



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 09:31 PM UTC

PDB ID : 6NHJ / pdb_00006nhj
EMDB ID : EMD-9366
Title : Atomic structures and deletion mutant reveal different capsid-binding patterns and functional significance of tegument protein pp150 in murine and human cytomegaloviruses with implications for therapeutic development
Authors : Liu, W.; Dai, X.H.; Jih, J.; Chan, K.; Trang, P.; Yu, X.K.; Balogun, R.; Mei, Y.; Liu, F.Y.; Zhou, Z.H.
Deposited on : 2018-12-22
Resolution : 5.00 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:

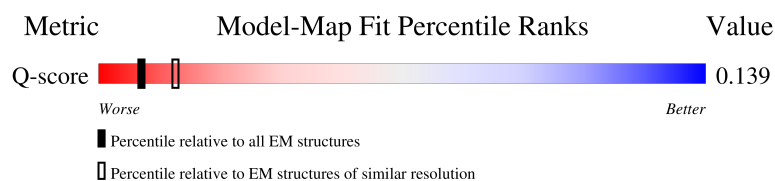
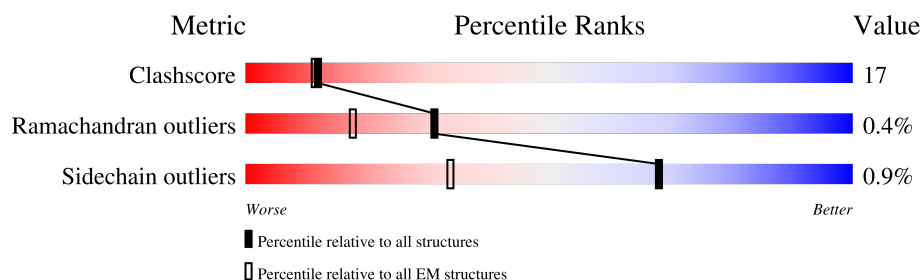
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 5.00 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	1057 (4.50 - 5.50)

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	1353	28% 69% 29% ..
1	B	1353	27% 68% 28% .
1	C	1353	30% 67% 29% ..
1	D	1353	30% 64% 32% ..

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Mol	Chain	Length	Quality of chain
1	E	1353	
1	F	1353	
1	G	1353	
1	H	1353	
1	I	1353	
1	k	1353	
1	l	1353	
1	m	1353	
1	n	1353	
1	o	1353	
1	p	1353	
1	q	1353	
2	2	718	
2	3	718	
2	e	718	
2	f	718	
2	g	718	
2	h	718	
2	i	718	
2	j	718	
3	J	98	
3	K	98	
3	L	98	
3	M	98	
3	N	98	

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Mol	Chain	Length	Quality of chain
3	O	98	
3	P	98	
3	Q	98	
3	R	98	
3	r	98	
3	s	98	
3	t	98	
3	u	98	
3	v	98	
3	w	98	
3	x	98	
4	S	294	
4	T	294	
4	U	294	
4	V	294	
4	y	294	
5	1	311	
5	W	311	
5	X	311	
5	Y	311	
5	Z	311	
5	a	311	
5	b	311	
5	c	311	
5	d	311	

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Mol	Chain	Length	Quality of chain
5	z	311	53% 55% 33% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 218639 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	1335	Total	C	N	O	S	0	0
			10537	6666	1856	1962	53		
1	B	1310	Total	C	N	O	S	0	0
			10351	6550	1822	1926	53		
1	C	1310	Total	C	N	O	S	0	0
			10350	6551	1822	1924	53		
1	D	1314	Total	C	N	O	S	0	0
			10375	6567	1826	1929	53		
1	E	1330	Total	C	N	O	S	0	0
			10495	6635	1852	1955	53		
1	F	1319	Total	C	N	O	S	0	0
			10407	6585	1831	1938	53		
1	G	1341	Total	C	N	O	S	0	0
			10580	6692	1864	1971	53		
1	H	1341	Total	C	N	O	S	0	0
			10580	6692	1864	1971	53		
1	I	1321	Total	C	N	O	S	0	0
			10421	6593	1834	1941	53		
1	k	1295	Total	C	N	O	S	0	0
			10209	6465	1795	1896	53		
1	l	1336	Total	C	N	O	S	0	0
			10548	6673	1859	1963	53		
1	m	1312	Total	C	N	O	S	0	0
			10364	6559	1824	1928	53		
1	n	1335	Total	C	N	O	S	0	0
			10538	6663	1858	1964	53		
1	o	1313	Total	C	N	O	S	0	0
			10368	6558	1828	1929	53		
1	p	1301	Total	C	N	O	S	0	0
			10252	6477	1813	1910	52		
1	q	1219	Total	C	N	O	S	0	0
			9621	6090	1690	1791	50		

- Molecule 2 is a protein called Tegument protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	174	Total 1469	C 929	N 279	O 255	S 6	0	0
2	3	200	Total 1665	C 1052	N 314	O 291	S 8	0	0
2	e	174	Total 1469	C 929	N 279	O 255	S 6	0	0
2	h	200	Total 1665	C 1052	N 314	O 291	S 8	0	0
2	f	174	Total 1469	C 929	N 279	O 255	S 6	0	0
2	i	200	Total 1665	C 1052	N 314	O 291	S 8	0	0
2	g	174	Total 1469	C 929	N 279	O 255	S 6	0	0
2	j	200	Total 1665	C 1052	N 314	O 291	S 8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	60	Total 471	C 300	N 83	O 83	S 5	0	0
3	K	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	L	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	M	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	N	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	O	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	P	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	Q	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	R	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	r	60	Total 471	C 300	N 83	O 83	S 5	0	0
3	s	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	t	59	Total 462	C 294	N 81	O 82	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	u	60	Total	C	N	O	S	0	0
			471	300	83	83	5		
3	v	60	Total	C	N	O	S	0	0
			471	300	83	83	5		
3	w	60	Total	C	N	O	S	0	0
			471	300	83	83	5		
3	x	57	Total	C	N	O	S	0	0
			450	287	79	79	5		

- Molecule 4 is a protein called Minor capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	y	249	Total	C	N	O	S	0	0
			1977	1261	350	356	10		
4	S	289	Total	C	N	O	S	0	0
			2305	1470	406	416	13		
4	T	289	Total	C	N	O	S	0	0
			2305	1470	406	416	13		
4	U	289	Total	C	N	O	S	0	0
			2305	1470	406	416	13		
4	V	289	Total	C	N	O	S	0	0
			2305	1470	406	416	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	z	284	Total	C	N	O	S	0	0
			2224	1403	382	419	20		
5	W	281	Total	C	N	O	S	0	0
			2201	1390	378	414	19		
5	X	277	Total	C	N	O	S	0	0
			2166	1367	373	407	19		
5	Y	282	Total	C	N	O	S	0	0
			2209	1395	379	415	20		
5	Z	281	Total	C	N	O	S	0	0
			2201	1390	378	414	19		
5	1	257	Total	C	N	O	S	0	0
			2009	1268	350	374	17		
5	a	267	Total	C	N	O	S	0	0
			2085	1314	363	389	19		
5	b	270	Total	C	N	O	S	0	0
			2109	1330	366	394	19		

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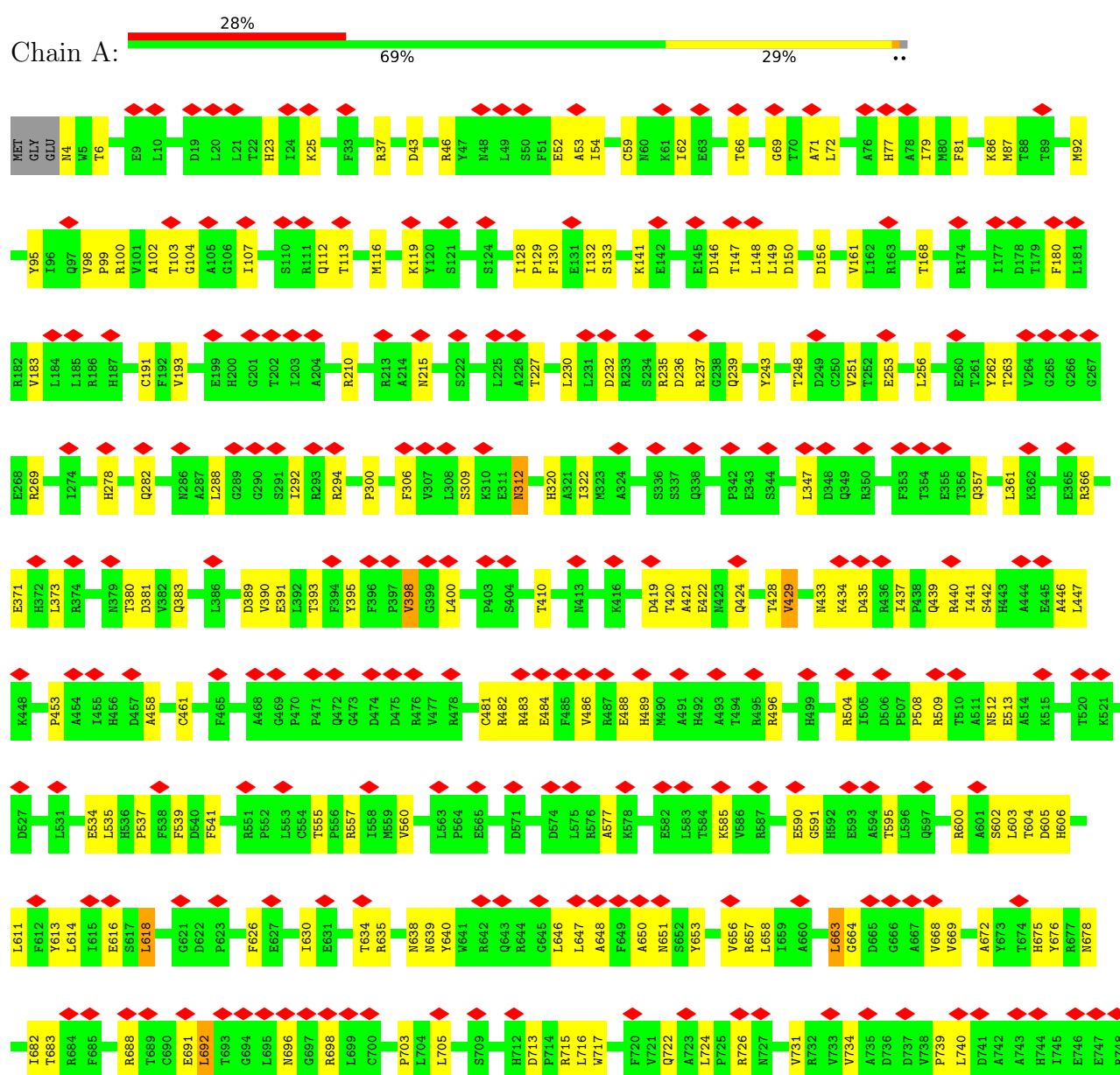
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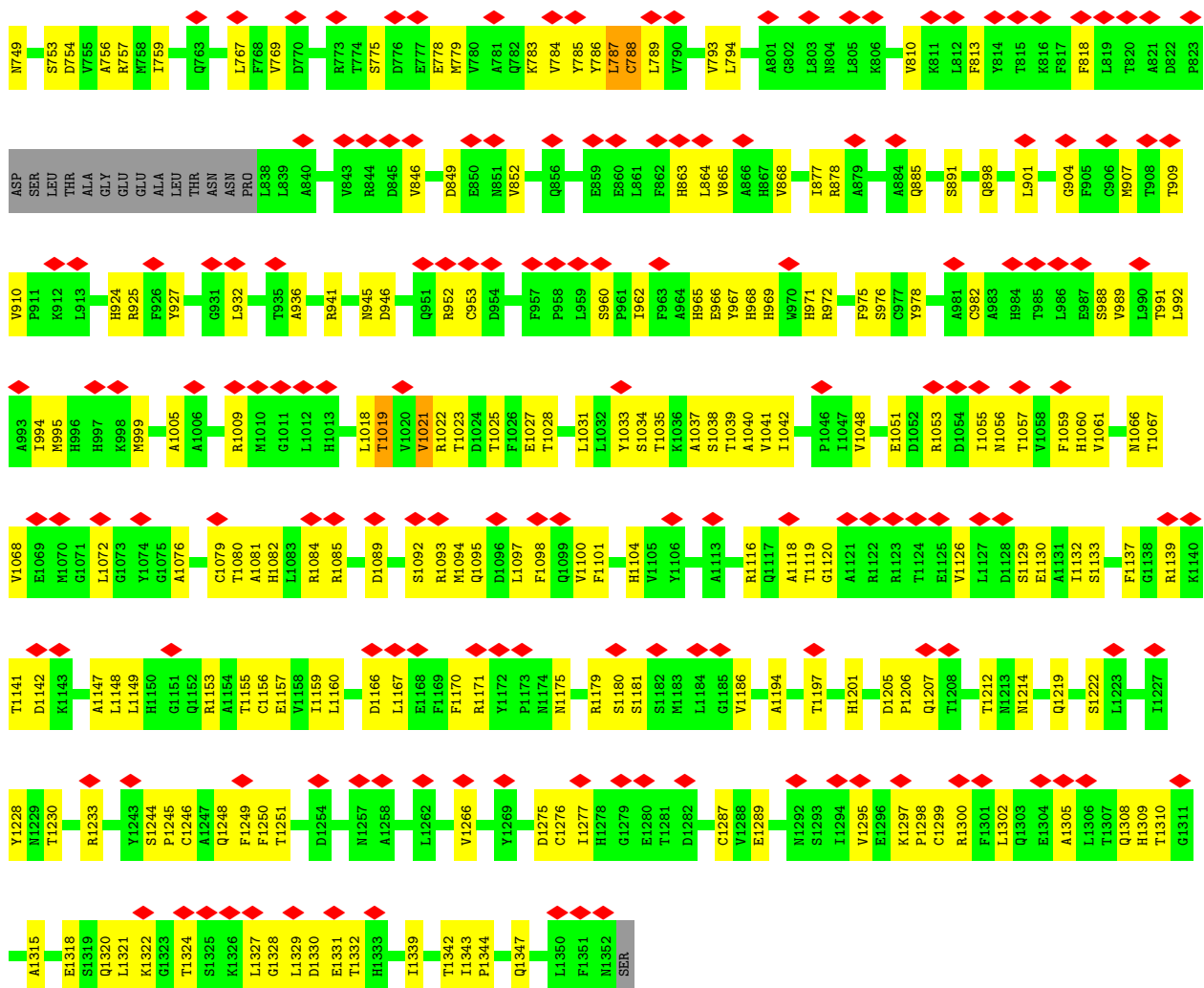
Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	274	Total	C	N	O	S	0	0
			2141	1349	371	401	20		
5	d	274	Total	C	N	O	S	0	0
			2140	1351	370	399	20		

3 Residue-property plots

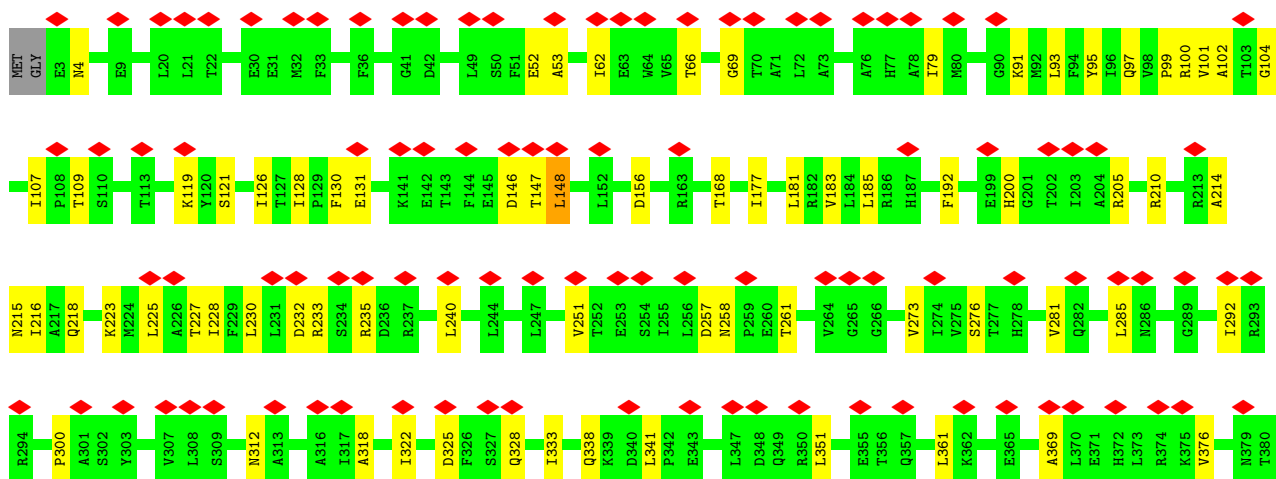
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

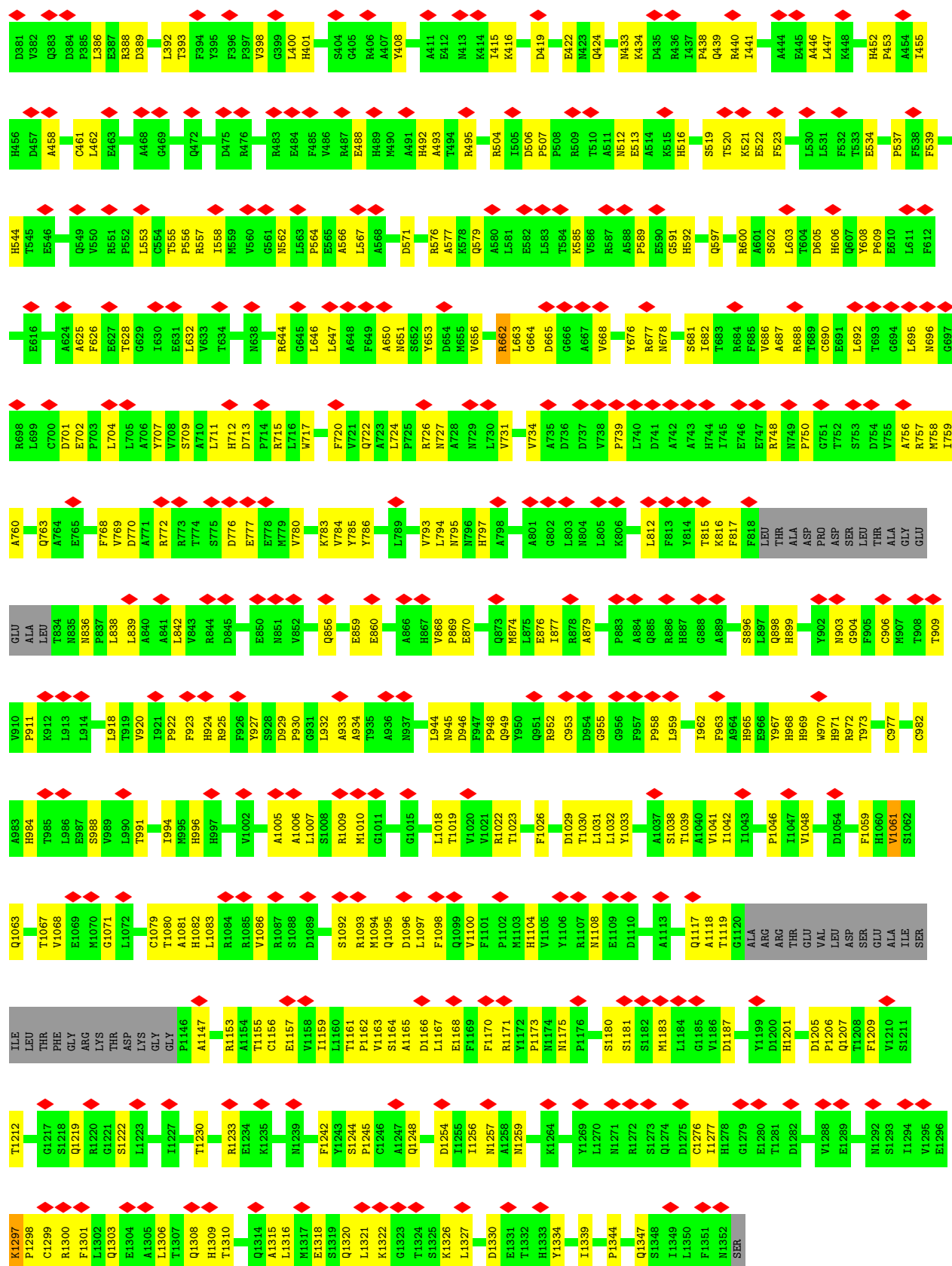
• Molecule 1: Major capsid protein



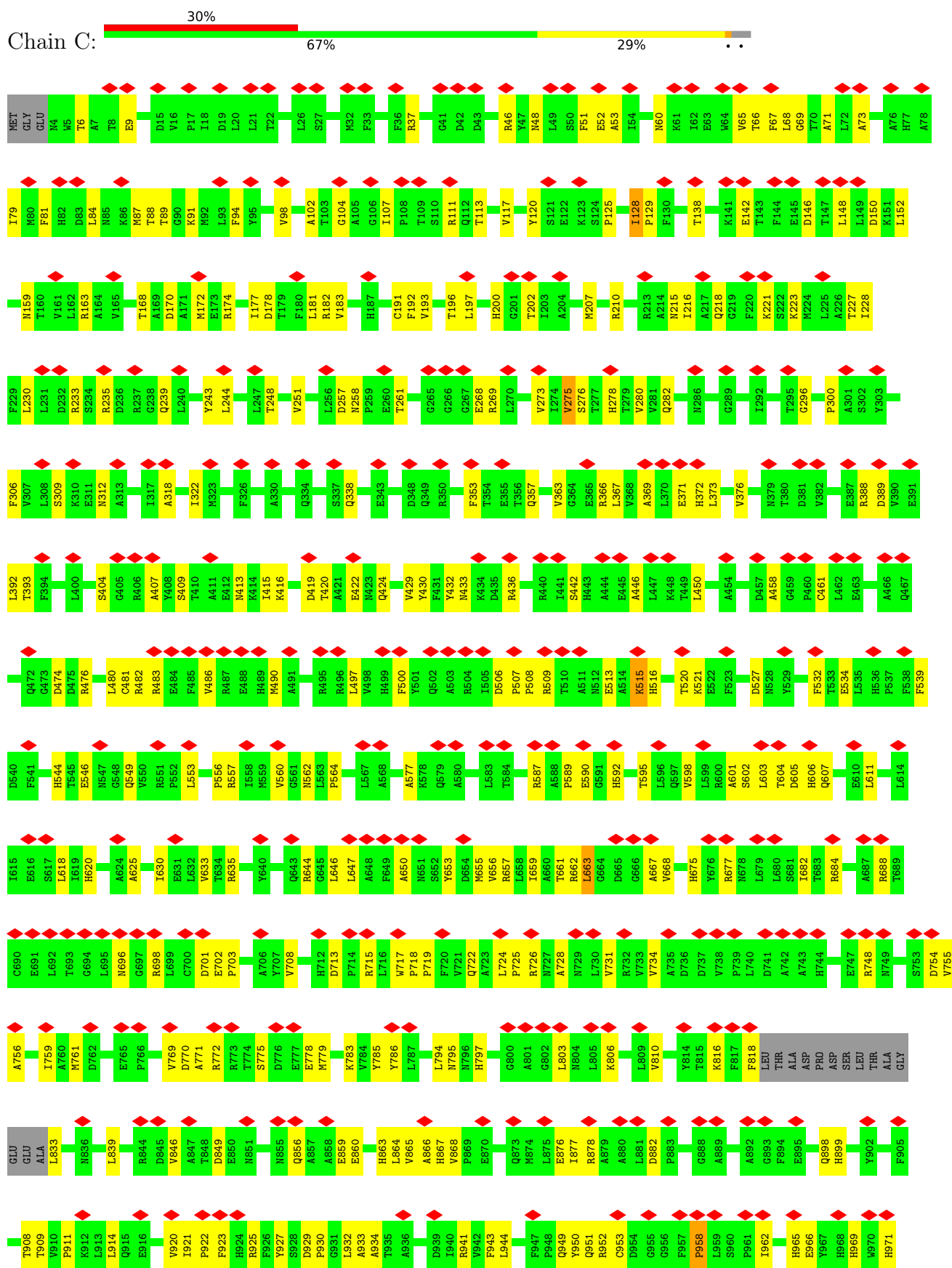


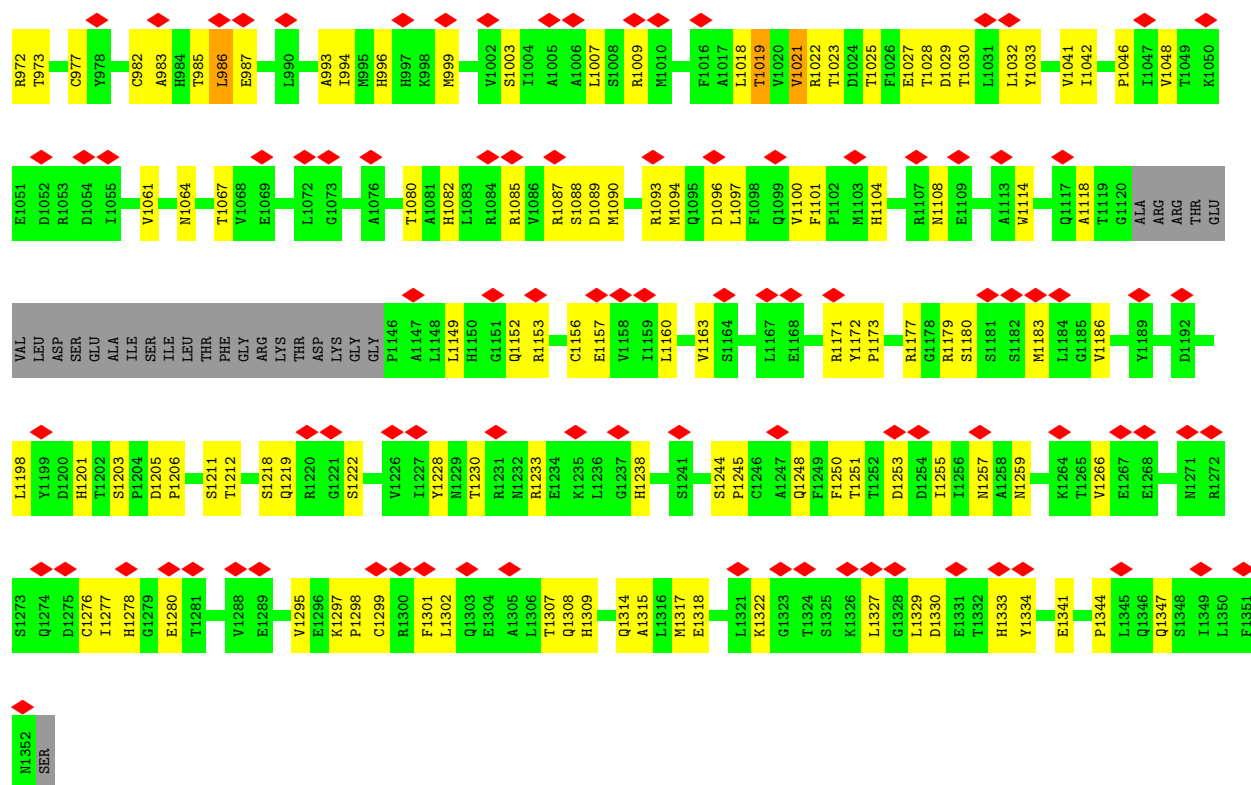
• Molecule 1: Major capsid protein



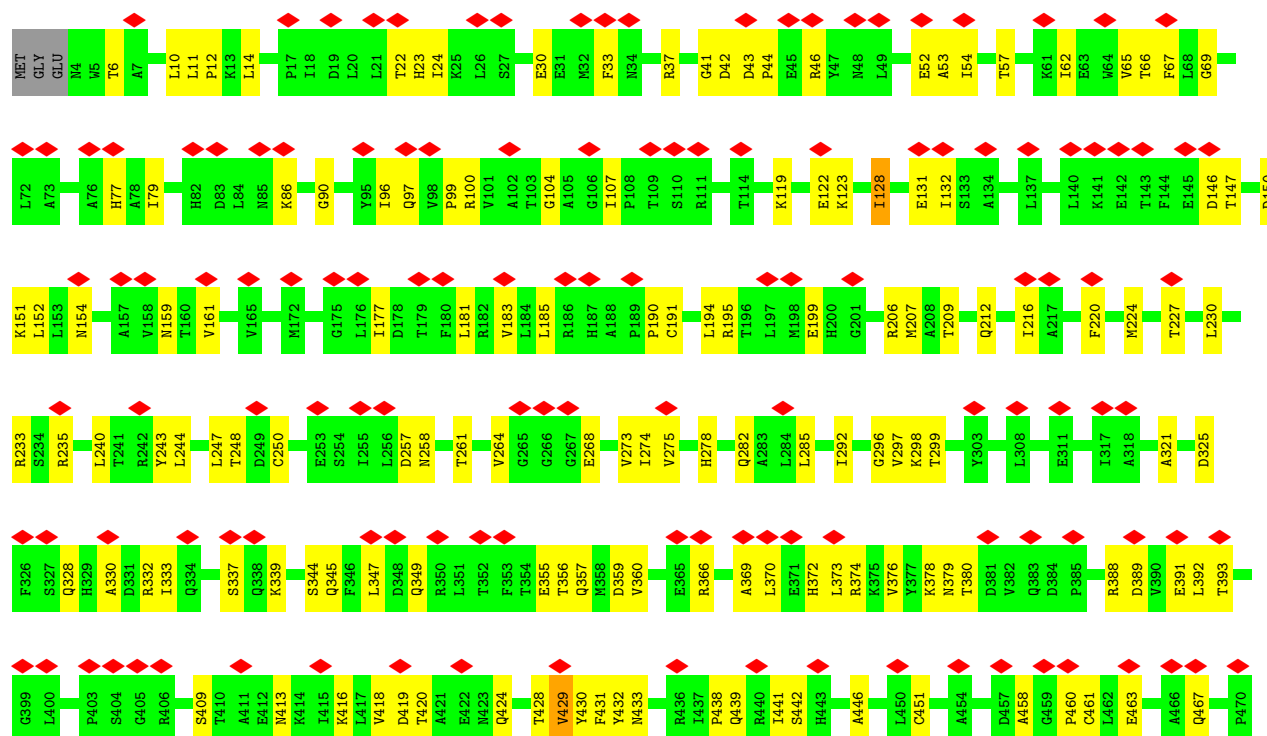


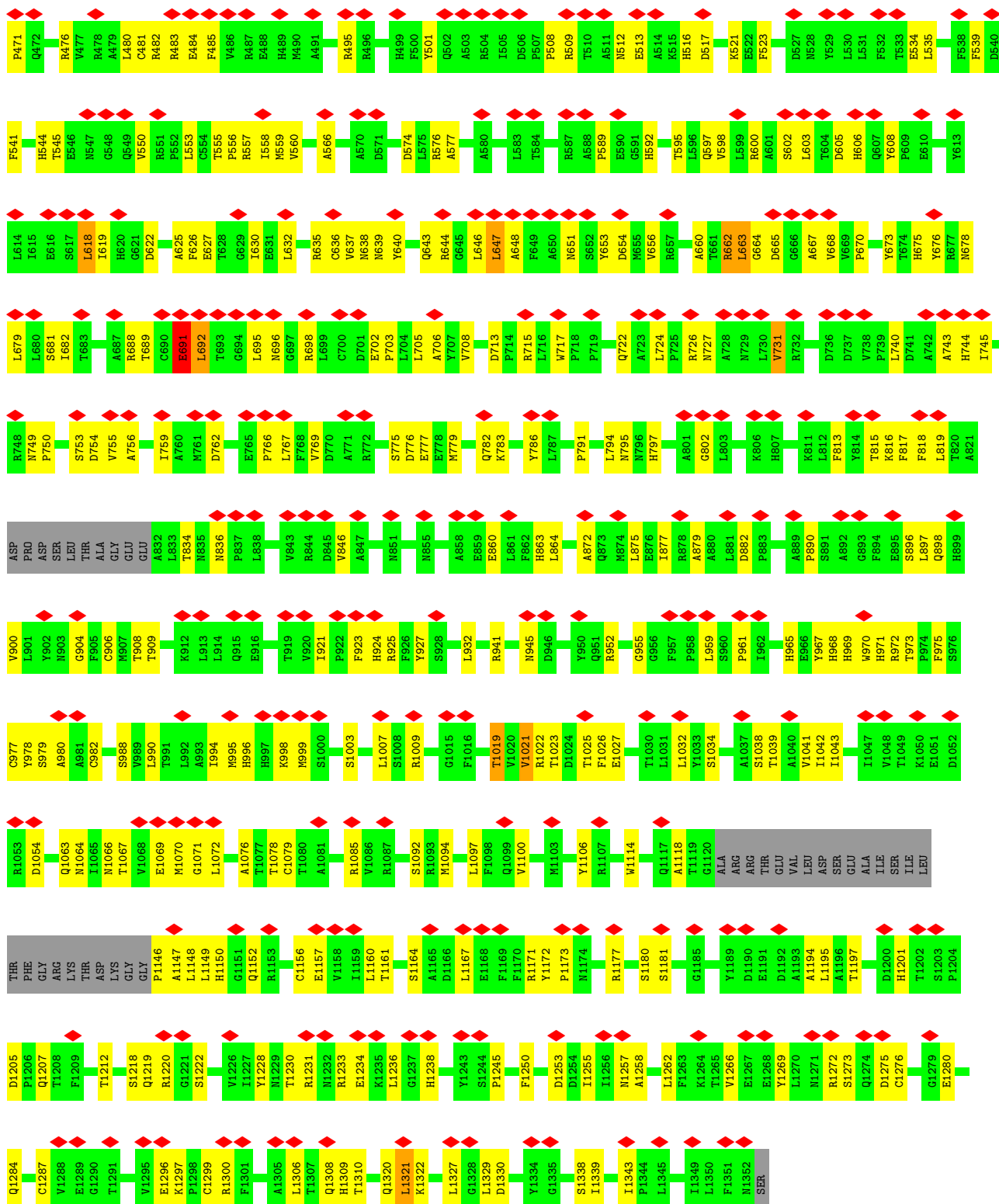
- Molecule 1: Major capsid protein





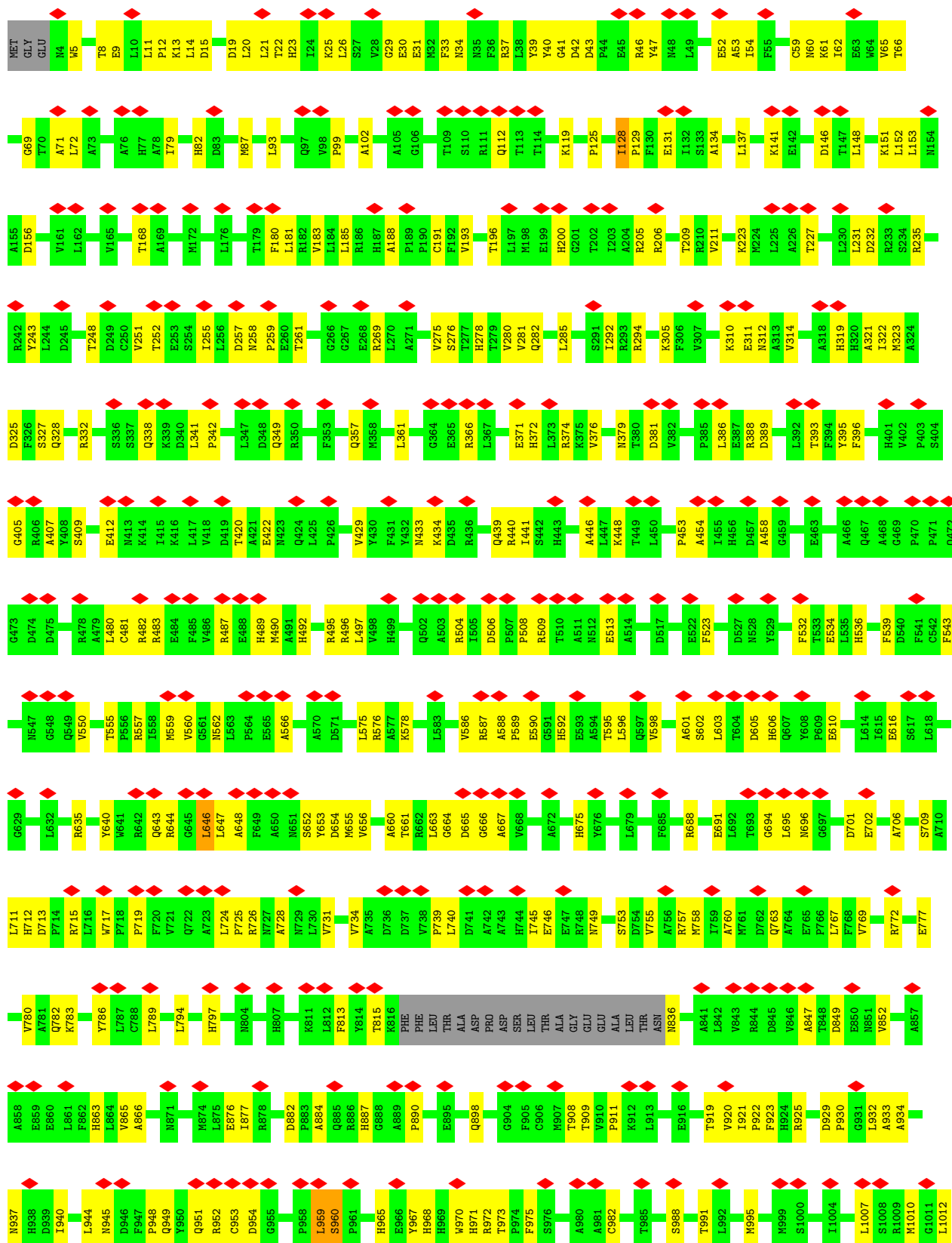
• Molecule 1: Major capsid protein

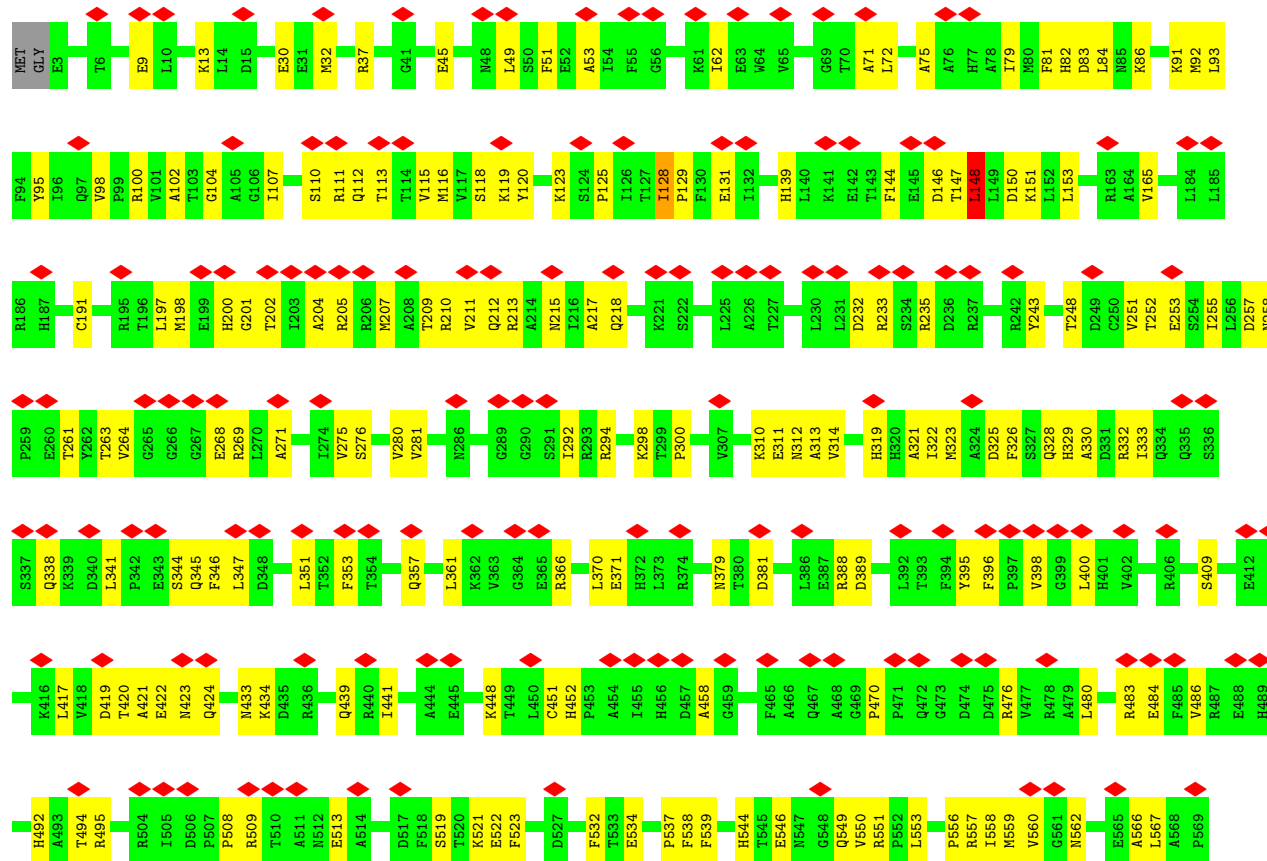


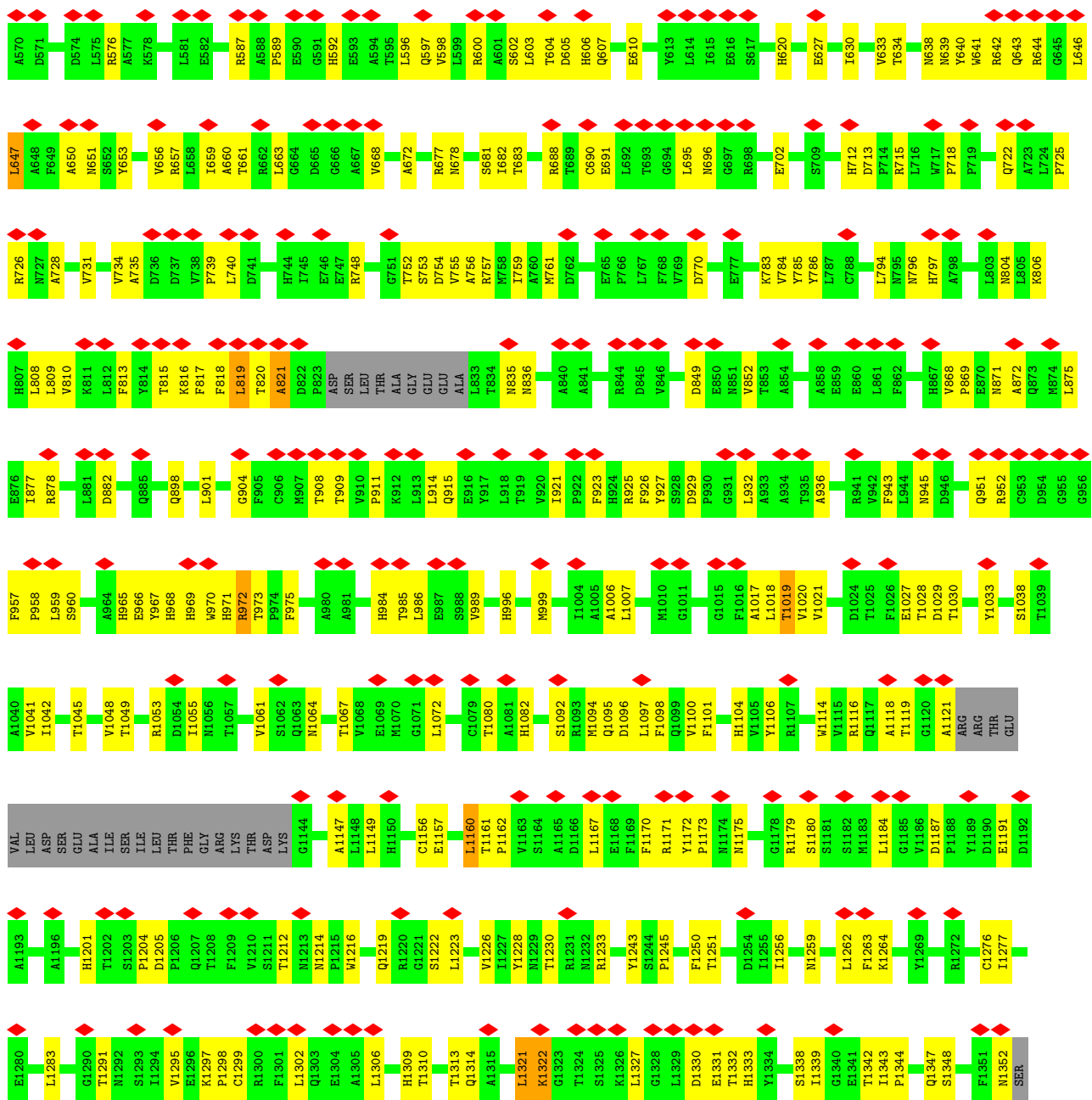


• Molecule 1: Major capsid protein

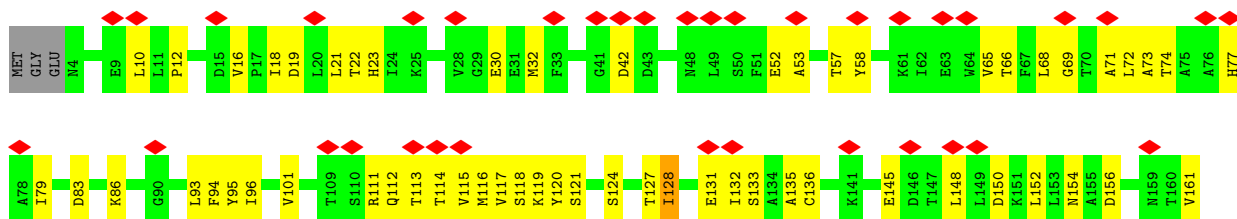




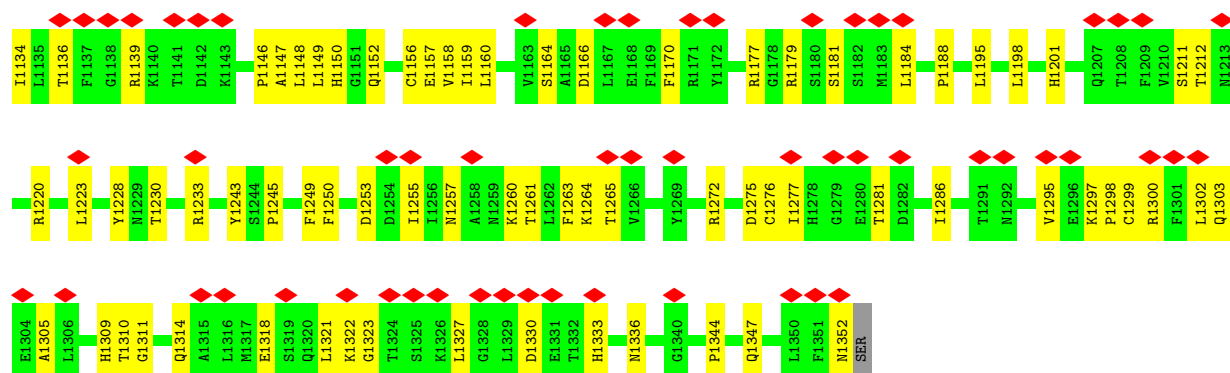




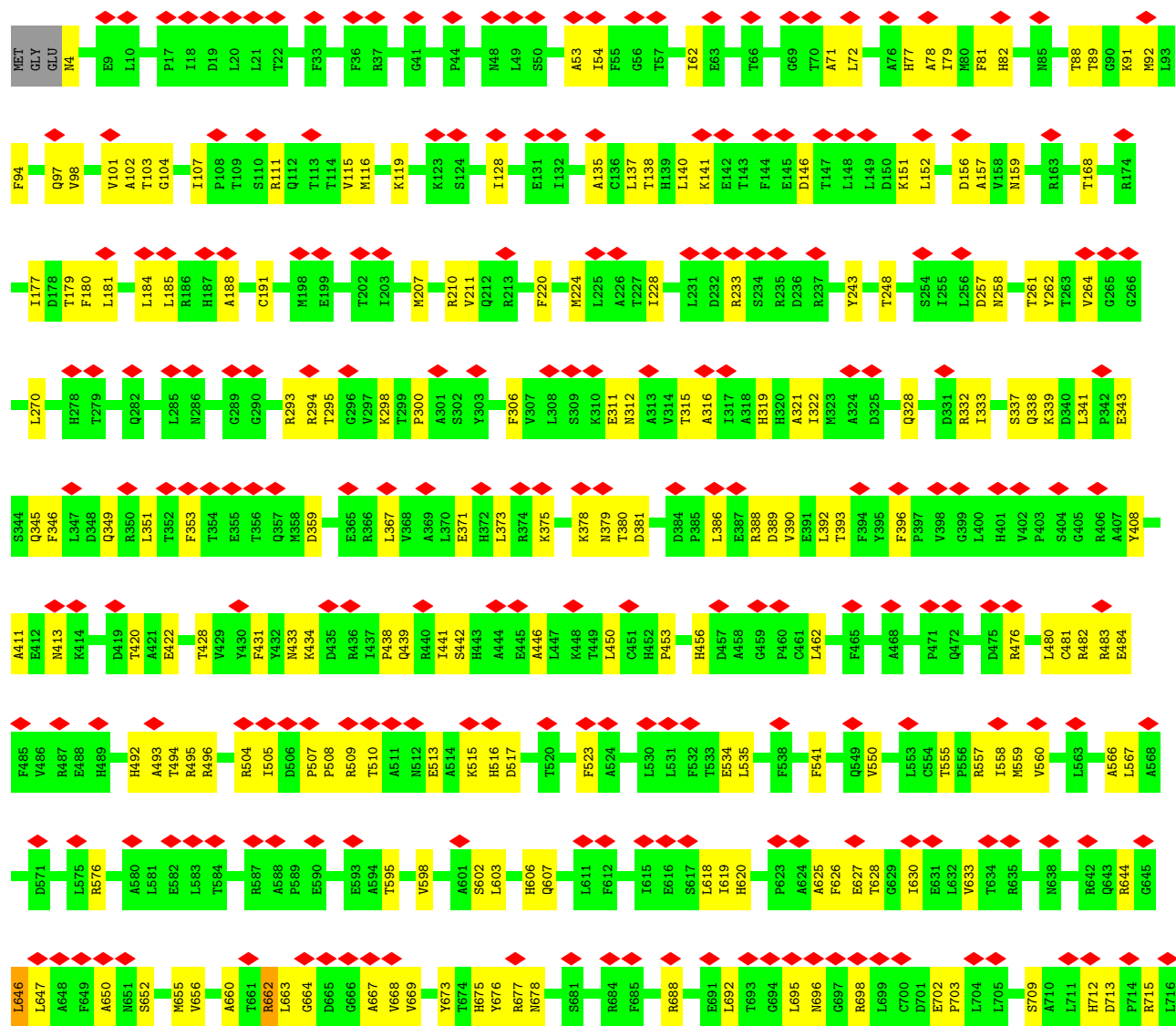
• Molecule 1: Major capsid protein

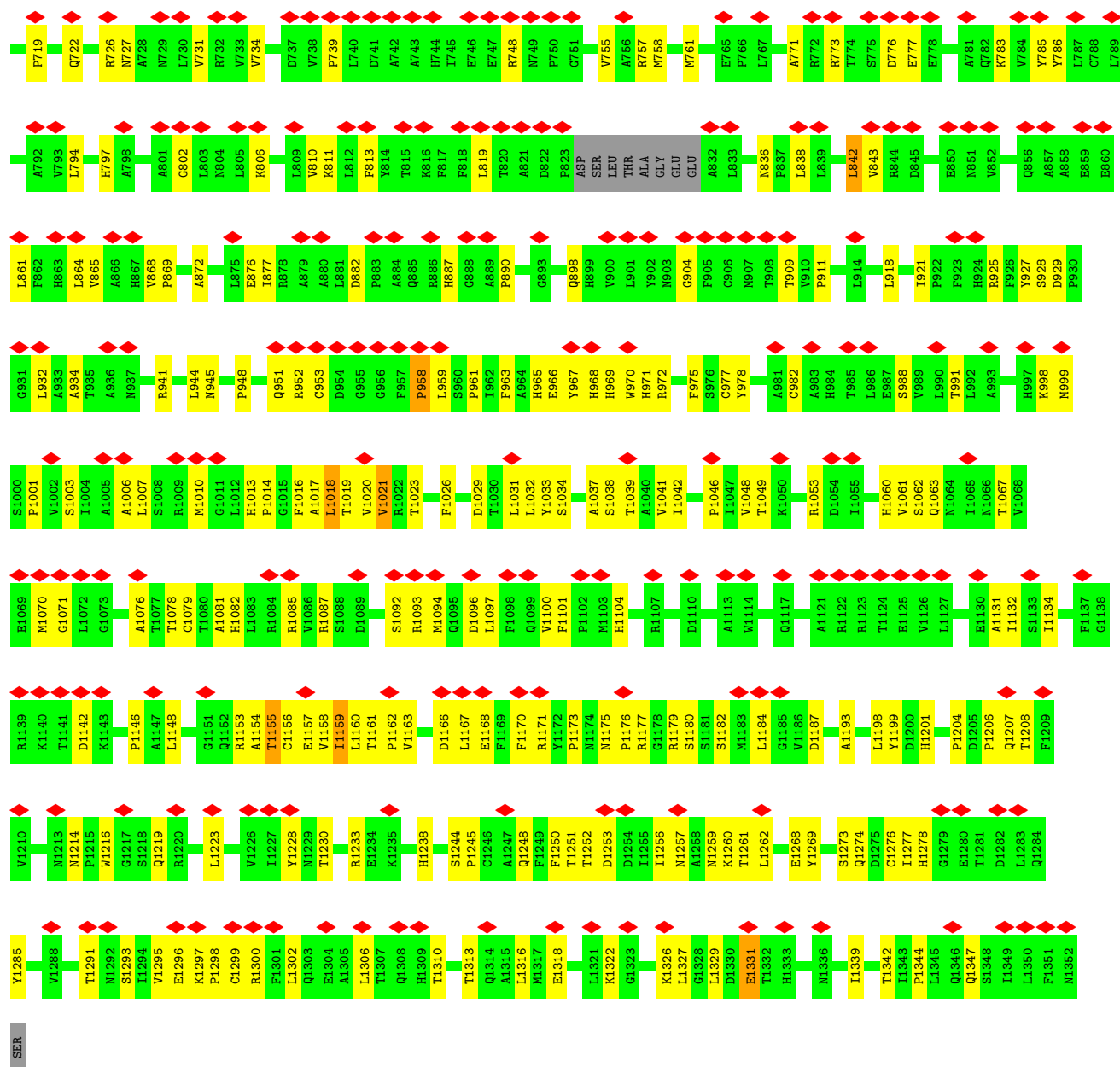


V1061	C982	M907	N835	F766	L699	E627	N563	V477	F396	A324	T248	L162
M1064	A983	T908	N836	L767	C700	E630	L563	R478	P397	D325	D249	R163
I1065	H984	T909	A840	R772	D701	E631	E565	A479	V398	F326	T252	K166
T1067	T985	V910	A841	R773	E702	E632	E566	L480	G399	H329	E253	R174
V1068	L986	P911	T774	R774	P703	L632	A566	C481	L400	A330	E254	I177
E1069	E987	K912	R844	S775	L705	V633	A570	R482	S404	D331	S255	F180
M1070	S988	L914	D845	D776	L706	R635	D571	E484	G405	Q332	L256	L181
G1071	T991	L914	V846	E777	V707	R635	F572	F485	R406	Q334	D257	L184
L1072	L992	T919	A847	E778	V708	N638	H573	V486	N413	Q335	N258	L185
G1073	A993	V920	T848	V780	S709	N639	D574	R487	N414	Q336	P259	A188
Y1074	M995	P922	E850	A781	A710	D574	L575	E488	K414	Q337	E260	C191
A1075	H996	F923	N851	K783	H712	H641	R576	H489	L417	Q338	T261	F192
G1076	H997	H924	A854	V784	D713	N638	K578	T494	D419	Q339	Y262	L197
C1079	K998	R925	A857	V785	L716	N639	E582	R495	T420	L341	G265	M198
T1080	M999	F927	A857	V786	W717	D574	L583	R496	Q424	D348	G266	E199
H1082	V1002	S928	E857	L787	P718	L646	L583	L497	Q424	D348	G267	H200
L1083	S1003	D929	E860	C788	P719	L647	K585	F500	Q424	D348	E268	G201
R1084	T1004	P930	L861	L789	F720	A648	V586	Y501	Q424	D348	R269	T202
R1085	A1005	G931	F862	V790	F721	F649	V586	R504	Q424	D348	L270	I203
S1088	A1006	L932	H863	A792	Q722	N651	E588	I505	Q424	D348	V275	R206
D1089	L1007	A933	L864	A793	A723	S652	P589	I506	Q424	D348	S276	A208
M1090	L1007	A933	V865	V793	A723	S652	E590	D506	Q424	D348	T277	T209
G1091	S1008	R936	A866	L794	L724	V653	E591	P507	Q424	D348	H278	Q212
S1092	R1009	A936	H867	H797	P725	V656	H592	P508	Q424	D348	T279	N215
R1093	M1010	A936	V868	H797	R726	V656	H592	R509	Q424	D348	V280	Q218
M1094	D946	F947	A801	A801	A728	L659	E593	N512	Q424	D348	Q282	G219
G1095	P948	P948	E870	G802	A728	L659	A594	N512	Q424	D348	Q282	S222
D1096	P948	P948	L803	L803	A728	L659	T595	N512	Q424	D348	Q282	K223
L1097	F1016	G955	N804	L804	A728	L659	L596	D517	Q424	D348	Q282	M224
V1100	A1017	G955	L805	L805	A728	L659	Q597	F518	Q424	D348	Q282	L225
V1105	L1018	G955	K806	K806	A728	L659	V598	S519	Q424	D348	Q282	A226
T1106	V1020	C953	V810	V810	A728	L659	L599	T520	Q424	D348	Q282	F306
R1107	V1021	D954	K811	K811	A728	L659	R600	K521	Q424	D348	Q282	V307
M1108	R1022	G955	A879	A879	A728	L659	A601	E522	Q424	D348	Q282	L308
W1114	T1023	G956	L881	L881	A728	L659	S602	E522	Q424	D348	Q282	S309
V1115	D1024	G956	D882	D882	A728	L659	T604	D527	Q424	D348	Q282	L231
R1116	F1026	L959	P883	P883	A728	L659	D605	L530	Q424	D348	Q282	D232
Q1117	E1027	L959	A884	A884	A728	L659	H606	L531	Q424	D348	Q282	R233
A1118	T1028	S960	Q885	Q885	A728	L659	Q607	L531	Q424	D348	Q282	S234
A1121	Y1033	P961	Q888	Q888	A728	L659	P609	E534	Q424	D348	Q282	R235
R1122	S1034	P962	Q888	Q888	A728	L659	E610	P537	Q424	D348	Q282	D236
T1123	A1037	E966	S891	S891	A728	L659	L611	F538	Q424	D348	Q282	R237
T1124	S1038	Y967	A892	A892	A728	L659	F612	D540	Q424	D348	Q282	R242
E1125	T1039	H968	S896	S896	A728	L659	T615	F539	Q424	D348	Q282	Y243
V1126	A1040	H969	L897	L897	A728	L659	E616	D540	Q424	D348	Q282	L247
L1127	I1042	W970	Q898	Q898	A728	L659	L618	H544	Q424	D348	Q282	
D1128	I1043	H971	Q898	Q898	A728	L659	L618	H544	Q424	D348	Q282	
S1129	V1048	R972	L901	L901	A728	L659	T619	L553	Q424	D348	Q282	
E1130	H1060	F975	Y902	Y902	A728	L659	G621	P566	Q424	D348	Q282	
S1133			G904	G904	A728	L659	D622	R567	Q424	D348	Q282	
			F905	F905	A728	L659	P623	I558	Q424	D348	Q282	
			A880	A880	A728	L659	A624	V560	Q424	D348	Q282	
			A981	A981	A728	L659	A625	G561	Q424	D348	Q282	
			L833	L833	A728	L659	F626		Q424	D348	Q282	
			T834	T834	A728	L659			Q424	D348	Q282	

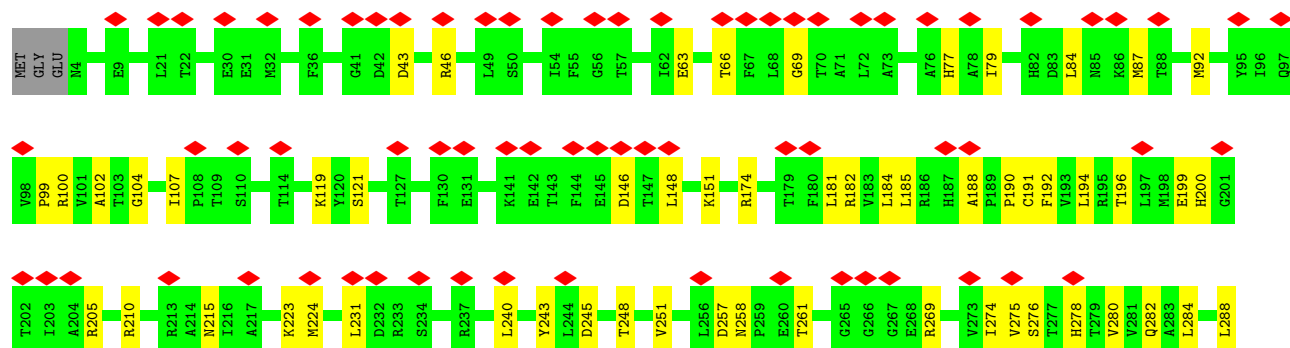


• Molecule 1: Major capsid protein

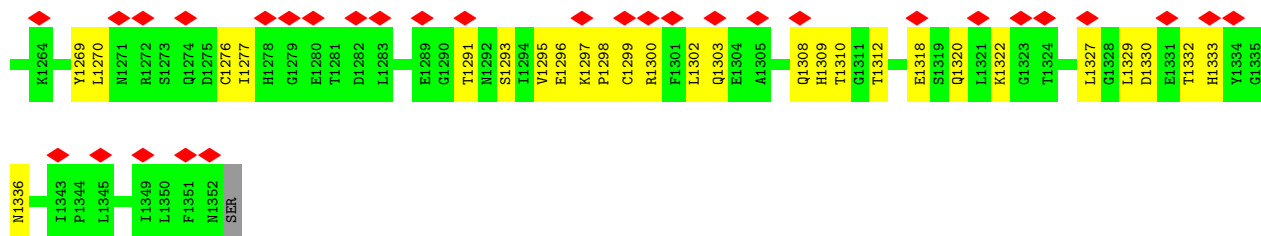




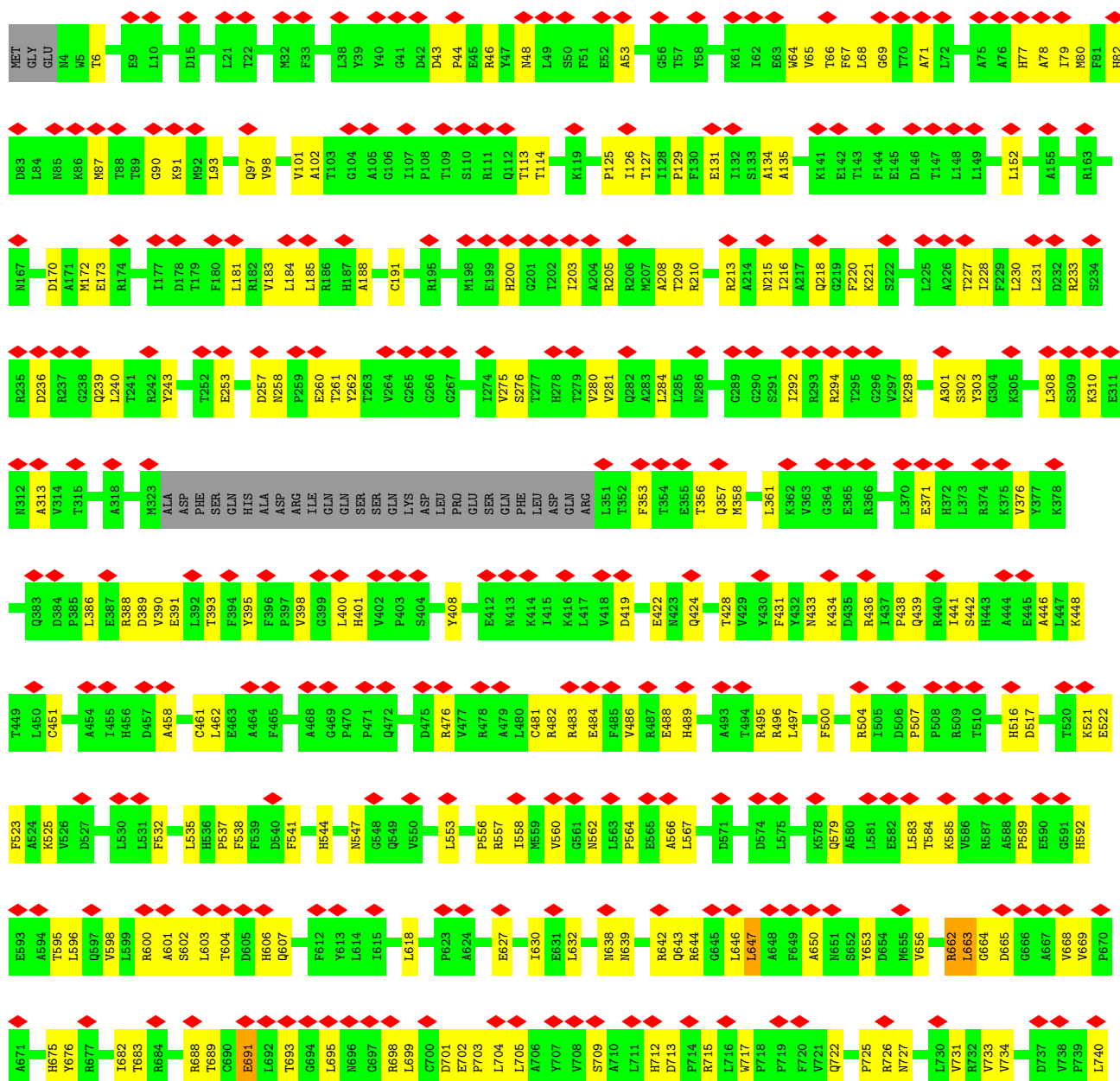
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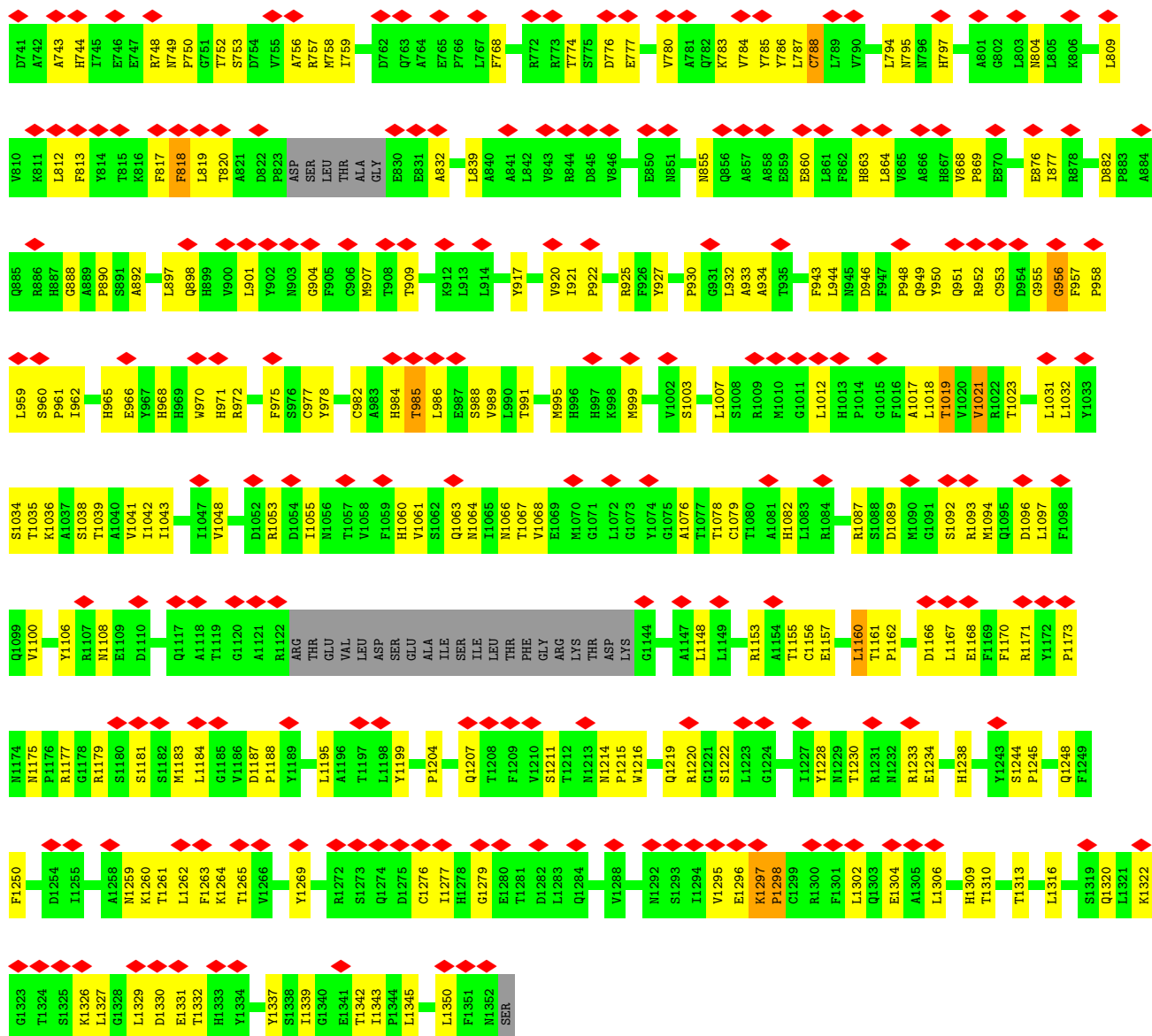




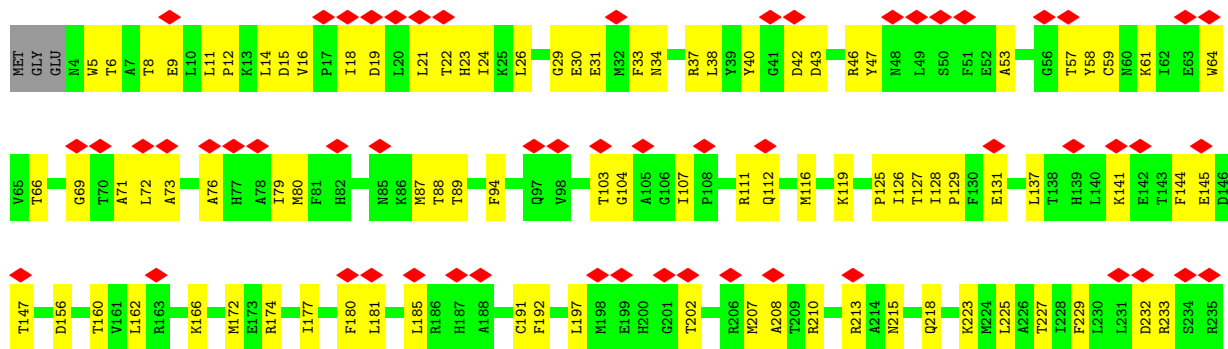


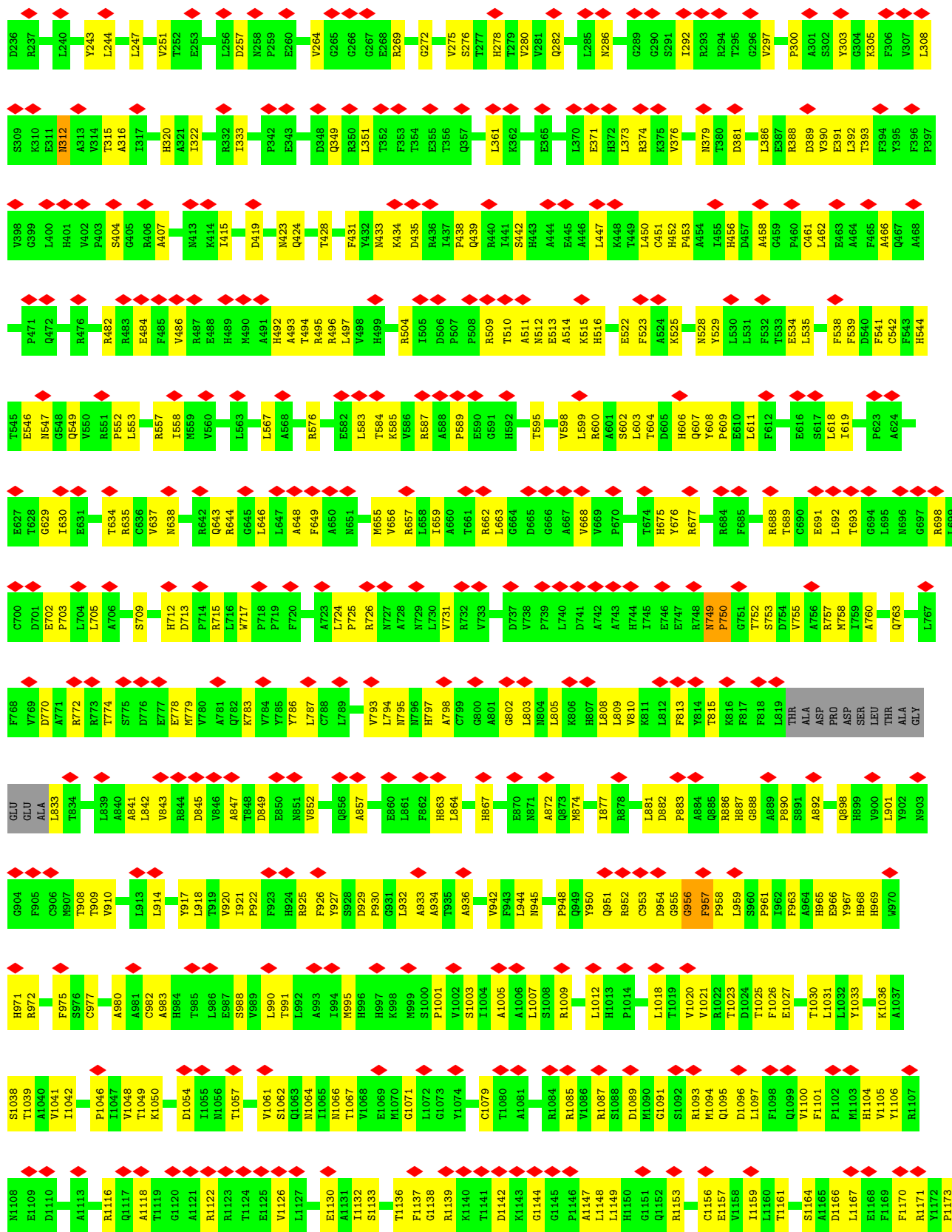
• Molecule 1: Major capsid protein

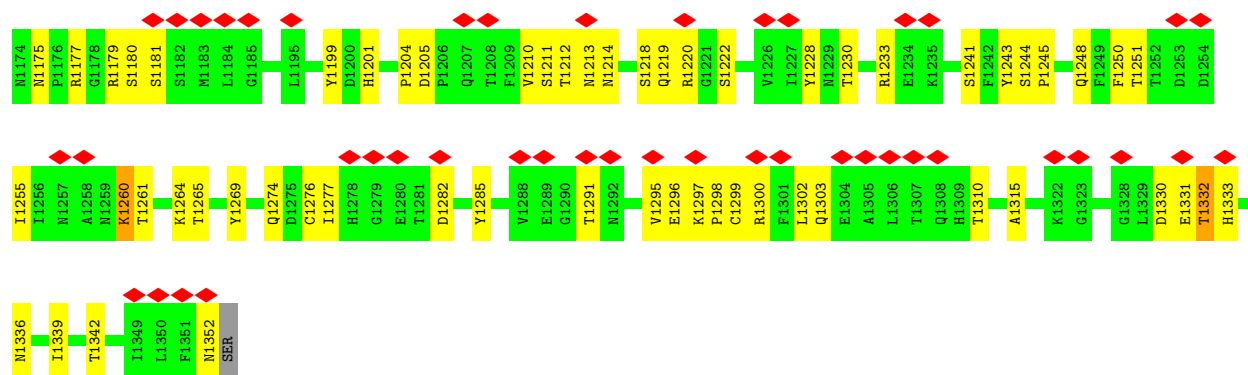




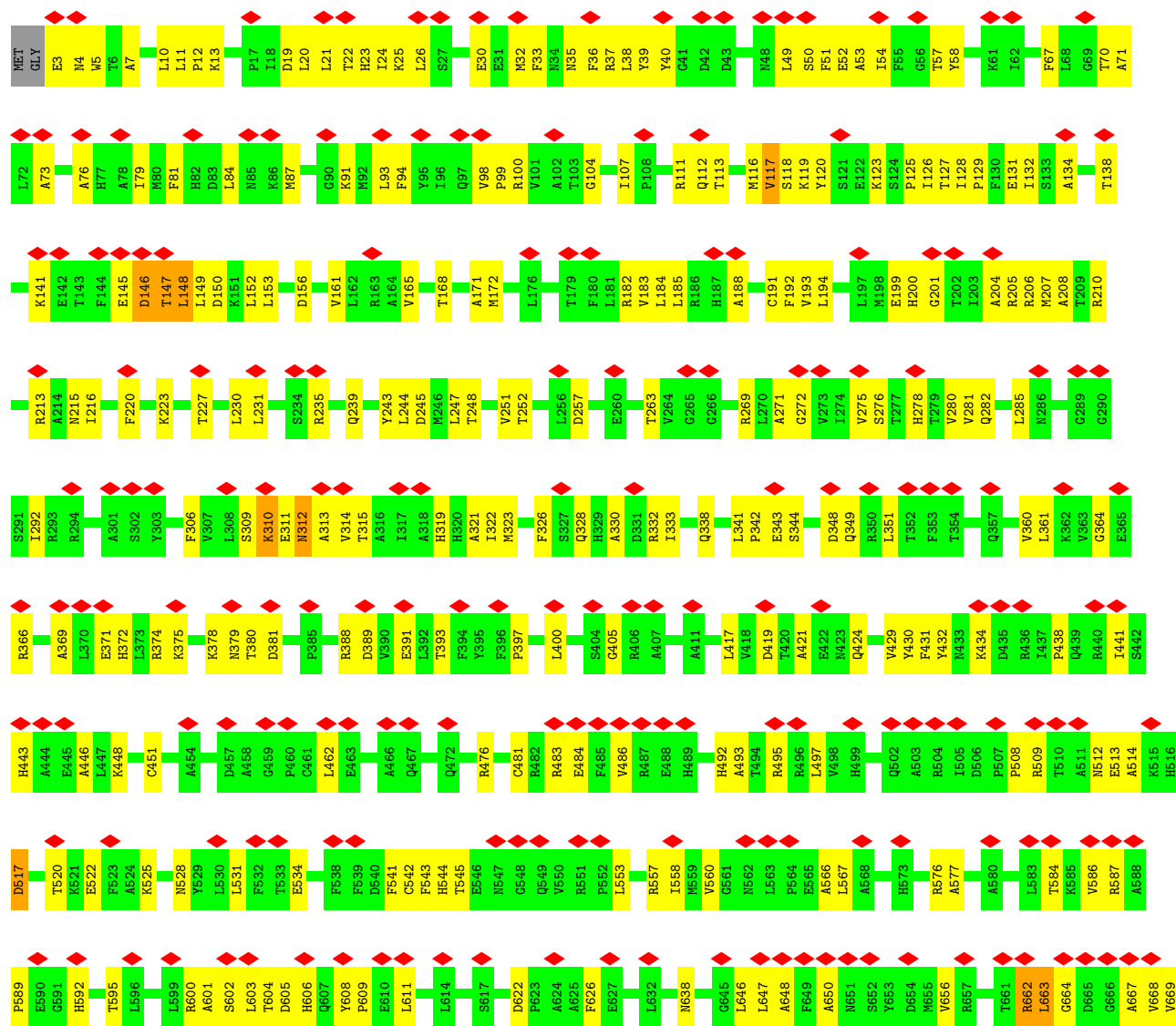
• Molecule 1: Major capsid protein

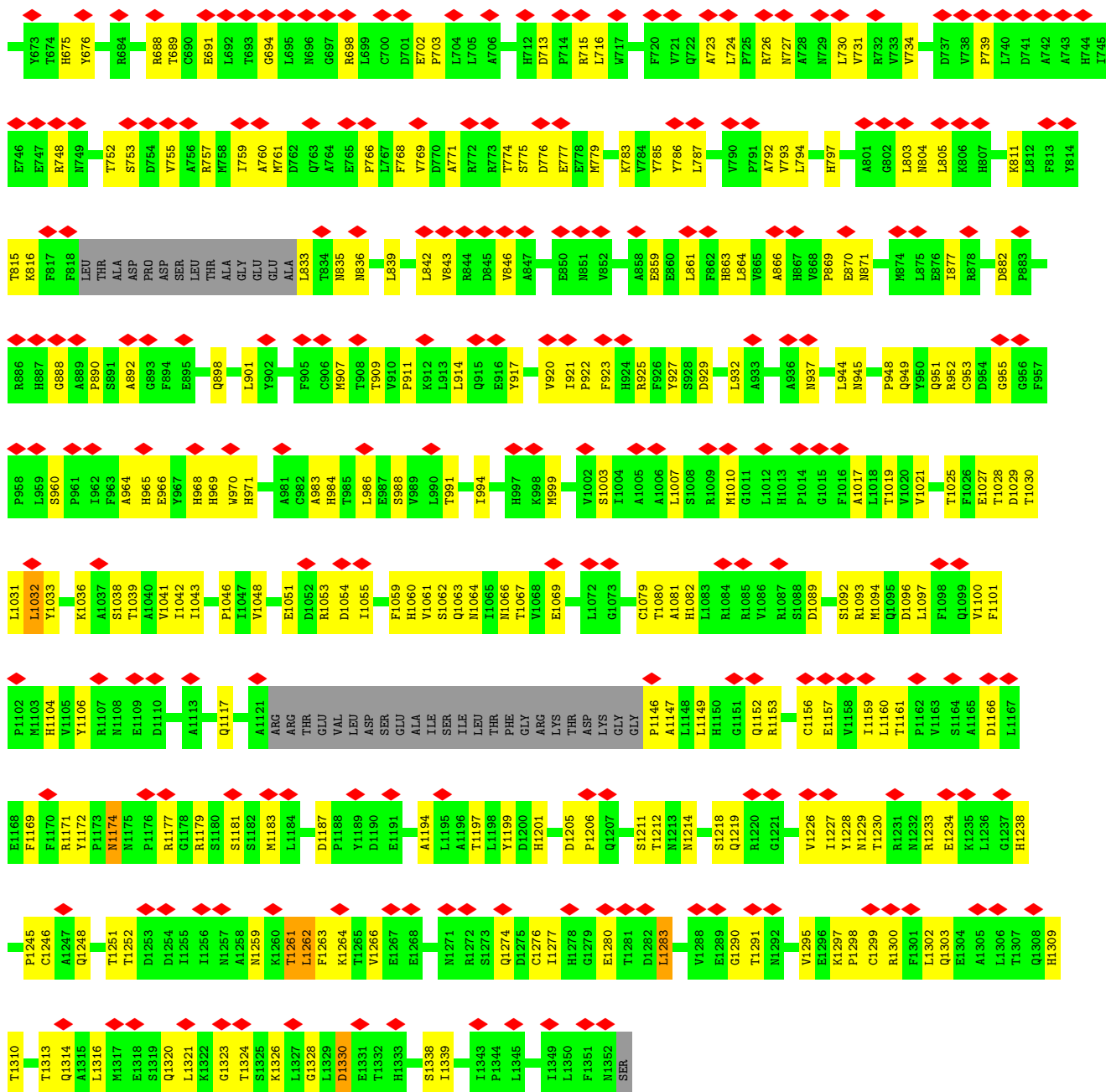




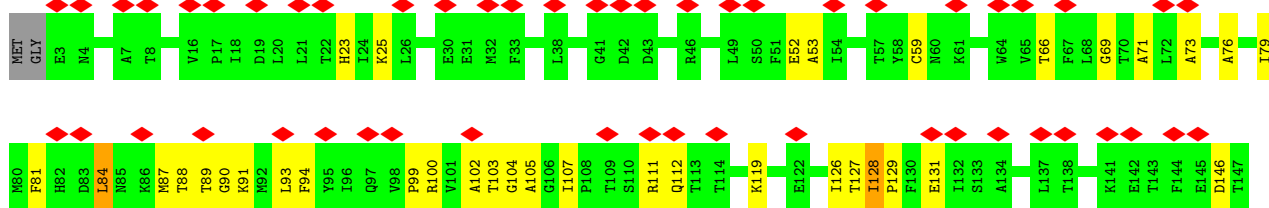


• Molecule 1: Major capsid protein

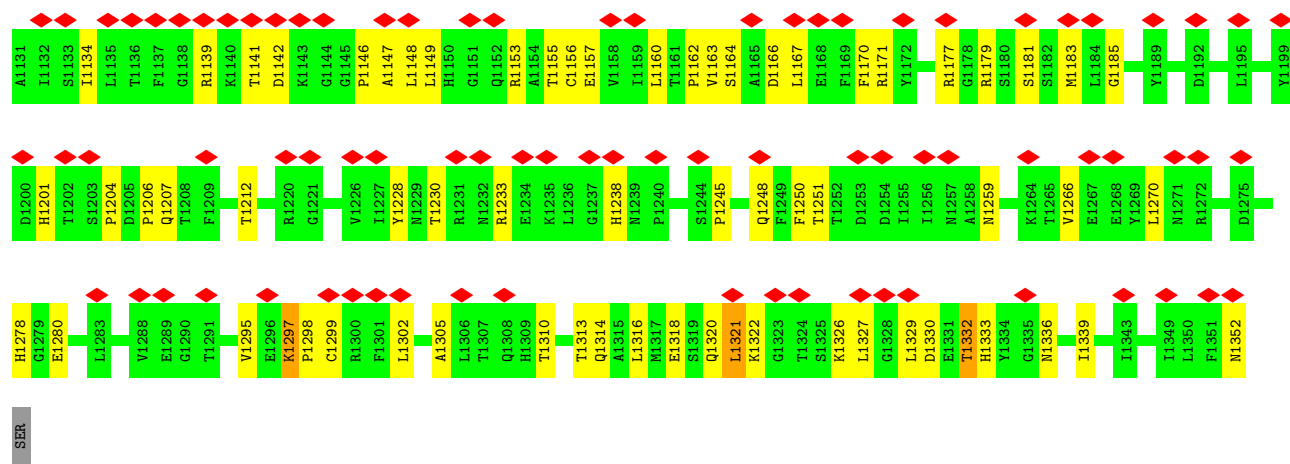




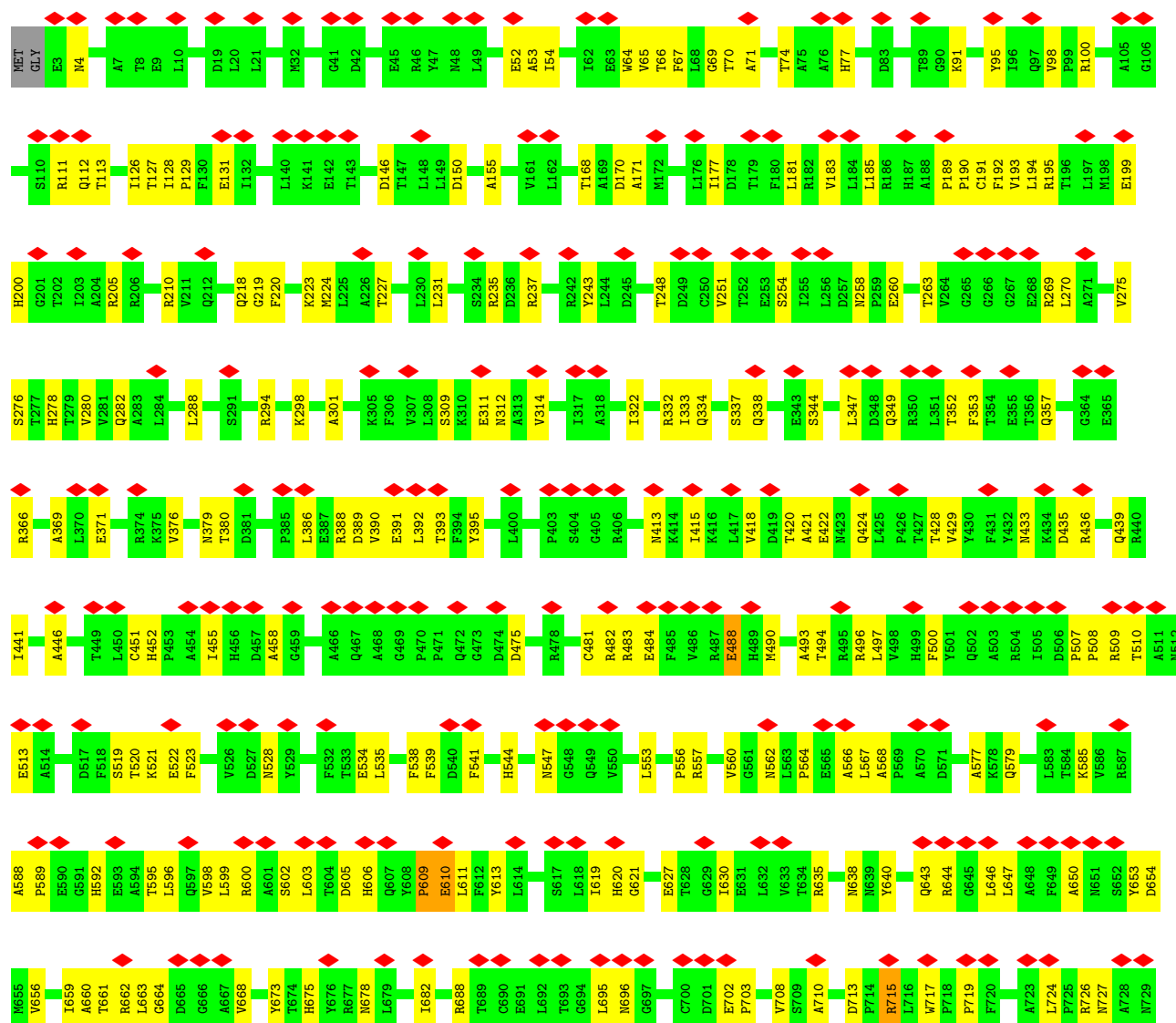
• Molecule 1: Major capsid protein

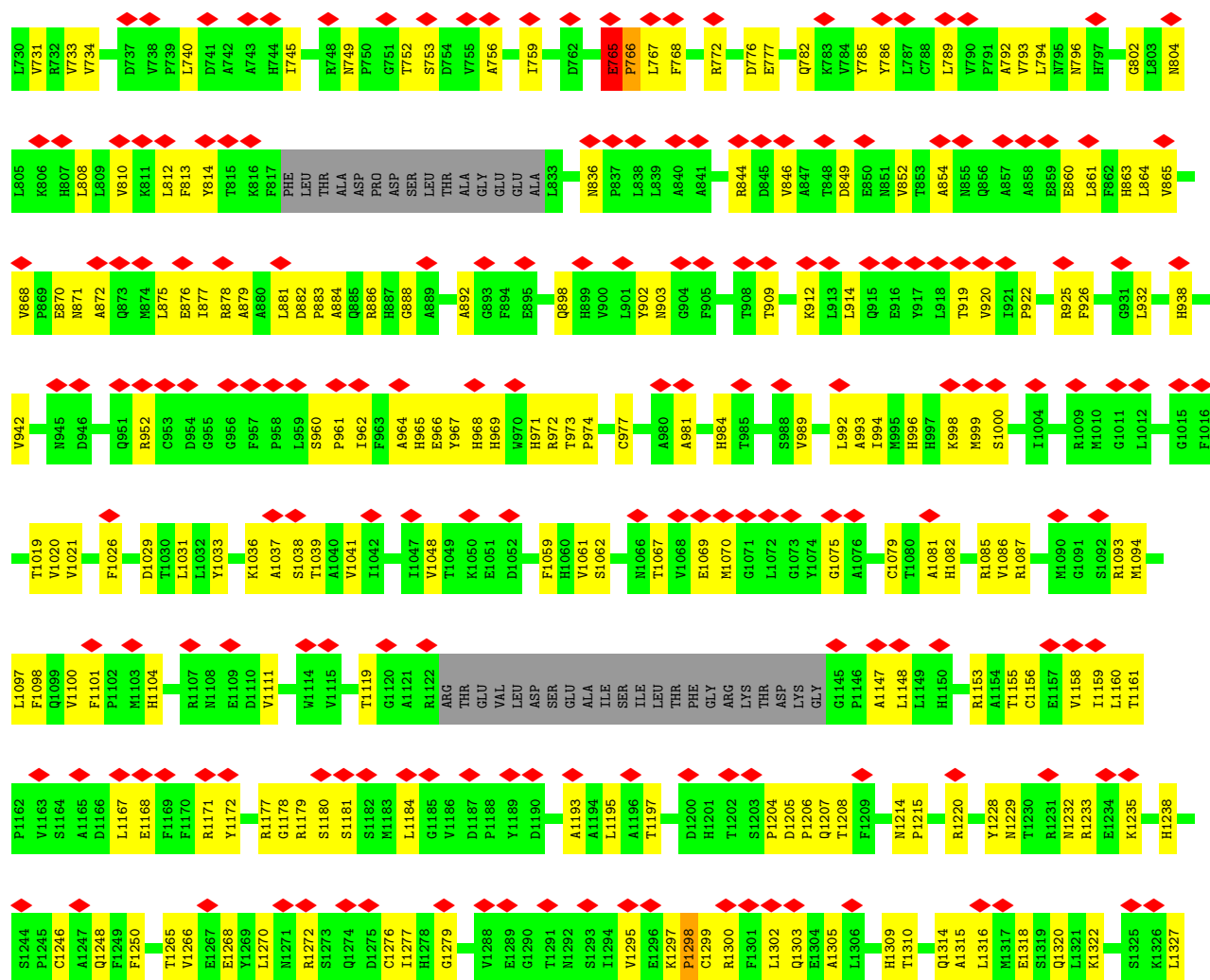


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E1051	E966	Q898	GLY	A756	R688	I615	L535	L462	T393	S309	T228	L152
D1052	Y967	H899	GLU	R757	T689	E616	H536	E463	F394	K310	T229	L153
R1053	H968		ALA	W758	C690	S617	P537	E311	Y395	E311	L230	H154
D1054	H969	Y902	L833	I759	E691	L618	F538	Q467	L400	A313	L231	
H1060	Q970	N903			L692	L619	F539	A468		V314	D232	
V1061	R972	Q904			T693	H620	D540	G469	P403	V314	D233	
S1062	R975	H907	N836	D762	G694	A624	F541	P471	S404	T315	D234	
T1067	Y978	T908	P837	E765	L695	G629	N547	Q472	R406	T317	R235	
V1068	S979	T909	L838	F766	R696	E630	G548	G473	A407	A318	L240	
E1069	A980	Y910	L839	L767	H697	E631	Q549	D474	Y408	H319	T241	
M1070	A981	P911	V843	F768	G697	L630	Q549	D475	A321	H320	D242	
G1071	C982	K912	R844	W769	C700	L632	R551			A318	T241	
L1072	M995	L913	D845	R772	D701	V633	P552			H319	D242	
D1073	C995	L914	V846	R773	L705	T634	L553	R478	A411	A321	Y243	
	H996	E916	A847	D776	A706	R635	L553	R482	E412	F326	Y244	
	H996	Y917	T848	E777	Y707	N638	R557	R483	E413	S327	D245	
	H997	L918	D849	E778	Y708	N639	I558	E484	E414	T333	T248	
	K998	T919	D849		Y708	E588		F485	L417	S337	D249	
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H1082	S1003	I921		H783	A710	R641	L563	E488	T420	E343	E253	
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D1089	E1008	R925	E859	Y786	P714	G645	L567	M490	Q424	L347	N258	
M1090	R1009	Y926	E860	L787	R715	L646	A570	A491	L425	D348	F180	
G1091	M1010	Y927	L861	W717	L716	L647			P426	Q349	T261	
S1092	G1011		F862	F790	F717	A648	L575	R495	V429	Q349	T262	
R1093	L1012	P930	H863	P791	P718	F649	R576	R496	Y430	T352	T263	
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F1101	V1100		P869	G802	Q722	D654	K585			E355	G267	
P1102	Y1020	H938	E870	L803	A723	M655	V586			D359	E268	
M1103	R1022	D939	M874	N804	L724	V656	R587			G364	R269	
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R1107	T1028	F947	R876	L808	A728	R662	H592			L367	G273	
N1108	D1029	P948	R876		H807	L663	P508			V368	G274	
E1109	T1030	Q949	A880		L808	G664	R509			A369	S276	
	R1116	Y950	L881	K811	V731	D665	T595			L370	V275	
Q1117	L1031	Q951	D882	L812	R732	G666	L596			E371	T277	
A1118	T1032	R952	F813	T815	V733	A667	A511			H372	L284	
T1119	K1036	C953	P883	Y614	W734	V668	H512			L373	L285	
G1120	A1037	D954	A884	T815	A735	V669	E513			L373	L288	
A1121	S1038	Q955	Q885	K816	A601	P670	A514			N379	L288	
R1122	T1039	G956	R886	PHE	A671	A671	K515			T380	T292	
R1123	A1040	H887	H887	LEU	D737	A672	C451			D381	R293	
T1124	I1041	G958	G888	THR	V738	Y673	L603			V382	R294	
E1125	V1042	P958	A889	ALA	P739	V676	D605					
V1126	I1047	S960	P890	ASP	D741	L679	H606					
L1127	V1048	P961	S891	PRO	T745		Q607					
D1128	T1049	I962	A892	SER	R748	T683	V526					
S1129		F963	R894	LEU	N748	R684	D457					
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			S896		S753	V686	P460					
					D754							

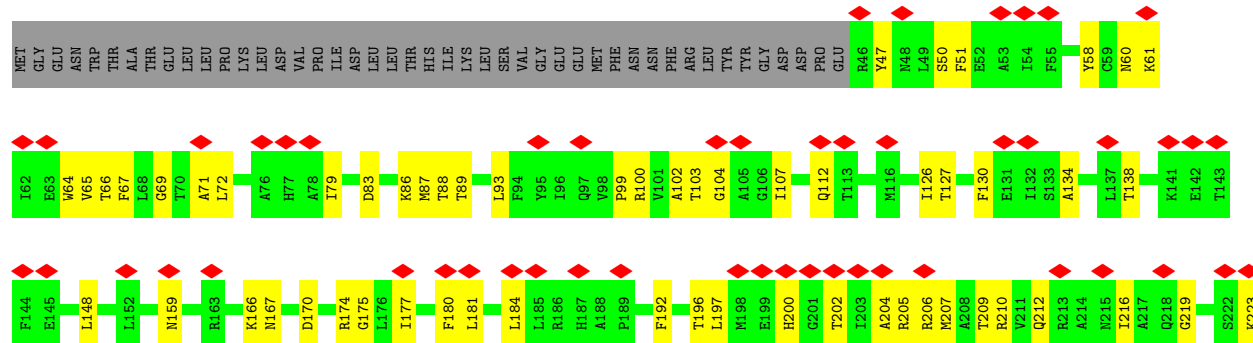


• Molecule 1: Major capsid protein

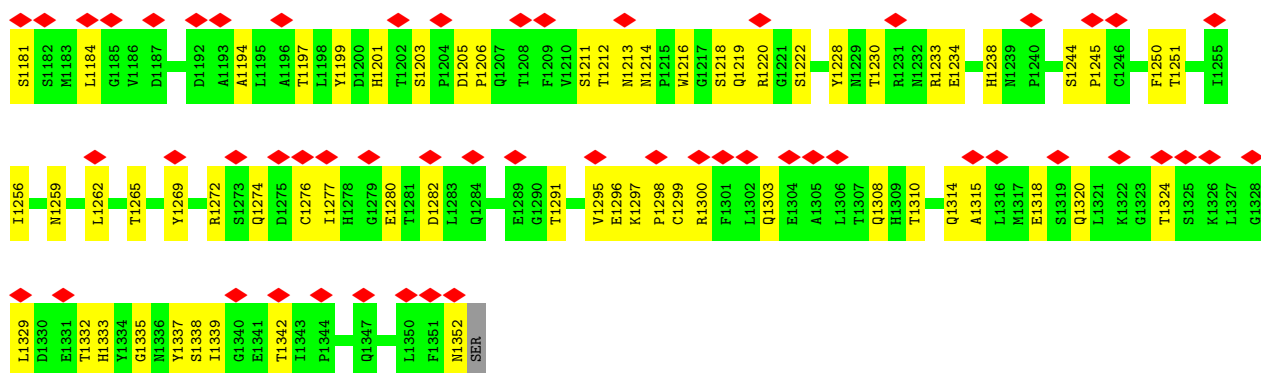




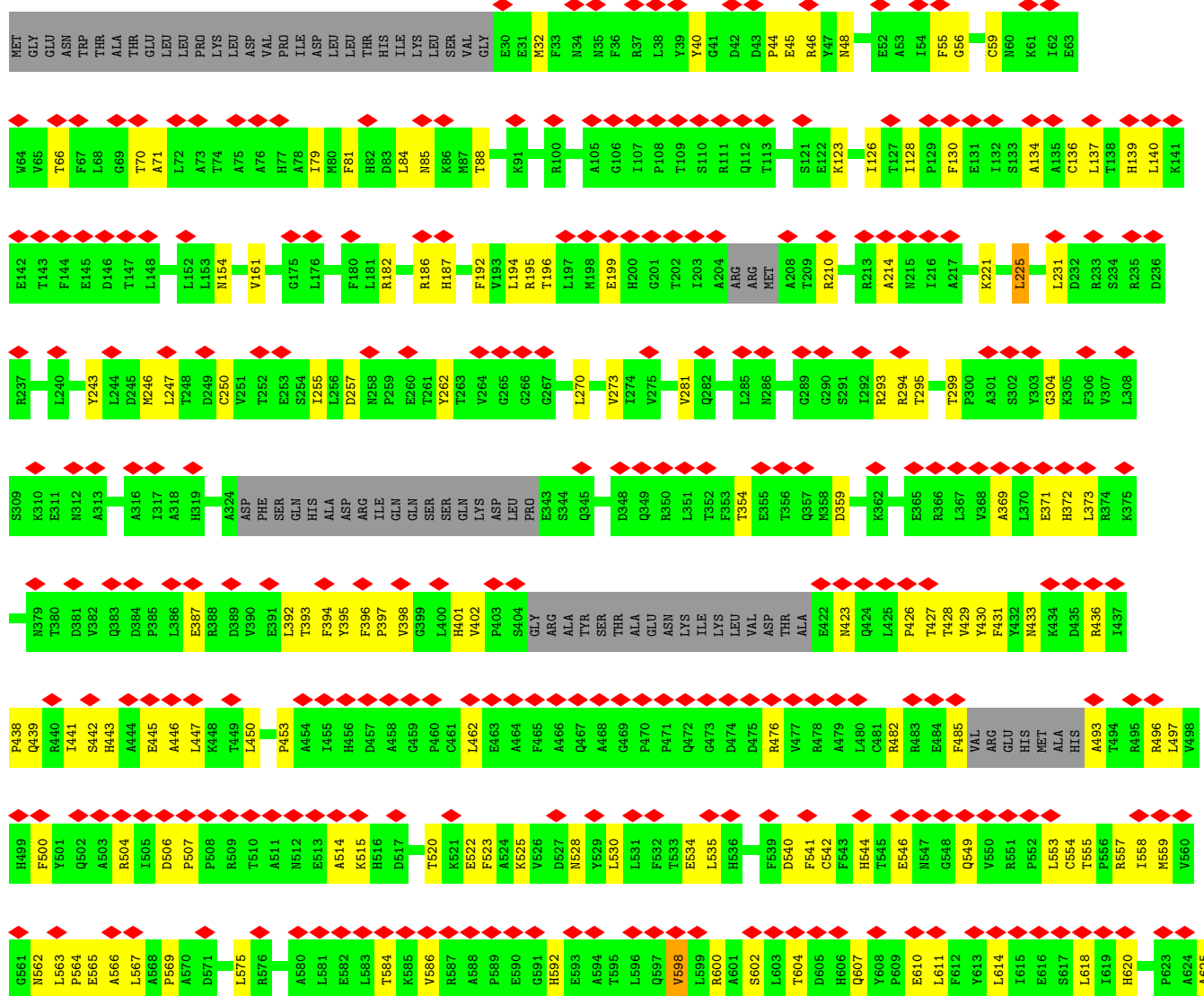
• Molecule 1: Major capsid protein

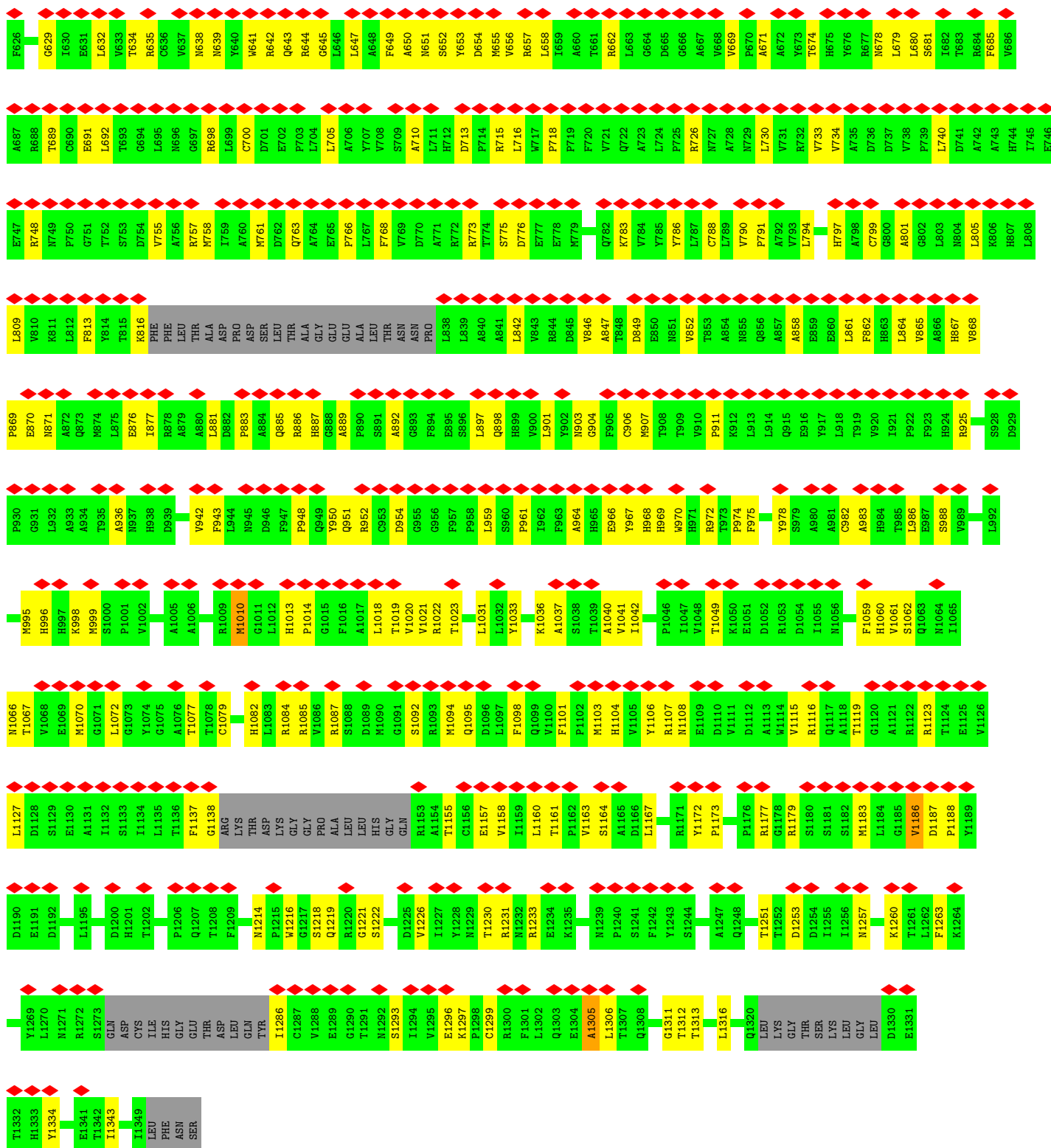






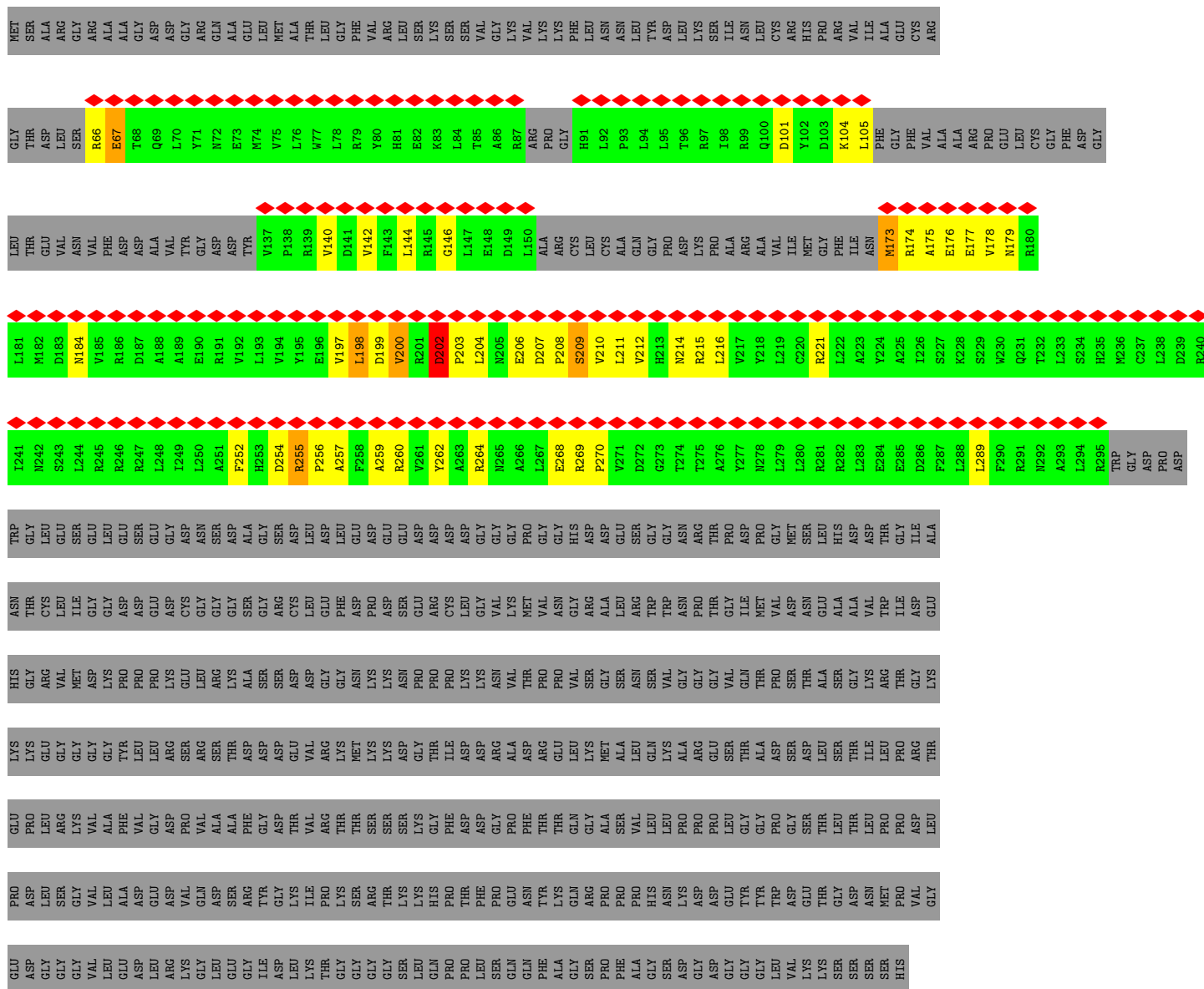
• Molecule 1: Major capsid protein



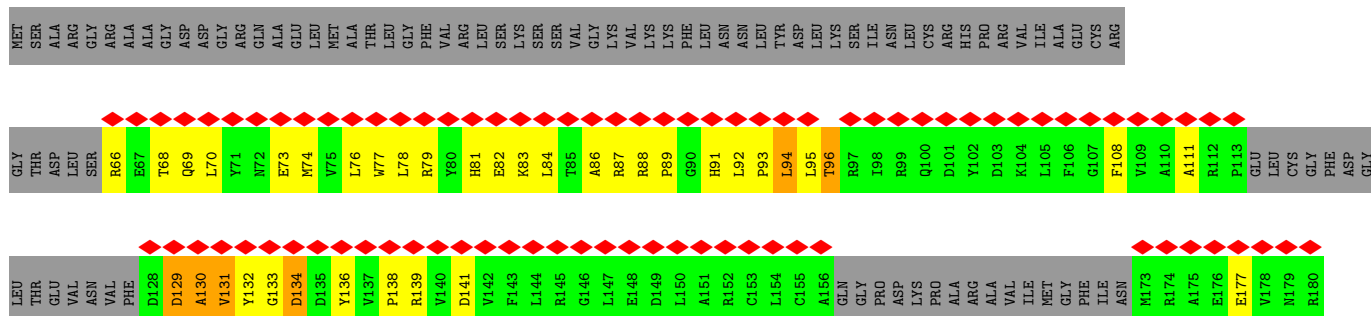


• Molecule 2: Tegument protein





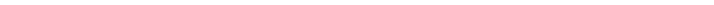
- Molecule 2: Tegument protein

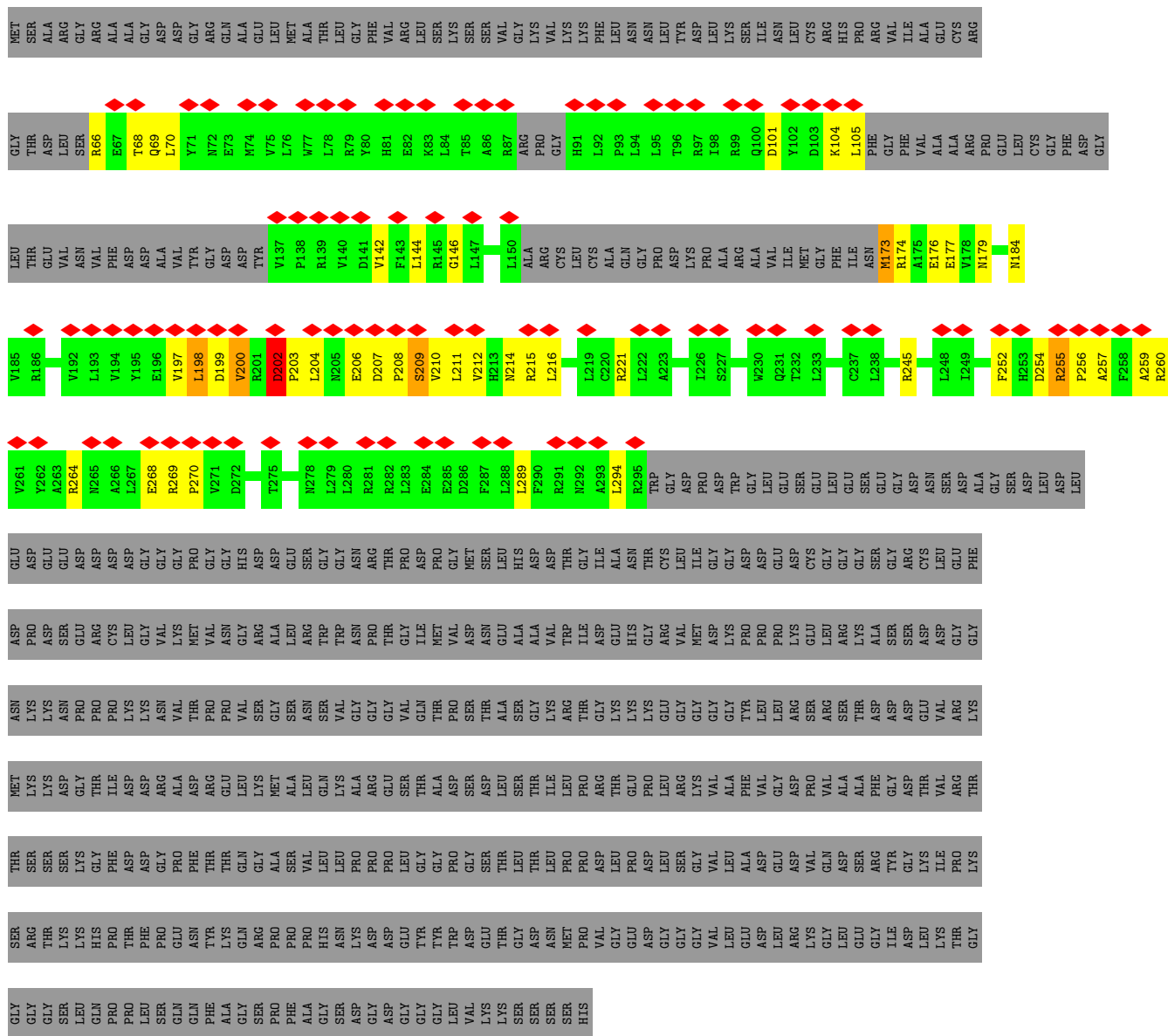


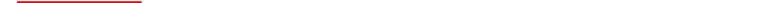


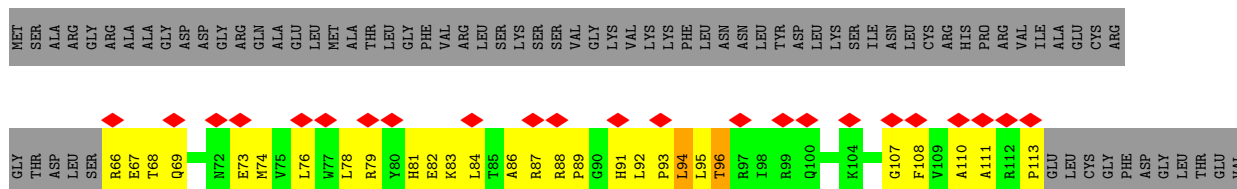
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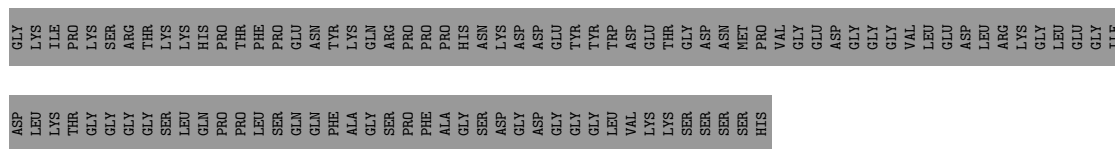
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Chain f: 

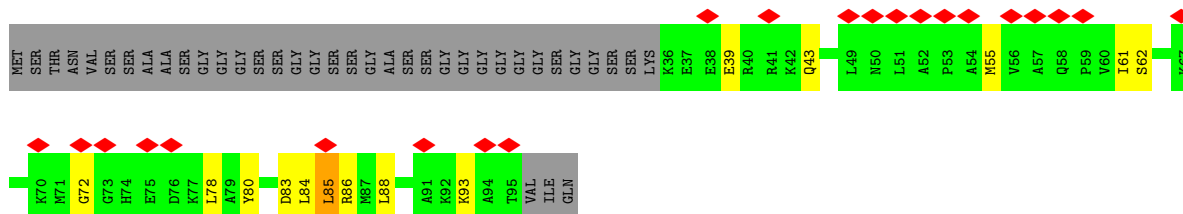


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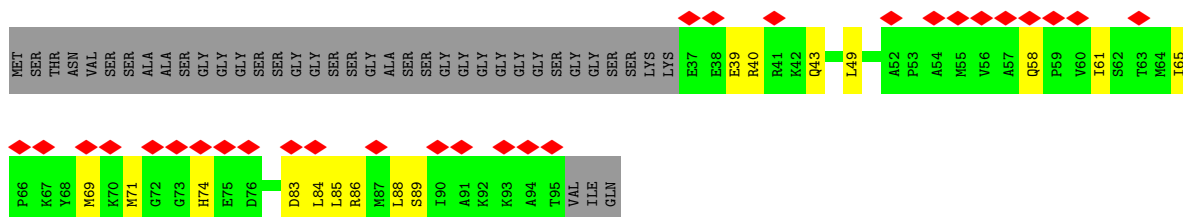
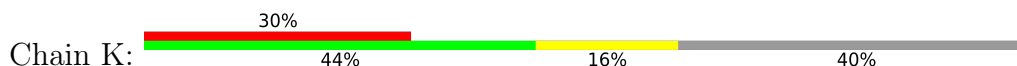




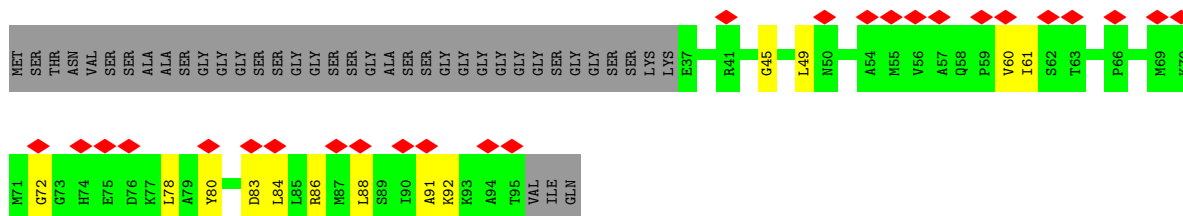
- Molecule 3: Small capsomere-interacting protein



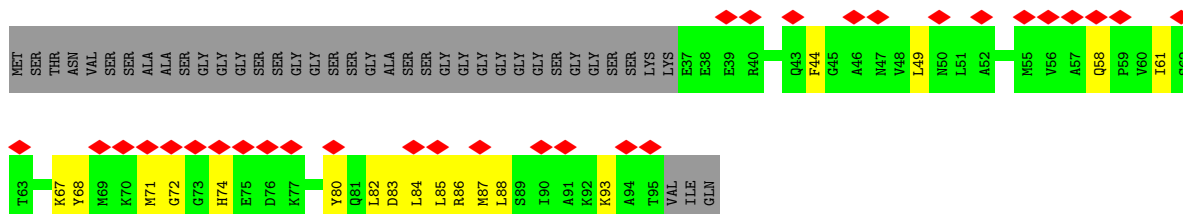
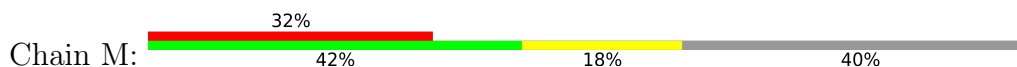
- Molecule 3: Small capsomere-interacting protein



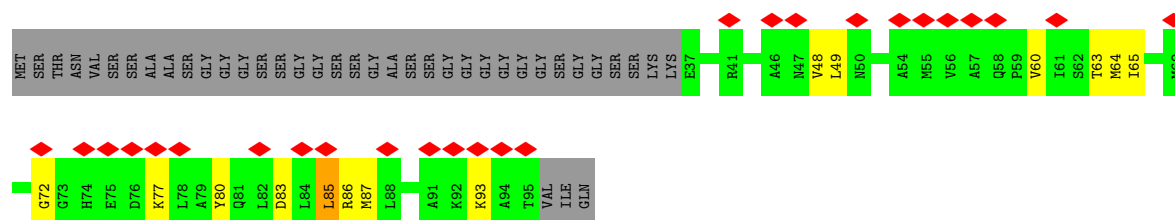
- Molecule 3: Small capsomere-interacting protein



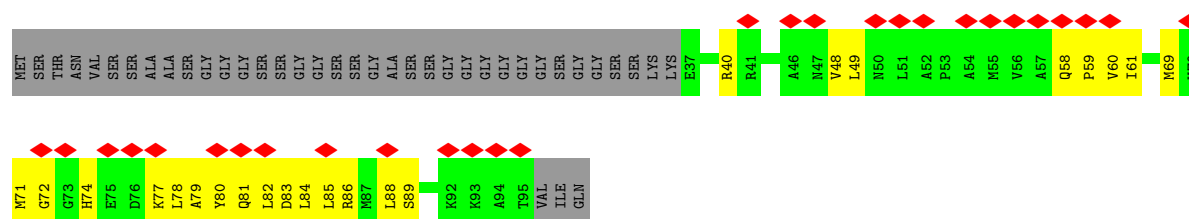
- Molecule 3: Small capsomere-interacting protein



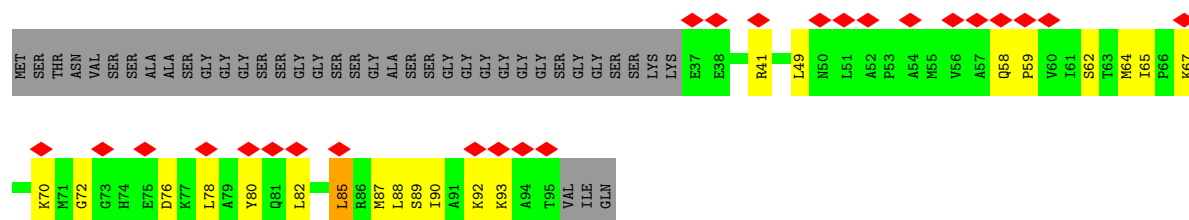
- Molecule 3: Small capsomere-interacting protein



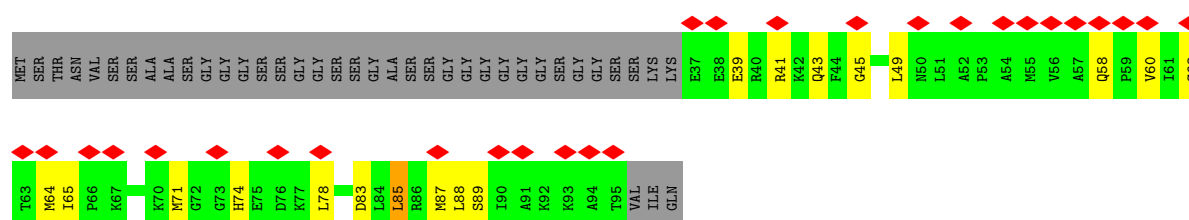
- Molecule 3: Small capsomere-interacting protein



- Molecule 3: Small capsomere-interacting protein

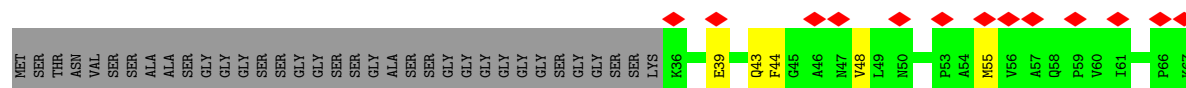


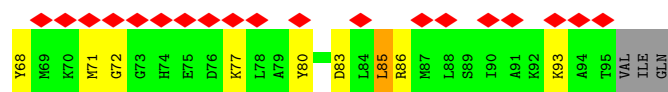
- Molecule 3: Small capsomere-interacting protein



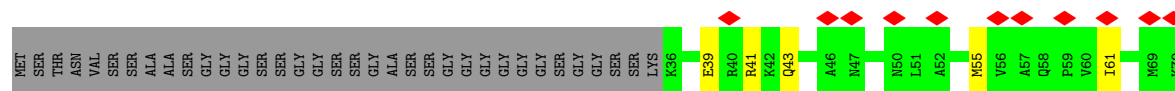
- Molecule 3: Small capsomere-interacting protein



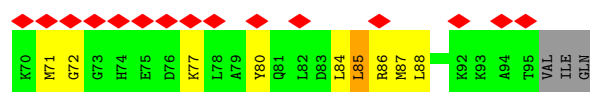
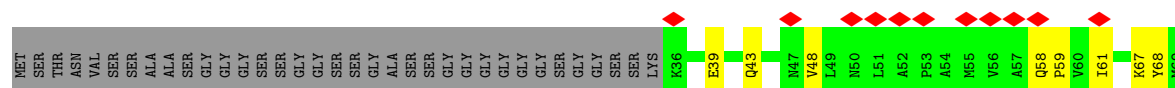
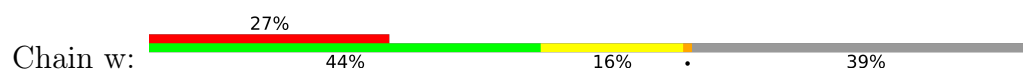




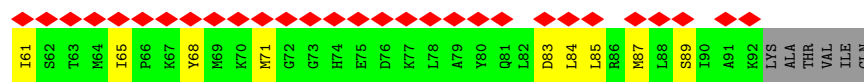
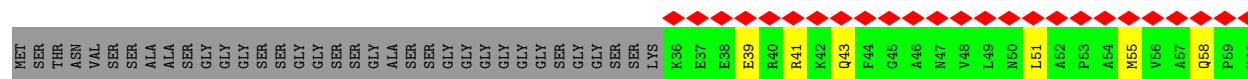
• Molecule 3: Small capsomere-interacting protein



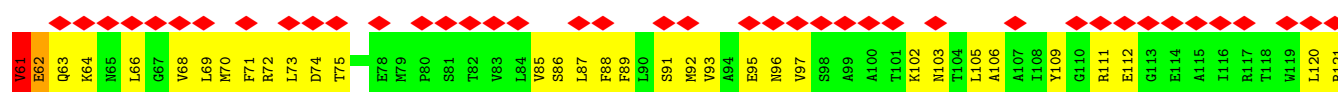
• Molecule 3: Small capsomere-interacting protein

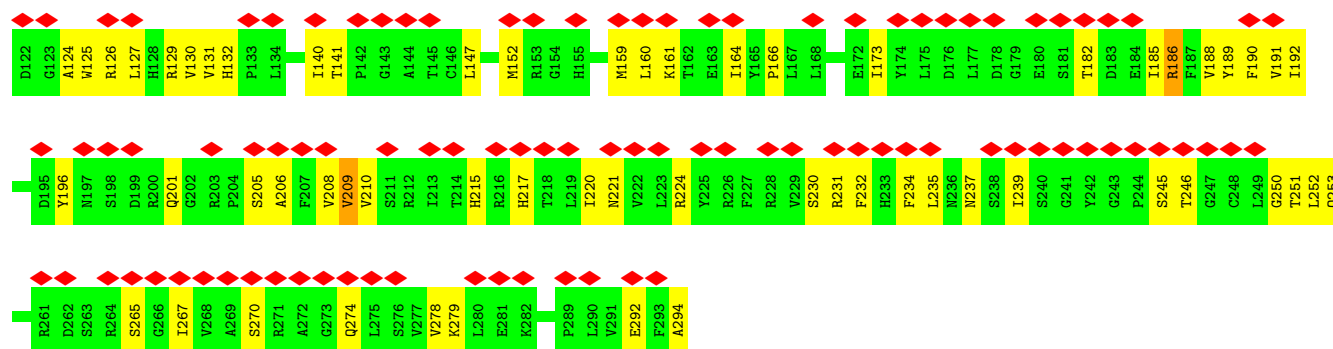


• Molecule 3: Small capsomere-interacting protein

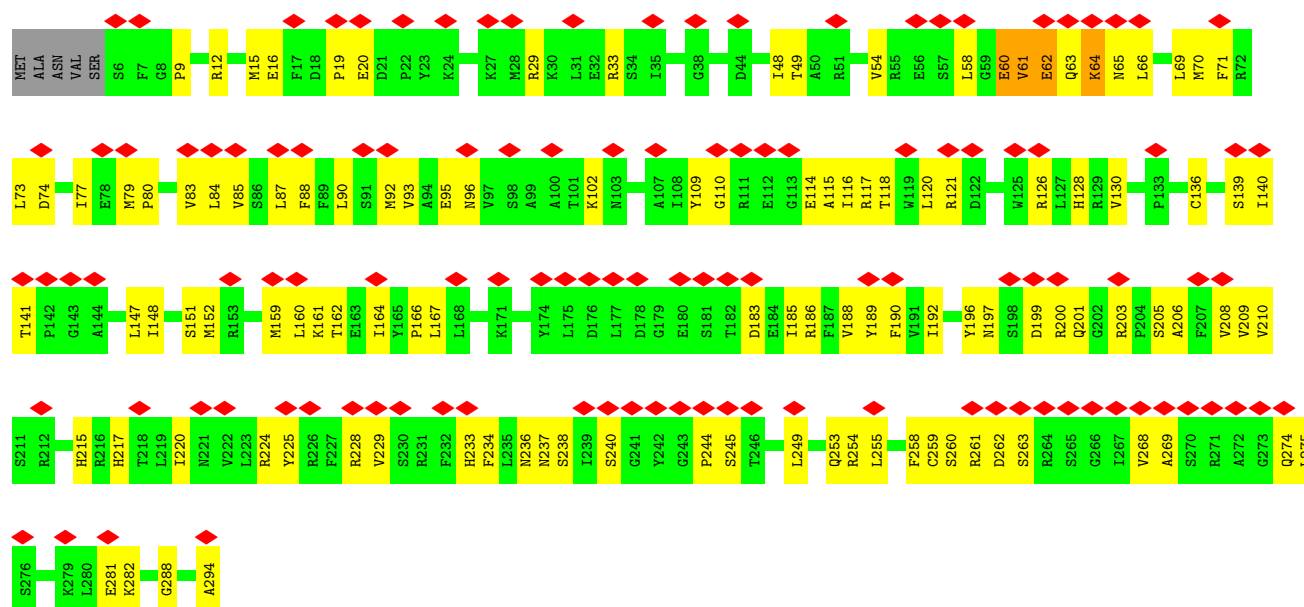


• Molecule 4: Minor capsid protein

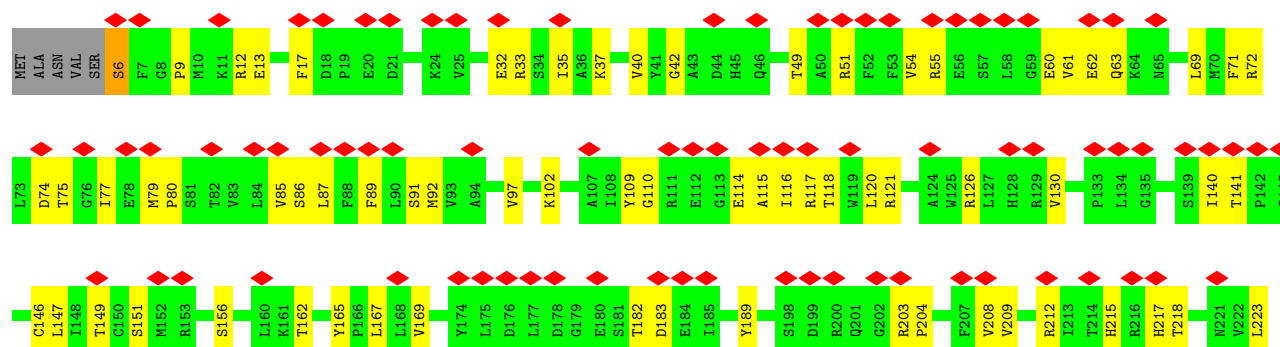
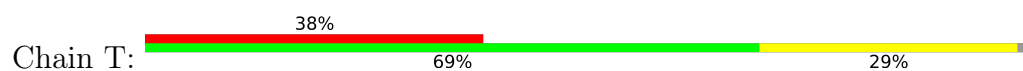




• Molecule 4: Minor capsid protein

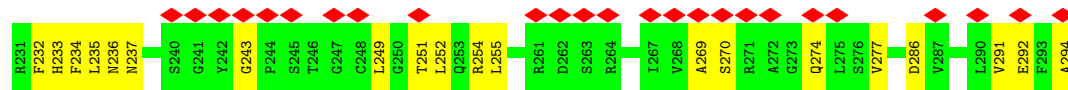
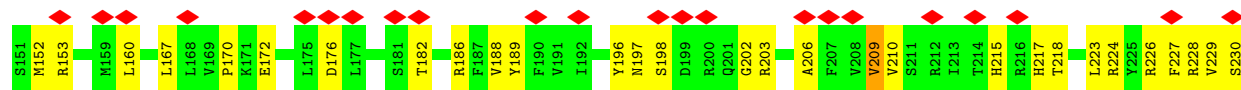


• Molecule 4: Minor capsid protein

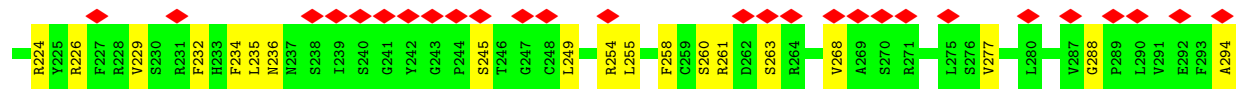
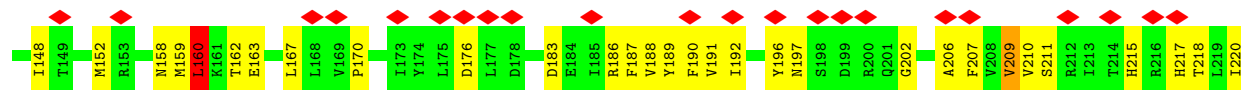




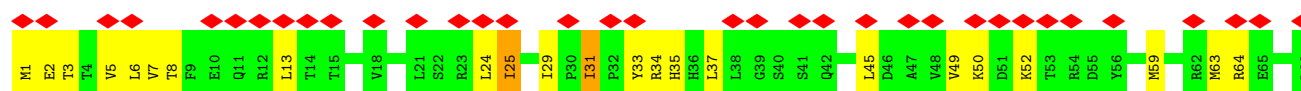
• Molecule 4: Minor capsid protein

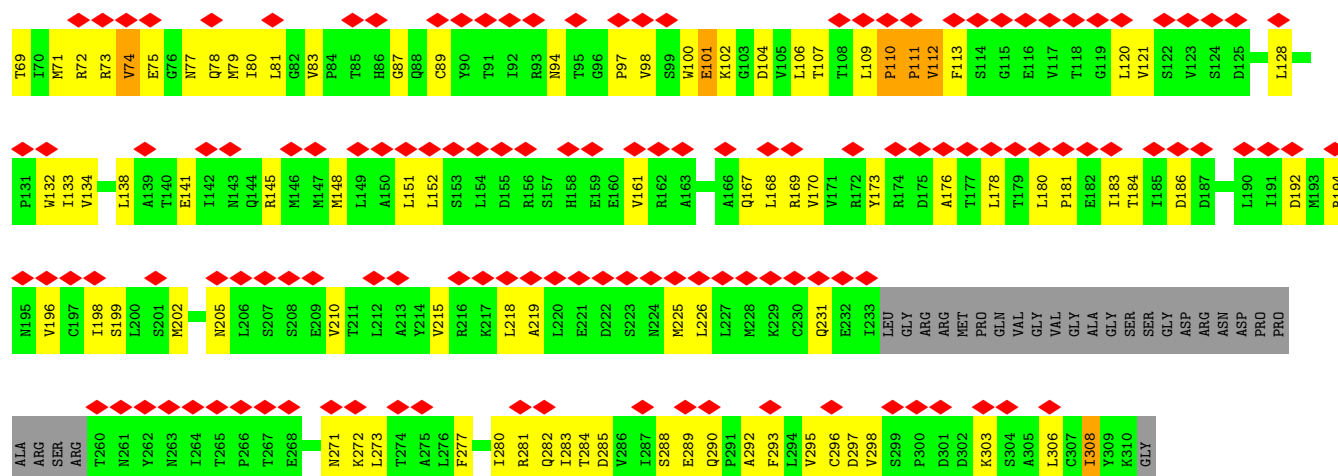


• Molecule 4: Minor capsid protein

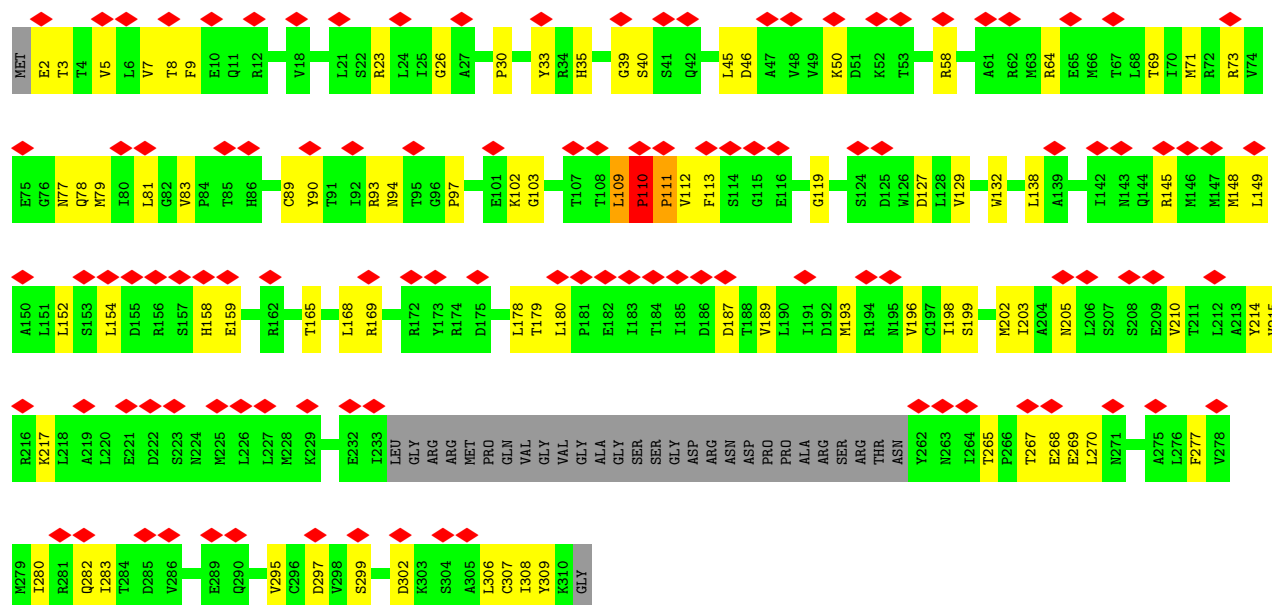


• Molecule 5: Triplex capsid protein 2

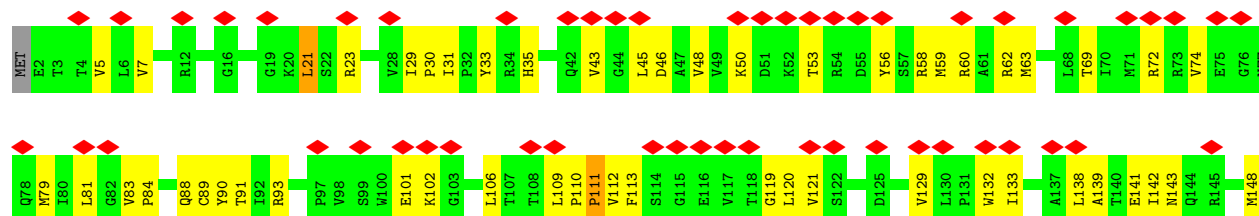


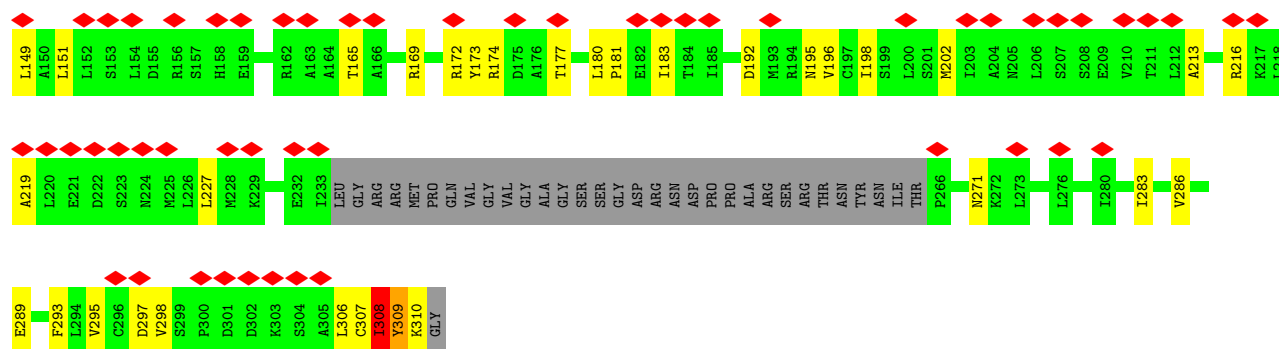


• Molecule 5: Triplex capsid protein 2

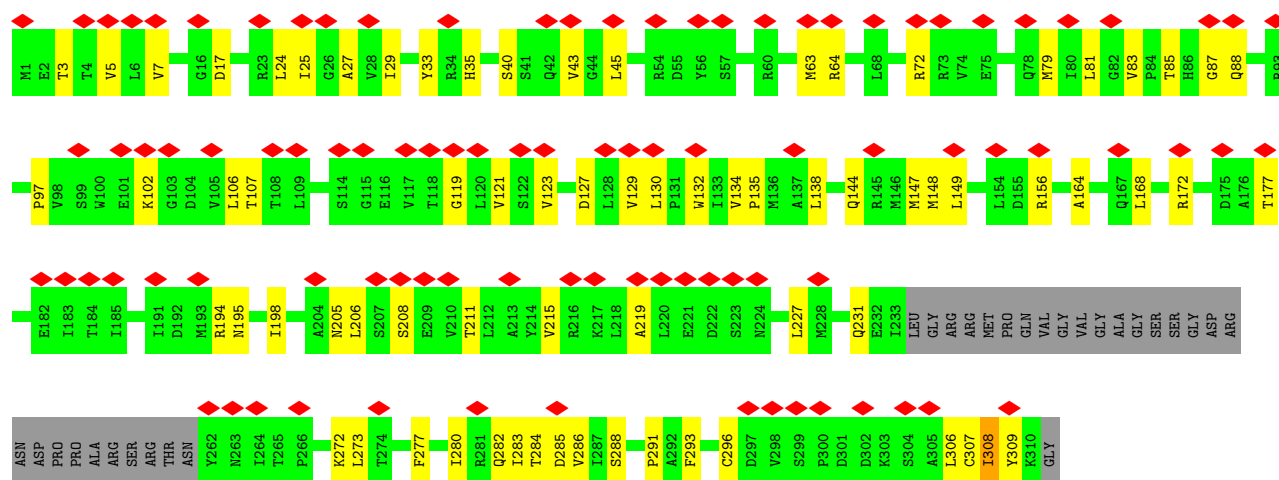


• Molecule 5: Triplex capsid protein 2

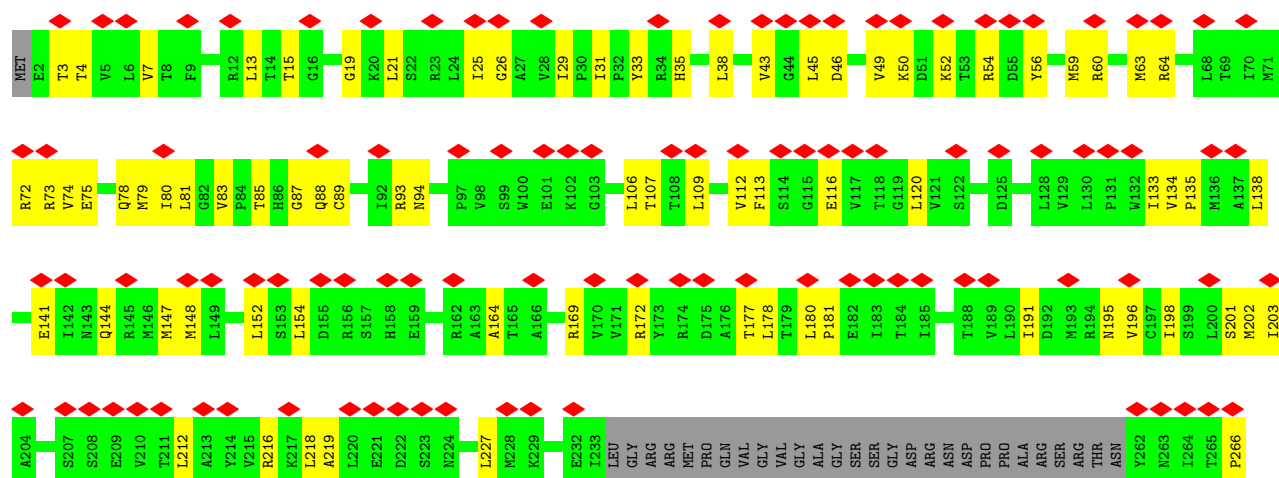
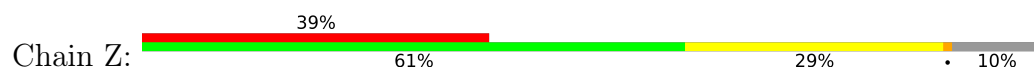


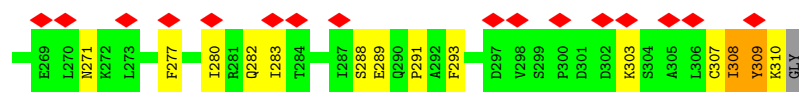


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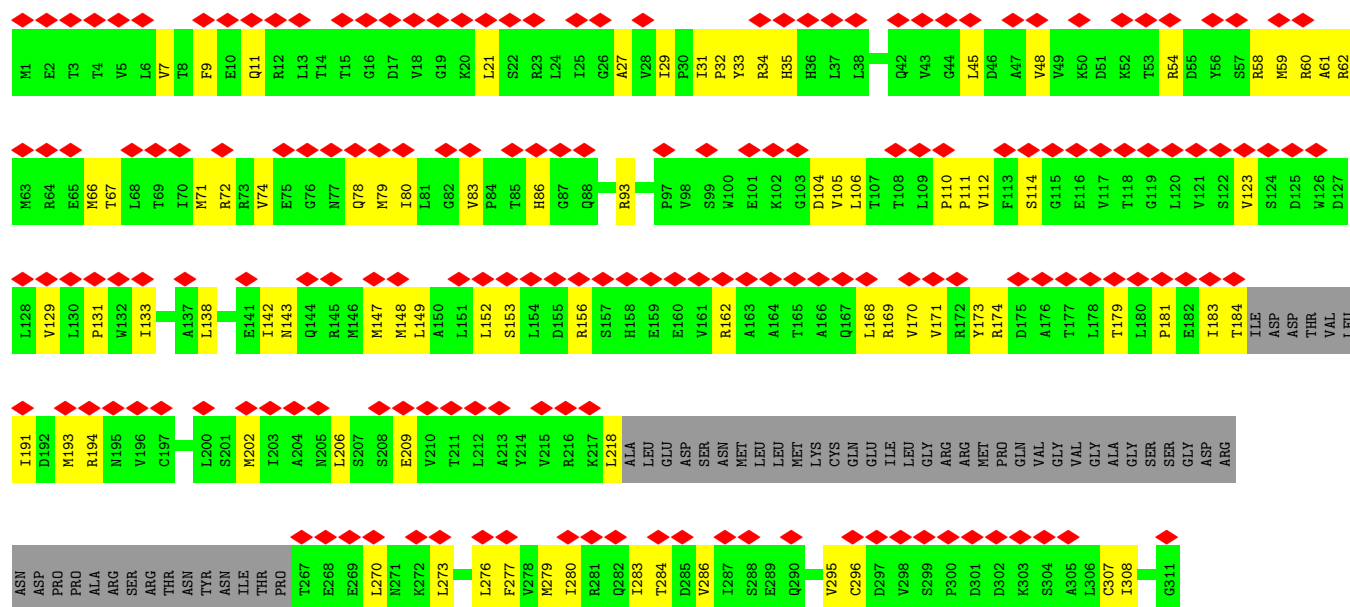


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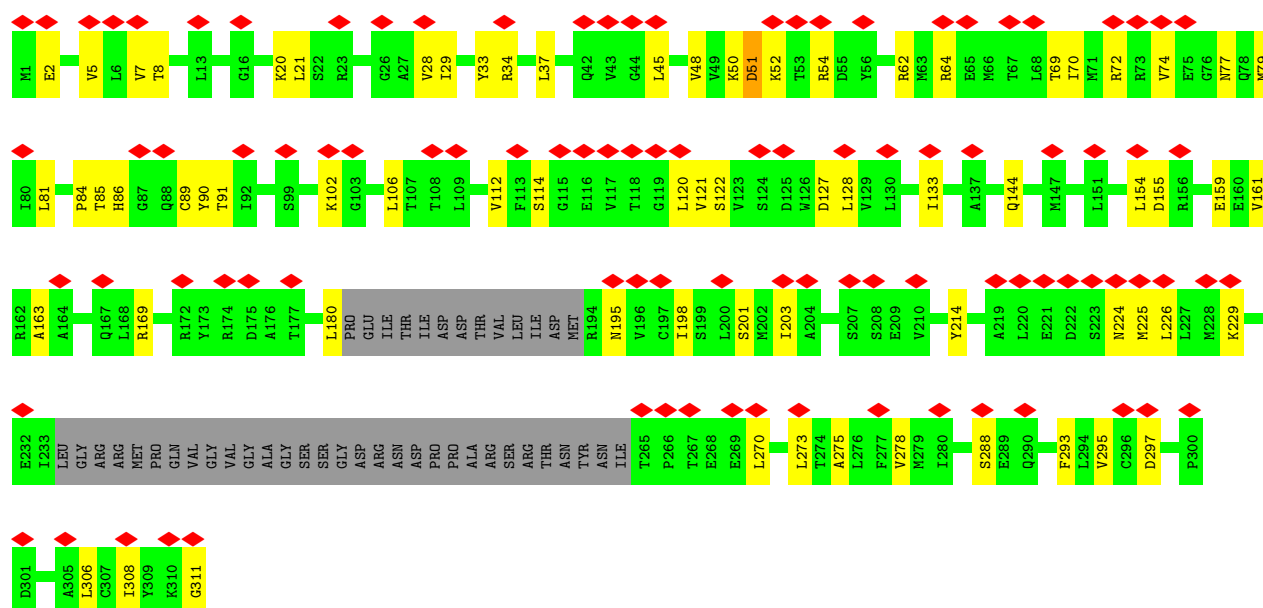




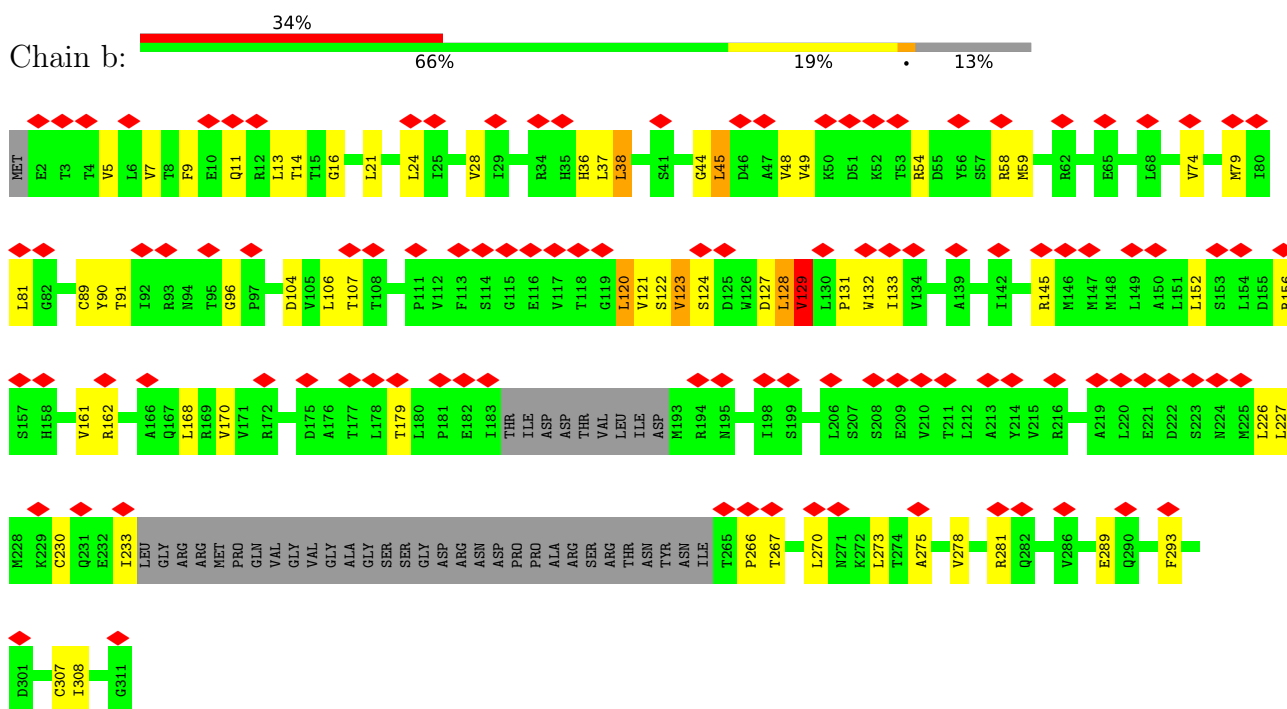
• Molecule 5: Triplex capsid protein 2



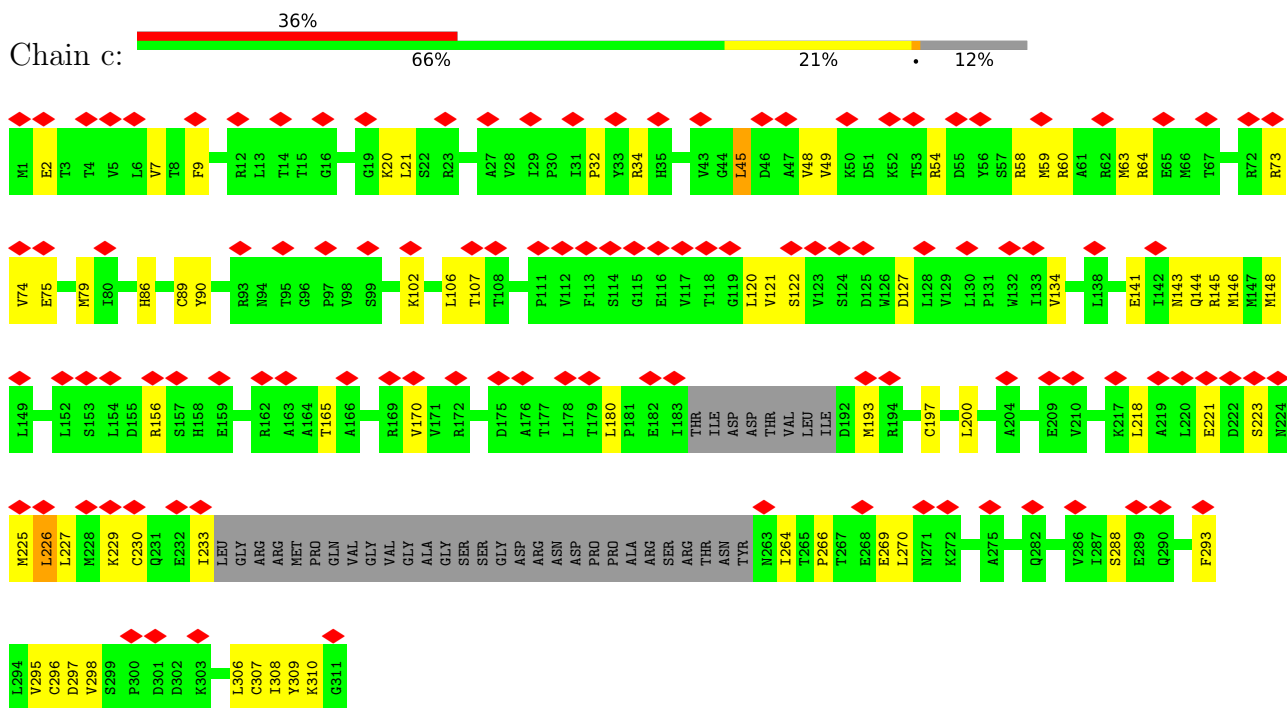
• Molecule 5: Triplex capsid protein 2



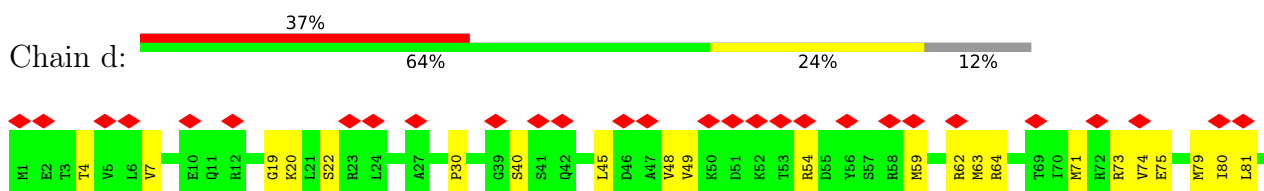
• Molecule 5: Triplex capsid protein 2

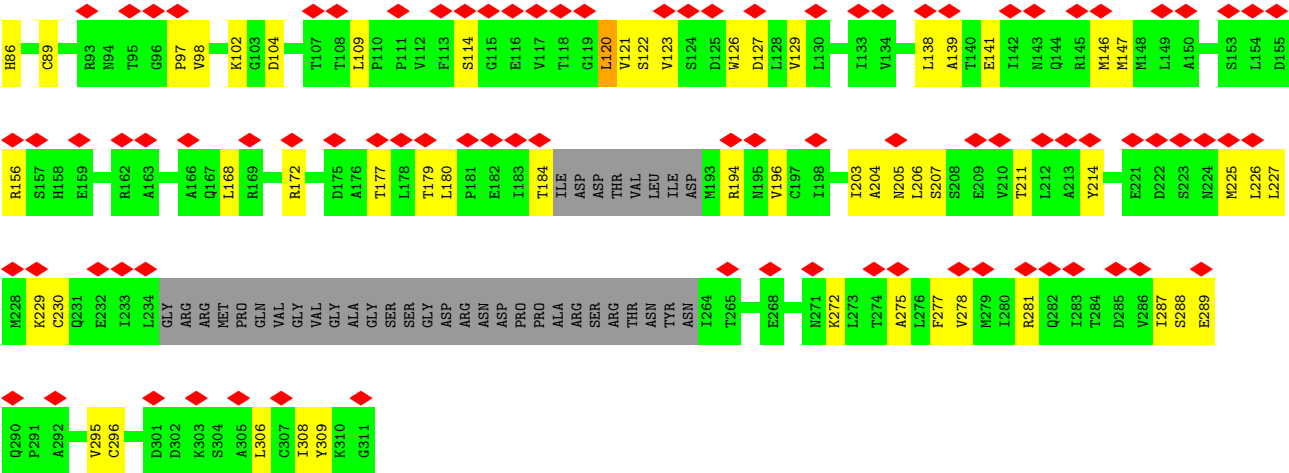


• Molecule 5: Triplex capsid protein 2



• 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	47982	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	47000	Depositor
Image detector	AGFA SCIENTA FILM	Depositor
Maximum map value	13.184	Depositor
Minimum map value	-7.318	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size ($\text{\AA}$)	1729.2799, 1729.2799, 1729.2799	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.351, 1.351, 1.351	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	0.34	0/10779	0.63	1/14662 (0.0%)
1	B	0.36	0/10591	0.65	2/14408 (0.0%)
1	C	0.41	0/10590	0.66	0/14407
1	D	0.41	0/10615	0.67	1/14442 (0.0%)
1	E	0.29	0/10735	0.61	2/14602 (0.0%)
1	F	0.35	0/10648	0.63	4/14488 (0.0%)
1	G	0.43	0/10823	0.69	0/14724
1	H	0.35	0/10823	0.65	4/14724 (0.0%)
1	I	0.32	0/10662	0.62	0/14506
1	k	0.35	0/10445	0.67	6/14213 (0.0%)
1	l	0.35	0/10790	0.67	6/14677 (0.0%)
1	m	0.36	0/10604	0.69	7/14426 (0.0%)
1	n	0.31	0/10779	0.67	4/14662 (0.0%)
1	o	0.33	0/10607	0.67	4/14430 (0.0%)
1	p	0.33	0/10485	0.68	2/14261 (0.0%)
1	q	0.28	0/9837	0.66	8/13377 (0.1%)
2	2	0.57	1/1493 (0.1%)	0.81	5/2016 (0.2%)
2	3	0.34	1/1696 (0.1%)	0.75	7/2294 (0.3%)
2	e	0.57	1/1493 (0.1%)	0.81	5/2016 (0.2%)
2	f	0.57	1/1493 (0.1%)	0.81	5/2016 (0.2%)
2	g	0.57	1/1493 (0.1%)	0.81	5/2016 (0.2%)
2	h	0.34	1/1696 (0.1%)	0.75	7/2294 (0.3%)
2	i	0.34	1/1696 (0.1%)	0.75	7/2294 (0.3%)
2	j	0.34	1/1696 (0.1%)	0.75	7/2294 (0.3%)
3	J	0.26	0/477	0.58	0/637
3	K	0.27	0/468	0.60	0/626
3	L	0.26	0/468	0.54	0/626
3	M	0.38	0/468	0.60	0/626
3	N	0.27	0/468	0.57	0/626
3	O	0.28	0/468	0.58	0/626
3	P	0.30	0/468	0.59	0/626
3	Q	0.28	0/468	0.54	0/626
3	R	0.29	0/468	0.58	0/626
3	r	0.30	0/477	0.75	0/637

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	s	0.27	0/468	0.65	0/626
3	t	0.30	0/468	0.64	0/626
3	u	0.28	0/477	0.66	0/637
3	v	0.26	0/477	0.65	0/637
3	w	0.31	0/477	0.69	0/637
3	x	0.32	0/456	0.78	1/609 (0.2%)
4	S	0.34	0/2357	0.66	0/3185
4	T	0.33	1/2357 (0.0%)	0.74	3/3185 (0.1%)
4	U	0.32	0/2357	0.70	1/3185 (0.0%)
4	V	0.30	0/2357	0.68	1/3185 (0.0%)
4	y	0.37	0/2020	0.78	2/2735 (0.1%)
5	1	0.29	0/2037	0.66	0/2761
5	W	0.28	0/2232	0.69	2/3031 (0.1%)
5	X	0.25	0/2196	0.63	1/2980 (0.0%)
5	Y	0.30	0/2240	0.68	0/3041
5	Z	0.27	0/2232	0.63	0/3031
5	a	0.31	0/2113	0.64	0/2862
5	b	0.26	0/2138	0.59	0/2897
5	c	0.30	0/2170	0.63	0/2940
5	d	0.31	0/2169	0.62	0/2939
5	z	0.30	0/2255	0.70	1/3062 (0.0%)
All	All	0.35	9/223320 (0.0%)	0.67	111/303322 (0.0%)

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
4	T	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	209	SER	C-N	18.71	1.56	1.33
2	2	209	SER	C-N	18.68	1.56	1.33
2	g	209	SER	C-N	18.68	1.56	1.33
2	f	209	SER	C-N	18.66	1.56	1.33
2	3	96	THR	C-N	-6.52	1.24	1.33

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	209	SER	O-C-N	-15.29	104.33	122.22
2	f	209	SER	O-C-N	-15.28	104.34	122.22
2	2	209	SER	O-C-N	-15.28	104.35	122.22
2	g	209	SER	O-C-N	-15.26	104.36	122.22
4	T	6	SER	CA-C-N	-12.09	103.24	122.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	T	203	ARG	Peptide
4	T	248	CYS	Peptide

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	10537	0	10392	346	0
1	B	10351	0	10195	286	0
1	C	10350	0	10200	286	0
1	D	10375	0	10228	434	0
1	E	10495	0	10355	423	0
1	F	10407	0	10250	454	0
1	G	10580	0	10431	524	0
1	H	10580	0	10436	352	0
1	I	10421	0	10266	276	0
1	k	10209	0	10068	465	0
1	l	10548	0	10408	523	0
1	m	10364	0	10209	672	0
1	n	10538	0	10394	379	0
1	o	10368	0	10219	338	0
1	p	10252	0	10114	386	0
1	q	9621	0	9467	280	0
2	2	1469	0	1492	149	0
2	3	1665	0	1672	199	0
2	e	1469	0	1492	181	0
2	f	1469	0	1493	134	0
2	g	1469	0	1493	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	h	1665	0	1672	207	0
2	i	1665	0	1672	184	0
2	j	1665	0	1672	169	0
3	J	471	0	502	33	0
3	K	462	0	489	11	0
3	L	462	0	489	13	0
3	M	462	0	489	67	0
3	N	462	0	489	17	0
3	O	462	0	489	34	0
3	P	462	0	489	57	0
3	Q	462	0	489	15	0
3	R	462	0	489	46	0
3	r	471	0	502	71	0
3	s	462	0	489	21	0
3	t	462	0	489	74	0
3	u	471	0	502	17	0
3	v	471	0	502	16	0
3	w	471	0	502	17	0
3	x	450	0	477	18	0
4	S	2305	0	2306	137	0
4	T	2305	0	2306	89	0
4	U	2305	0	2306	98	0
4	V	2305	0	2306	84	0
4	y	1977	0	1983	113	0
5	1	2009	0	2086	57	0
5	W	2201	0	2278	92	0
5	X	2166	0	2246	90	0
5	Y	2209	0	2290	64	0
5	Z	2201	0	2278	72	0
5	a	2085	0	2165	69	0
5	b	2109	0	2186	46	0
5	c	2141	0	2219	71	0
5	d	2140	0	2227	54	0
5	z	2224	0	2303	99	0
All	All	218639	0	217652	7576	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 17.

The worst 5 of 7576 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)
2:3:258:PHE:CE1	3:r:90:ILE:HG22	1.25	1.65
1:D:429:VAL:HG12	1:D:431:PHE:CE2	1.32	1.64
1:G:431:PHE:CZ	1:G:1310:THR:HG23	1.15	1.64
2:i:111:ALA:HB2	4:U:232:PHE:CE2	1.16	1.62
1:D:431:PHE:CE1	1:D:1310:THR:HA	1.29	1.62

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	1331/1353 (98%)	1204 (90%)	126 (10%)	1 (0%)	48	83
1	B	1304/1353 (96%)	1209 (93%)	92 (7%)	3 (0%)	43	77
1	C	1304/1353 (96%)	1182 (91%)	119 (9%)	3 (0%)	43	77
1	D	1308/1353 (97%)	1184 (90%)	123 (9%)	1 (0%)	48	83
1	E	1326/1353 (98%)	1186 (89%)	138 (10%)	2 (0%)	43	77
1	F	1313/1353 (97%)	1216 (93%)	92 (7%)	5 (0%)	30	67
1	G	1337/1353 (99%)	1223 (92%)	112 (8%)	2 (0%)	48	83
1	H	1337/1353 (99%)	1193 (89%)	142 (11%)	2 (0%)	48	83
1	I	1315/1353 (97%)	1190 (90%)	123 (9%)	2 (0%)	43	77
1	k	1287/1353 (95%)	1164 (90%)	117 (9%)	6 (0%)	24	63
1	l	1332/1353 (98%)	1211 (91%)	120 (9%)	1 (0%)	48	83
1	m	1306/1353 (96%)	1175 (90%)	125 (10%)	6 (0%)	24	63
1	n	1331/1353 (98%)	1202 (90%)	128 (10%)	1 (0%)	48	83
1	o	1307/1353 (97%)	1173 (90%)	130 (10%)	4 (0%)	36	72
1	p	1297/1353 (96%)	1167 (90%)	127 (10%)	3 (0%)	43	77
1	q	1201/1353 (89%)	1058 (88%)	143 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	166/718 (23%)	153 (92%)	9 (5%)	4 (2%)	4	26
2	3	194/718 (27%)	177 (91%)	13 (7%)	4 (2%)	5	29
2	e	166/718 (23%)	153 (92%)	10 (6%)	3 (2%)	6	32
2	f	166/718 (23%)	154 (93%)	9 (5%)	3 (2%)	6	32
2	g	166/718 (23%)	154 (93%)	9 (5%)	3 (2%)	6	32
2	h	194/718 (27%)	177 (91%)	13 (7%)	4 (2%)	5	29
2	i	194/718 (27%)	176 (91%)	14 (7%)	4 (2%)	5	29
2	j	194/718 (27%)	176 (91%)	14 (7%)	4 (2%)	5	29
3	J	58/98 (59%)	54 (93%)	4 (7%)	0	100	100
3	K	57/98 (58%)	55 (96%)	2 (4%)	0	100	100
3	L	57/98 (58%)	57 (100%)	0	0	100	100
3	M	57/98 (58%)	57 (100%)	0	0	100	100
3	N	57/98 (58%)	54 (95%)	3 (5%)	0	100	100
3	O	57/98 (58%)	56 (98%)	1 (2%)	0	100	100
3	P	57/98 (58%)	56 (98%)	1 (2%)	0	100	100
3	Q	57/98 (58%)	54 (95%)	3 (5%)	0	100	100
3	R	57/98 (58%)	56 (98%)	1 (2%)	0	100	100
3	r	58/98 (59%)	57 (98%)	1 (2%)	0	100	100
3	s	57/98 (58%)	55 (96%)	2 (4%)	0	100	100
3	t	57/98 (58%)	56 (98%)	1 (2%)	0	100	100
3	u	58/98 (59%)	54 (93%)	4 (7%)	0	100	100
3	v	58/98 (59%)	56 (97%)	2 (3%)	0	100	100
3	w	58/98 (59%)	56 (97%)	2 (3%)	0	100	100
3	x	55/98 (56%)	52 (94%)	3 (6%)	0	100	100
4	S	287/294 (98%)	254 (88%)	30 (10%)	3 (1%)	12	47
4	T	287/294 (98%)	255 (89%)	30 (10%)	2 (1%)	18	55
4	U	287/294 (98%)	256 (89%)	28 (10%)	3 (1%)	12	47
4	V	287/294 (98%)	242 (84%)	40 (14%)	5 (2%)	7	34
4	y	247/294 (84%)	211 (85%)	33 (13%)	3 (1%)	10	42
5	1	251/311 (81%)	233 (93%)	17 (7%)	1 (0%)	30	67
5	W	277/311 (89%)	239 (86%)	36 (13%)	2 (1%)	18	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	X	273/311 (88%)	250 (92%)	21 (8%)	2 (1%)	18	55
5	Y	278/311 (89%)	251 (90%)	27 (10%)	0	100	100
5	Z	277/311 (89%)	253 (91%)	23 (8%)	1 (0%)	30	67
5	a	261/311 (84%)	241 (92%)	20 (8%)	0	100	100
5	b	264/311 (85%)	249 (94%)	14 (5%)	1 (0%)	30	67
5	c	268/311 (86%)	248 (92%)	20 (8%)	0	100	100
5	d	268/311 (86%)	253 (94%)	15 (6%)	0	100	100
5	z	280/311 (90%)	255 (91%)	23 (8%)	2 (1%)	18	55
All	All	27383/33540 (82%)	24832 (91%)	2455 (9%)	96 (0%)	31	67

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	692	LEU
1	E	960	SER
1	k	1262	LEU
1	l	750	PRO
1	m	148	LEU

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	1142/1156 (99%)	1132 (99%)	10 (1%)	70	77
1	B	1123/1156 (97%)	1114 (99%)	9 (1%)	73	78
1	C	1123/1156 (97%)	1111 (99%)	12 (1%)	65	74
1	D	1125/1156 (97%)	1112 (99%)	13 (1%)	63	74
1	E	1138/1156 (98%)	1134 (100%)	4 (0%)	84	83
1	F	1128/1156 (98%)	1120 (99%)	8 (1%)	76	80
1	G	1147/1156 (99%)	1139 (99%)	8 (1%)	76	80
1	H	1147/1156 (99%)	1138 (99%)	9 (1%)	73	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	1130/1156 (98%)	1123 (99%)	7 (1%)	78	81
1	k	1105/1156 (96%)	1093 (99%)	12 (1%)	65	74
1	l	1144/1156 (99%)	1140 (100%)	4 (0%)	86	84
1	m	1124/1156 (97%)	1115 (99%)	9 (1%)	73	78
1	n	1143/1156 (99%)	1130 (99%)	13 (1%)	65	74
1	o	1124/1156 (97%)	1119 (100%)	5 (0%)	84	83
1	p	1110/1156 (96%)	1103 (99%)	7 (1%)	78	81
1	q	1042/1156 (90%)	1037 (100%)	5 (0%)	81	82
2	2	159/596 (27%)	156 (98%)	3 (2%)	50	66
2	3	177/596 (30%)	173 (98%)	4 (2%)	44	63
2	e	159/596 (27%)	156 (98%)	3 (2%)	50	66
2	f	159/596 (27%)	156 (98%)	3 (2%)	50	66
2	g	159/596 (27%)	156 (98%)	3 (2%)	50	66
2	h	177/596 (30%)	173 (98%)	4 (2%)	44	63
2	i	177/596 (30%)	173 (98%)	4 (2%)	44	63
2	j	177/596 (30%)	173 (98%)	4 (2%)	44	63
3	J	50/71 (70%)	49 (98%)	1 (2%)	48	66
3	K	49/71 (69%)	49 (100%)	0	100	100
3	L	49/71 (69%)	49 (100%)	0	100	100
3	M	49/71 (69%)	49 (100%)	0	100	100
3	N	49/71 (69%)	48 (98%)	1 (2%)	48	66
3	O	49/71 (69%)	48 (98%)	1 (2%)	48	66
3	P	49/71 (69%)	48 (98%)	1 (2%)	48	66
3	Q	49/71 (69%)	48 (98%)	1 (2%)	48	66
3	R	49/71 (69%)	49 (100%)	0	100	100
3	r	50/71 (70%)	48 (96%)	2 (4%)	28	49
3	s	49/71 (69%)	48 (98%)	1 (2%)	48	66
3	t	49/71 (69%)	47 (96%)	2 (4%)	27	49
3	u	50/71 (70%)	49 (98%)	1 (2%)	48	66
3	v	50/71 (70%)	49 (98%)	1 (2%)	48	66
3	w	50/71 (70%)	49 (98%)	1 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	x	48/71 (68%)	48 (100%)	0	100	100
4	S	251/255 (98%)	250 (100%)	1 (0%)	84	83
4	T	251/255 (98%)	251 (100%)	0	100	100
4	U	251/255 (98%)	248 (99%)	3 (1%)	63	74
4	V	251/255 (98%)	244 (97%)	7 (3%)	38	59
4	y	216/255 (85%)	212 (98%)	4 (2%)	50	66
5	1	229/275 (83%)	229 (100%)	0	100	100
5	W	253/275 (92%)	251 (99%)	2 (1%)	73	78
5	X	249/275 (90%)	247 (99%)	2 (1%)	73	78
5	Y	254/275 (92%)	253 (100%)	1 (0%)	84	83
5	Z	253/275 (92%)	251 (99%)	2 (1%)	73	78
5	a	238/275 (86%)	233 (98%)	5 (2%)	47	65
5	b	241/275 (88%)	235 (98%)	6 (2%)	42	62
5	c	245/275 (89%)	242 (99%)	3 (1%)	63	74
5	d	245/275 (89%)	242 (99%)	3 (1%)	63	74
5	z	256/275 (93%)	250 (98%)	6 (2%)	44	63
All	All	23810/28425 (84%)	23589 (99%)	221 (1%)	68	77

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	n	1297	LYS
2	e	200	VAL
5	d	123	VAL
5	X	21	LEU
1	o	488	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 528 such sidechains are listed below:

Mol	Chain	Res	Type
2	j	91	HIS
3	t	43	GLN
2	g	214	ASN
5	a	167	GLN
1	H	443	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

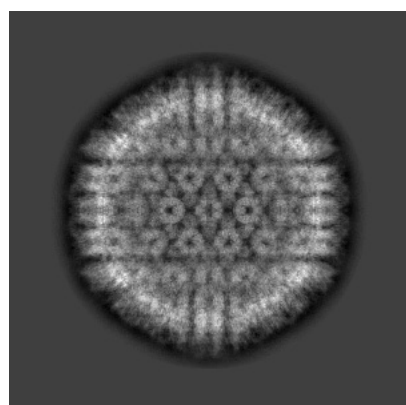
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9366. These allow visual inspection of the internal detail of the map and identification of artifacts.

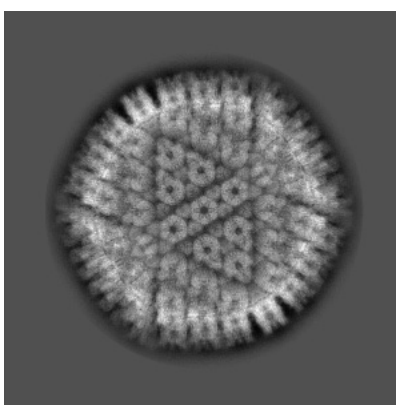
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

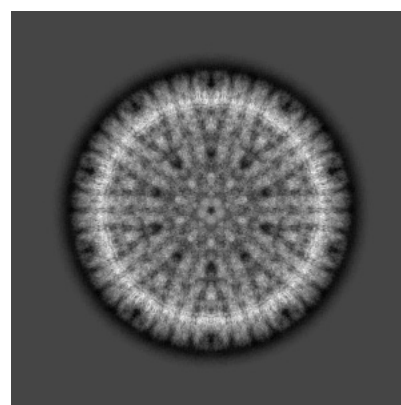
6.1.1 Primary map



X



Y

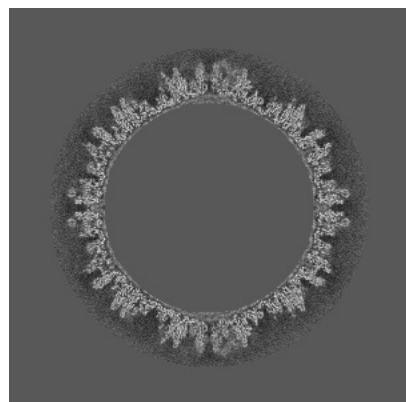


Z

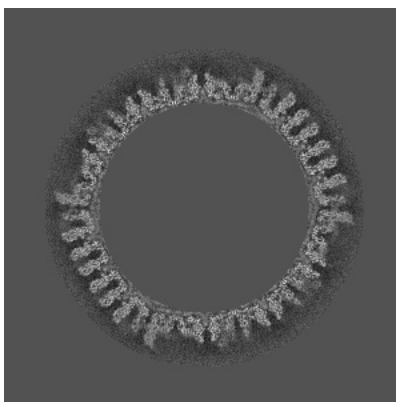
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

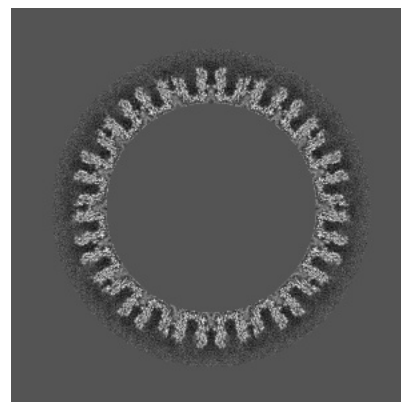
6.2.1 Primary map



X Index: 640



Y Index: 640

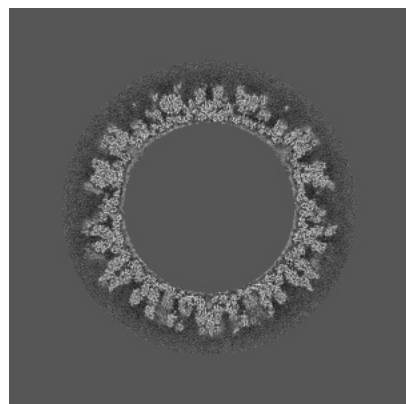


Z Index: 640

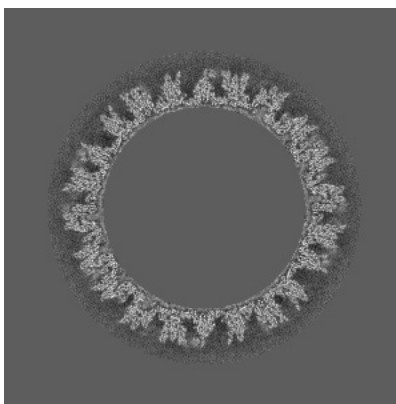
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

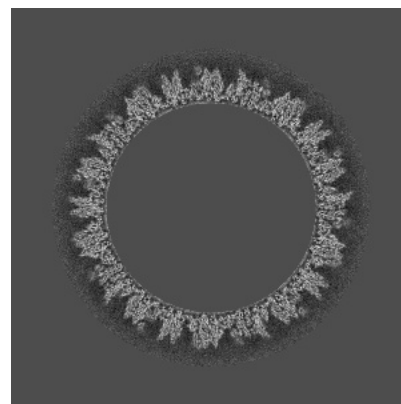
6.3.1 Primary map



X Index: 445



Y Index: 731

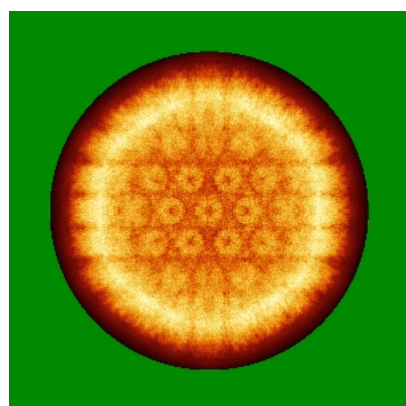


Z Index: 618

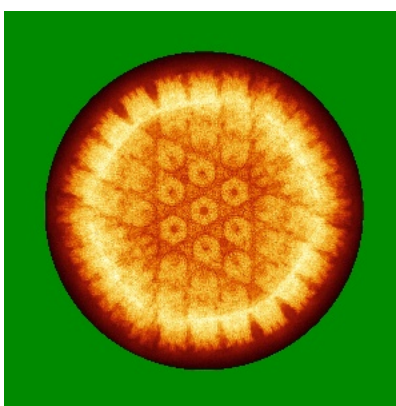
The images above show the largest variance slices of the map in three orthogonal directions.

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

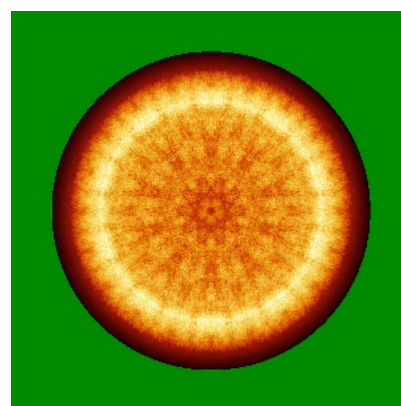
6.4.1 Primary map



X



Y

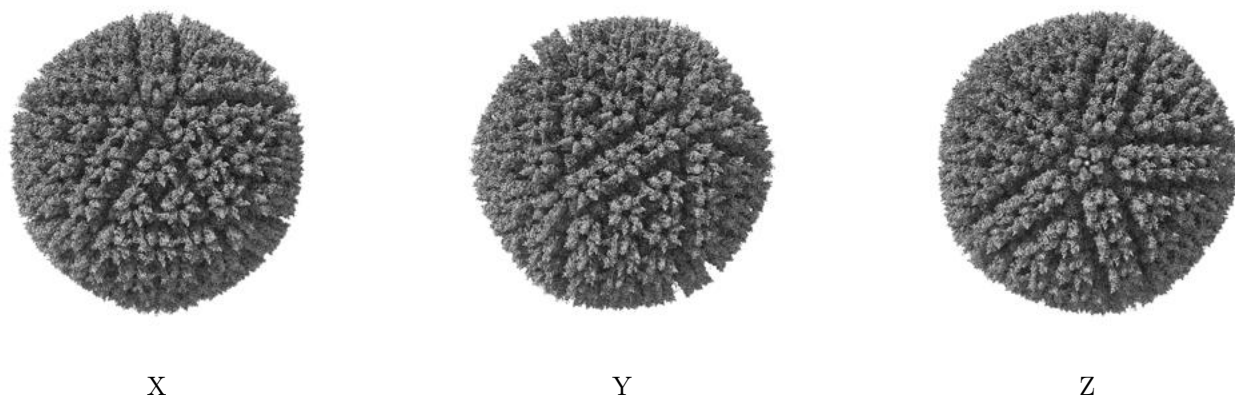


Z

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

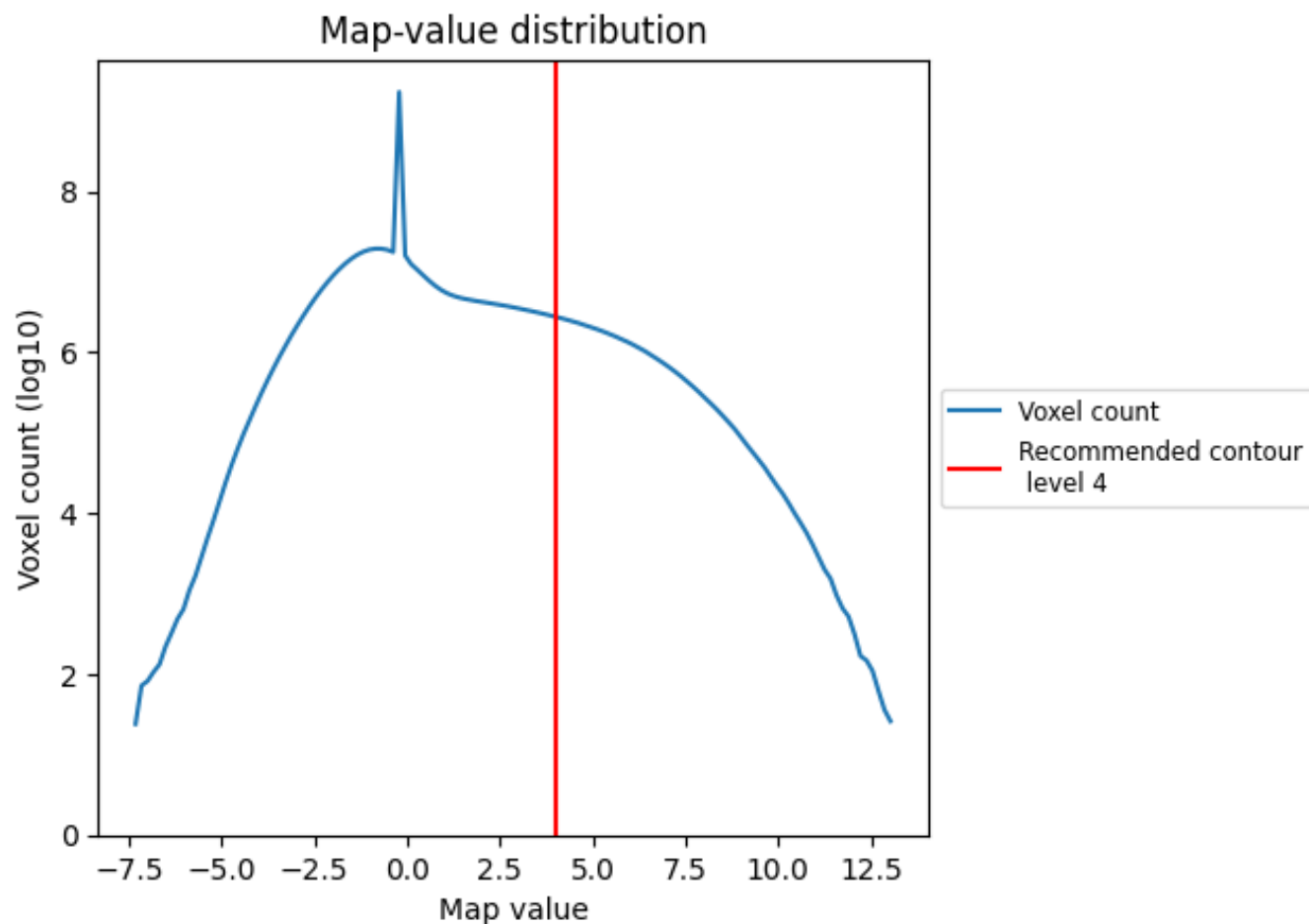
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

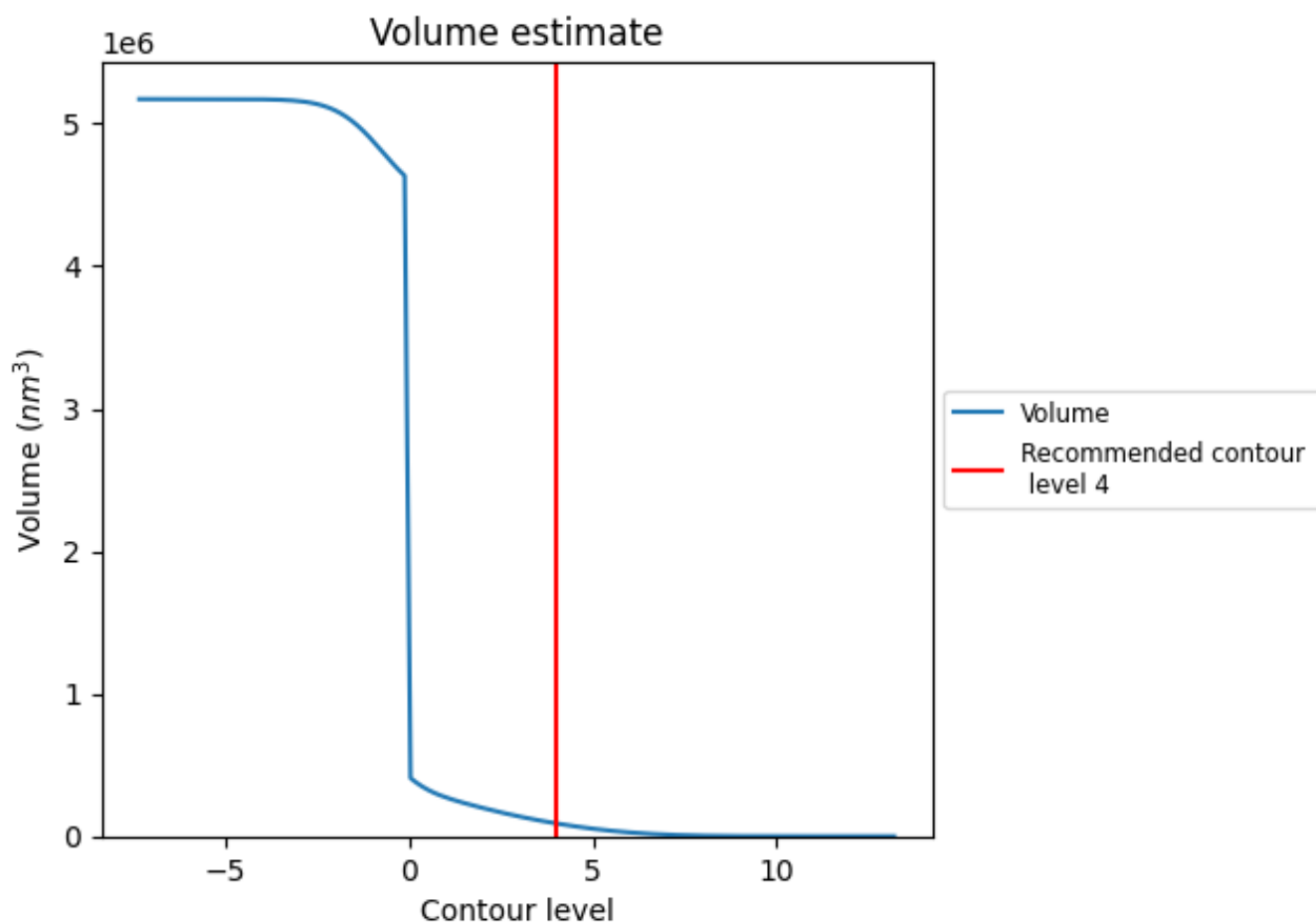
This section contains the results of statistical analysis of the map.

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.

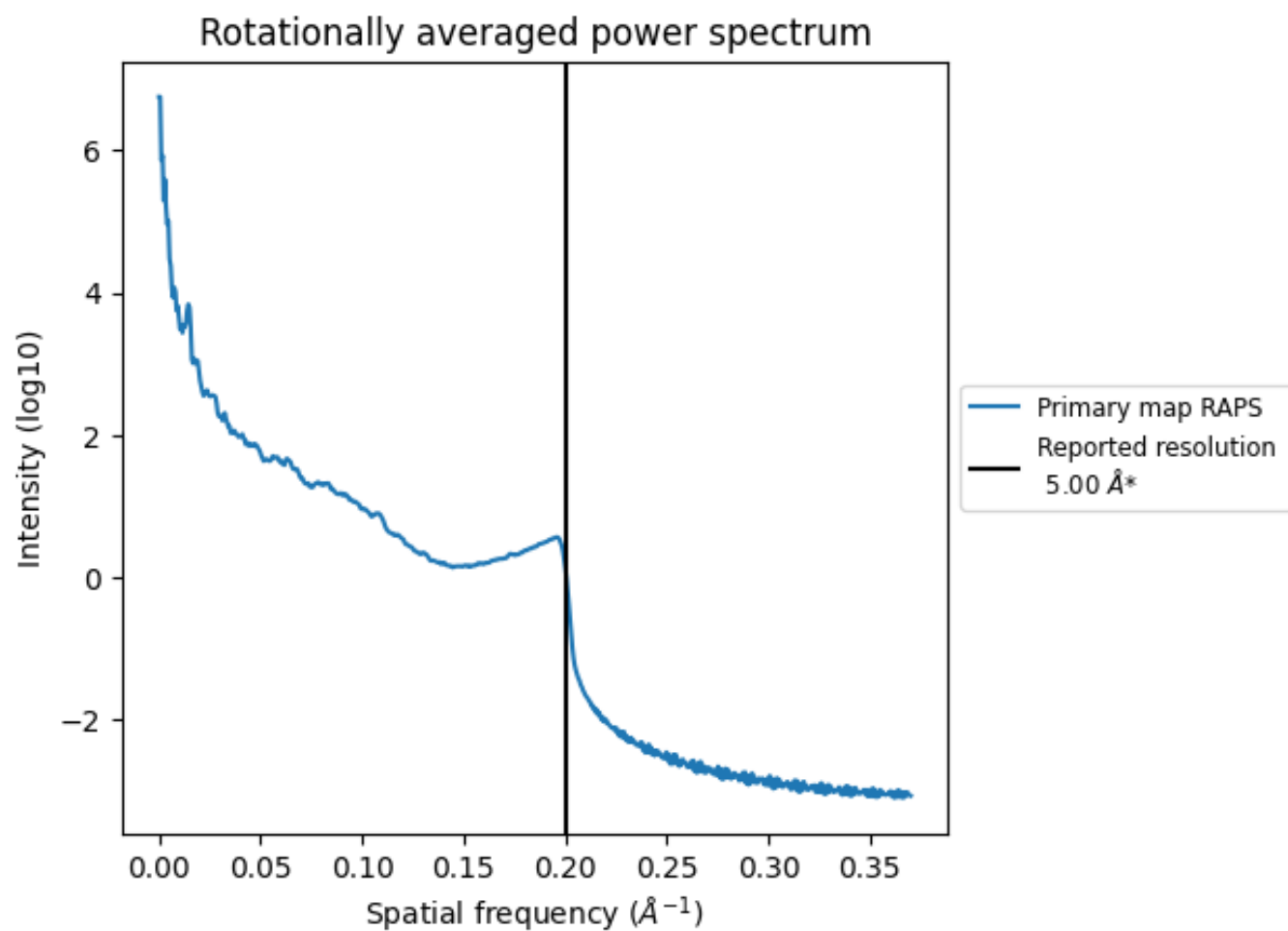
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90561 nm^3 ; this corresponds to an approximate mass of 81806 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 0.200 Å⁻¹

8 Fourier-Shell correlation

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

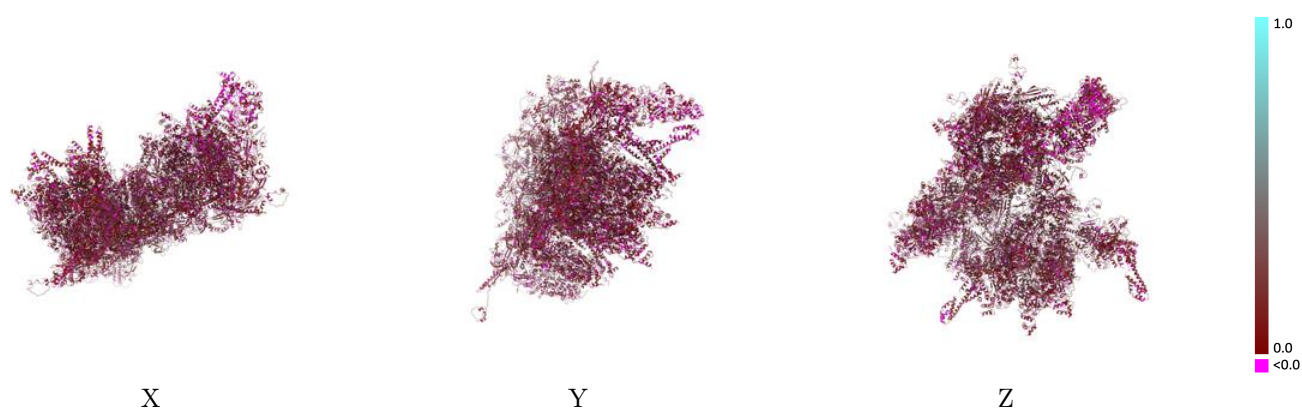
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9366 and PDB model 6NHJ. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)

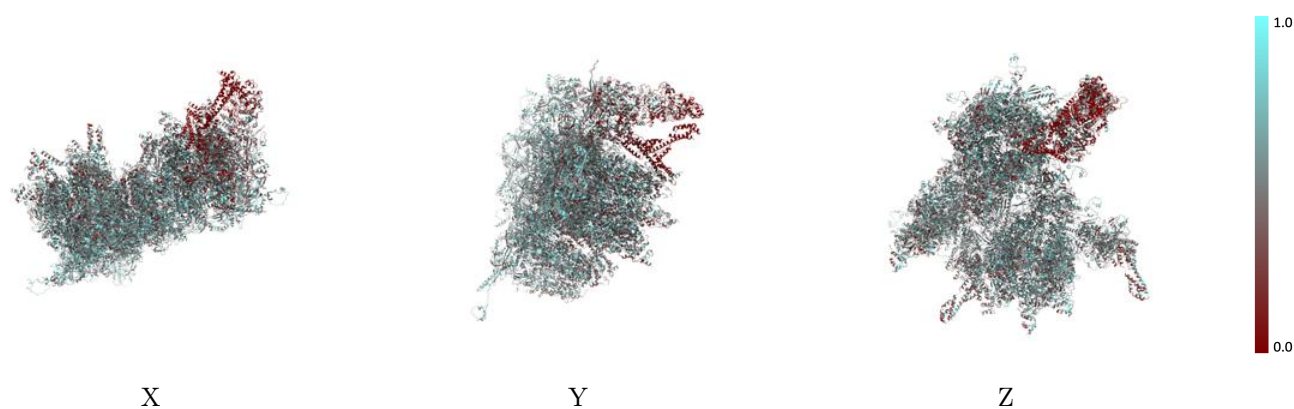
This section was not generated.

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



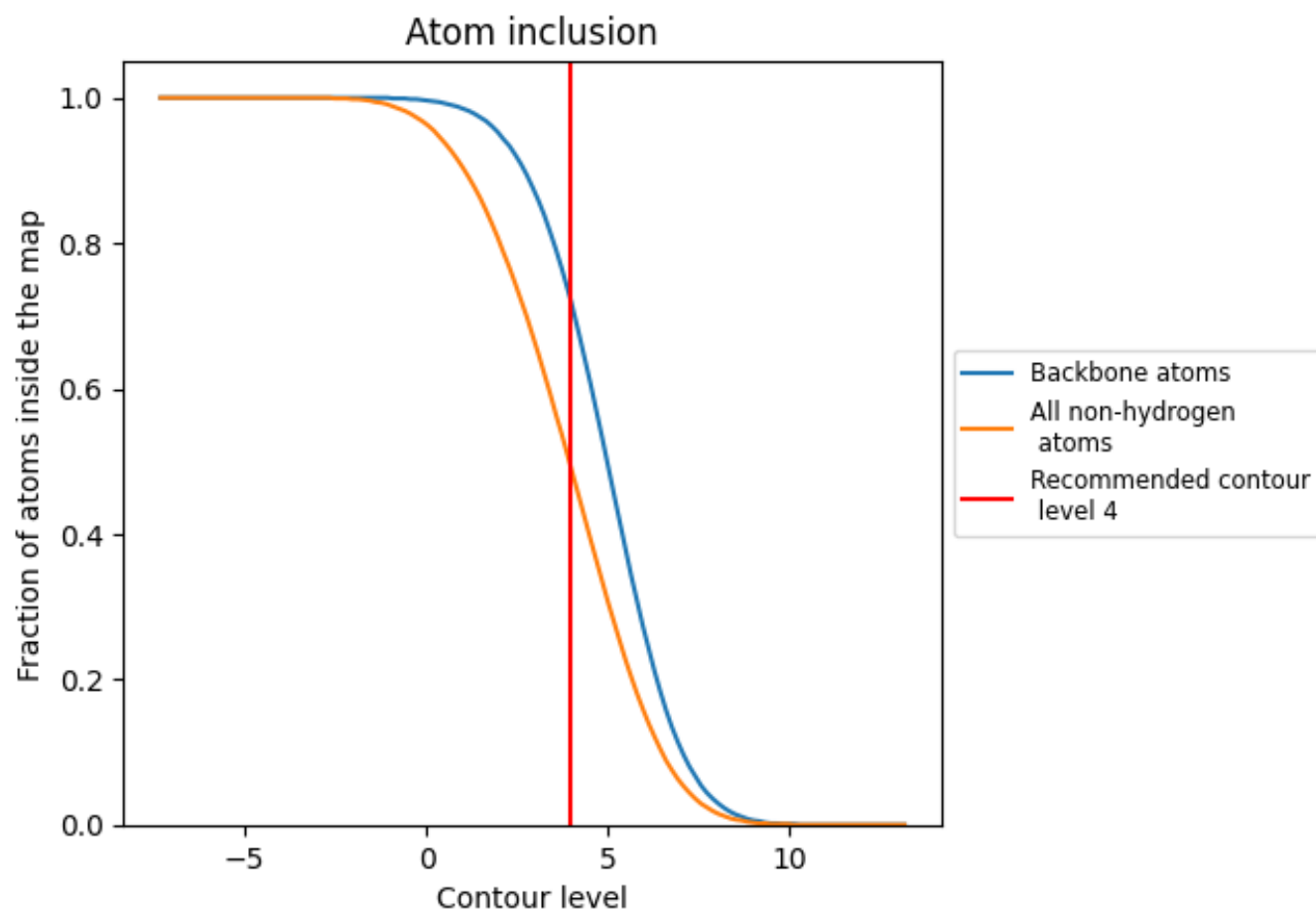
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 49% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4900	 0.1390
1	 0.2890	 0.1150
2	 0.0080	 0.0720
3	 0.0220	 0.0940
A	 0.5450	 0.1570
B	 0.5470	 0.1490
C	 0.5370	 0.1410
D	 0.5280	 0.1390
E	 0.5370	 0.1490
F	 0.5400	 0.1530
G	 0.5260	 0.1470
H	 0.5170	 0.1340
I	 0.5190	 0.1270
J	 0.4730	 0.1410
K	 0.4540	 0.1350
L	 0.4360	 0.1300
M	 0.4120	 0.1250
N	 0.4520	 0.1270
O	 0.4340	 0.1210
P	 0.4470	 0.1160
Q	 0.4540	 0.1730
R	 0.4410	 0.0880
S	 0.4790	 0.1310
T	 0.4810	 0.1380
U	 0.5040	 0.1500
V	 0.4940	 0.1260
W	 0.4890	 0.1610
X	 0.4740	 0.1550
Y	 0.4990	 0.1580
Z	 0.4640	 0.1350
a	 0.4880	 0.1430
b	 0.4740	 0.1530
c	 0.4670	 0.1350
d	 0.4430	 0.1250
e	 0.4230	 0.1290



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Chain	Atom inclusion	Q-score
f	 0.3670	 0.1160
g	 0.3650	 0.1090
h	 0.4260	 0.1230
i	 0.4090	 0.1310
j	 0.4000	 0.1230
k	 0.5010	 0.1470
l	 0.5270	 0.1480
m	 0.5250	 0.1390
n	 0.5140	 0.1360
o	 0.5220	 0.1370
p	 0.5090	 0.1490
q	 0.3280	 0.1180
r	 0.4080	 0.1110
s	 0.4340	 0.1440
t	 0.4340	 0.1220
u	 0.3970	 0.1250
v	 0.4470	 0.1270
w	 0.4170	 0.1250
x	 0.0570	 0.0410
y	 0.3460	 0.1190
z	 0.3360	 0.1290