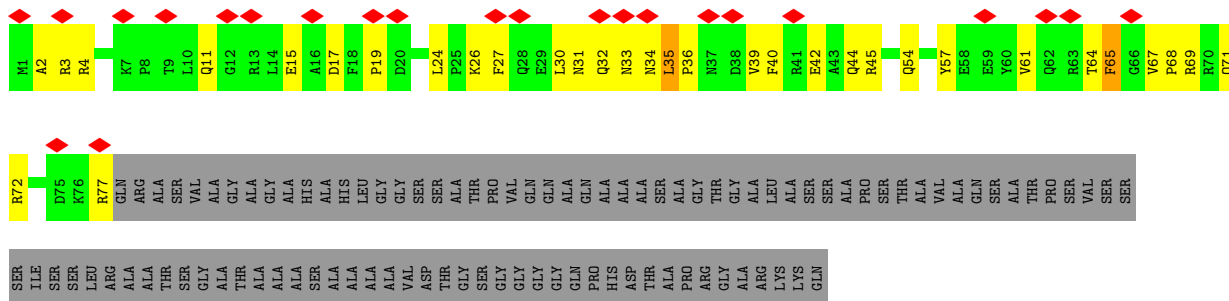
- Molecule 2: Small capsomere-interacting protein



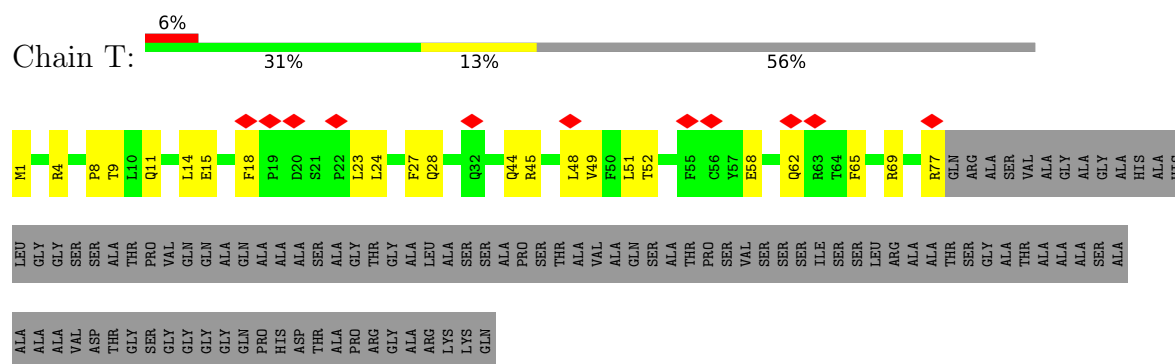
- Molecule 2: Small capsomere-interacting protein



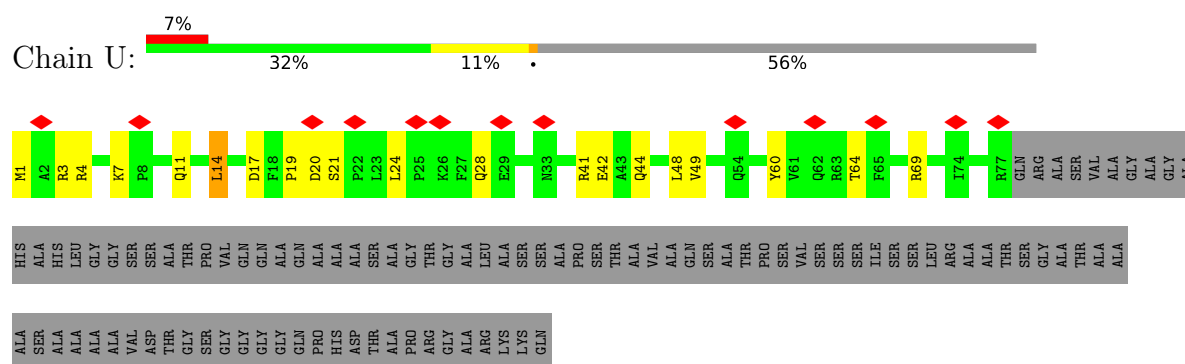
- Molecule 2: Small capsomere-interacting protein



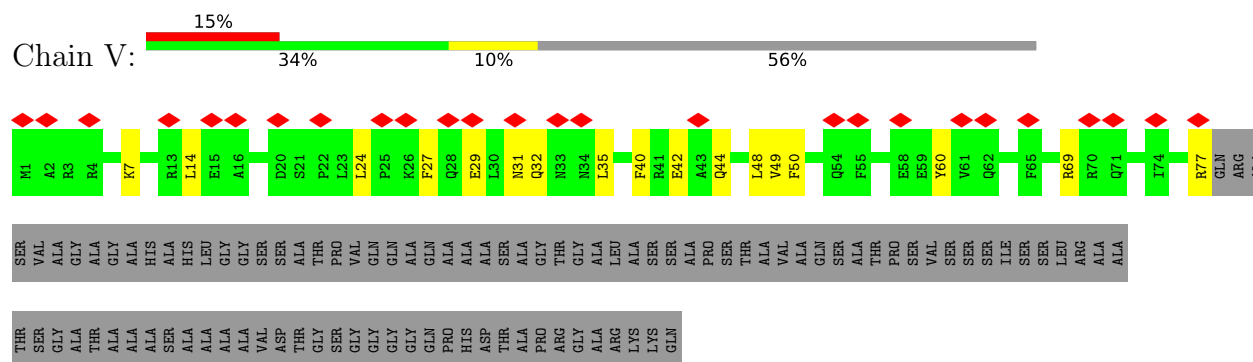
- Molecule 2: Small capsomere-interacting protein



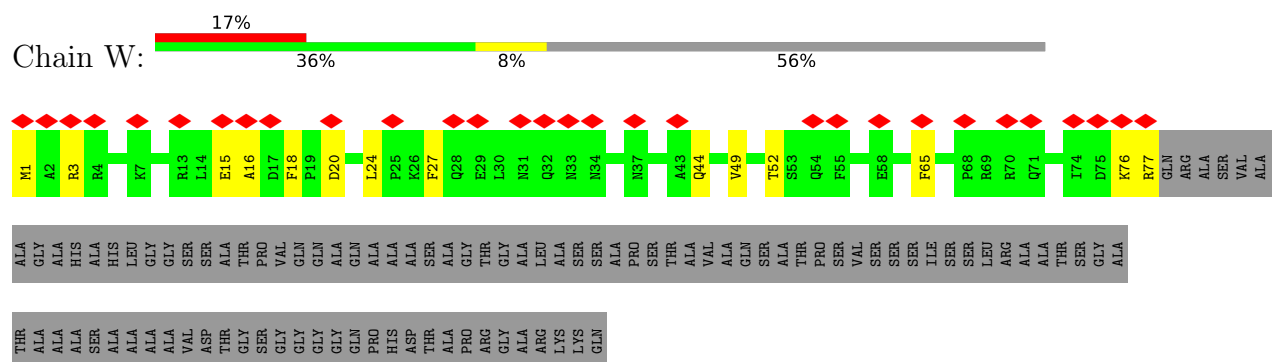
- Molecule 2: Small capsomere-interacting protein

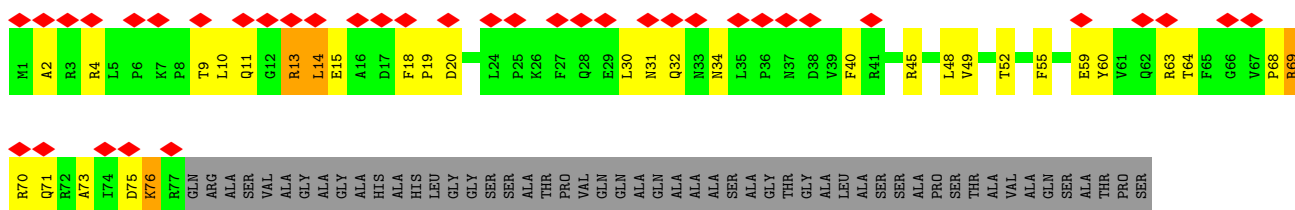


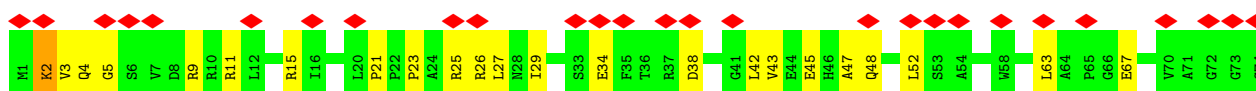
- Molecule 2: Small capsomere-interacting protein

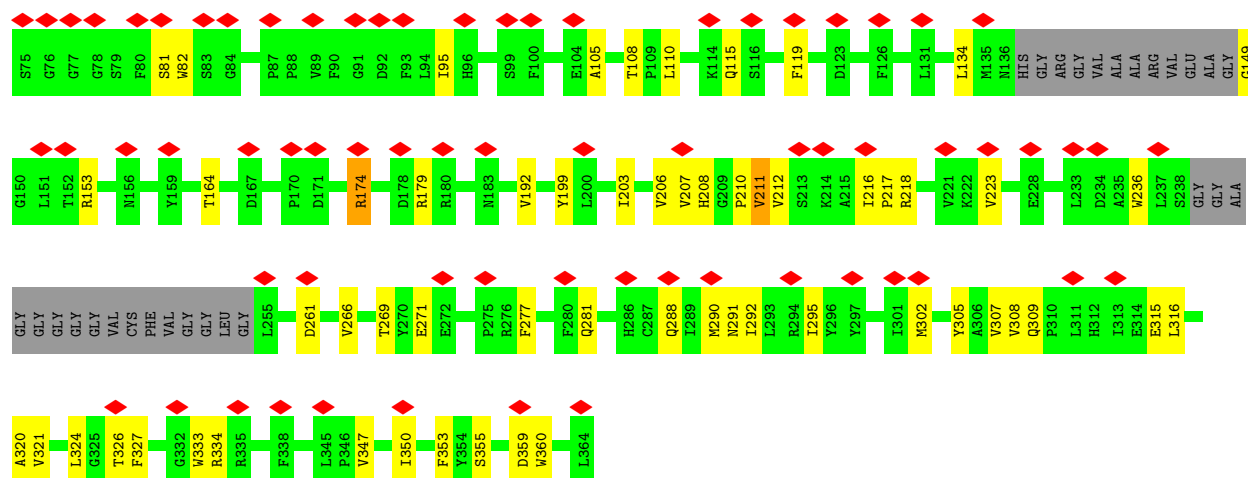


- Molecule 2: Small capsomere-interacting protein

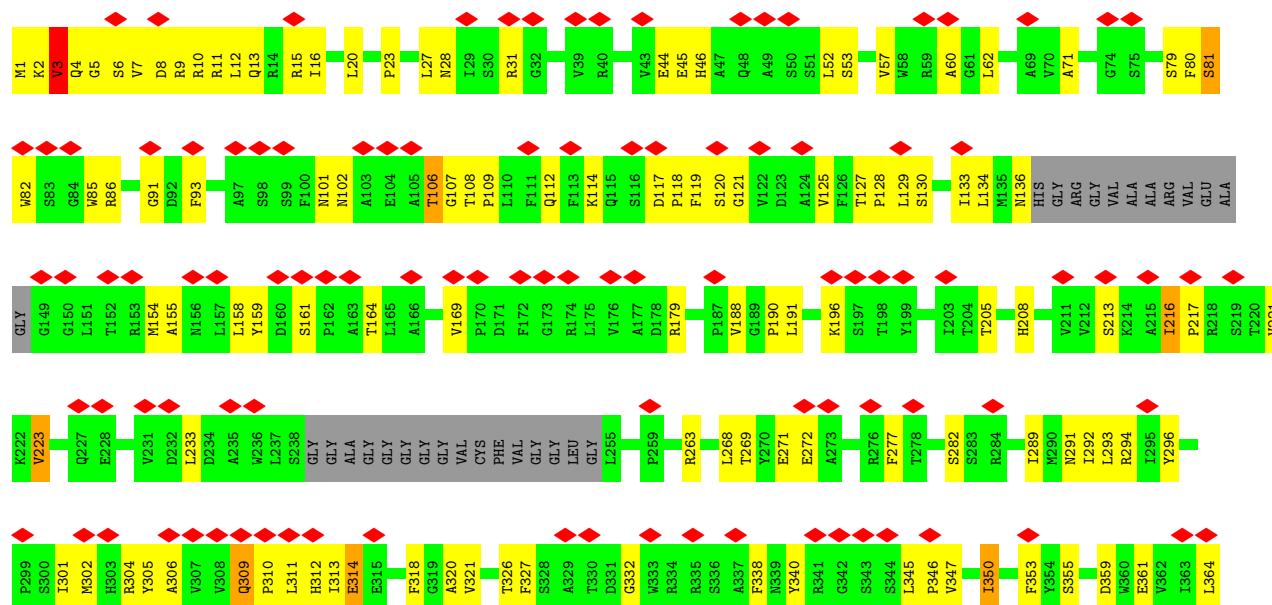




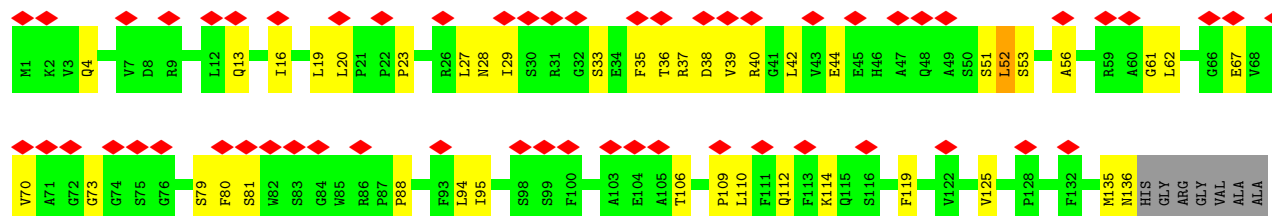


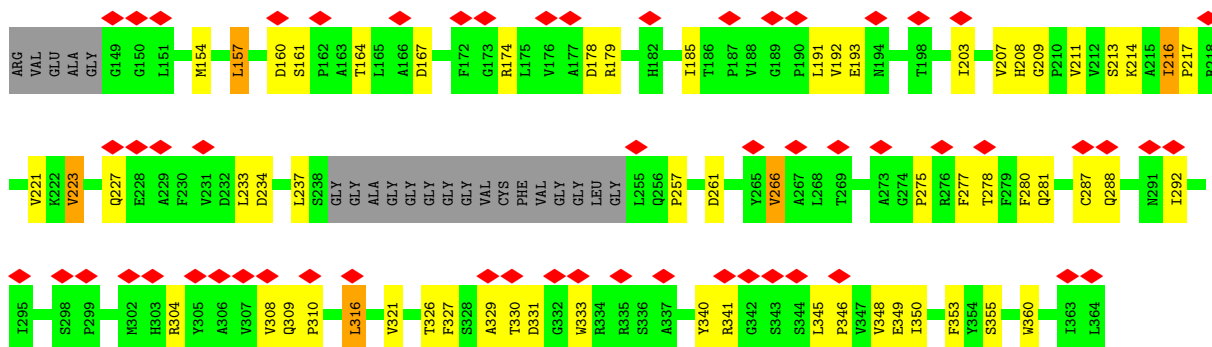


• Molecule 3: Triplex capsid protein 1

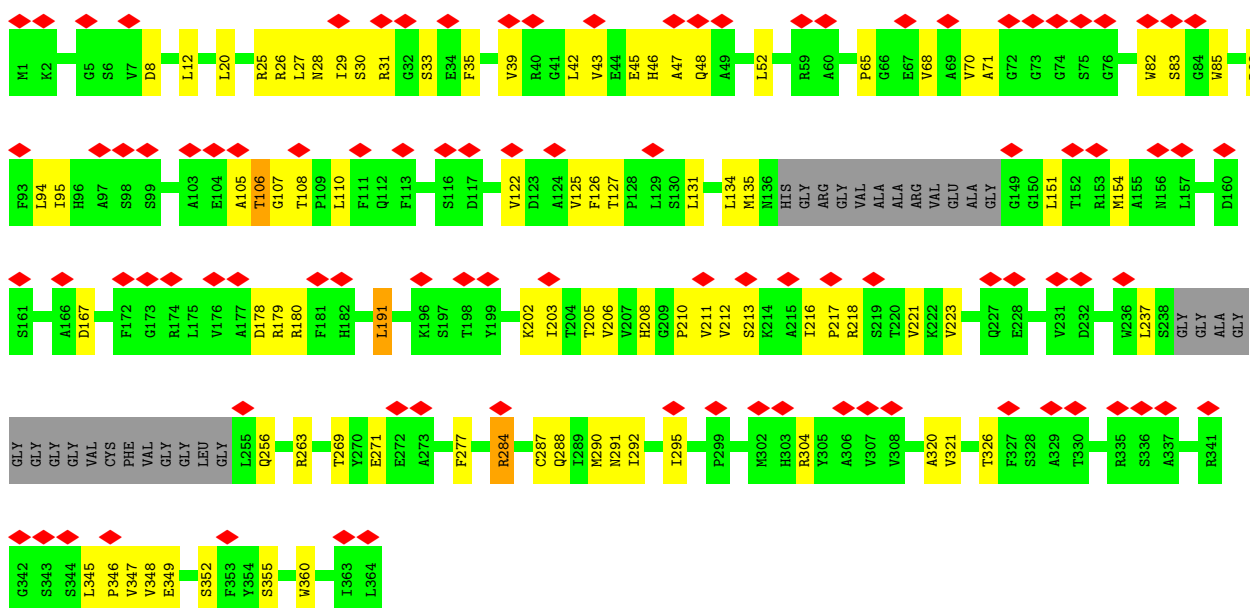


• Molecule 3: Triplex capsid protein 1

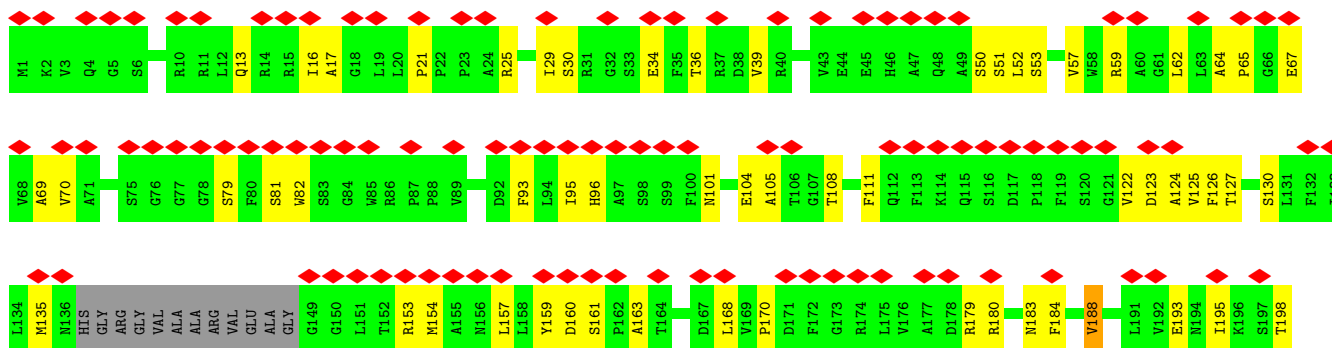
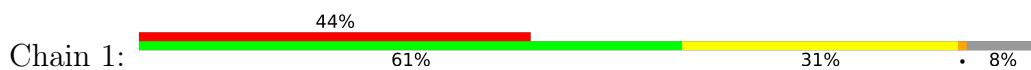


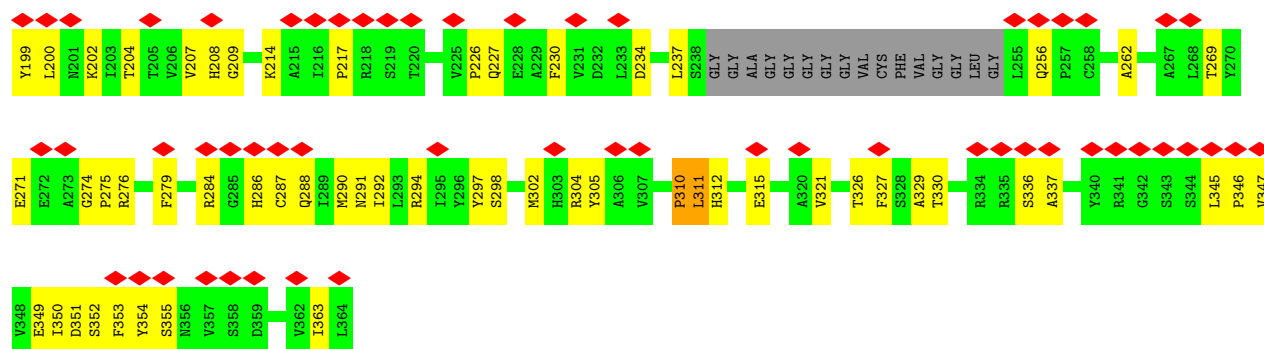


• Molecule 3: Triplex capsid protein 1

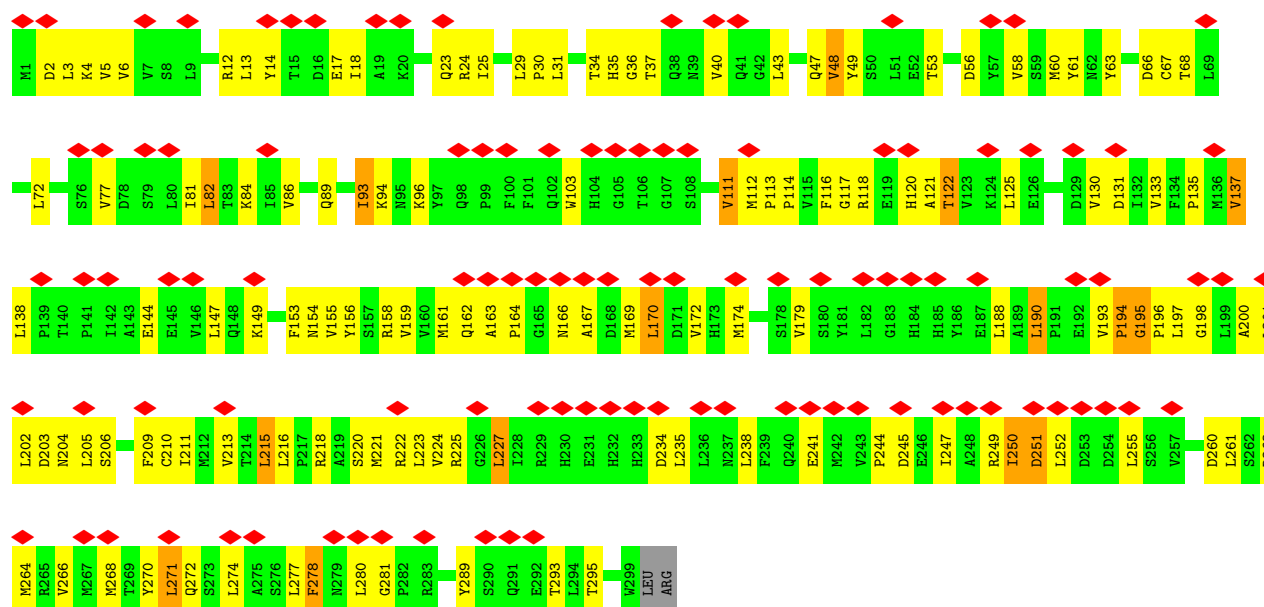


• Molecule 3: Triplex capsid protein 1

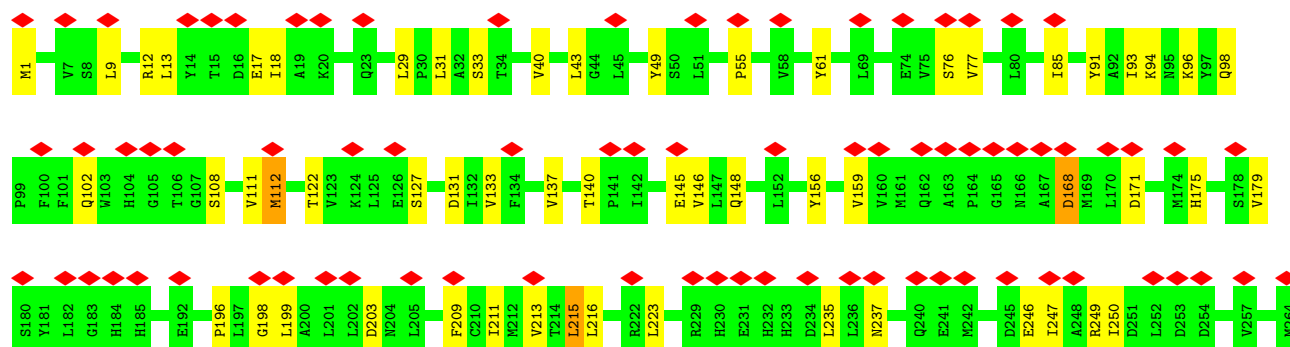
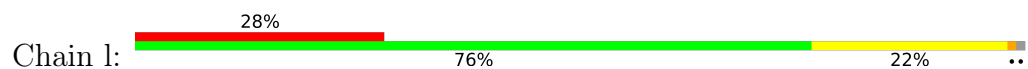




• Molecule 4: Triplex capsid protein 2

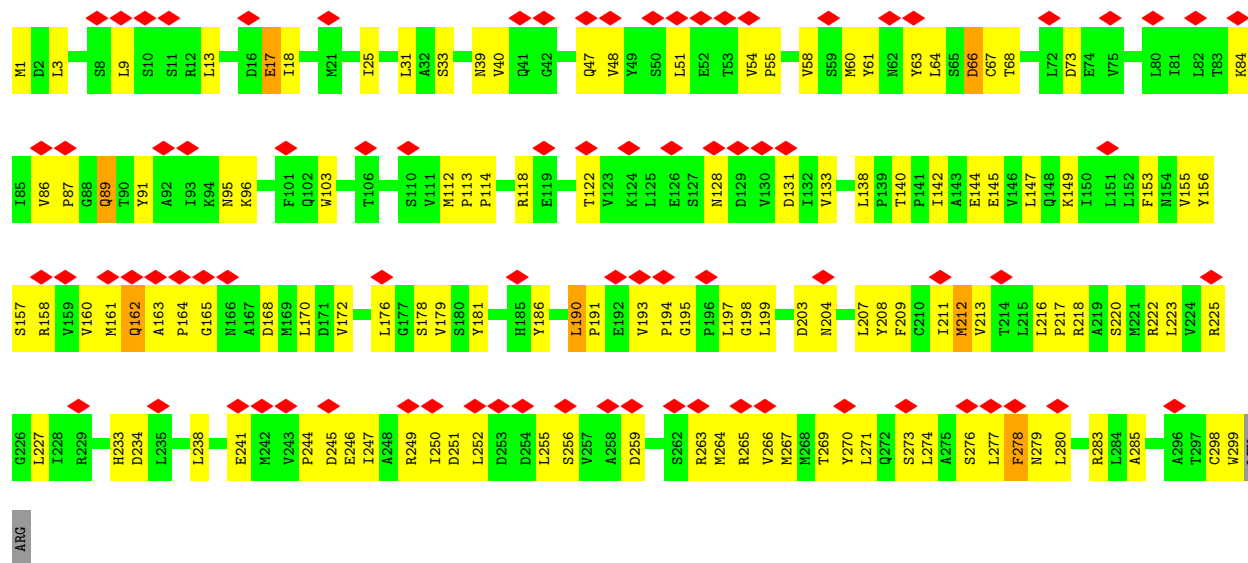


• Molecule 4: Triplex capsid protein 2

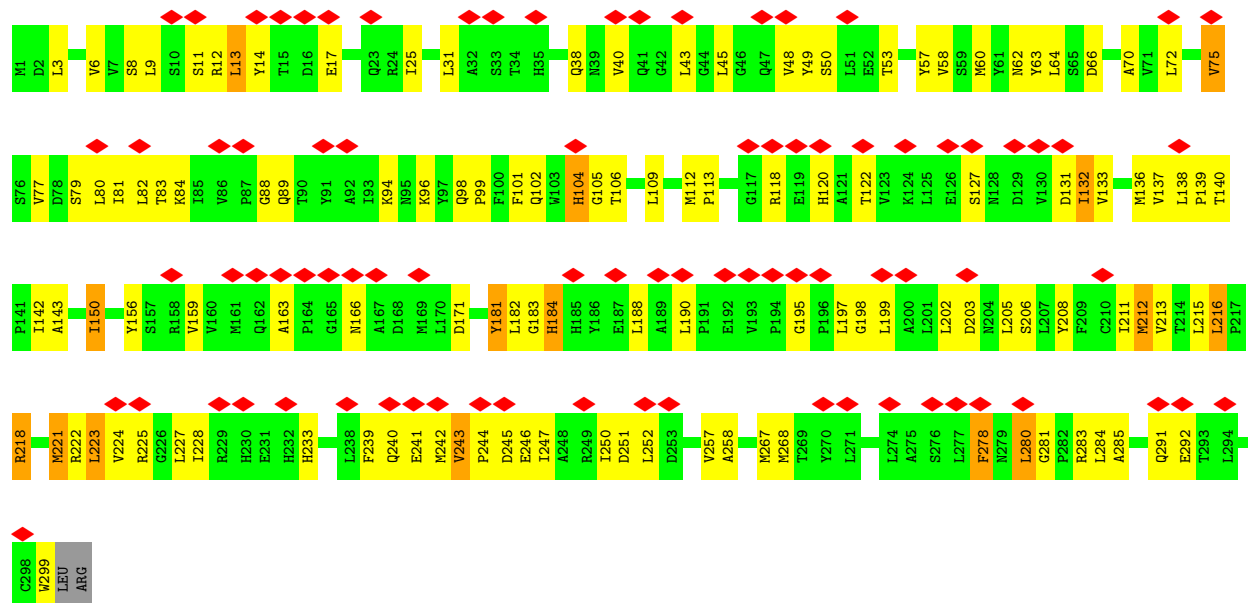




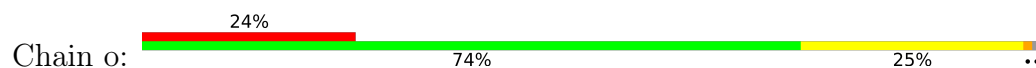
• Molecule 4: Triplex capsid protein 2

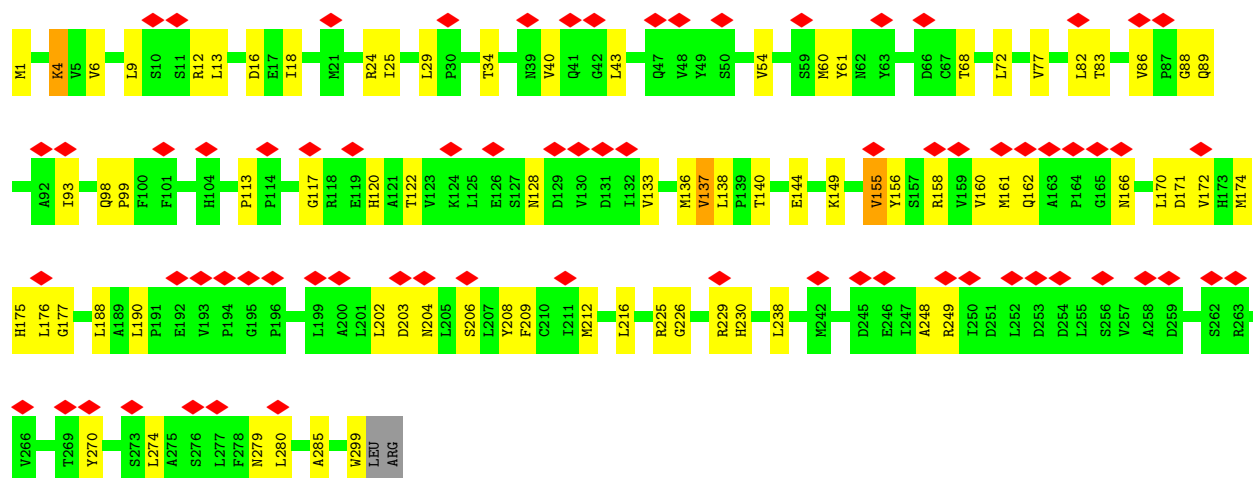


• Molecule 4: Triplex capsid protein 2

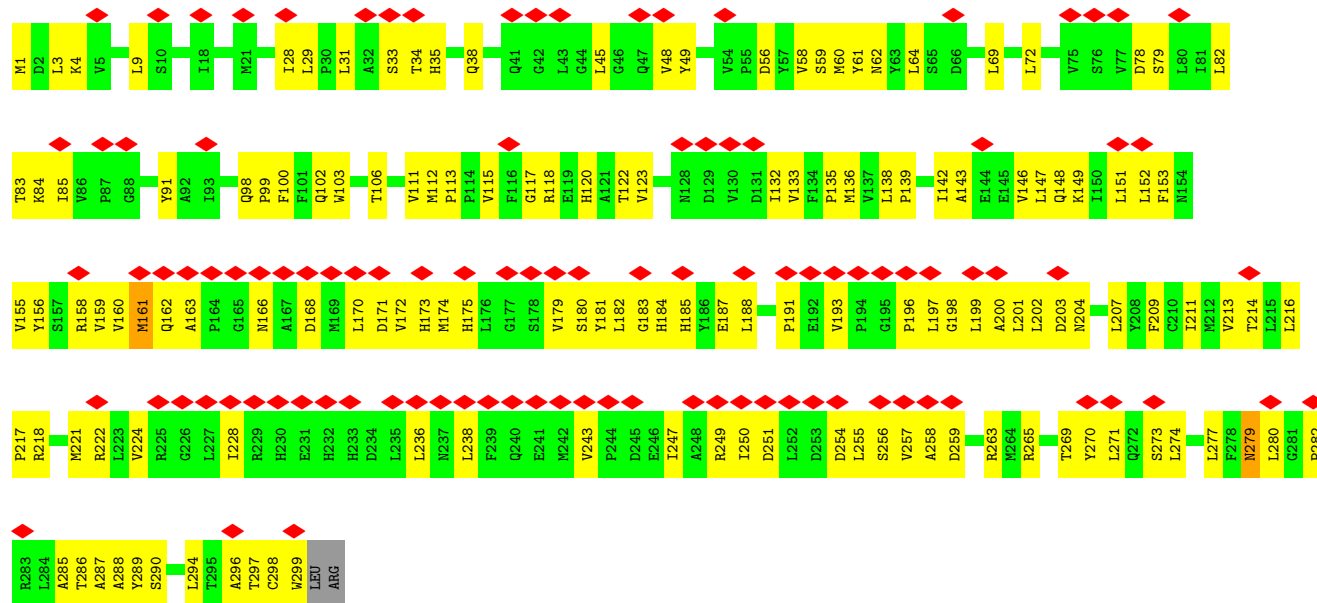


• Molecule 4: Triplex capsid protein 2

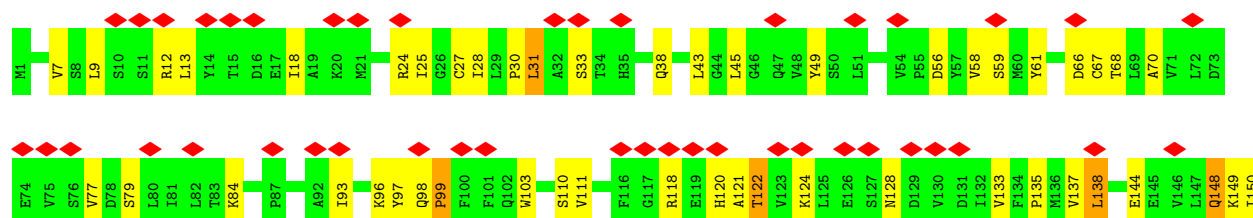


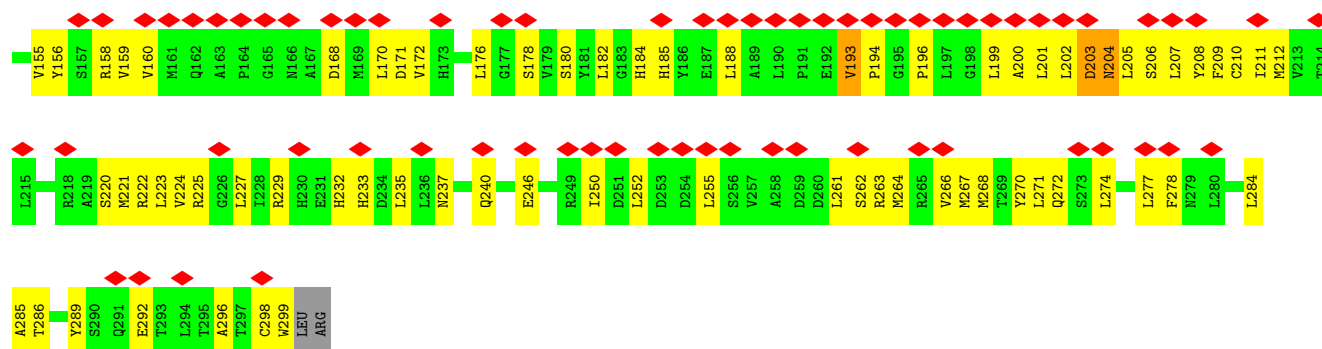


• Molecule 4: Triplex capsid protein 2

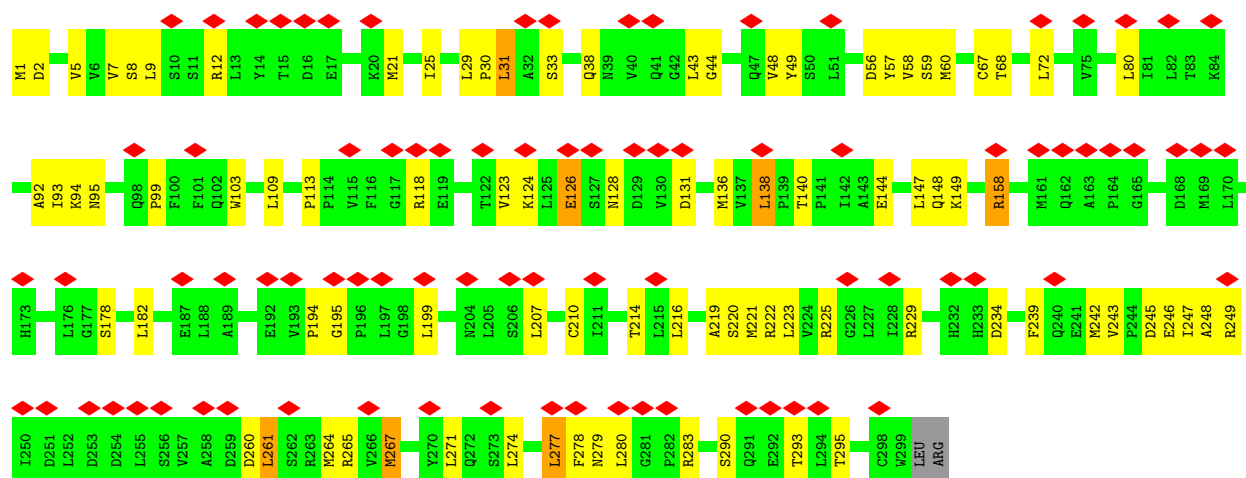


• Molecule 4: Triplex capsid protein 2

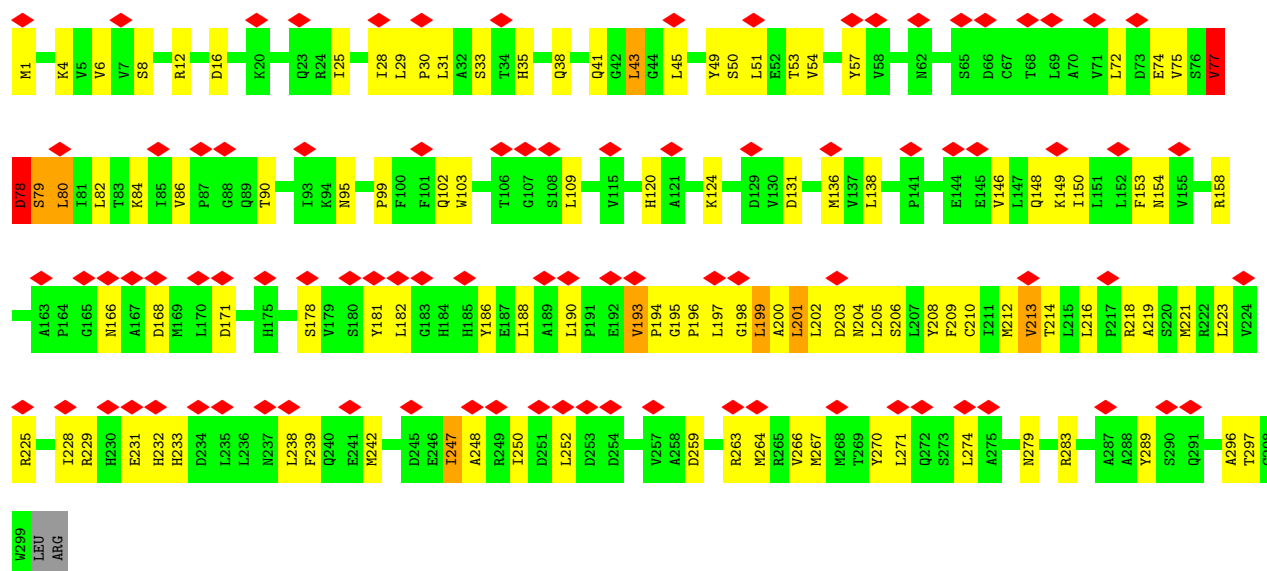




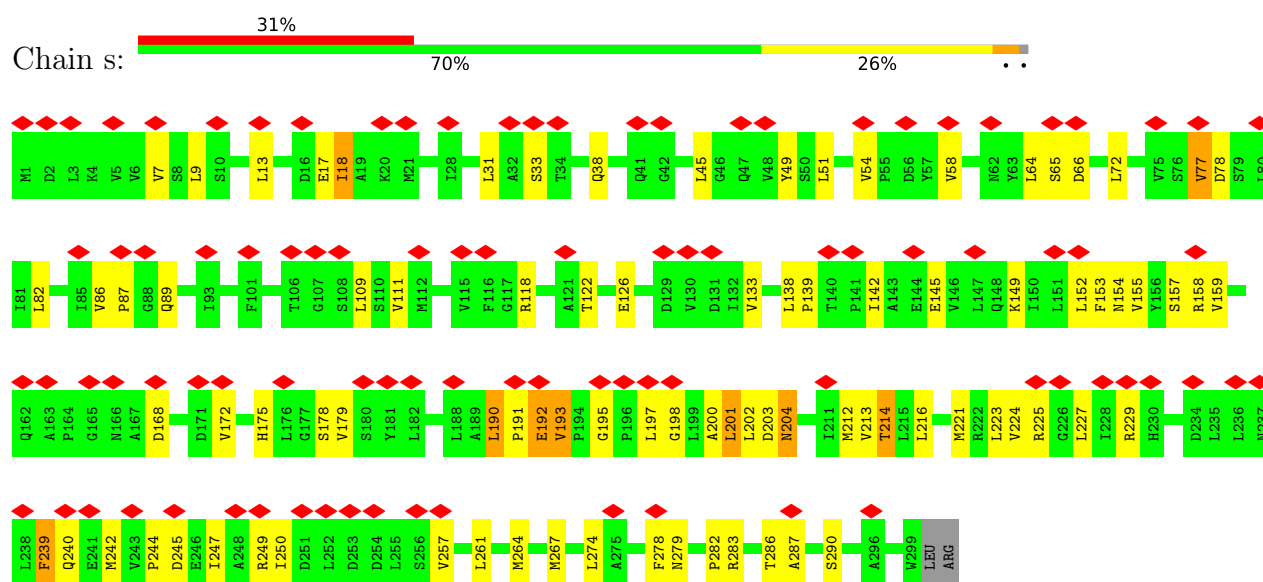
• Molecule 4: Triplex capsid protein 2



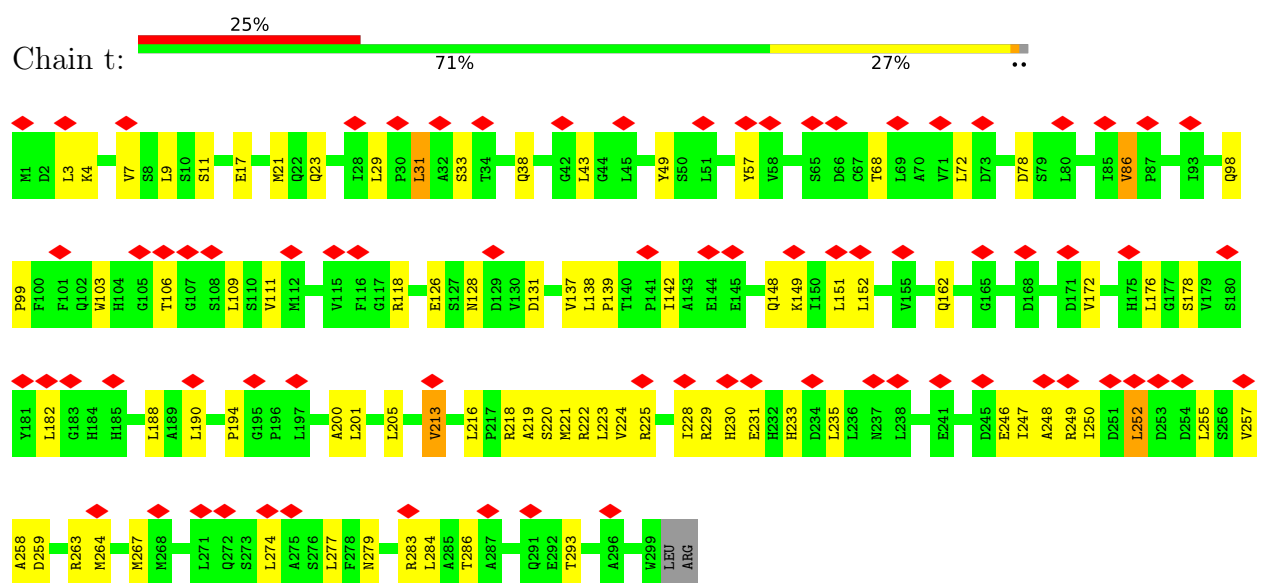
• Molecule 4: Triplex capsid protein 2



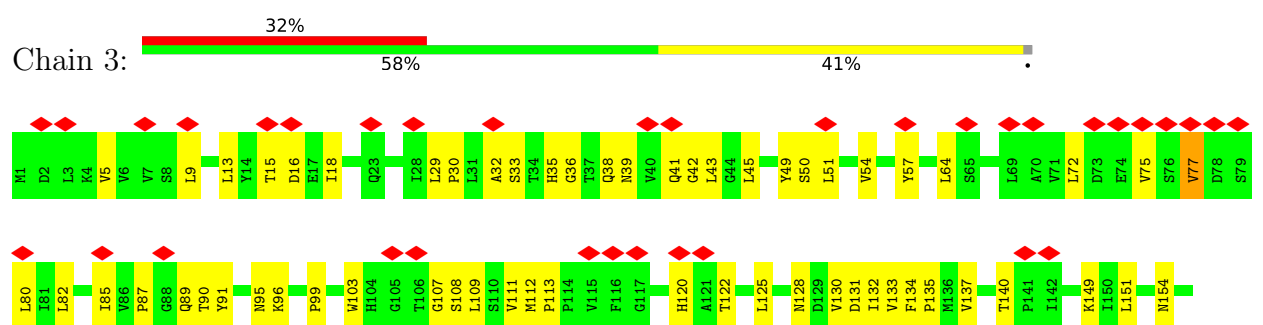
- Molecule 4: Triplex capsid protein 2

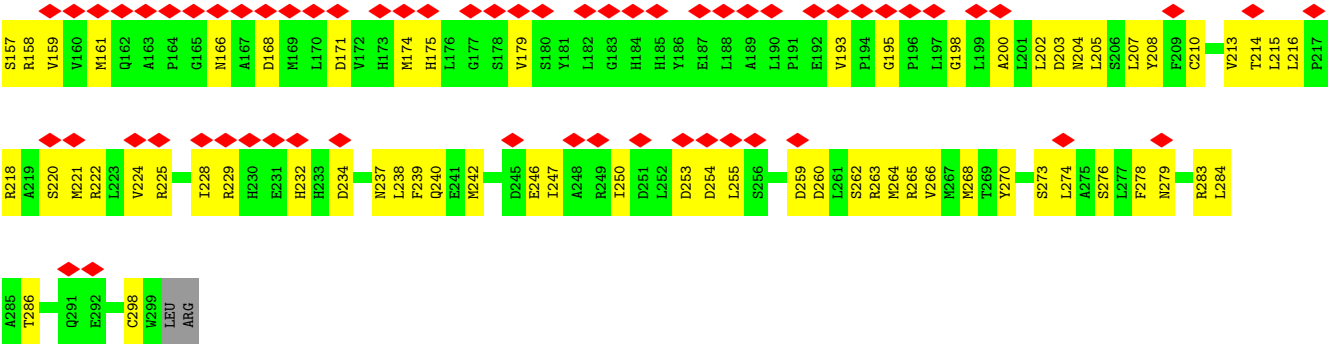


- Molecule 4: Triplex capsid protein 2



- Molecule 4: Triplex capsid protein 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2048	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 ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	1387.52, 1387.52, 1387.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.71, 2.71, 2.71	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	0.35	0/11085	0.54	9/15066 (0.1%)
1	B	0.37	0/10951	0.57	21/14882 (0.1%)
1	C	0.36	0/10940	0.54	6/14868 (0.0%)
1	D	0.37	0/11085	0.58	14/15066 (0.1%)
1	E	0.36	0/11085	0.52	8/15066 (0.1%)
1	F	0.34	0/10933	0.51	4/14858 (0.0%)
1	G	0.31	0/11084	0.49	4/15065 (0.0%)
1	H	0.30	0/11085	0.45	5/15066 (0.0%)
1	I	0.30	0/10952	0.45	3/14883 (0.0%)
1	J	0.47	0/10850	0.55	2/14745 (0.0%)
1	K	0.46	0/11085	0.51	2/15066 (0.0%)
1	L	0.27	0/10955	0.45	4/14887 (0.0%)
1	M	0.27	0/11085	0.43	3/15066 (0.0%)
1	N	0.33	0/10933	0.63	15/14858 (0.1%)
1	O	0.35	0/10719	0.66	27/14565 (0.2%)
1	P	0.39	0/10410	0.53	1/14140 (0.0%)
2	Q	0.22	0/664	0.41	0/896
2	R	0.26	0/664	0.57	1/896 (0.1%)
2	S	0.41	0/664	0.74	2/896 (0.2%)
2	T	0.26	0/664	0.52	0/896
2	U	0.28	0/664	0.46	0/896
2	V	0.25	0/664	0.49	0/896
2	W	0.21	0/664	0.40	0/896
2	X	0.21	0/664	0.34	0/896
2	Y	0.21	0/664	0.36	0/896
2	Z	0.29	0/664	0.45	0/896
2	a	0.31	0/664	0.48	0/896
2	b	0.18	0/664	0.37	0/896
2	c	0.20	0/664	0.38	0/896
2	d	0.24	0/664	0.63	1/896 (0.1%)
2	e	0.29	0/664	0.63	1/896 (0.1%)
2	u	0.23	0/542	0.44	0/735
3	l	0.26	0/2672	0.52	0/3635
3	f	0.35	0/2537	0.47	0/3450

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	g	0.27	0/2672	0.42	1/3635 (0.0%)
3	h	0.34	0/2672	0.62	2/3635 (0.1%)
3	i	0.32	0/2672	0.55	6/3635 (0.2%)
3	j	0.27	0/2672	0.46	0/3635
4	2	0.31	0/2388	0.57	0/3254
4	3	0.30	0/2388	0.50	0/3254
4	k	0.32	0/2388	0.75	10/3254 (0.3%)
4	l	0.28	0/2388	0.41	0/3254
4	m	0.29	0/2388	0.63	3/3254 (0.1%)
4	n	0.36	0/2388	0.69	12/3254 (0.4%)
4	o	0.26	0/2388	0.40	0/3254
4	p	0.28	0/2388	0.63	8/3254 (0.2%)
4	q	0.27	0/2388	0.38	0/3254
4	r	0.31	0/2388	0.54	4/3254 (0.1%)
4	s	0.33	0/2388	0.57	5/3254 (0.2%)
4	t	0.27	0/2388	0.38	0/3254
All	All	0.34	0/230292	0.53	184/312995 (0.1%)

There are no bond length outliers.

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	199	ASP	CA-C-N	13.16	133.20	118.85
1	O	199	ASP	C-N-CA	13.16	133.20	118.85
1	D	359	VAL	N-CA-C	11.88	122.74	110.62
1	B	1114	THR	N-CA-C	11.28	123.33	111.14
4	m	278	PHE	N-CA-C	10.95	123.22	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10832	0	10655	464	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	10701	0	10521	426	0
1	C	10690	0	10505	560	0
1	D	10832	0	10655	479	0
1	E	10832	0	10652	450	0
1	F	10683	0	10498	576	0
1	G	10831	0	10652	408	0
1	H	10832	0	10655	389	0
1	I	10702	0	10519	301	0
1	J	10601	0	10428	532	0
1	K	10832	0	10655	458	0
1	L	10705	0	10521	401	0
1	M	10832	0	10652	349	0
1	N	10683	0	10497	805	0
1	O	10473	0	10298	682	0
1	P	10173	0	10014	425	0
2	Q	649	0	649	19	0
2	R	649	0	649	33	0
2	S	649	0	649	93	0
2	T	649	0	649	86	0
2	U	649	0	649	24	0
2	V	649	0	649	16	0
2	W	649	0	649	14	0
2	X	649	0	649	11	0
2	Y	649	0	649	21	0
2	Z	649	0	649	55	0
2	a	649	0	649	85	0
2	b	649	0	649	77	0
2	c	649	0	647	55	0
2	d	649	0	649	145	0
2	e	649	0	649	122	0
2	u	528	0	510	23	0
3	l	2604	0	2576	329	0
3	f	2474	0	2459	99	0
3	g	2604	0	2577	82	0
3	h	2604	0	2573	290	0
3	i	2604	0	2575	109	0
3	j	2604	0	2577	92	0
4	2	2338	0	2364	127	0
4	3	2338	0	2364	104	0
4	k	2338	0	2362	288	0
4	l	2338	0	2364	68	0
4	m	2338	0	2364	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	n	2338	0	2364	201	0
4	o	2338	0	2364	72	0
4	p	2338	0	2363	180	0
4	q	2338	0	2364	84	0
4	r	2338	0	2362	233	0
4	s	2338	0	2364	157	0
4	t	2338	0	2364	76	0
All	All	225047	0	222320	9709	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 22.

The worst 5 of 9709 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:N:1347:MET:HE1	1:N:1375:PHE:CD1	1.24	1.67
4:k:13:LEU:HD21	4:k:17:GLU:CG	1.21	1.67
4:k:122:THR:CG2	4:k:133:VAL:HG22	1.23	1.65
1:C:1072:PRO:CG	3:1:52:LEU:HD22	1.20	1.60
1:F:165:LEU:HB3	3:h:12:LEU:CD2	1.20	1.60

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1379/1381 (100%)	1297 (94%)	78 (6%)	4 (0%)	36	72
1	B	1360/1381 (98%)	1287 (95%)	72 (5%)	1 (0%)	48	83
1	C	1359/1381 (98%)	1277 (94%)	80 (6%)	2 (0%)	48	83
1	D	1379/1381 (100%)	1301 (94%)	78 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	1379/1381 (100%)	1286 (93%)	91 (7%)	2 (0%)	48	83
1	F	1358/1381 (98%)	1272 (94%)	84 (6%)	2 (0%)	48	83
1	G	1379/1381 (100%)	1296 (94%)	80 (6%)	3 (0%)	43	78
1	H	1379/1381 (100%)	1301 (94%)	75 (5%)	3 (0%)	43	78
1	I	1360/1381 (98%)	1288 (95%)	70 (5%)	2 (0%)	48	83
1	J	1344/1381 (97%)	1238 (92%)	104 (8%)	2 (0%)	48	83
1	K	1379/1381 (100%)	1268 (92%)	110 (8%)	1 (0%)	48	83
1	L	1361/1381 (99%)	1299 (95%)	60 (4%)	2 (0%)	48	83
1	M	1379/1381 (100%)	1299 (94%)	79 (6%)	1 (0%)	48	83
1	N	1358/1381 (98%)	1312 (97%)	42 (3%)	4 (0%)	36	72
1	O	1331/1381 (96%)	1274 (96%)	52 (4%)	5 (0%)	30	67
1	P	1284/1381 (93%)	1183 (92%)	97 (8%)	4 (0%)	36	72
2	Q	75/176 (43%)	68 (91%)	7 (9%)	0	100	100
2	R	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
2	S	75/176 (43%)	68 (91%)	6 (8%)	1 (1%)	9	41
2	T	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
2	U	75/176 (43%)	69 (92%)	6 (8%)	0	100	100
2	V	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
2	W	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
2	X	75/176 (43%)	73 (97%)	2 (3%)	0	100	100
2	Y	75/176 (43%)	72 (96%)	3 (4%)	0	100	100
2	Z	75/176 (43%)	69 (92%)	6 (8%)	0	100	100
2	a	75/176 (43%)	70 (93%)	5 (7%)	0	100	100
2	b	75/176 (43%)	69 (92%)	6 (8%)	0	100	100
2	c	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
2	d	75/176 (43%)	71 (95%)	2 (3%)	2 (3%)	4	25
2	e	75/176 (43%)	75 (100%)	0	0	100	100
2	u	61/176 (35%)	56 (92%)	5 (8%)	0	100	100
3	l	330/364 (91%)	303 (92%)	25 (8%)	2 (1%)	21	59
3	f	307/364 (84%)	280 (91%)	27 (9%)	0	100	100
3	g	330/364 (91%)	308 (93%)	22 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	h	330/364 (91%)	318 (96%)	10 (3%)	2 (1%)	21	59
3	i	330/364 (91%)	306 (93%)	23 (7%)	1 (0%)	36	72
3	j	330/364 (91%)	299 (91%)	31 (9%)	0	100	100
4	2	297/301 (99%)	253 (85%)	42 (14%)	2 (1%)	18	56
4	3	297/301 (99%)	279 (94%)	17 (6%)	1 (0%)	36	72
4	k	297/301 (99%)	284 (96%)	12 (4%)	1 (0%)	36	72
4	l	297/301 (99%)	286 (96%)	11 (4%)	0	100	100
4	m	297/301 (99%)	287 (97%)	10 (3%)	0	100	100
4	n	297/301 (99%)	277 (93%)	20 (7%)	0	100	100
4	o	297/301 (99%)	275 (93%)	22 (7%)	0	100	100
4	p	297/301 (99%)	293 (99%)	3 (1%)	1 (0%)	36	72
4	q	297/301 (99%)	283 (95%)	14 (5%)	0	100	100
4	r	297/301 (99%)	279 (94%)	15 (5%)	3 (1%)	12	48
4	s	297/301 (99%)	283 (95%)	12 (4%)	2 (1%)	18	56
4	t	297/301 (99%)	284 (96%)	12 (4%)	1 (0%)	36	72
All	All	28475/30708 (93%)	26770 (94%)	1648 (6%)	57 (0%)	44	78

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	978	ARG
1	K	1011	SER
1	O	1284	ASN
1	P	1179	GLN
2	d	19	PRO

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	1171/1171 (100%)	1135 (97%)	36 (3%)	35	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1157/1171 (99%)	1111 (96%)	46 (4%)	28	49
1	C	1156/1171 (99%)	1121 (97%)	35 (3%)	36	57
1	D	1171/1171 (100%)	1122 (96%)	49 (4%)	26	48
1	E	1171/1171 (100%)	1128 (96%)	43 (4%)	30	51
1	F	1155/1171 (99%)	1110 (96%)	45 (4%)	28	49
1	G	1170/1171 (100%)	1117 (96%)	53 (4%)	24	46
1	H	1171/1171 (100%)	1144 (98%)	27 (2%)	44	63
1	I	1157/1171 (99%)	1120 (97%)	37 (3%)	34	55
1	J	1146/1171 (98%)	1093 (95%)	53 (5%)	24	45
1	K	1171/1171 (100%)	1107 (94%)	64 (6%)	19	41
1	L	1157/1171 (99%)	1119 (97%)	38 (3%)	33	55
1	M	1171/1171 (100%)	1121 (96%)	50 (4%)	26	47
1	N	1155/1171 (99%)	1112 (96%)	43 (4%)	30	51
1	O	1131/1171 (97%)	1091 (96%)	40 (4%)	32	53
1	P	1100/1171 (94%)	1058 (96%)	42 (4%)	29	50
2	Q	71/128 (56%)	70 (99%)	1 (1%)	59	72
2	R	71/128 (56%)	71 (100%)	0	100	100
2	S	71/128 (56%)	70 (99%)	1 (1%)	59	72
2	T	71/128 (56%)	71 (100%)	0	100	100
2	U	71/128 (56%)	70 (99%)	1 (1%)	59	72
2	V	71/128 (56%)	69 (97%)	2 (3%)	38	59
2	W	71/128 (56%)	69 (97%)	2 (3%)	38	59
2	X	71/128 (56%)	71 (100%)	0	100	100
2	Y	71/128 (56%)	71 (100%)	0	100	100
2	Z	71/128 (56%)	71 (100%)	0	100	100
2	a	71/128 (56%)	67 (94%)	4 (6%)	19	40
2	b	71/128 (56%)	71 (100%)	0	100	100
2	c	71/128 (56%)	68 (96%)	3 (4%)	26	48
2	d	71/128 (56%)	69 (97%)	2 (3%)	38	59
2	e	71/128 (56%)	70 (99%)	1 (1%)	59	72
2	u	59/128 (46%)	58 (98%)	1 (2%)	53	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1	278/289 (96%)	277 (100%)	1 (0%)	84	83
3	f	267/289 (92%)	243 (91%)	24 (9%)	9	27
3	g	278/289 (96%)	264 (95%)	14 (5%)	22	43
3	h	278/289 (96%)	270 (97%)	8 (3%)	37	57
3	i	278/289 (96%)	269 (97%)	9 (3%)	34	55
3	j	278/289 (96%)	261 (94%)	17 (6%)	17	38
4	2	265/267 (99%)	265 (100%)	0	100	100
4	3	265/267 (99%)	265 (100%)	0	100	100
4	k	265/267 (99%)	249 (94%)	16 (6%)	17	39
4	l	265/267 (99%)	255 (96%)	10 (4%)	29	50
4	m	265/267 (99%)	256 (97%)	9 (3%)	32	54
4	n	265/267 (99%)	252 (95%)	13 (5%)	22	43
4	o	265/267 (99%)	253 (96%)	12 (4%)	24	46
4	p	265/267 (99%)	255 (96%)	10 (4%)	29	50
4	q	265/267 (99%)	253 (96%)	12 (4%)	24	46
4	r	265/267 (99%)	253 (96%)	12 (4%)	24	46
4	s	265/267 (99%)	253 (96%)	12 (4%)	24	46
4	t	265/267 (99%)	252 (95%)	13 (5%)	22	43
All	All	24471/25722 (95%)	23560 (96%)	911 (4%)	31	51

5 of 911 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	1190	THR
4	s	18	ILE
1	M	1351	GLN
4	r	43	LEU
4	k	137	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 715 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	1022	HIS
1	P	908	GLN
1	N	289	GLN

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Mol	Chain	Res	Type
1	M	997	HIS
1	O	389	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.

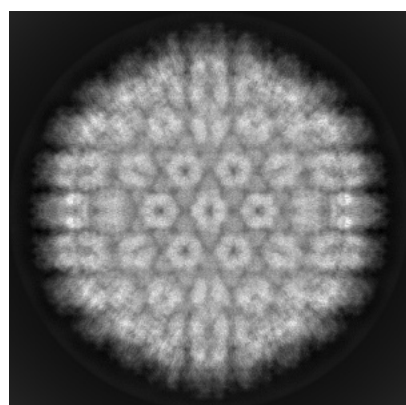
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21504. These allow visual inspection of the internal detail of the map and identification of artifacts.

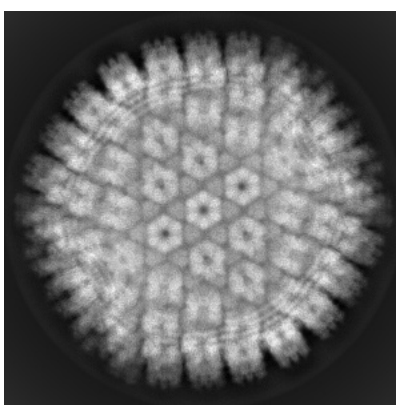
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

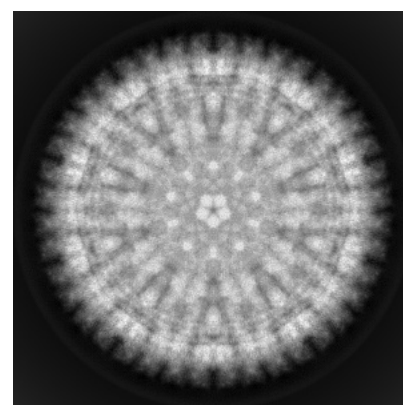
6.1.1 Primary map



X



Y

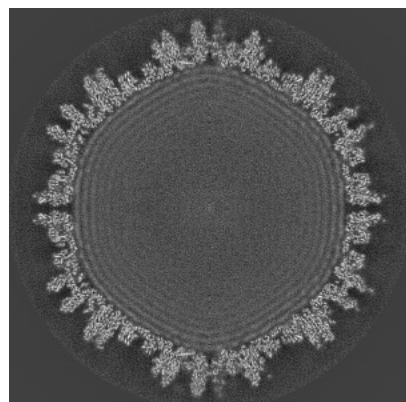


Z

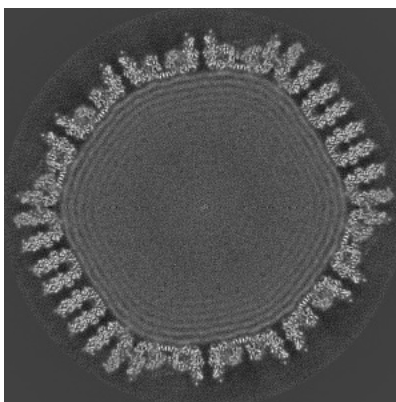
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

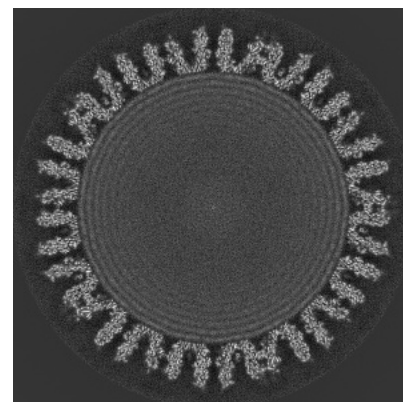
6.2.1 Primary map



X Index: 256



Y Index: 256

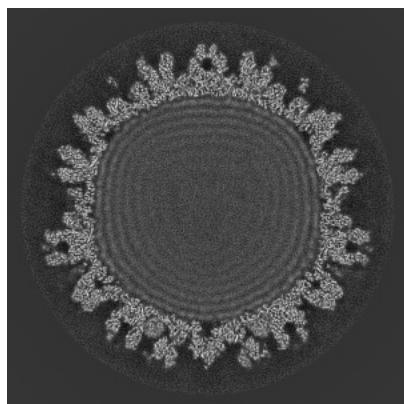


Z Index: 256

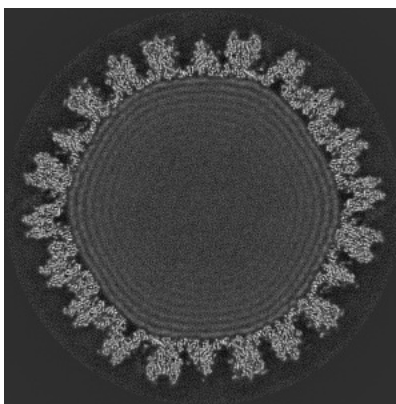
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

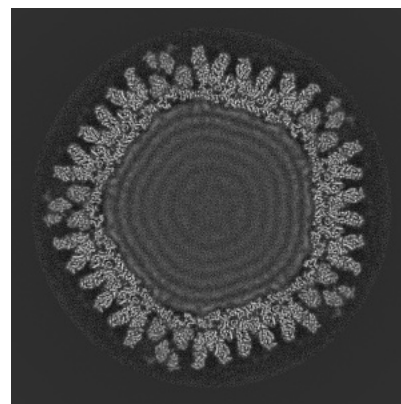
6.3.1 Primary map



X Index: 160



Y Index: 212

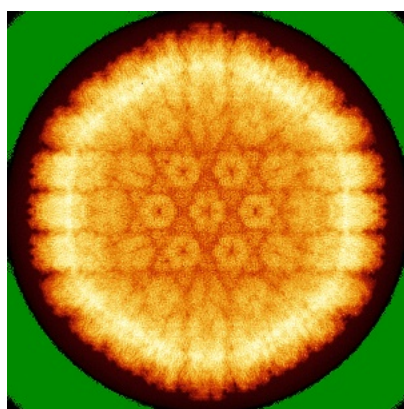


Z Index: 140

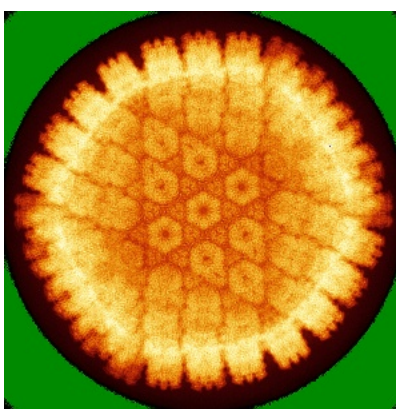
The images above show the largest variance slices of the map in three orthogonal directions.

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

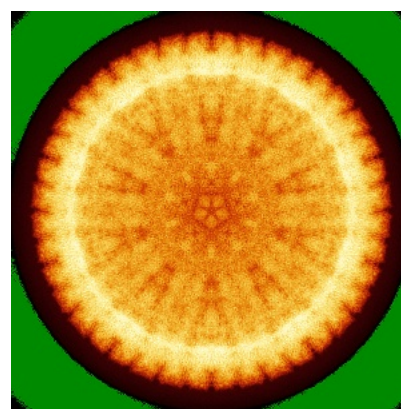
6.4.1 Primary map



X



Y

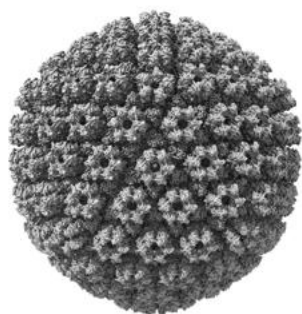


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

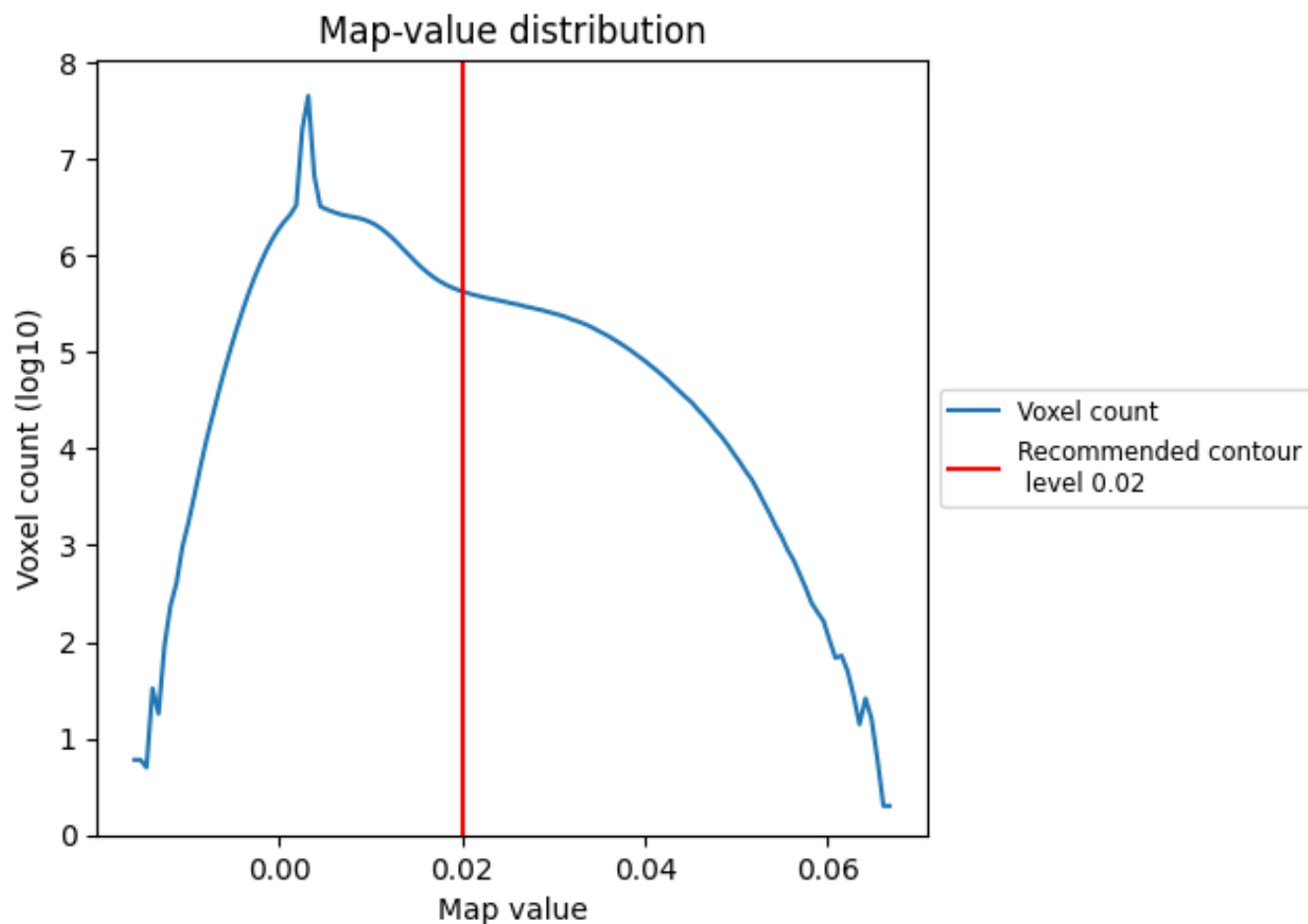
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

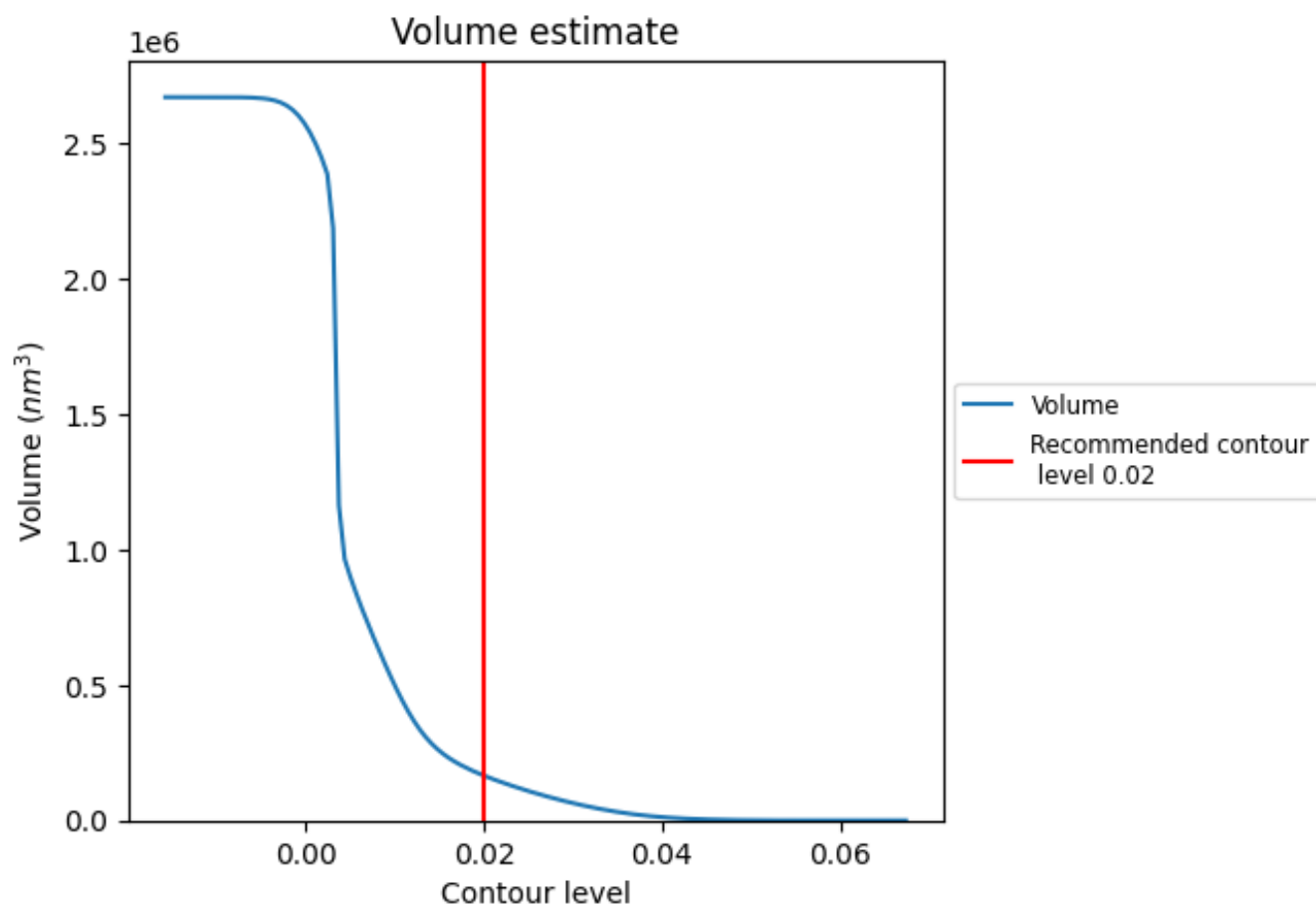
This section contains the results of statistical analysis of the map.

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.

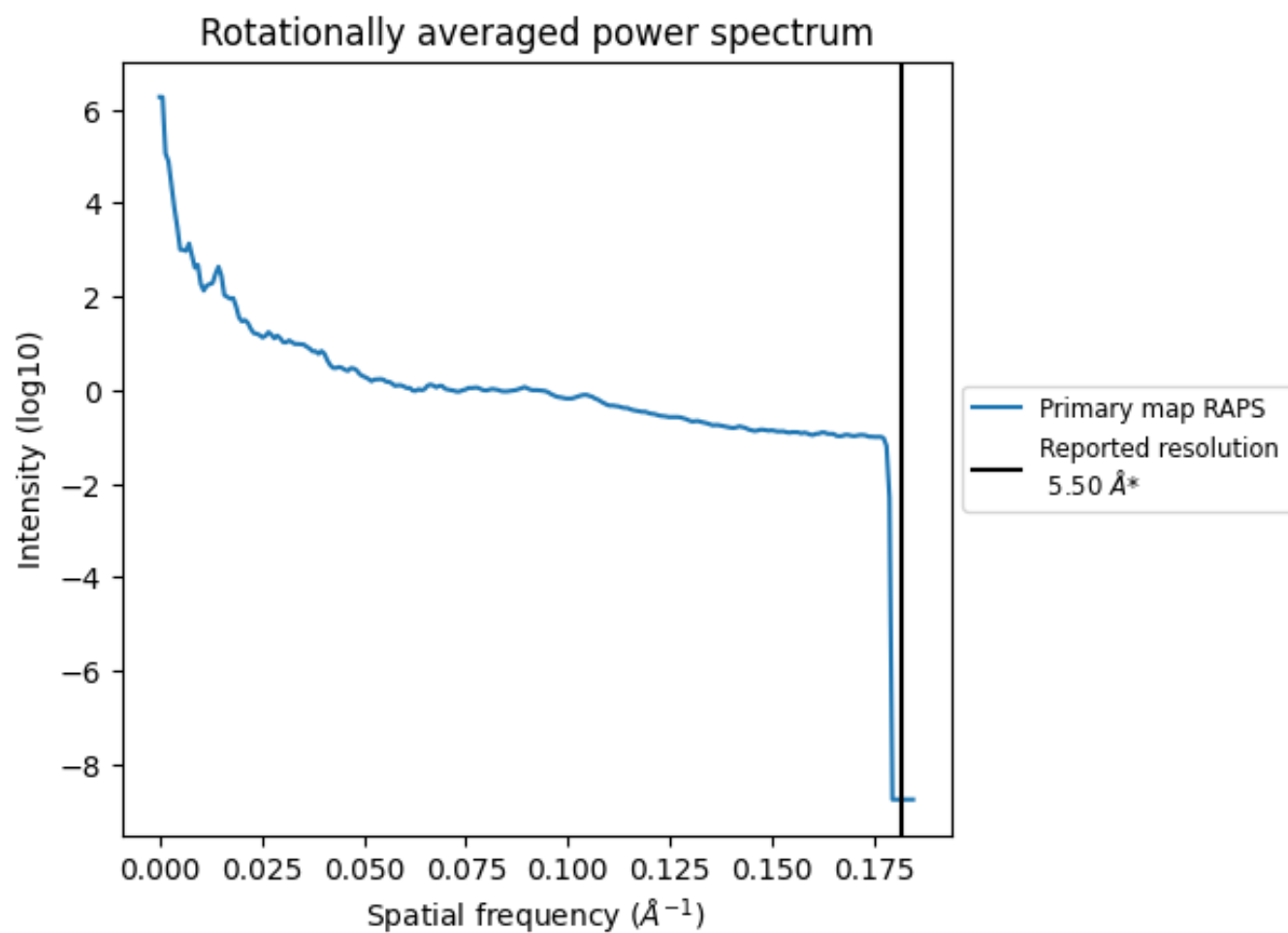
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165404 nm³; this corresponds to an approximate mass of 149413 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 0.182 Å⁻¹

8 Fourier-Shell correlation

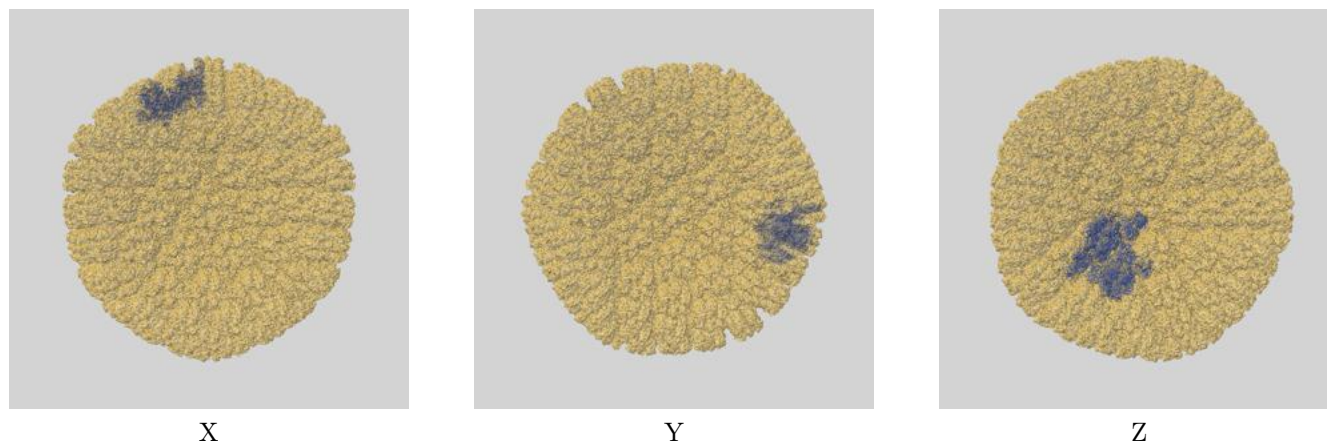
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

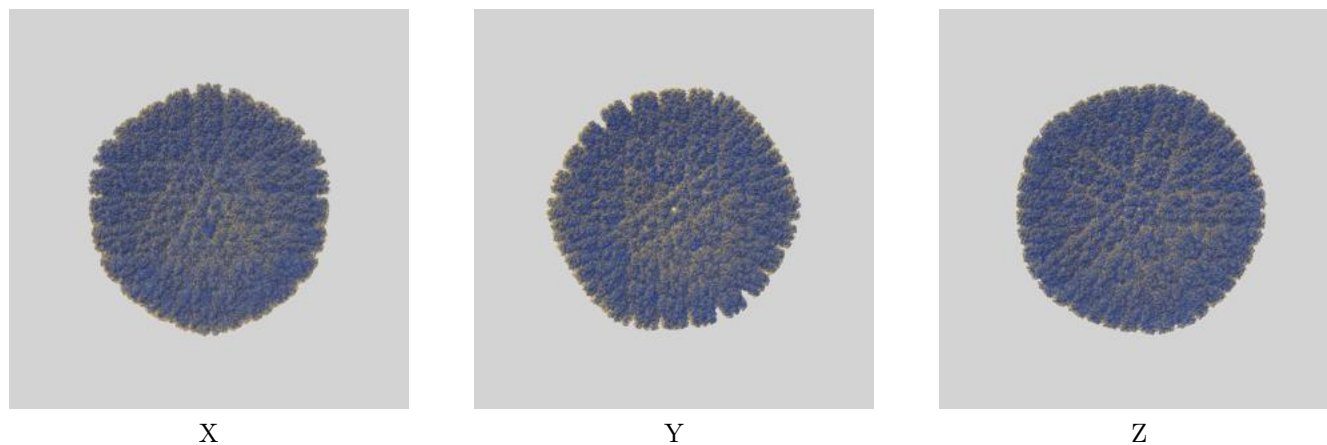
This section contains information regarding the fit between EMDB map EMD-21504 and PDB model 6W19. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

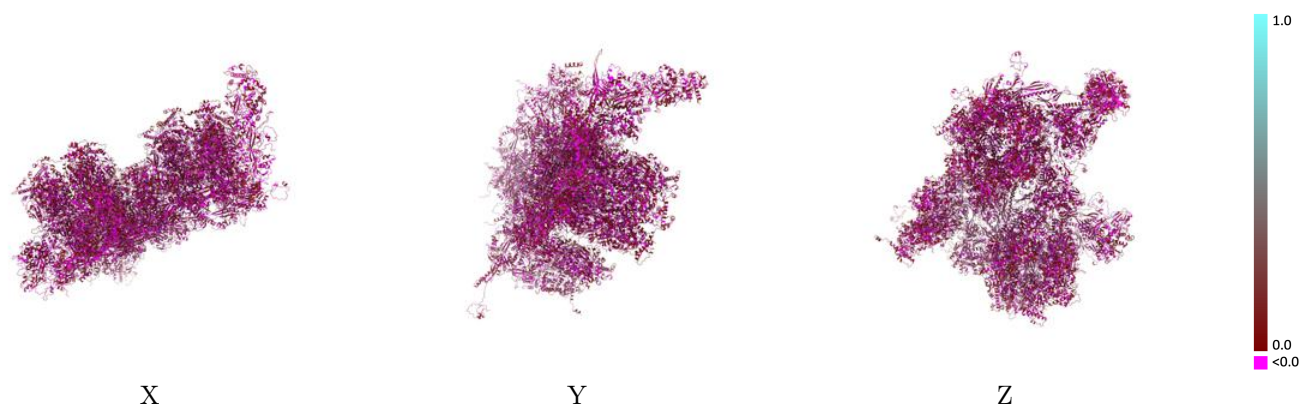


9.1.2 Map-model assembly overlay [i](#)



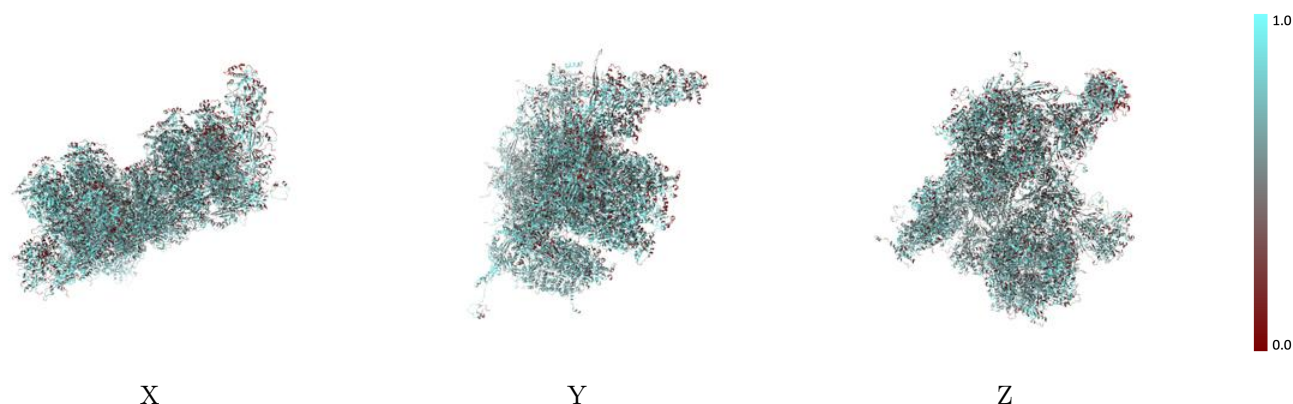
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



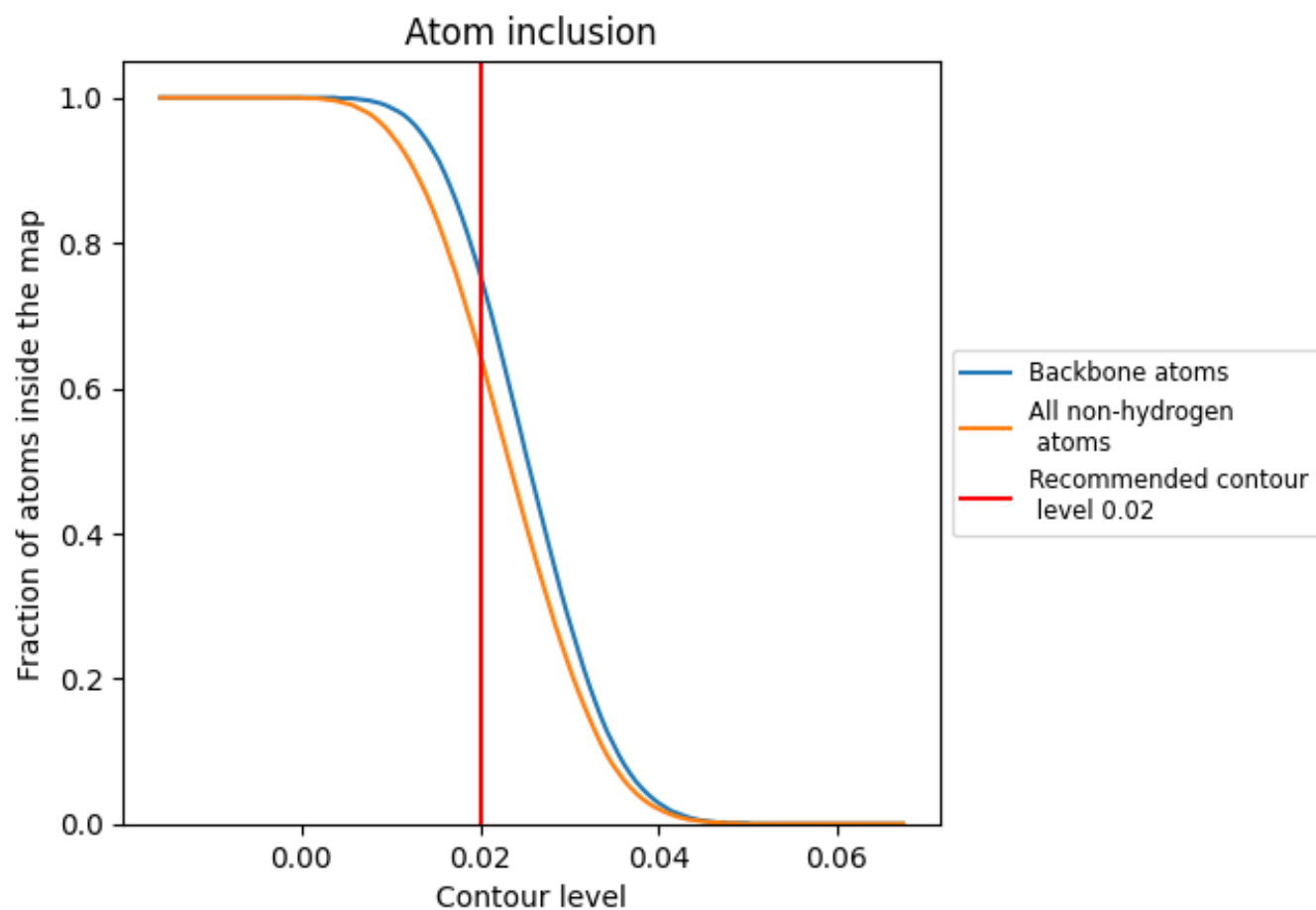
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6470	 0.0590
1	 0.4660	 0.0150
2	 0.5820	 0.0800
3	 0.5820	 0.0610
A	 0.6700	 0.0500
B	 0.6840	 0.0600
C	 0.6810	 0.0690
D	 0.6720	 0.0640
E	 0.6780	 0.0610
F	 0.6750	 0.0550
G	 0.6790	 0.0570
H	 0.6970	 0.0670
I	 0.6980	 0.0740
J	 0.6480	 0.0460
K	 0.6630	 0.0490
L	 0.6580	 0.0520
M	 0.6500	 0.0520
N	 0.6520	 0.0510
O	 0.6360	 0.0420
P	 0.5860	 0.0490
Q	 0.5370	 0.1020
R	 0.5220	 0.0960
S	 0.6090	 0.0930
T	 0.6900	 0.1310
U	 0.6680	 0.1130
V	 0.5700	 0.1040
W	 0.5410	 0.0980
X	 0.5350	 0.1070
Y	 0.5960	 0.0940
Z	 0.4250	 0.0730
a	 0.4460	 0.0770
b	 0.5430	 0.0820
c	 0.6710	 0.1110
d	 0.6450	 0.1120
e	 0.5180	 0.1020



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Chain	Atom inclusion	Q-score
f	 0.5760	 0.0400
g	 0.6310	 0.0530
h	 0.6140	 0.0670
i	 0.6070	 0.0560
j	 0.6320	 0.0800
k	 0.5420	 0.0550
l	 0.6040	 0.0700
m	 0.6340	 0.0690
n	 0.6110	 0.0670
o	 0.6660	 0.0770
p	 0.5620	 0.0750
q	 0.6180	 0.0710
r	 0.6130	 0.0630
s	 0.5970	 0.0560
t	 0.6500	 0.0670
u	 0.3200	 0.0440