wwPDB EM Validation Summary Report (i)

Nov 13, 2022 – 12:35 AM EST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

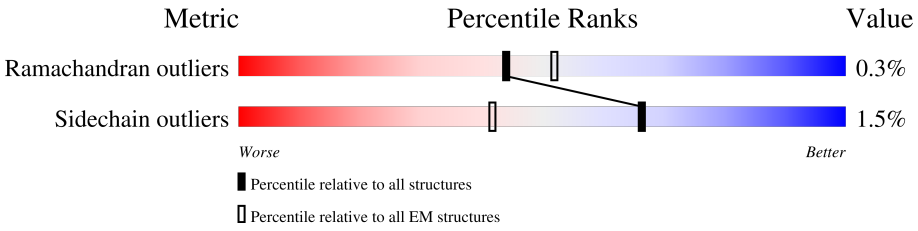
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1345	39% 99%
1	B	1345	41% 98%
1	C	1345	42% 97%
1	D	1345	38% 98%
1	E	1345	37% 98%
1	F	1345	43% 98%
1	G	1345	42% 98%
1	H	1345	34% 98%
1	I	1345	40% 99%

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Mol	Chain	Length	Quality of chain
1	q	1345	54% 95%
1	r	1345	49% 99%
1	s	1345	47% 99%
1	t	1345	45% 99%
1	u	1345	49% 99%
1	v	1345	51% 96%
1	w	1345	77% 92% 7%
2	e	858	27% 31% 69%
2	f	858	28% 31% 69%
2	g	858	25% 30% 69%
2	h	858	29% 31% 69%
2	i	858	26% 30% 69%
2	j	858	29% 30% 69%
2	k	858	25% 30% 69%
2	l	858	30% 30% 69%
2	m	858	24% 31% 69%
2	n	858	22% 30% 69%
2	o	858	21% 30% 69%
2	p	858	25% 31% 69%
3	1	89	45% 67% 31%
3	2	89	53% 67% 31%
3	3	89	61% 67% 31%
3	4	89	65% 64% 35%
3	J	89	48% 65% 31%
3	K	89	47% 67% 31%

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Mol	Chain	Length	Quality of chain
3	L	89	53% 66% 31%
3	M	89	49% 67% 31%
3	N	89	47% 67% 31%
3	O	89	58% 67% 31%
3	P	89	45% 67% 31%
3	Q	89	54% 67% 31%
3	R	89	49% 67% 31%
3	x	89	64% 67% 31%
3	y	89	61% 67% 31%
3	z	89	57% 67% 31%
4	5	299	56% 83% 16%
4	S	299	45% 98%
4	T	299	57% 99%
4	U	299	48% 97%
4	V	299	47% 97%
5	6	296	69% 95% 5%
5	7	296	71% 98%
5	W	296	48% 98%
5	X	296	58% 99%
5	Y	296	50% 98%
5	Z	296	46% 96%
5	a	296	48% 98%
5	b	296	54% 97%
5	c	296	46% 98%
5	d	296	47% 97%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 238552 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major capsid protein.

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

- Molecule 2 is a protein called Large structural phosphoprotein.

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

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

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

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

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

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

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

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

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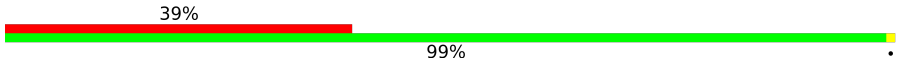
Mol	Chain	Residues	Atoms					AltConf	Trace
5	Z	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		
5	7	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		
5	a	295	Total	C	N	O	S	0	0
			2329	1481	392	436	20		
5	b	295	Total	C	N	O	S	0	0
			2329	1481	392	436	20		
5	c	295	Total	C	N	O	S	0	0
			2329	1481	392	436	20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

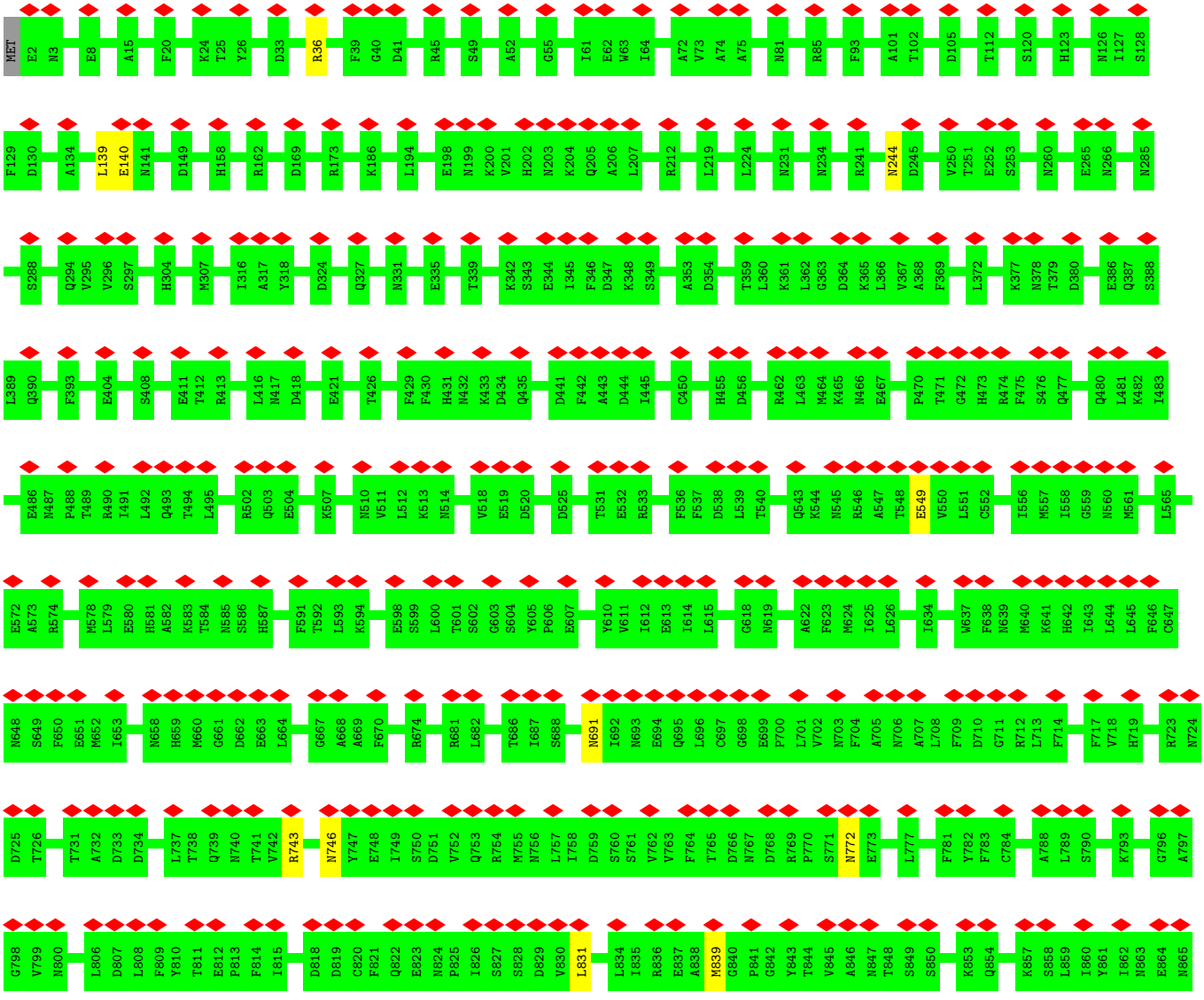
3 Residue-property plots (i)

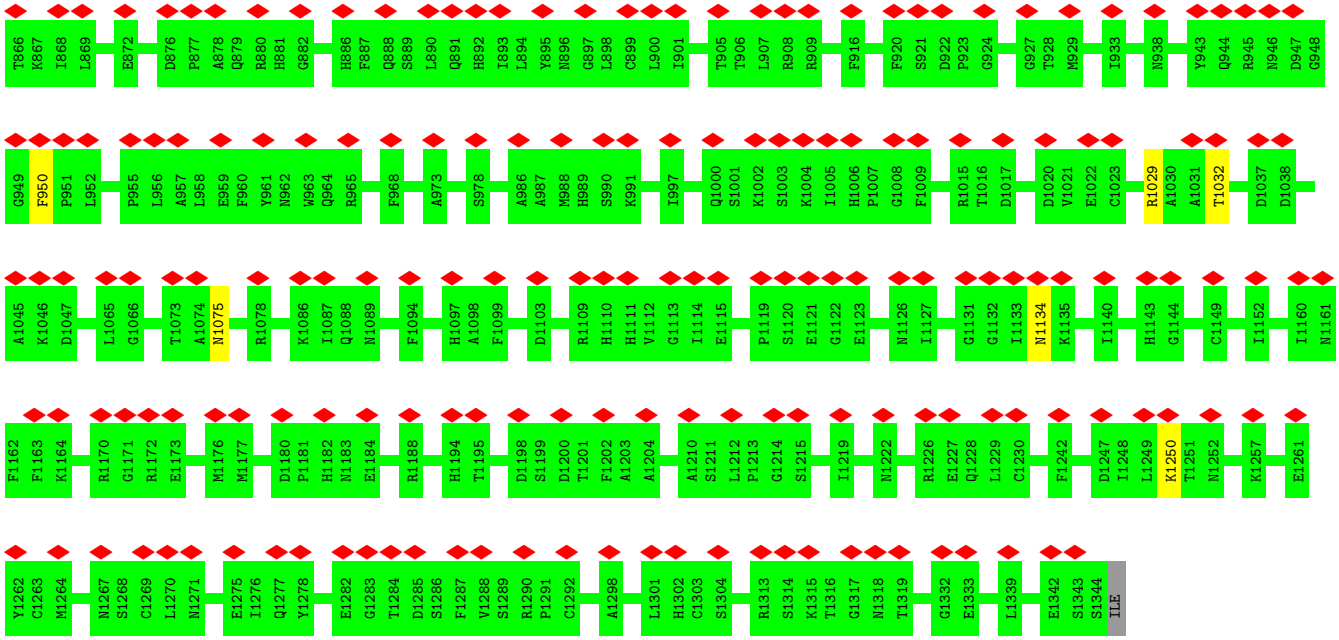
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:

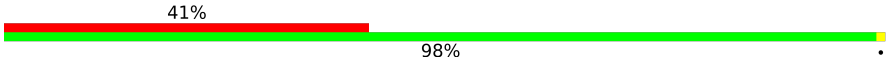


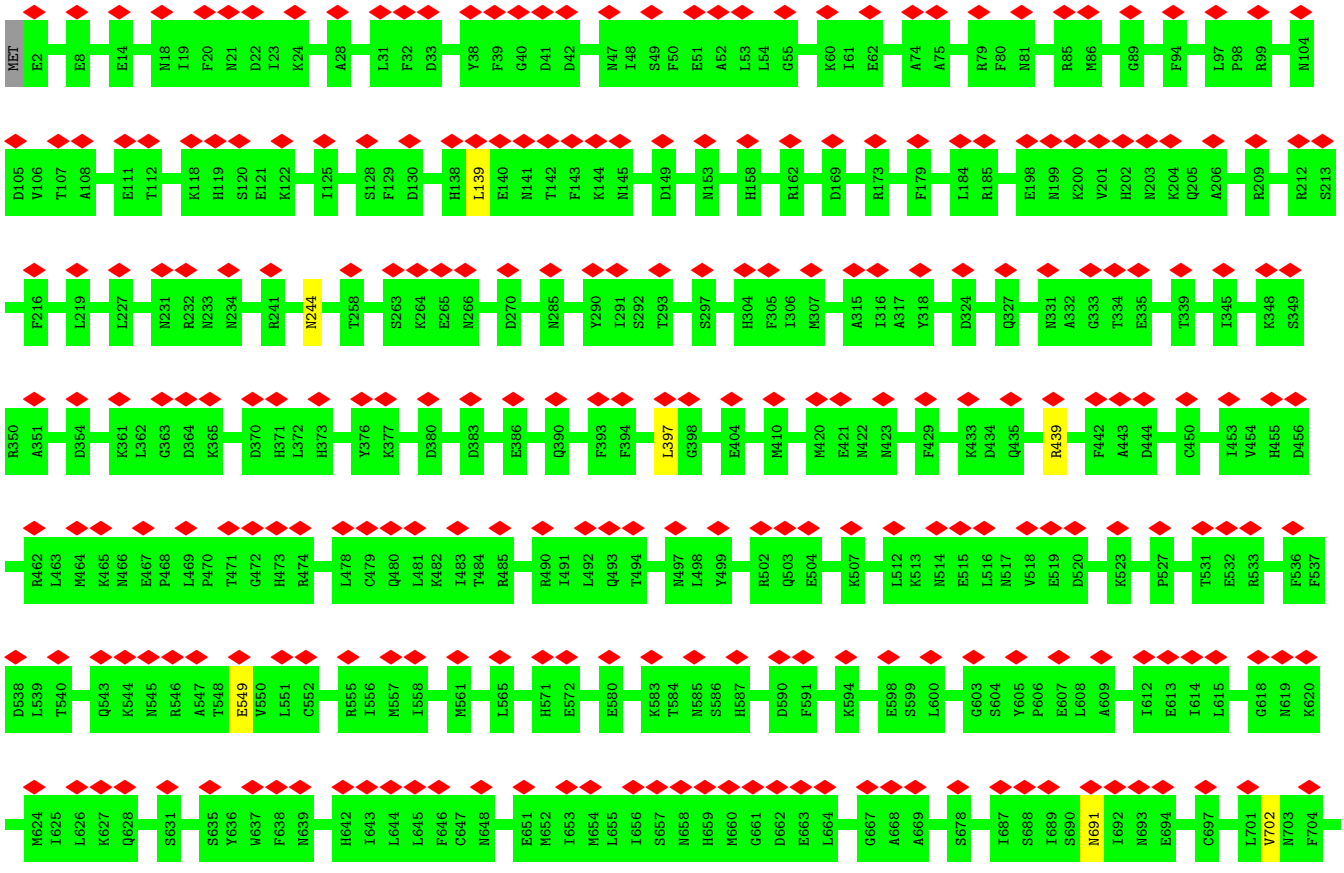


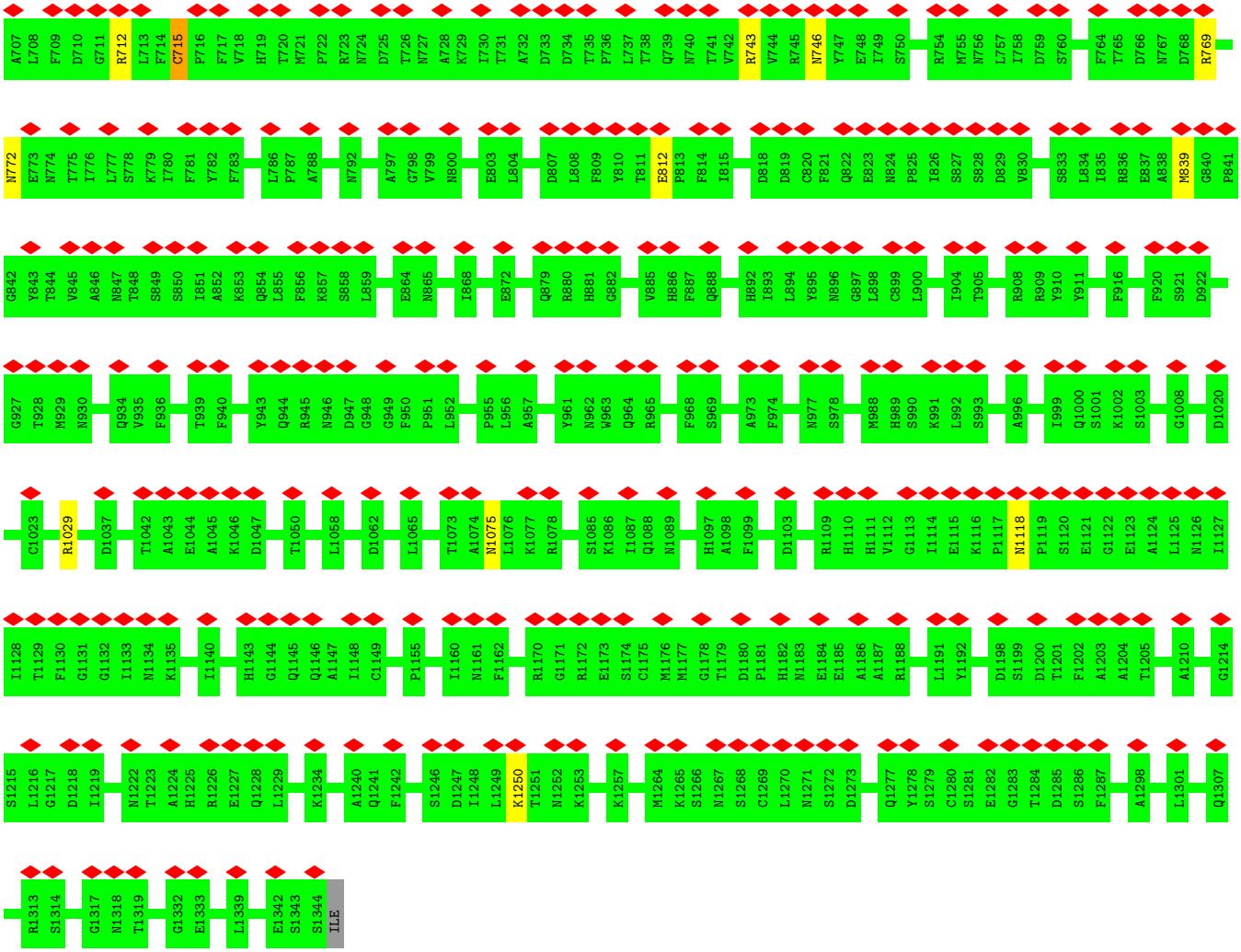


- Molecule 1: Major capsid protein

Chain B:

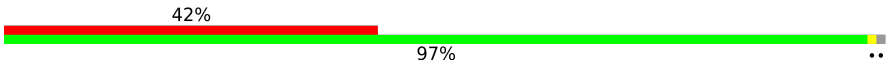


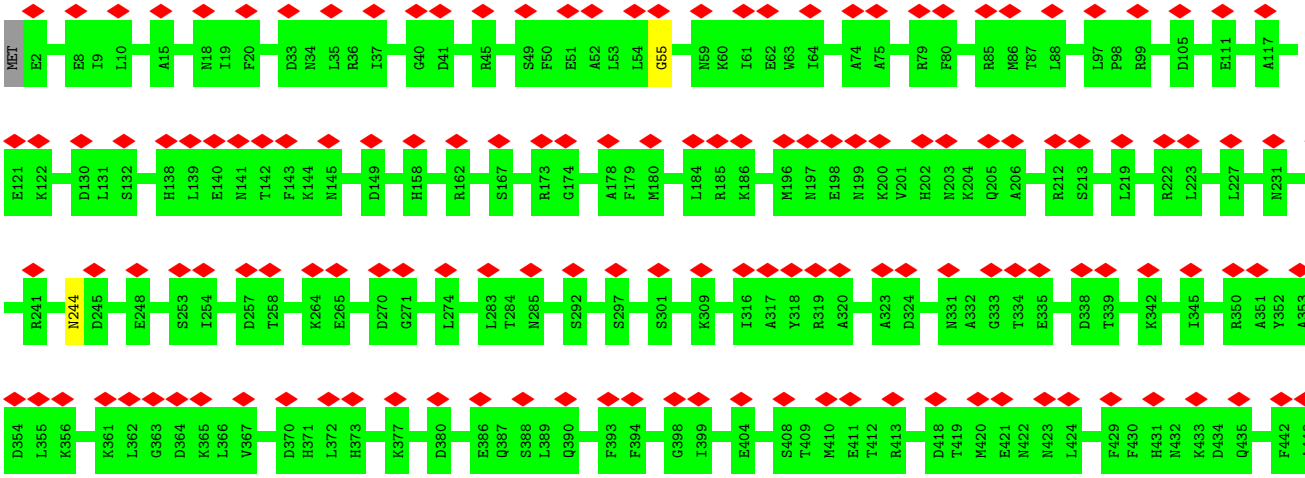




- Molecule 1: Major capsid protein

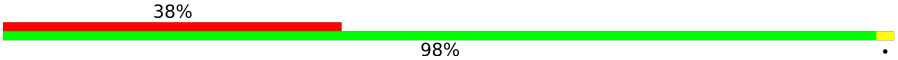
Chain C:

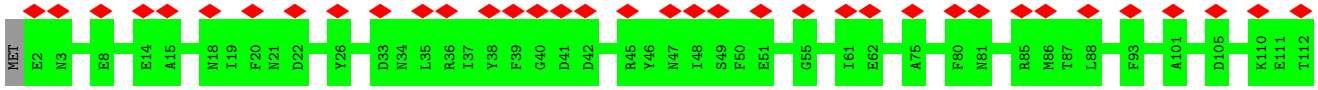


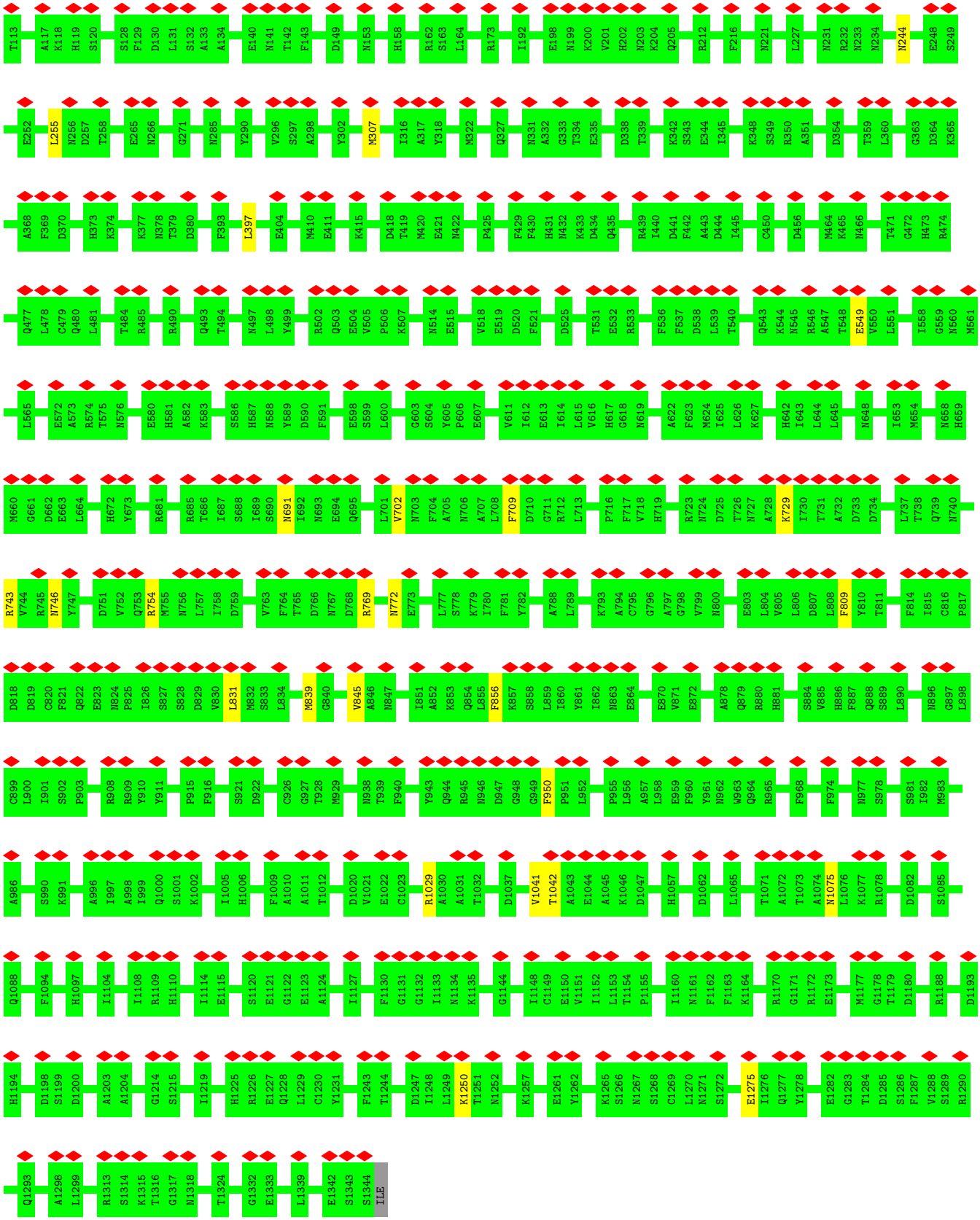


• Molecule 1: Major capsid protein

Chain D:



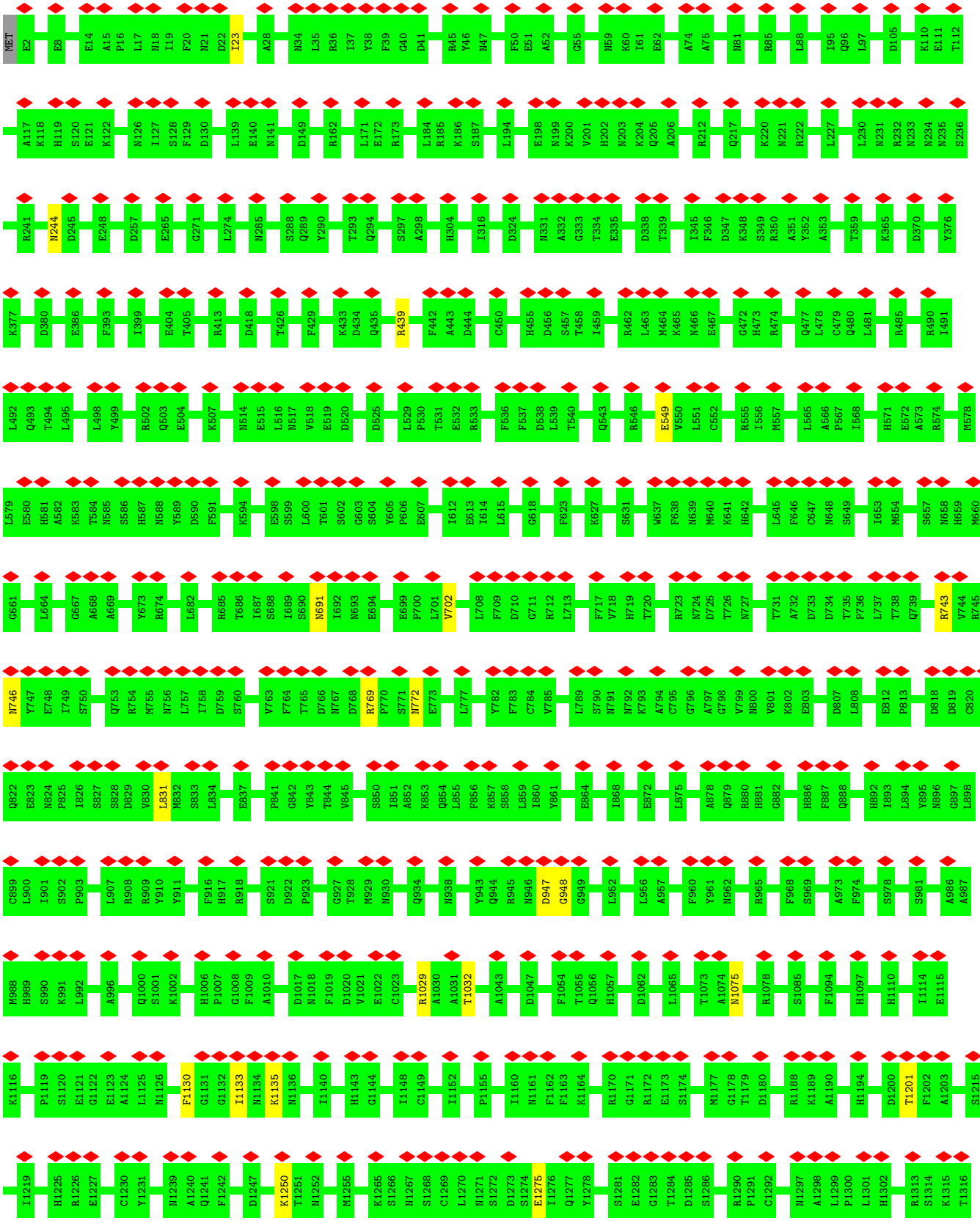


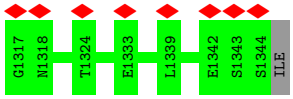


- Molecule 1: Major capsid protein

Chain E:

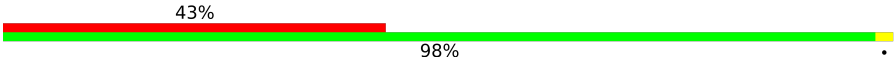
37%
98%

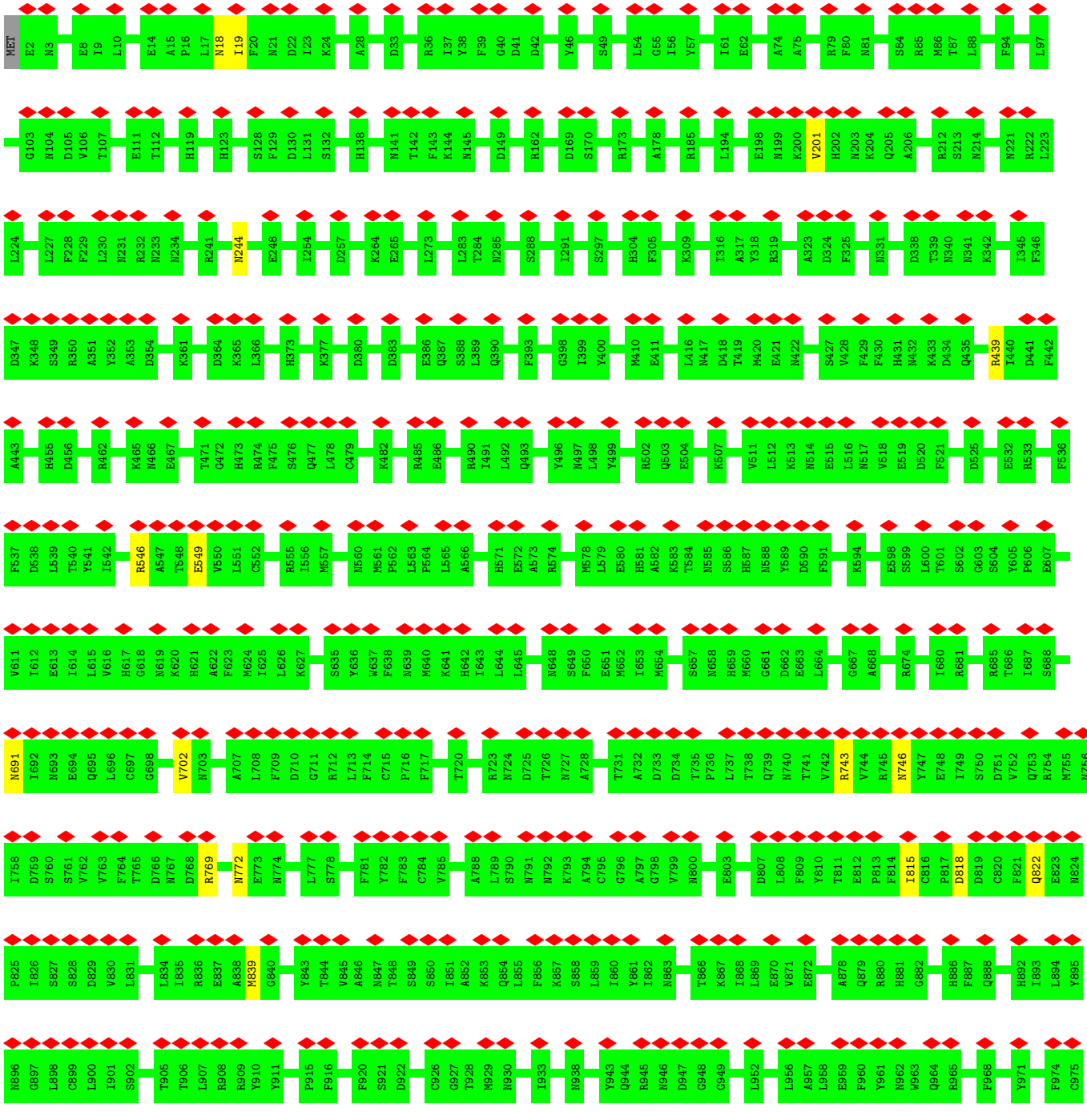

MET E2 E3 E14 A15 P16 L17 N18 I19 F20 N21 D22 I23 A28 N34 L35 R36 I37 Y38 F39 G40 D41 R45 Y46 N47 F50 E51 A52 G55 N59 K60 I61 E62 A74 A75 N81 R85 L88 I95 Q96 L97 D105 K110 E111 T112
A117 K118 H119 S120 E121 K122 N126 I127 S128 F129 D130 L139 E140 N141 D149 R162 L171 E172 R173 L184 R185 K186 S187 L194 E198 N199 K200 V201 H202 N203 K204 Q205 A206 R212 Q217 K220 N221 R222 L227 L230 N231 R232 N233 N234 N235 S236
R241 N244 D245 E248 D257 E265 G271 L274 N285 S288 Q289 Y290 T293 Q294 S297 A298 H304 I316 D324 N331 A332 G333 T334 E335 D338 T339 I345 F346 D347 K348 S349 R350 A351 Y352 A353 T359 K365 D370 Y376
K377 D380 E386 F393 I399 E404 T405 R413 D418 T426 F429 K433 D434 Q435 R439 F442 A443 D444 C450 H455 D456 S457 T458 I459 R462 L463 M464 K465 N466 E467 G472 H473 R474 Q477 L478 C479 Q480 L481 R485 R490 I491
L492 Q493 T494 L495 L498 Y499 R502 Q503 E504 K507 N514 E515 L516 N517 V518 E519 D520 D525 L529 P530 T531 E532 R533 F536 F537 D538 L539 T540 Q543 R546 E549 V550 L551 C552 R555 I556 M557 L565 A566 F567 I568 H571 E572 A573 R574 M578
L579 E580 H581 A582 K583 T584 N585 S586 H587 N588 Y589 D590 F591 K594 E598 S599 L600 T601 S602 G603 S604 Y605 P606 E607 I612 E613 I614 L615 G618 F623 K627 S631 W637 F638 N639 M640 K641 H642 L645 F646 C647 N648 S649 I653 M654 S657 N658 H659 M660
G661 L664 G667 A668 A669 Y673 R674 L682 R685 T686 I687 S688 I689 S690 N691 I692 N693 E694 E699 P700 L701 V702 L708 F709 D710 G711 R712 L713 F717 V718 H719 T720 R723 N724 D725 T726 N727 T731 A732 D733 D734 T735 P736 L737 T738 Q739 R743 V744 R745
N746 Y747 E748 I749 S750 Q753 R754 M755 N756 L757 I758 D759 S760 V763 F764 T765 D766 N767 D768 R769 P770 S771 N772 E773 L777 Y782 F783 C784 V785 L789 S790 N791 N792 K793 A794 C795 G796 A797 G798 V799 N800 V801 K802 E803 D807 L808 E812 P813 D818 D819 C820 F821
Q822 E823 N824 P825 I826 S827 S828 D829 V830 L831 M832 S833 L834 E837 P841 G842 Y843 T844 V845 S850 I851 A852 K853 Q854 L855 F856 K857 S858 L859 I860 Y861 E864 I868 E872 L875 A878 Q879 R880 H881 G882 H886 F887 Q888 H892 I893 L894 Y895 N896 G897 L898
C899 L900 I901 S902 P903 L907 R908 R909 Y910 Y911 F916 H917 R918 S921 D922 P923 G927 T928 M929 N930 Q934 N938 Y943 Q944 R945 N946 D947 G948 G949 L952 L956 A957 F960 Y961 N962 R965 F968 S969 A973 F974 S978 S981 A986 A987
M988 H989 S990 K991 L992 A996 Q1000 S1001 K1002 H1006 P1007 G1008 F1009 A1010 D1017 N1018 F1019 D1020 V1021 E1022 C1023 R1029 A1030 A1031 T1032 A1043 D1047 F1054 T1055 Q1056 H1057 D1062 L1065 T1073 A1074 N1075 R1078 S1085 F1094 H1097 H1110 I1114 E1115
K1116 P1119 S1120 E1121 G1122 E1123 A1124 L1125 N1126 F1130 G1131 G1132 I1133 N1134 K1135 N1136 I1140 H1143 G1144 I1148 C1149 I1152 P1155 I1160 N1161 F1162 F1163 K1164 R1170 G1171 R1172 E1173 S1174 M1177 G1178 T1179 D1180 R1188 K1189 A1190 H1194 D1200 T1201 F1202 A1203 S1215
I1219 H1225 R1226 E1227 C1230 Y1231 N1239 A1240 Q1241 F1242 D1247 K1250 T1251 N1252 M1255 K1265 S1266 N1267 S1268 C1269 L1270 N1271 S1272 D1273 S1274 E1275 I1276 Q1277 Y1278 S1281 E1282 G1283 T1284 D1285 S1286 R1290 P1291 C1292 N1297 A1298 L1299 P1300 L1301 H1302 R1313 S1314 K1315 T1316

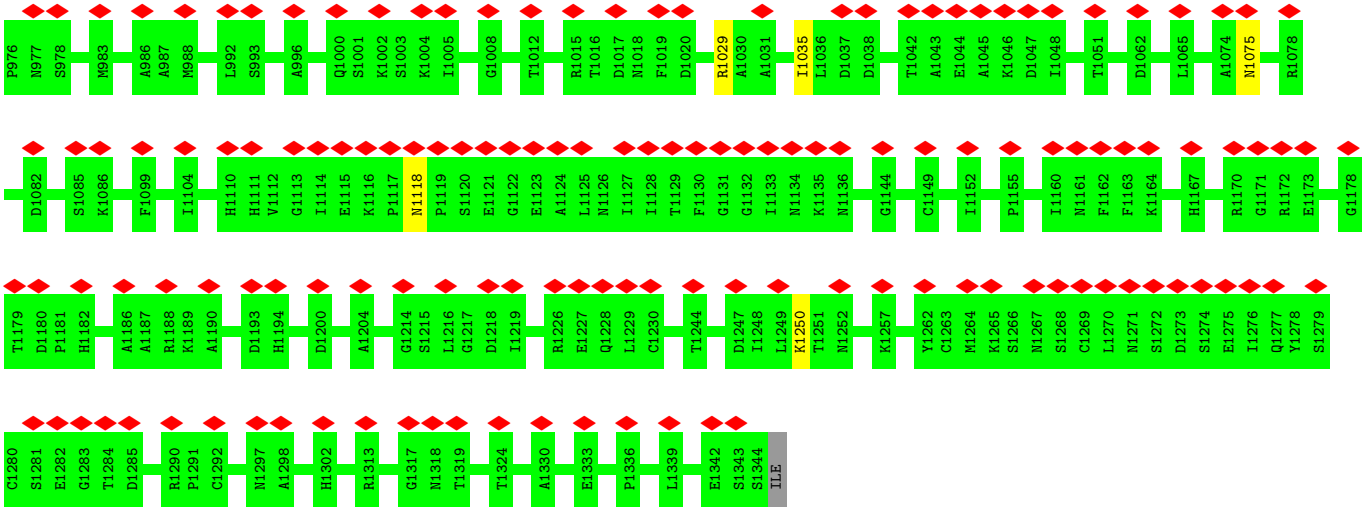


• Molecule 1: Major capsid protein

Chain F:

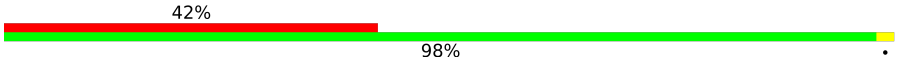


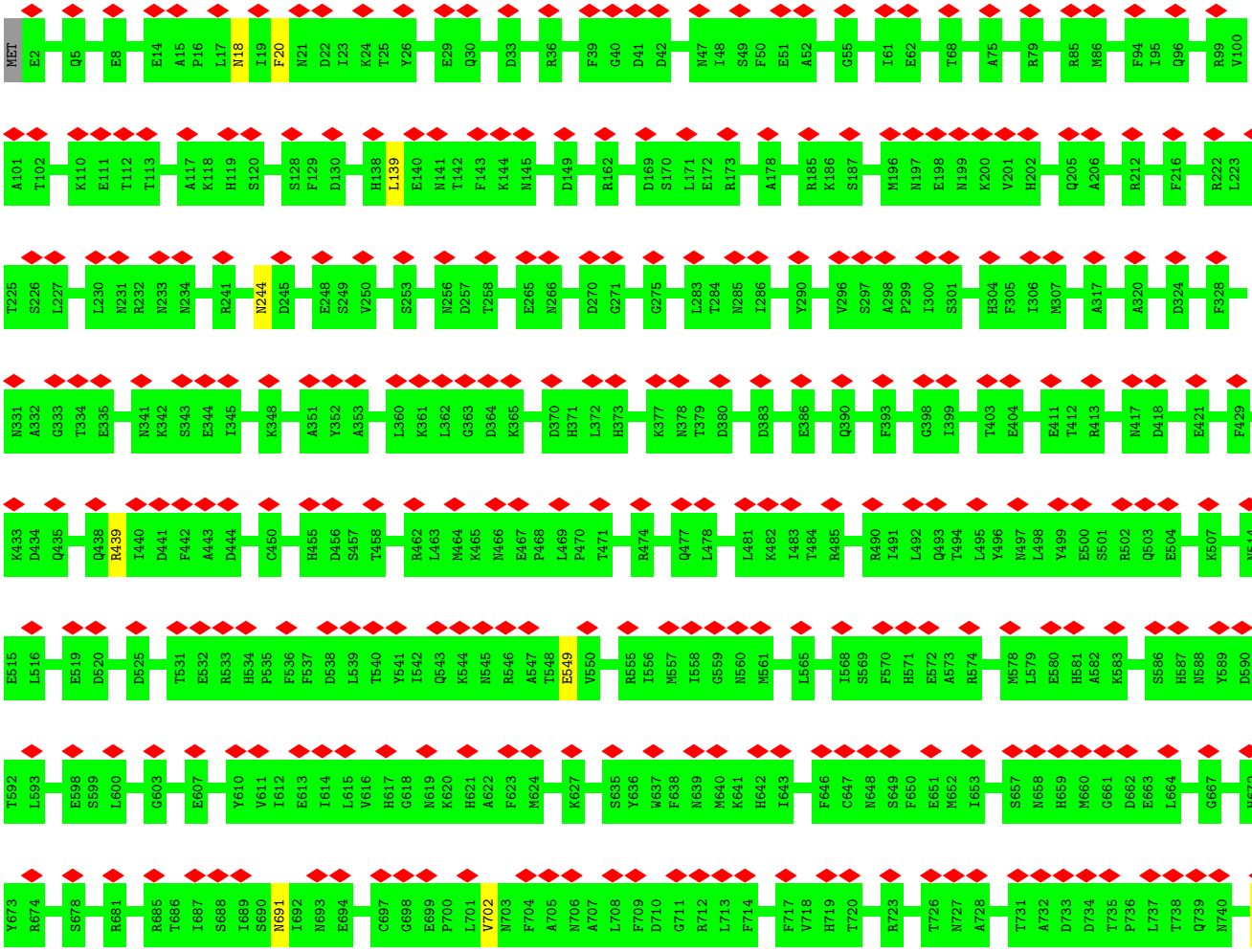


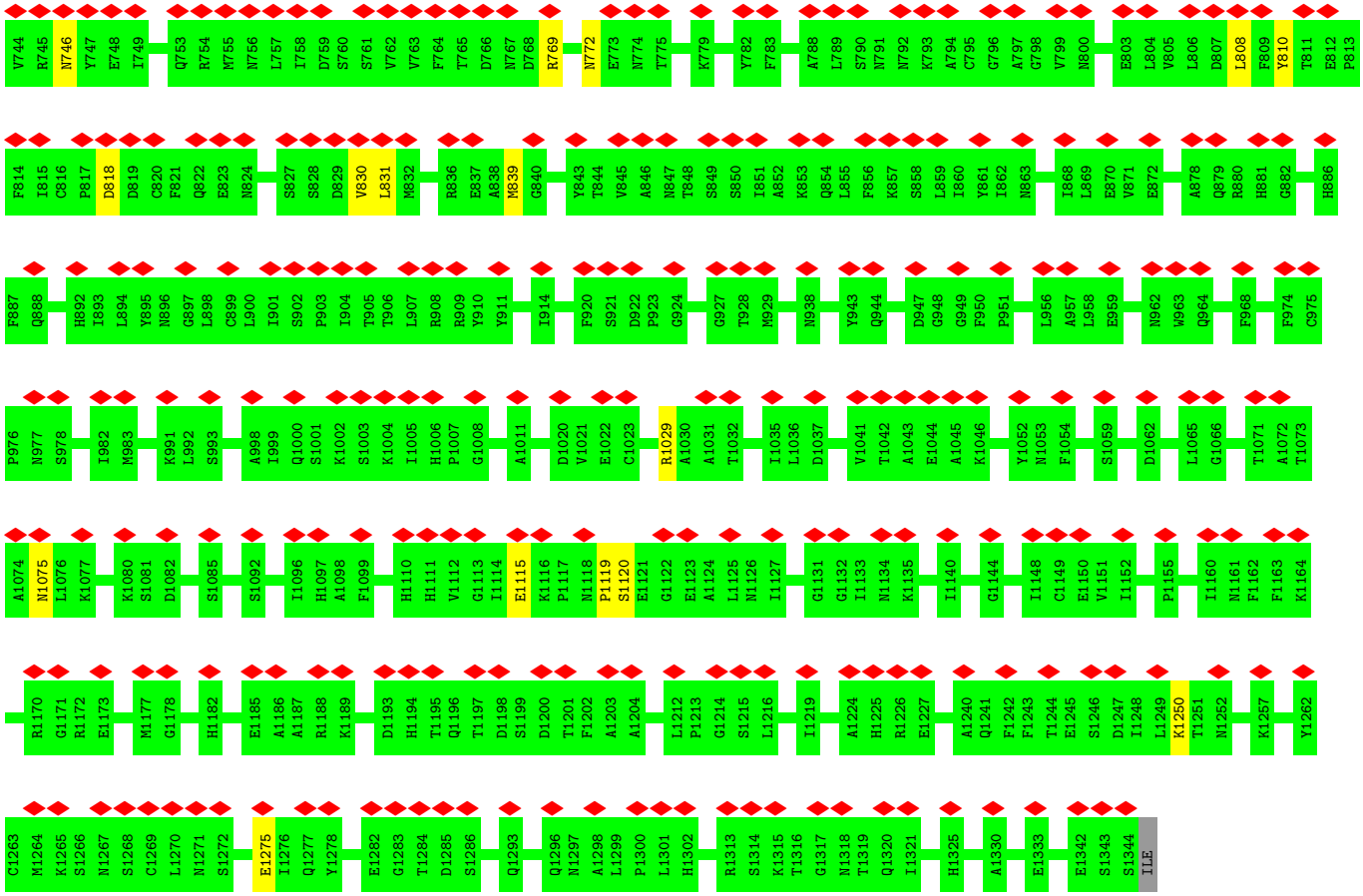


- Molecule 1: Major capsid protein

Chain G:

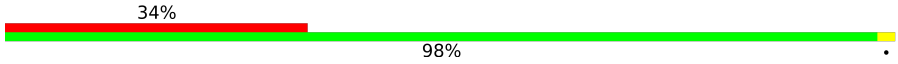


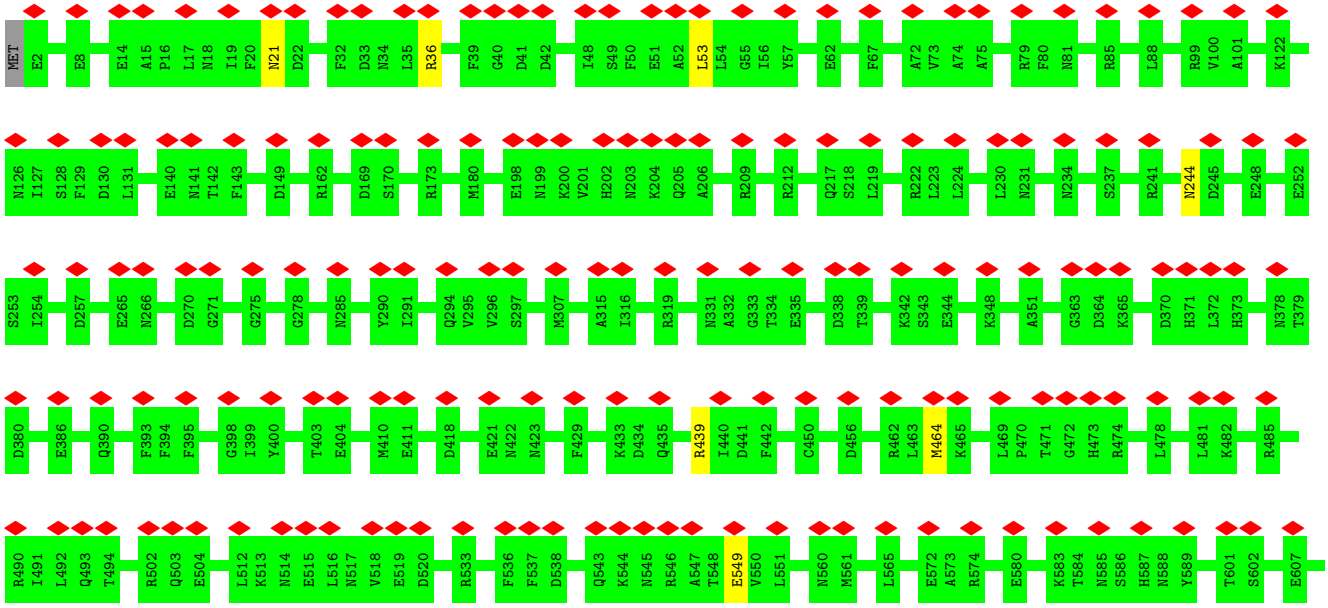


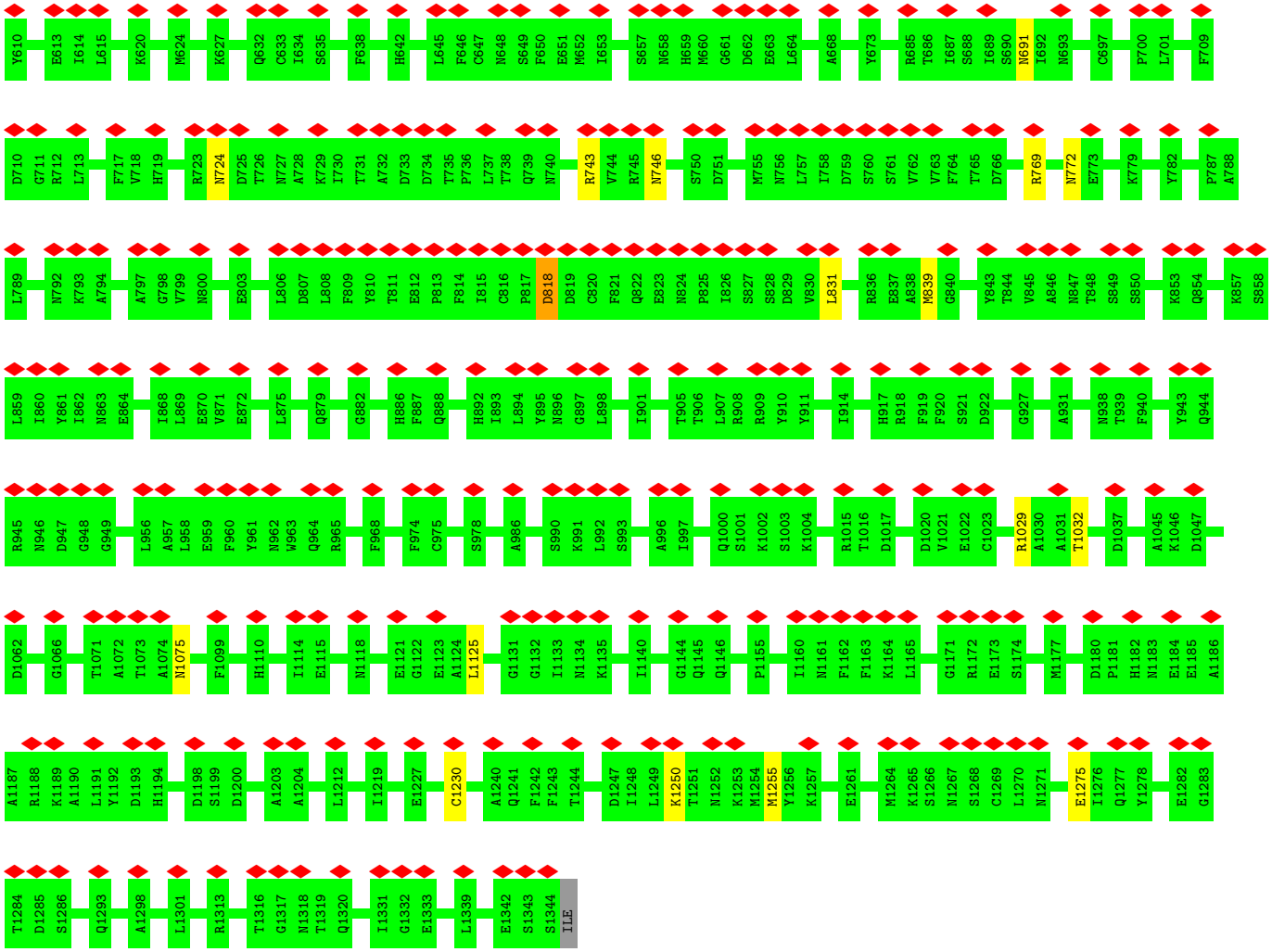


- Molecule 1: Major capsid protein

Chain H:

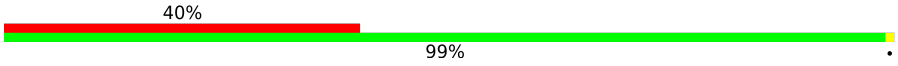


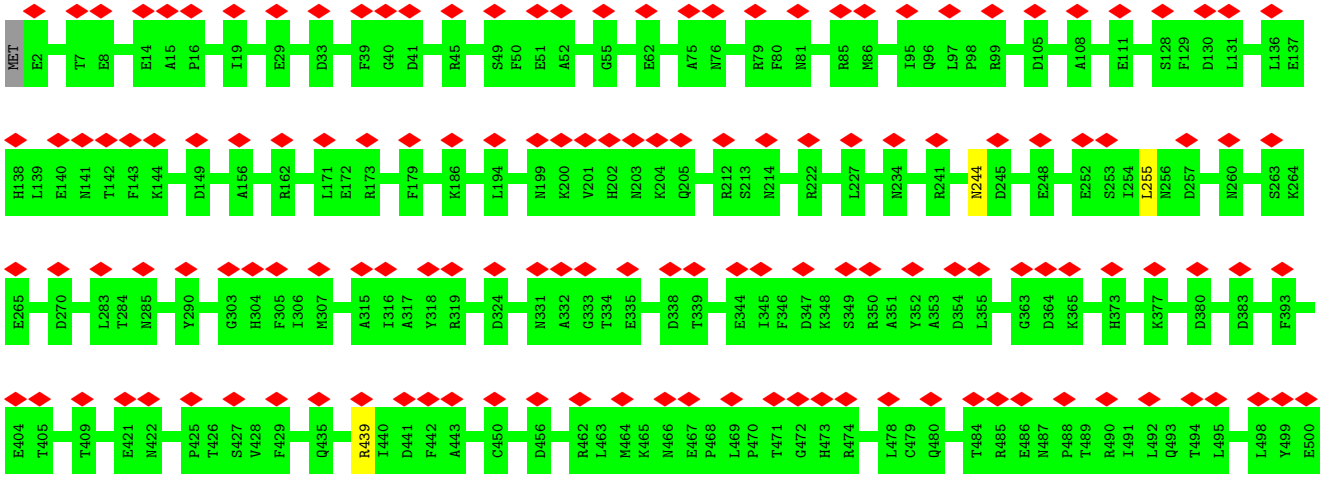


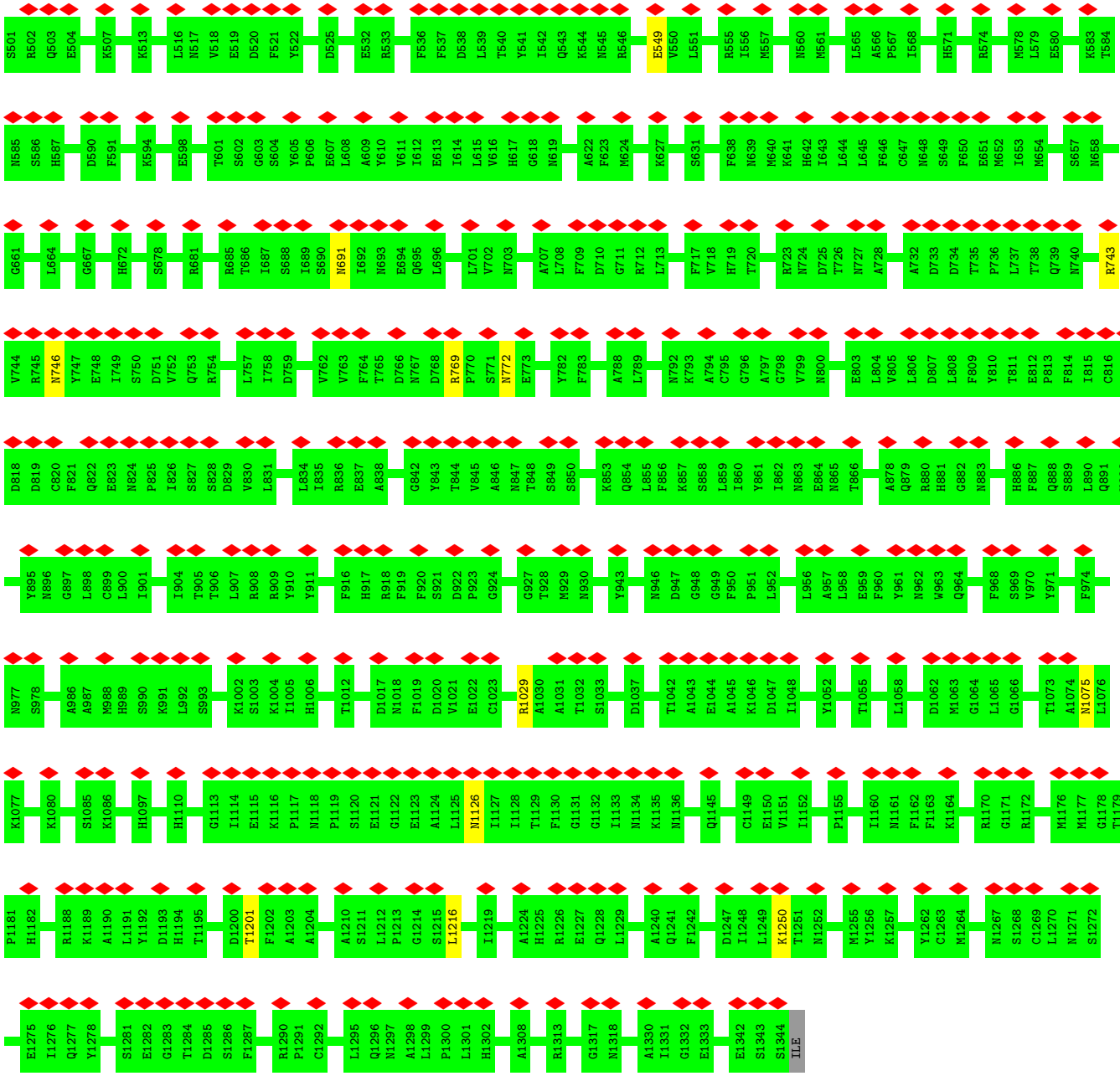


- Molecule 1: Major capsid protein

Chain I:

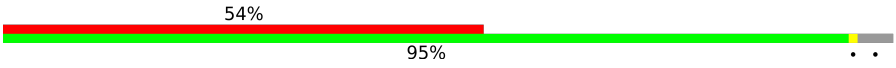


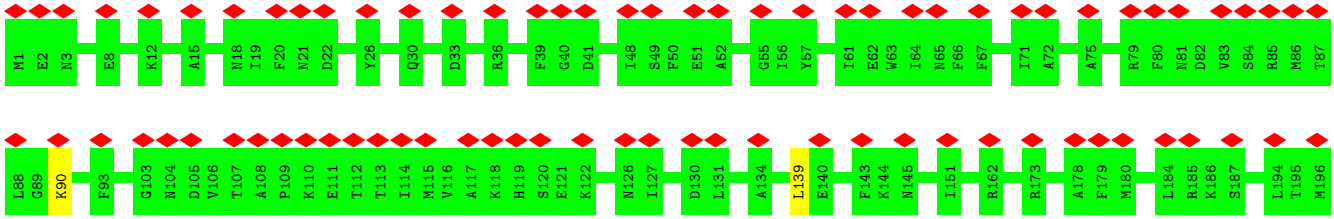


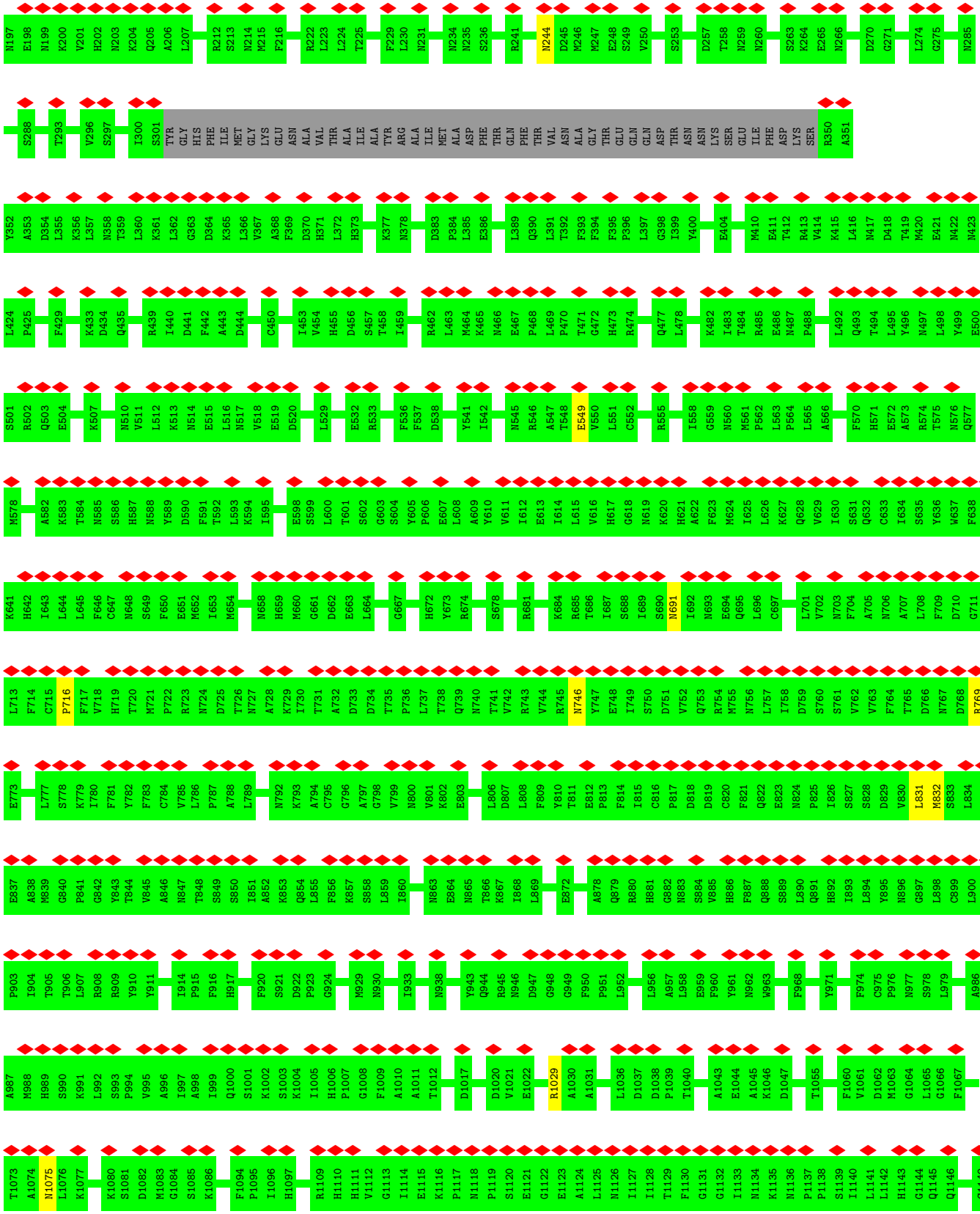


- Molecule 1: Major capsid protein

Chain q:



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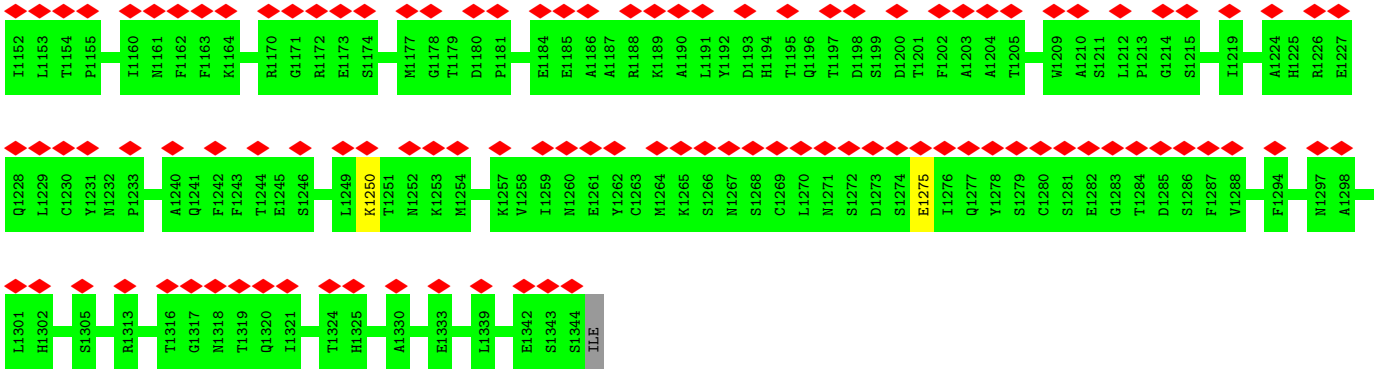
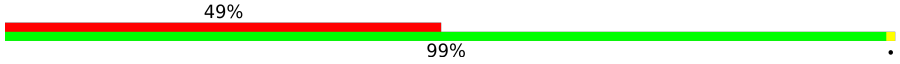
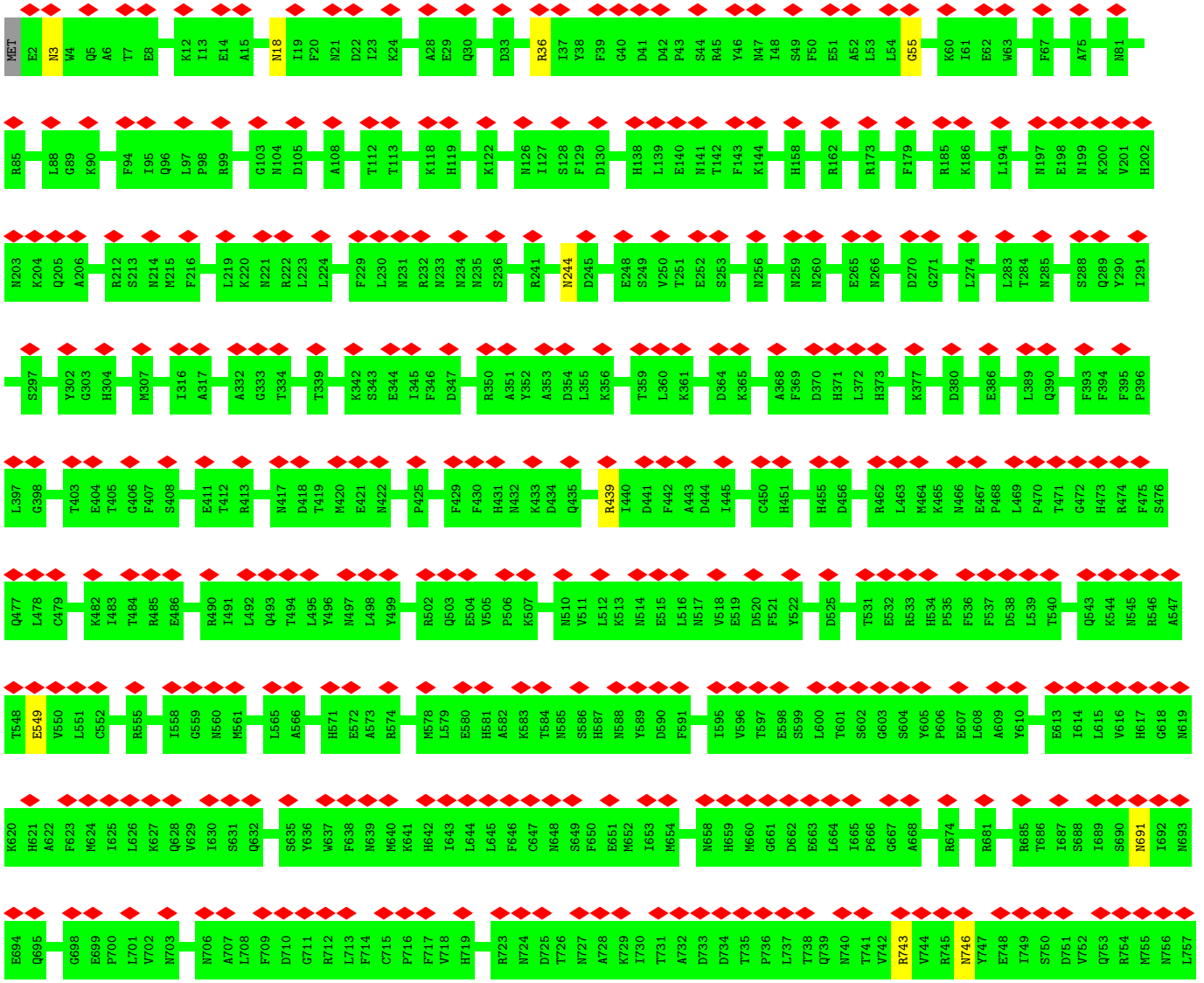
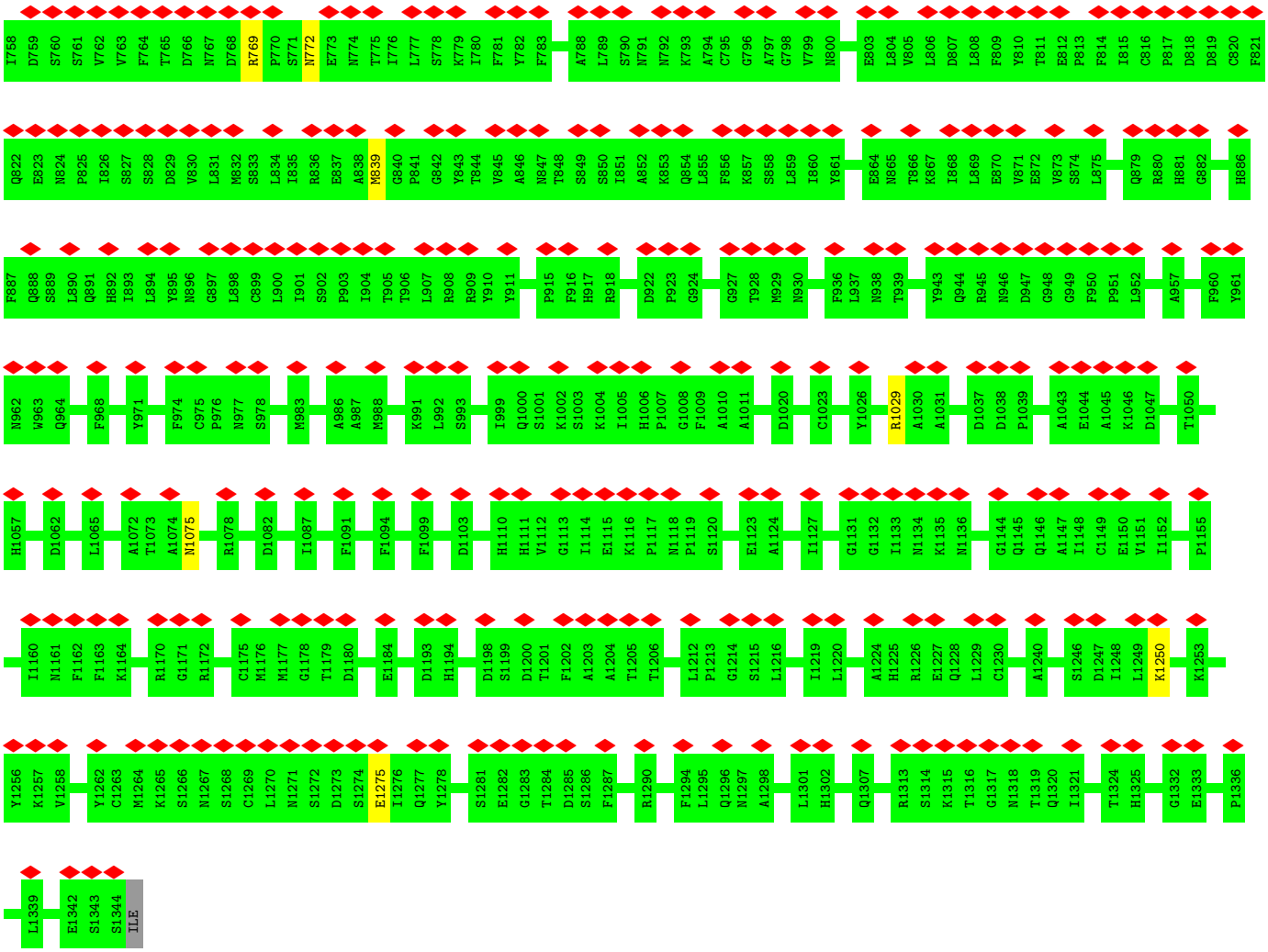


• Molecule 1: Major capsid protein

Chain r:

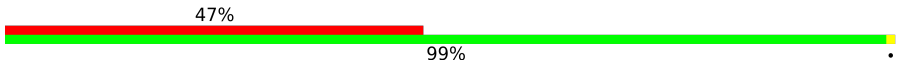


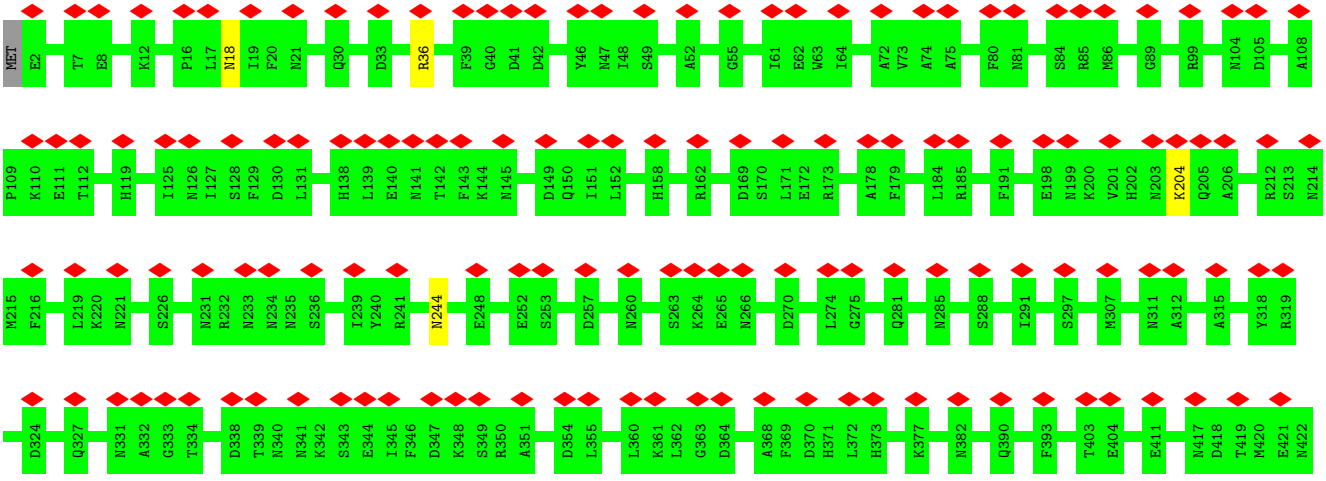


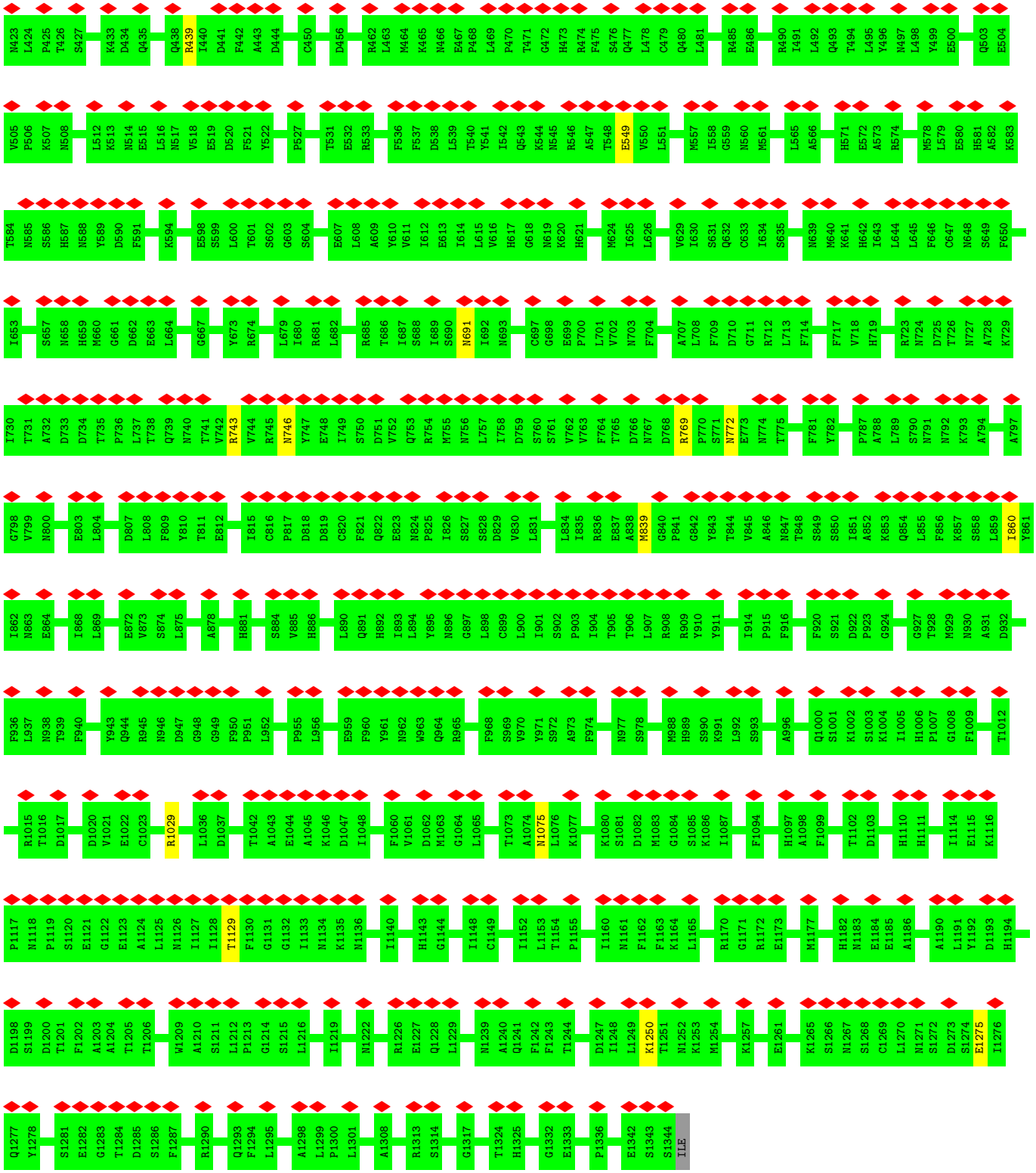


• Molecule 1: Major capsid protein

Chain s:

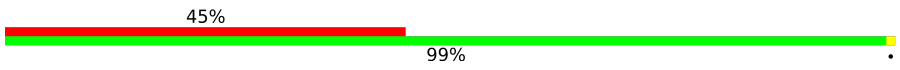


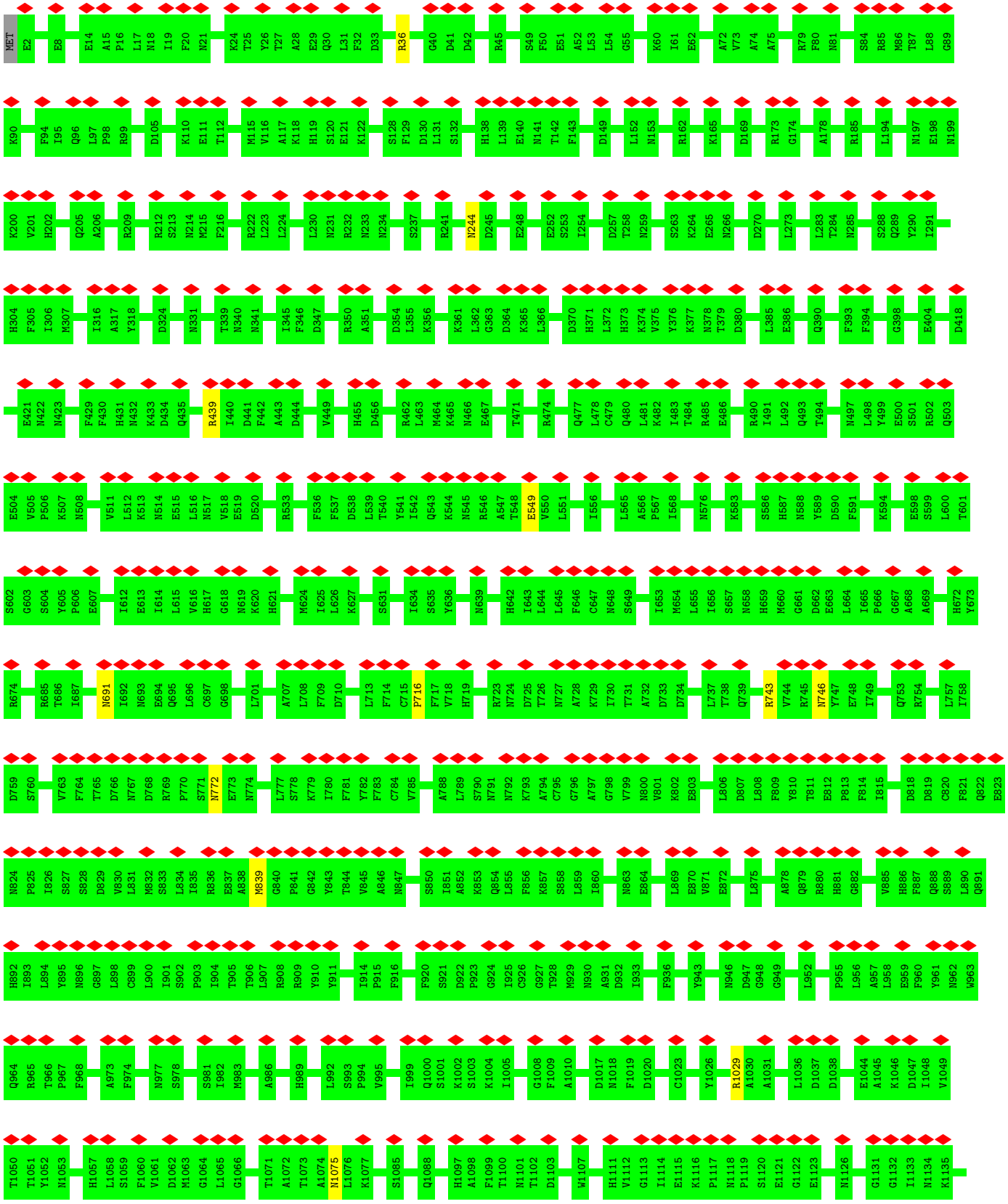




• Molecule 1: Major capsid protein

Chain t:

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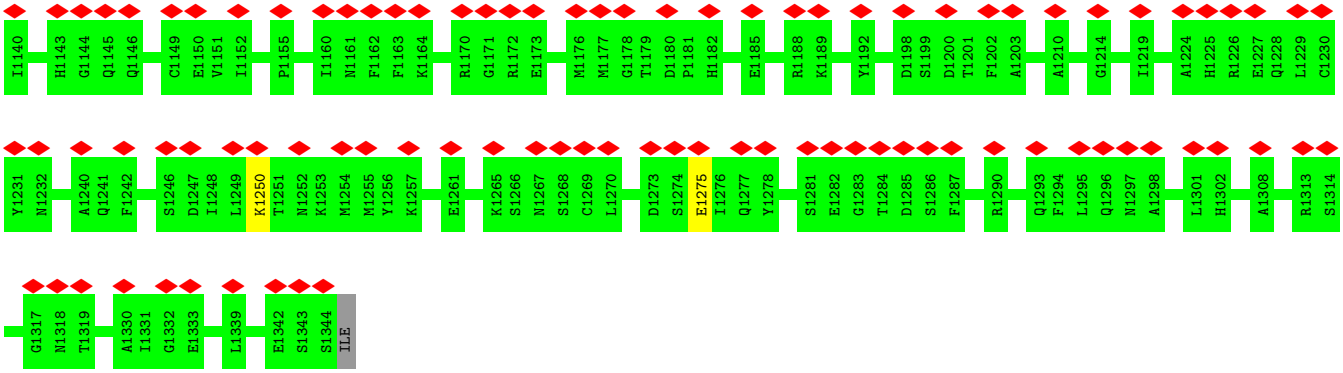
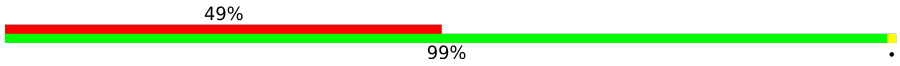
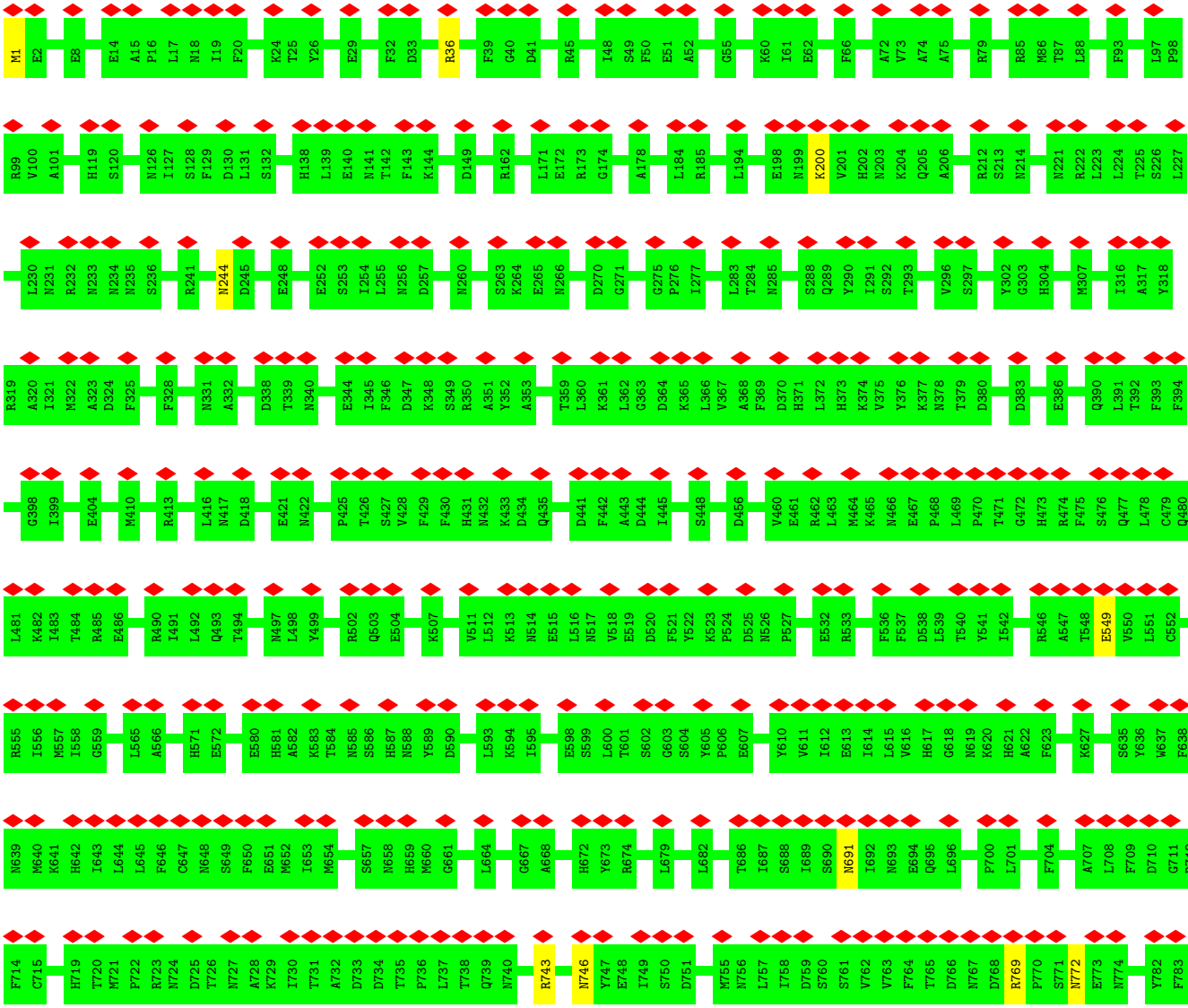
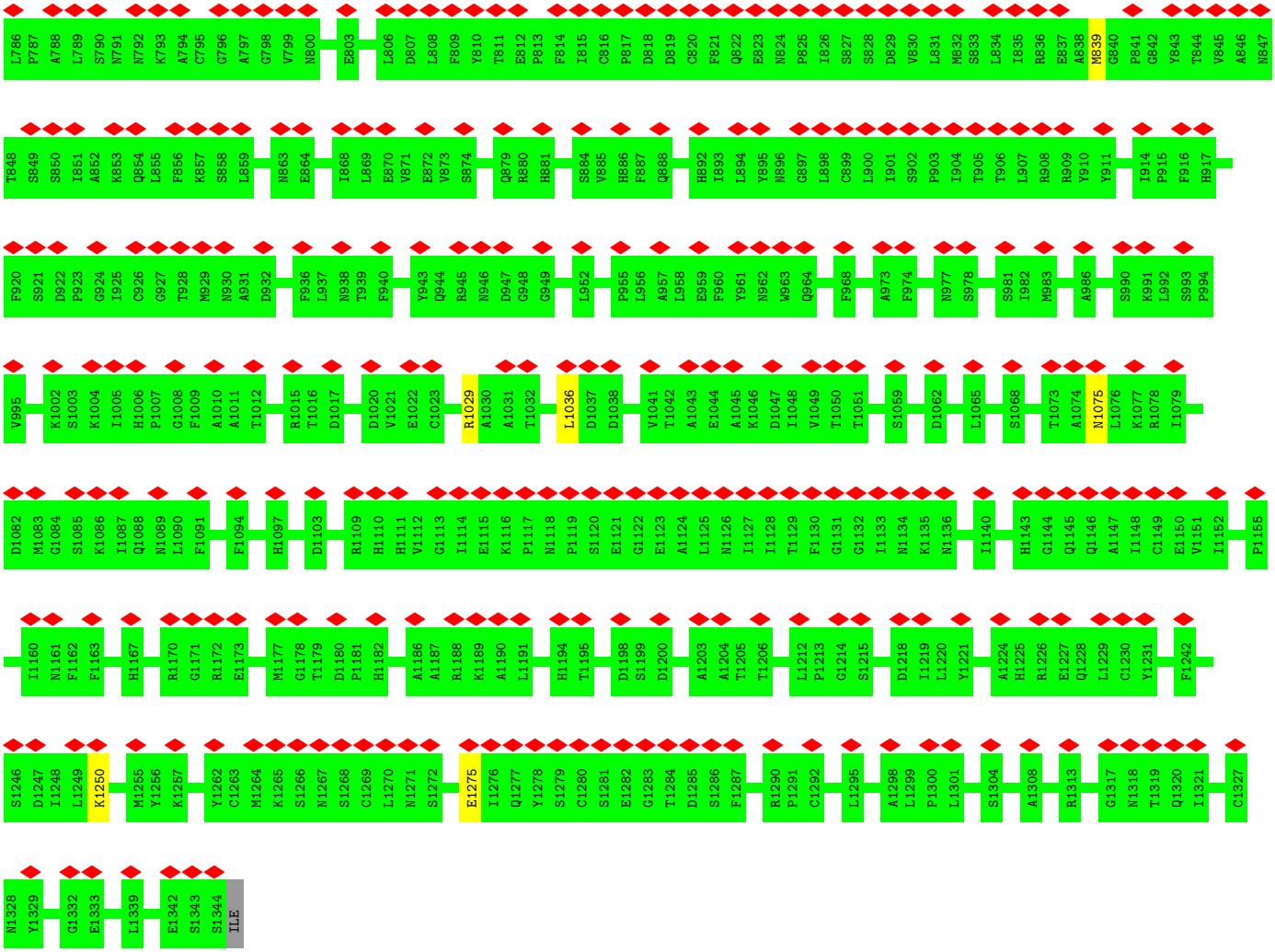


• Molecule 1: Major capsid protein

Chain u:

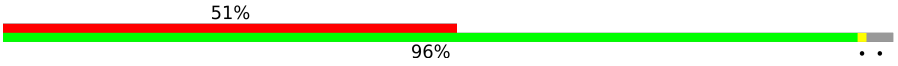


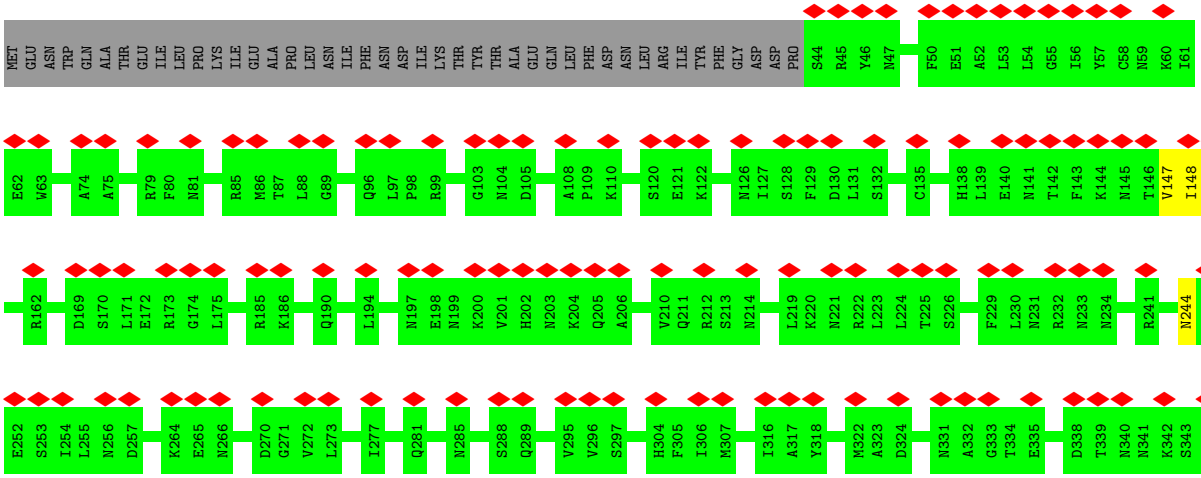


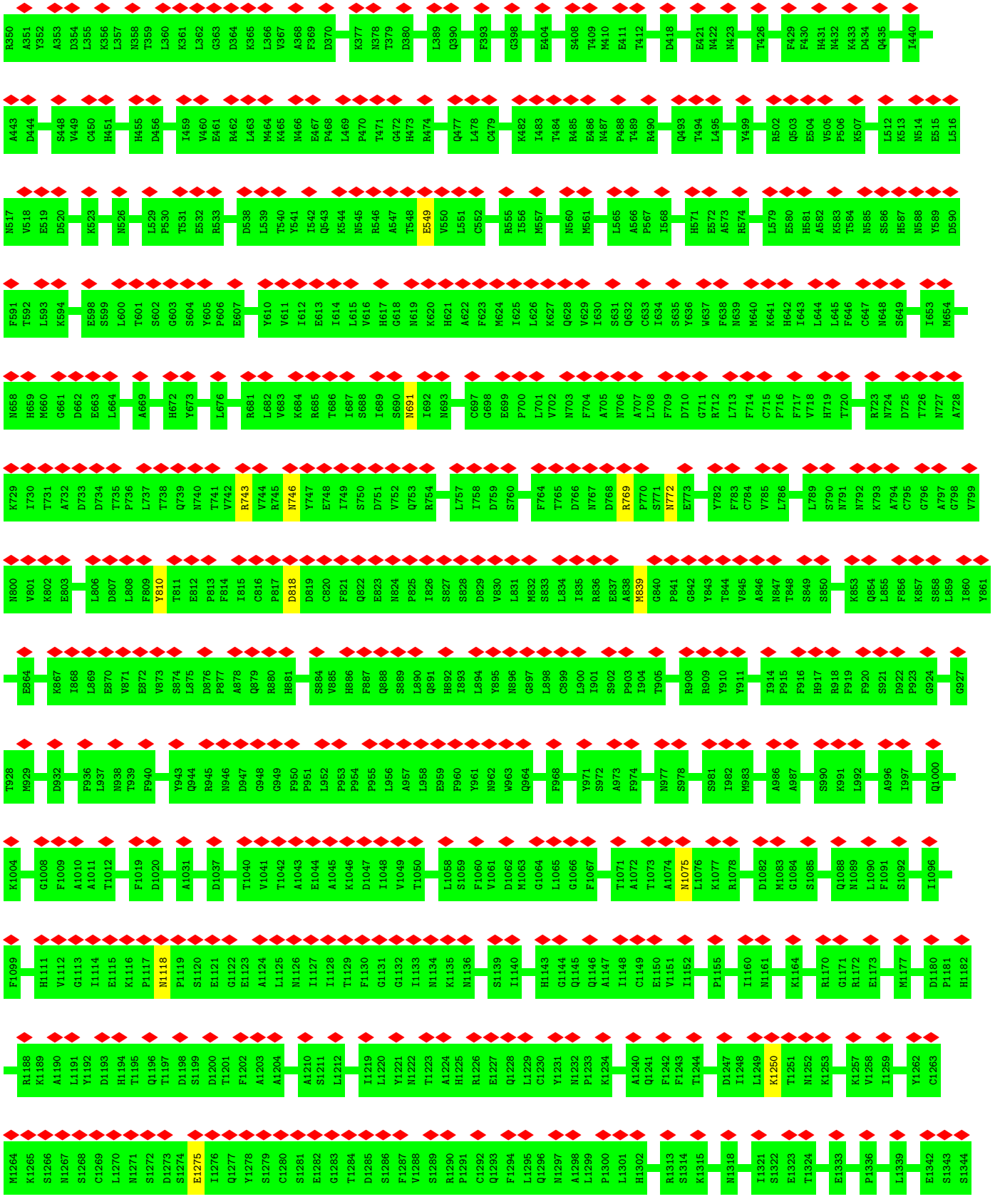


• Molecule 1: Major capsid protein

Chain v:



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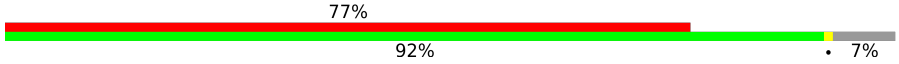
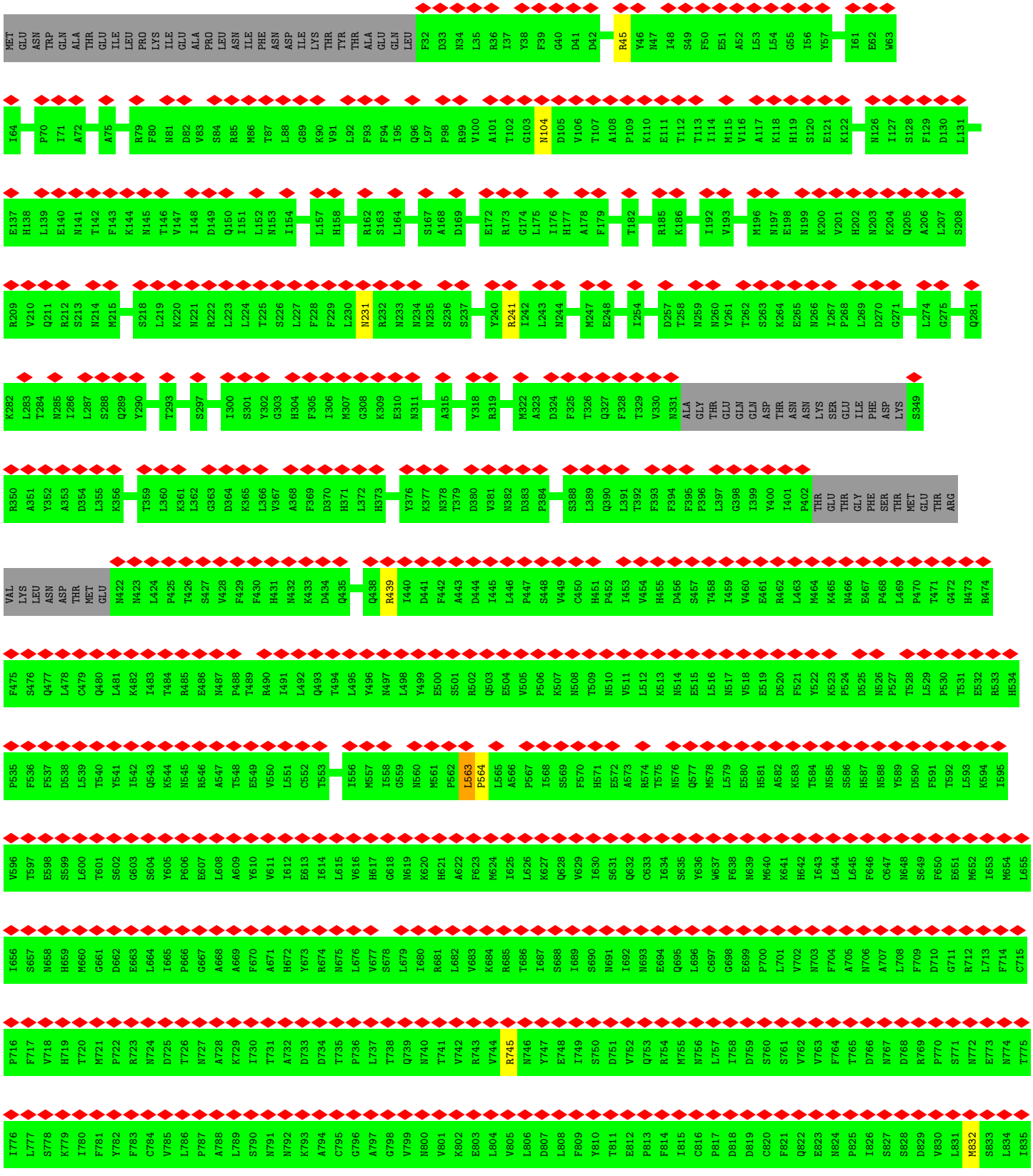
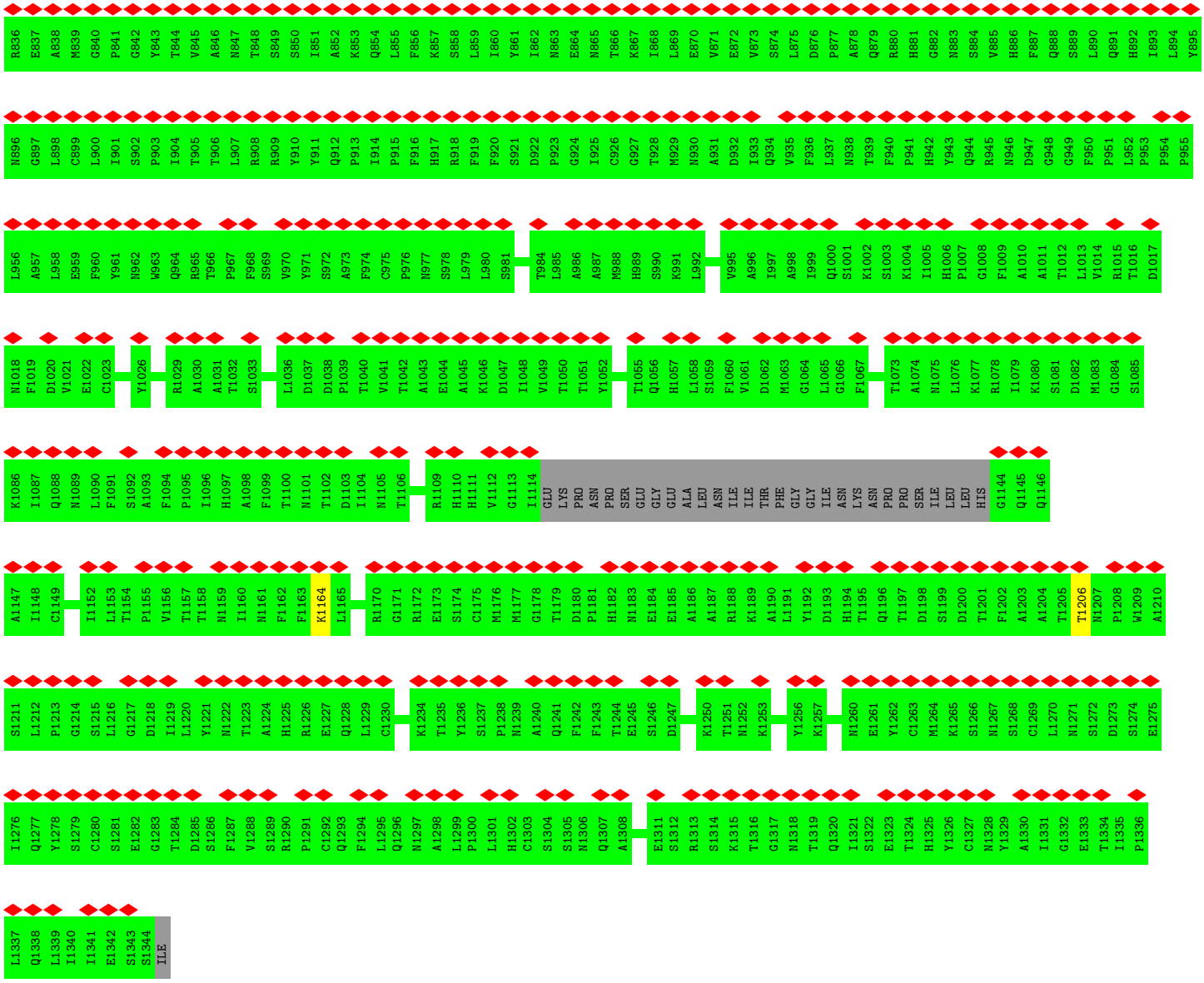
ILE

• Molecule 1: Major capsid protein

Chain w:

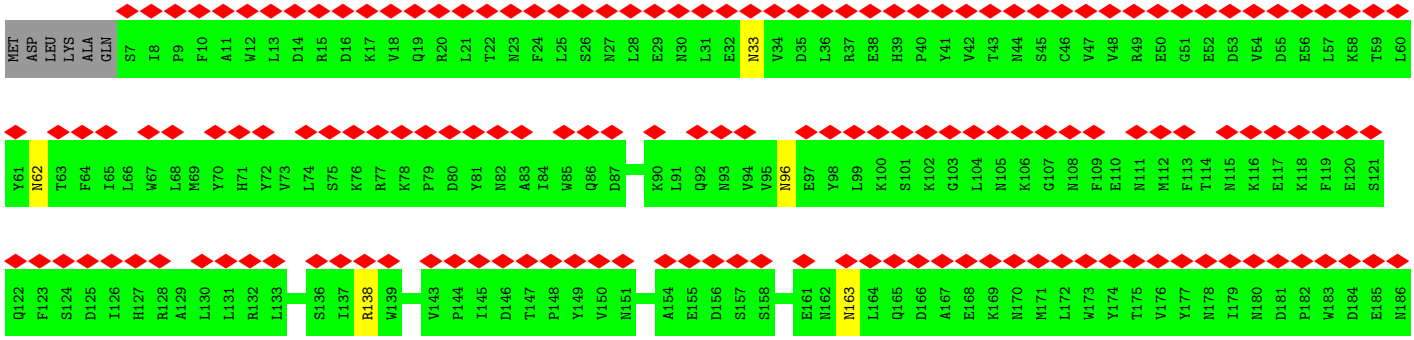


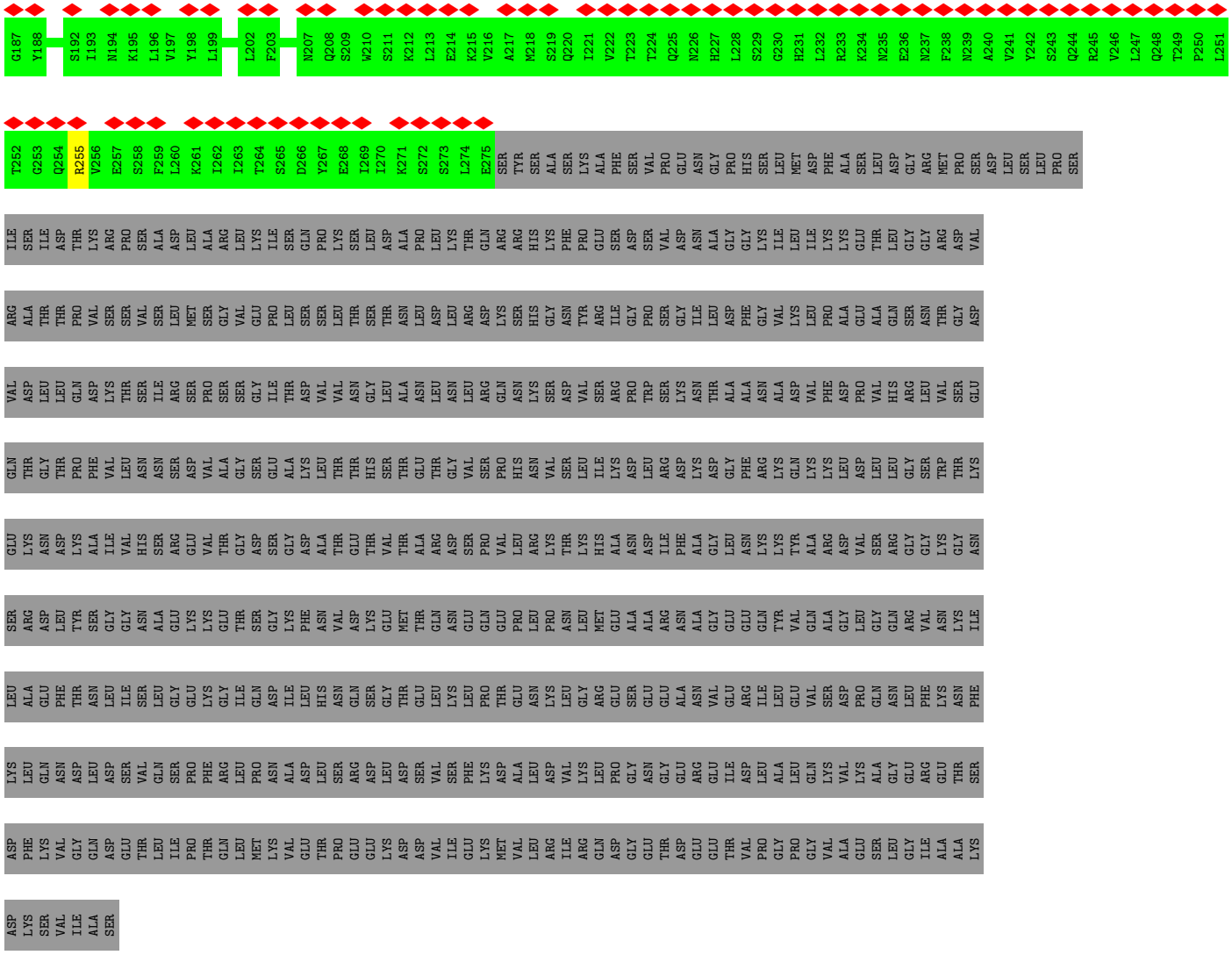




• Molecule 2: Large structural phosphoprotein

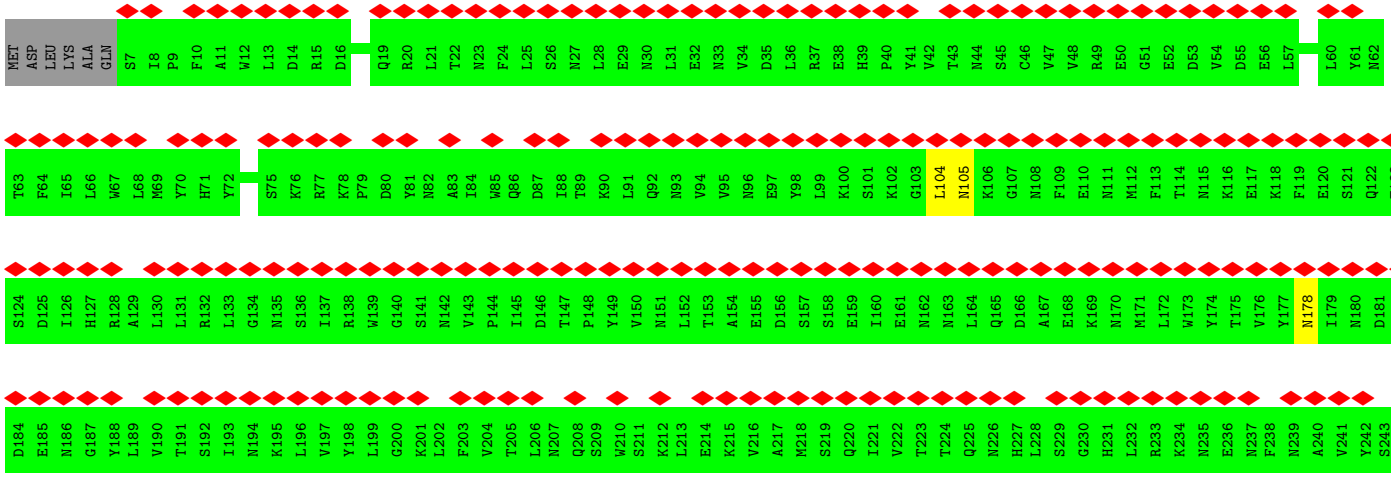
Chain e:

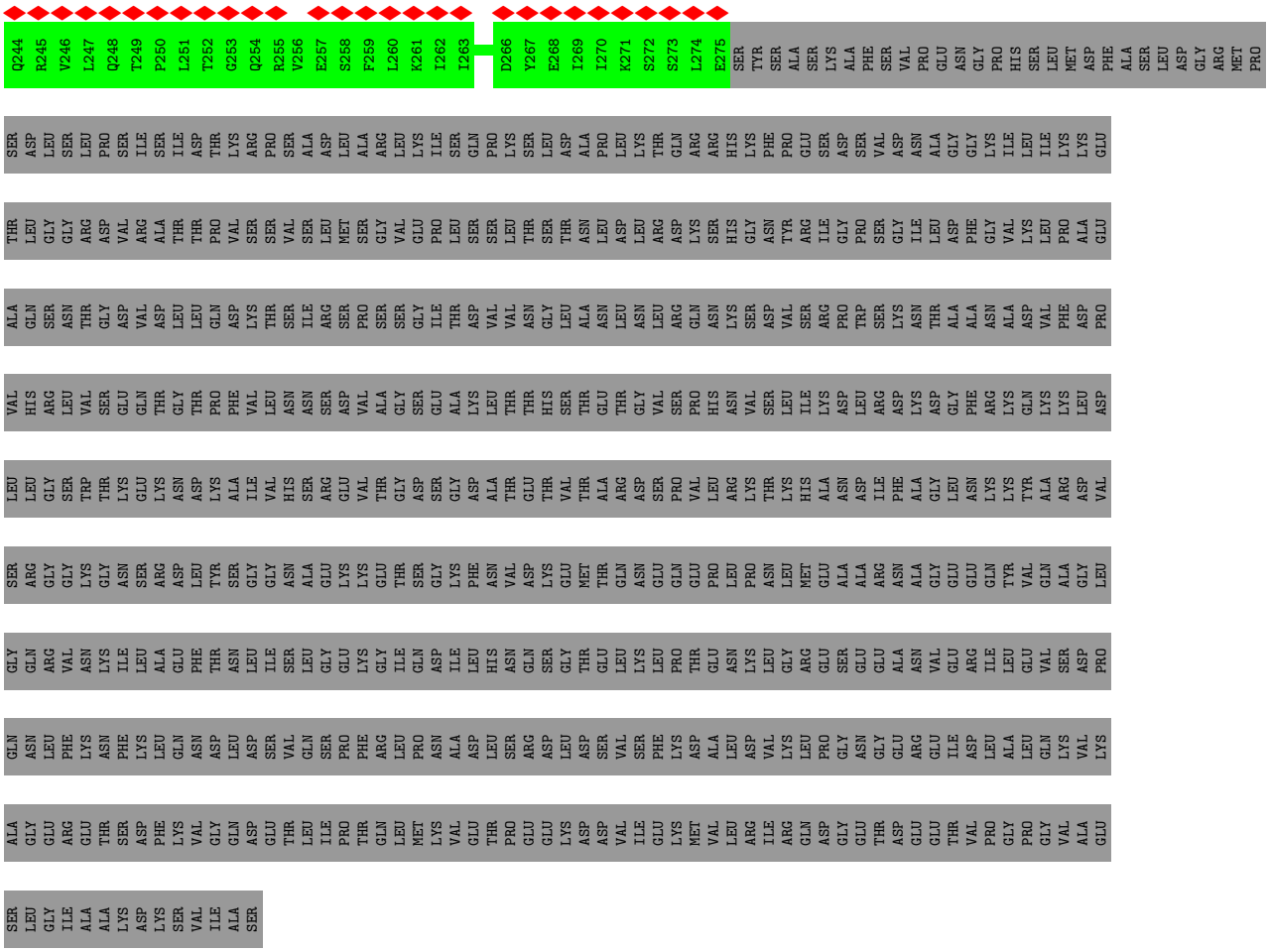




• Molecule 2: Large structural phosphoprotein

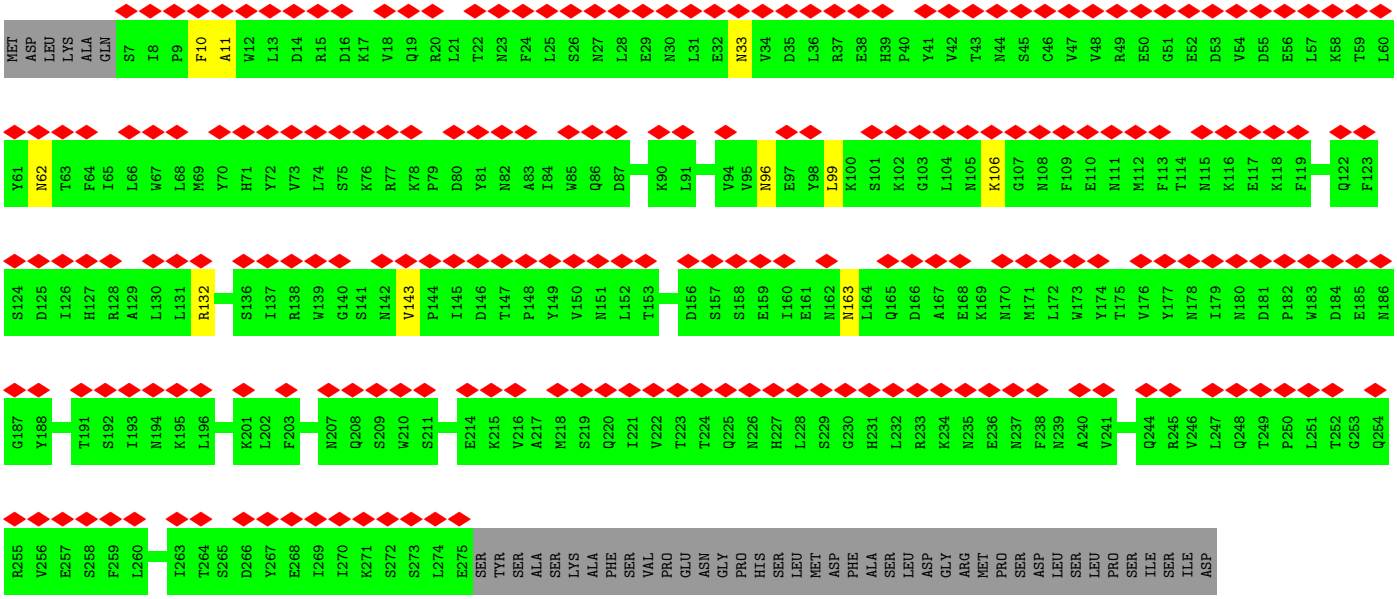
Chain f:

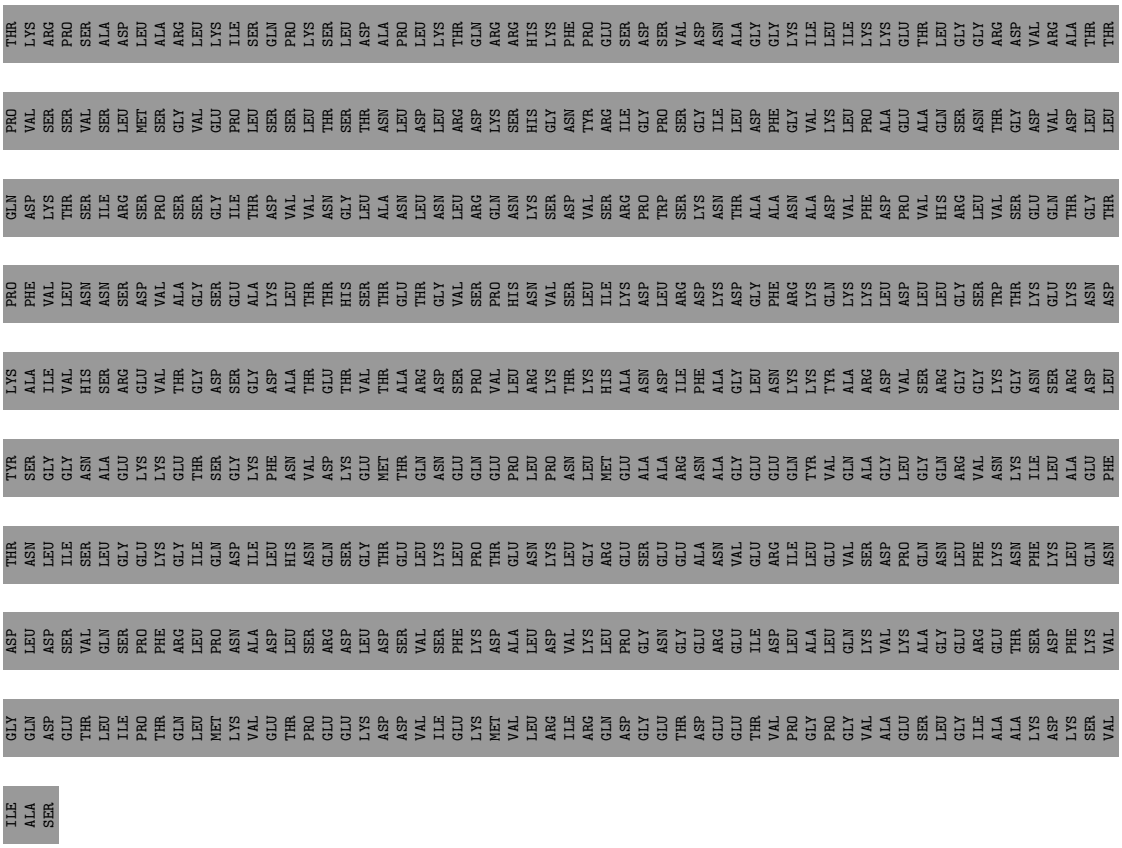




• Molecule 2: Large structural phosphoprotein

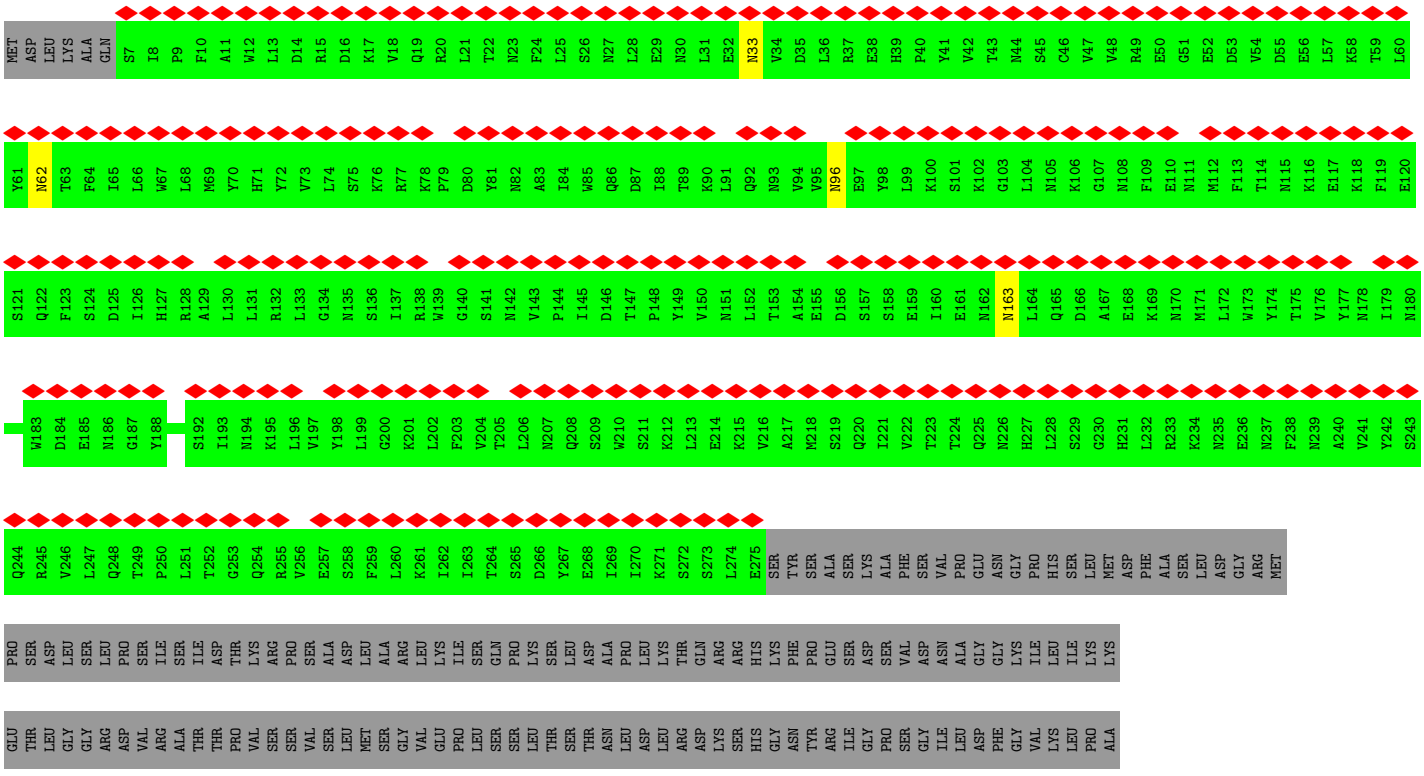
Chain g:

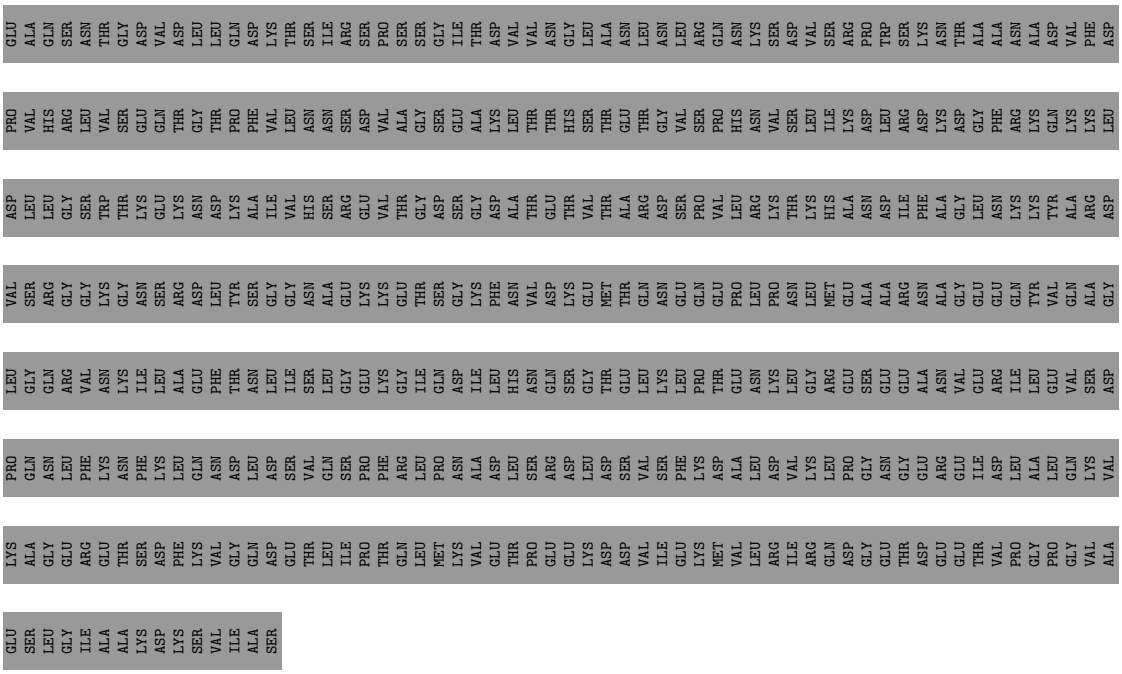




• Molecule 2: Large structural phosphoprotein

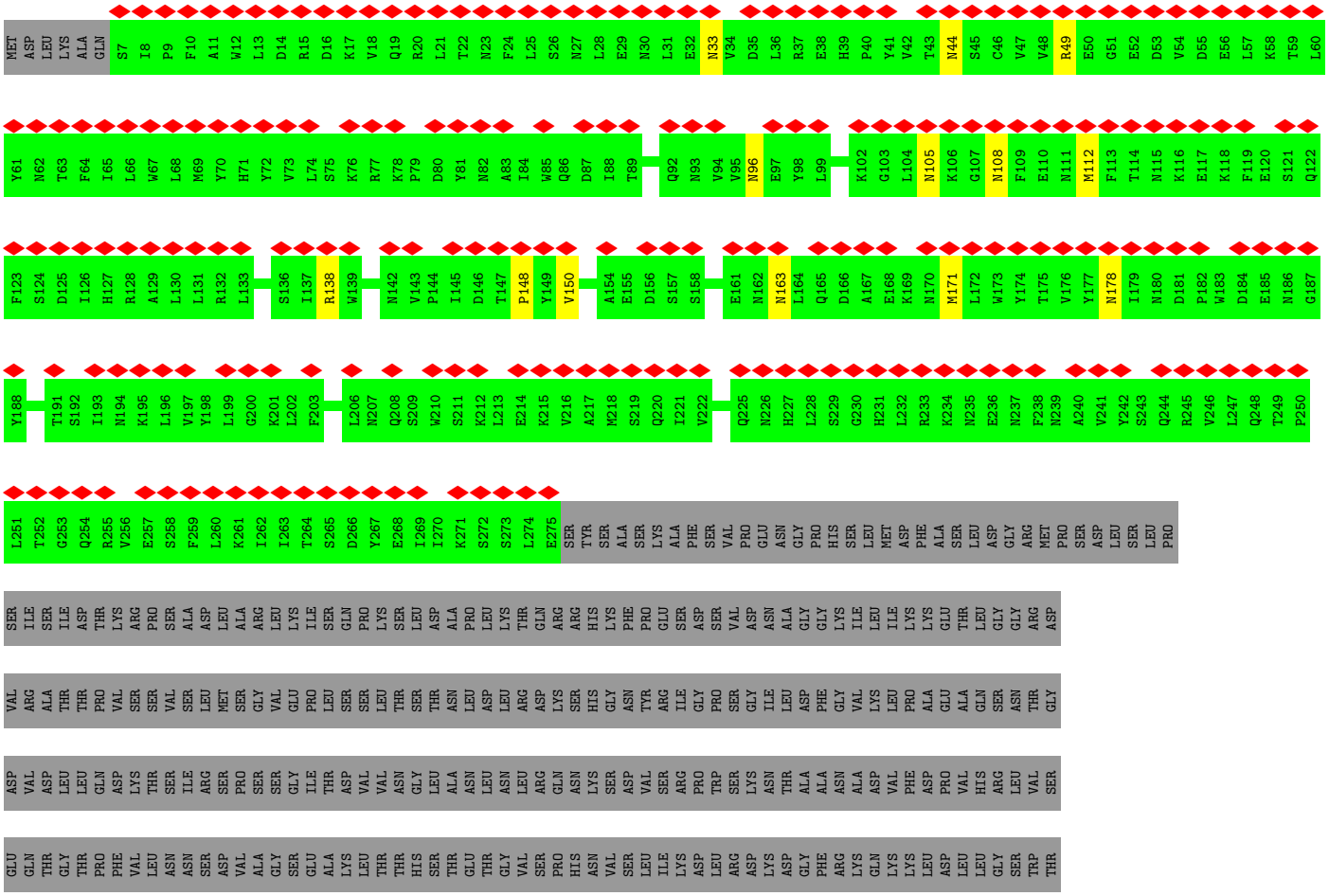
Chain h:





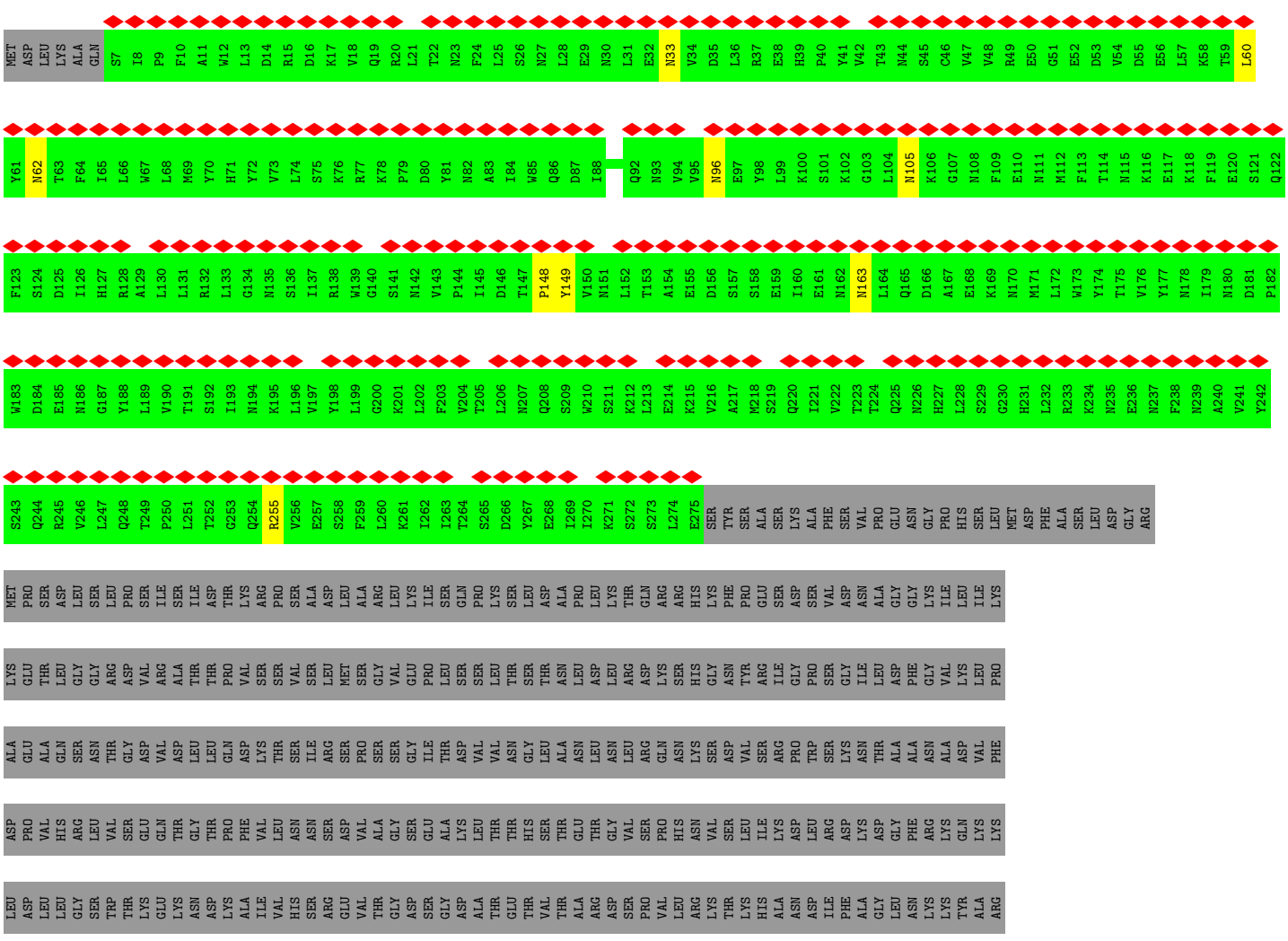
• Molecule 2: Large structural phosphoprotein

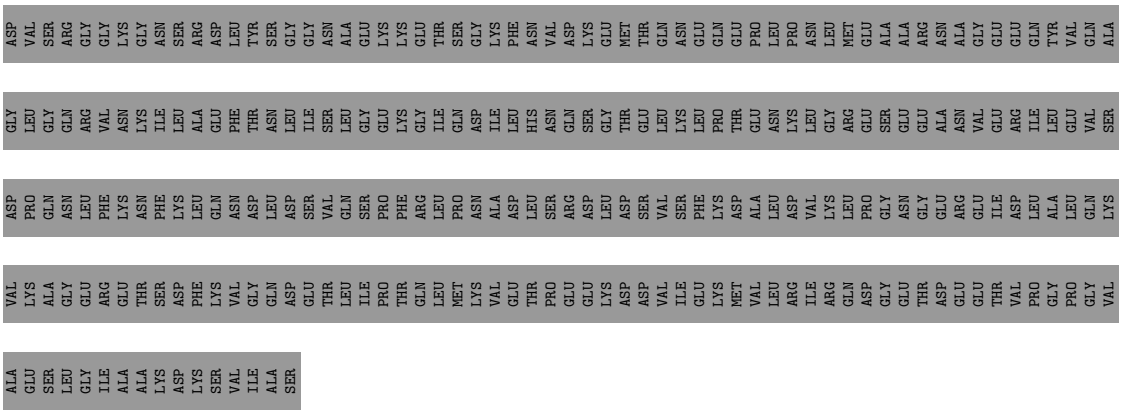
Chain i:



• Molecule 2: Large structural phosphoprotein

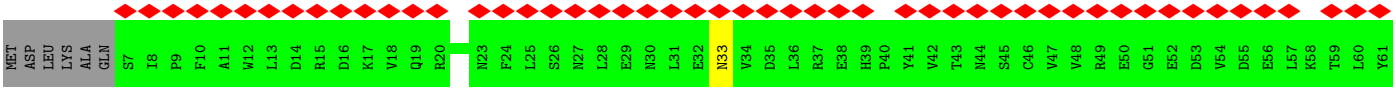
Chain j:

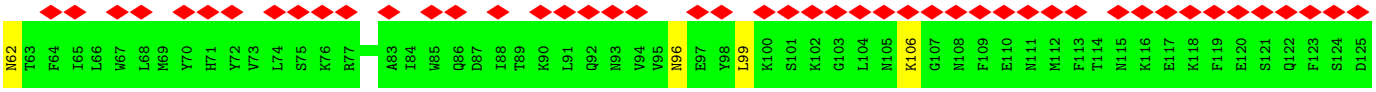


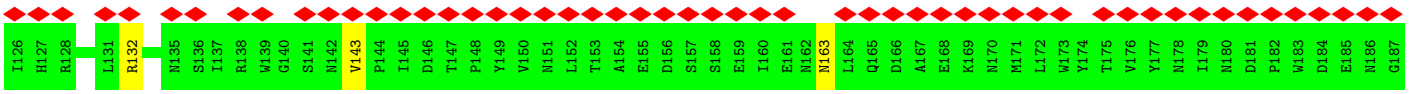


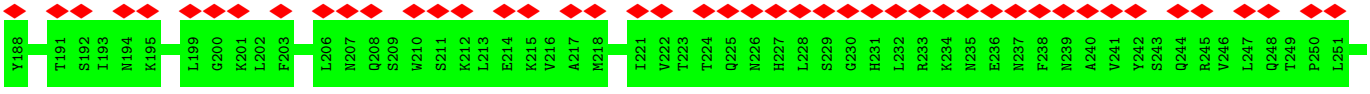
• Molecule 2: Large structural phosphoprotein

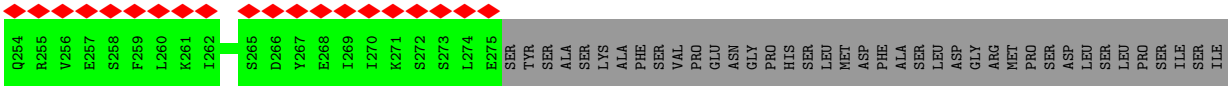
Chain k:

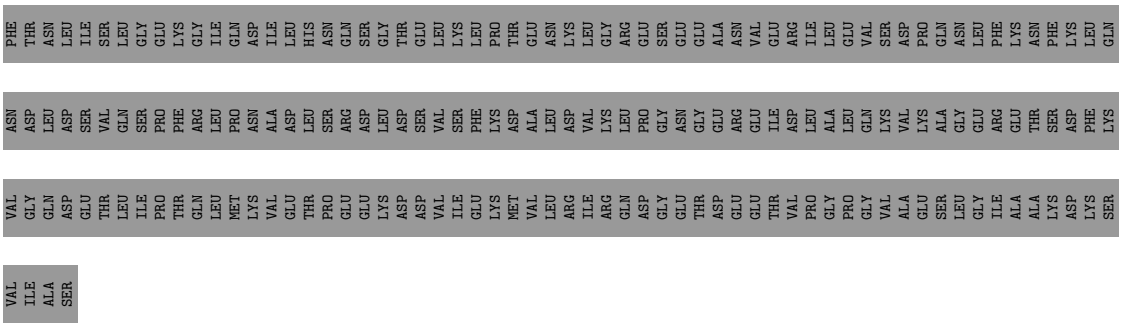






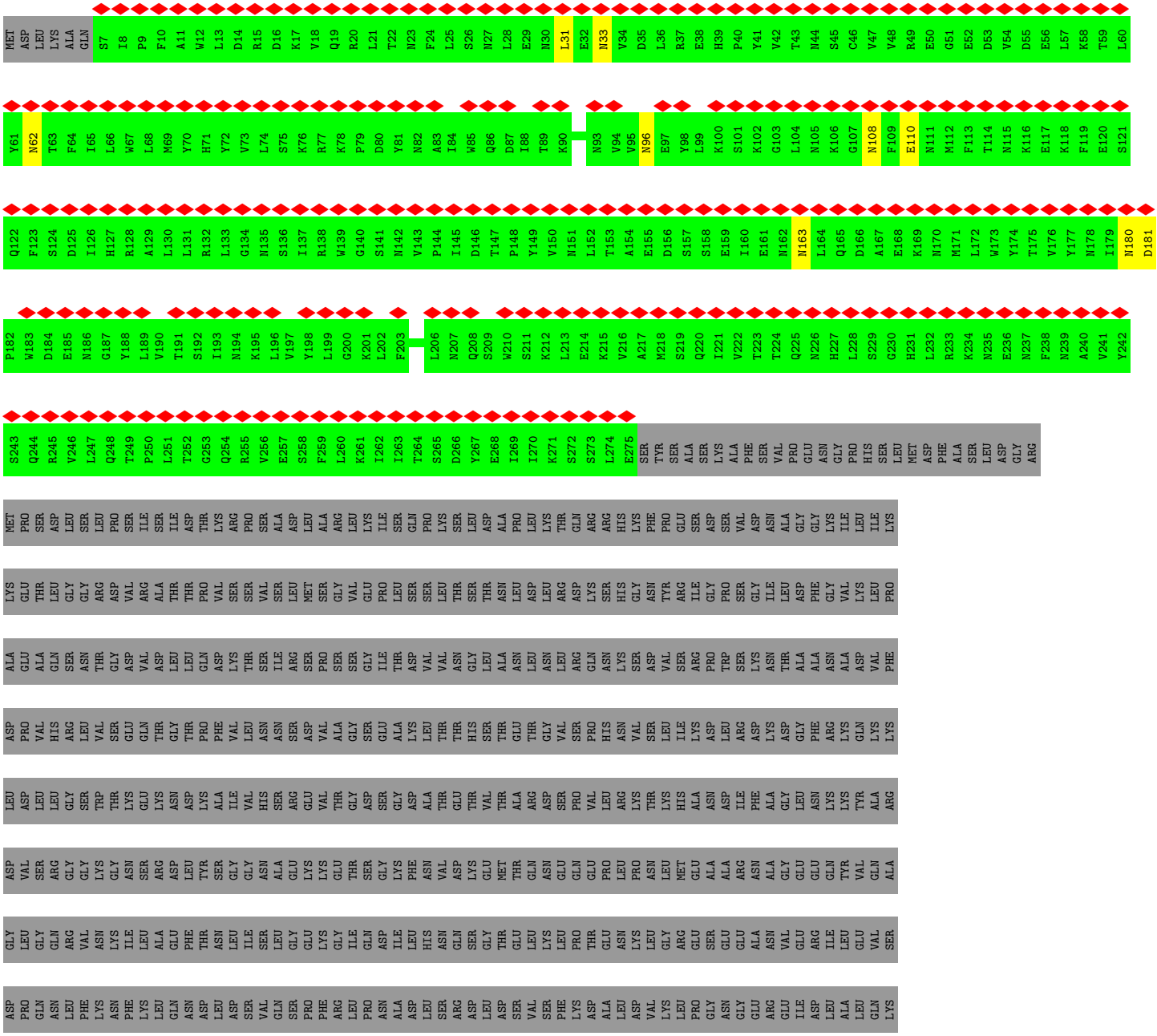


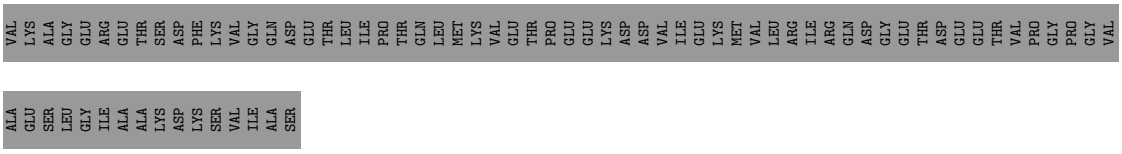




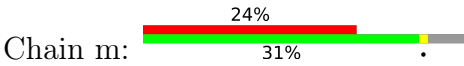
• Molecule 2: Large structural phosphoprotein

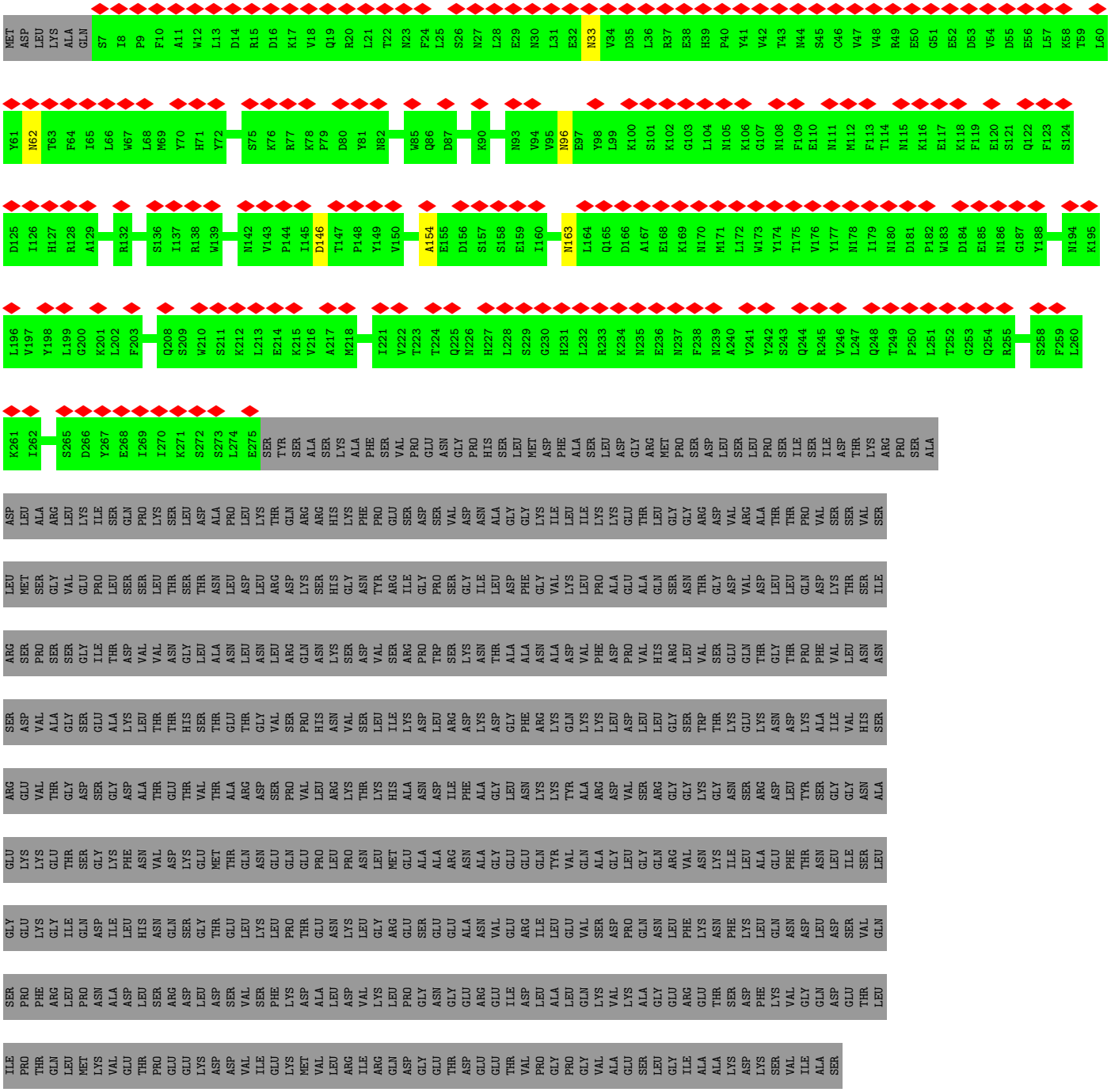
Chain l:



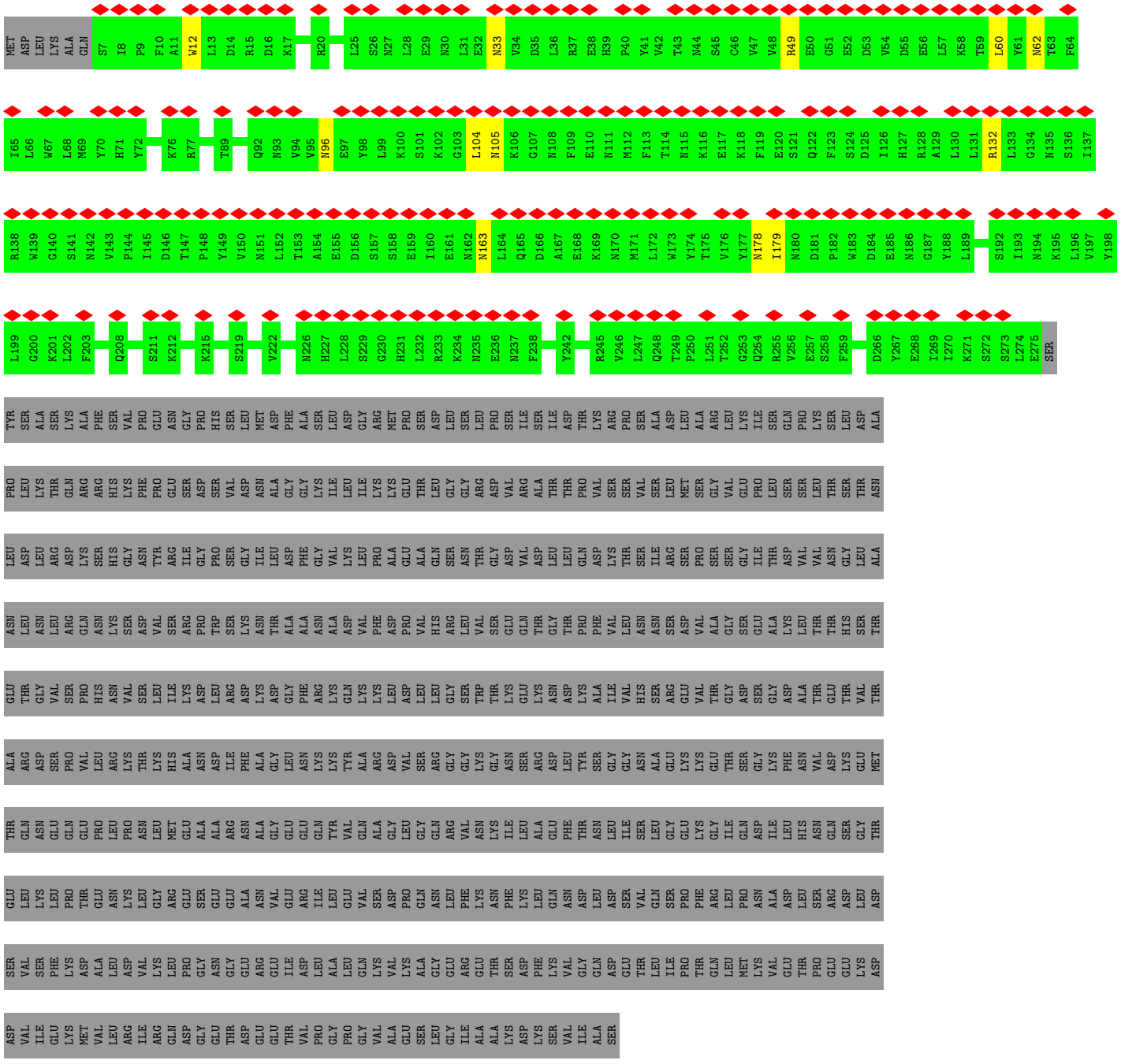


• Molecule 2: Large structural phosphoprotein

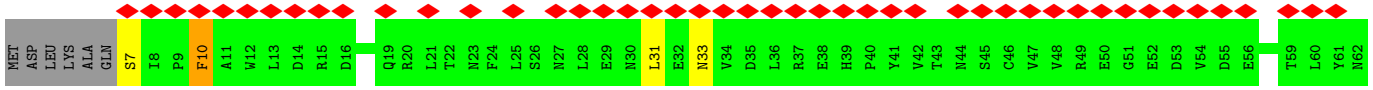


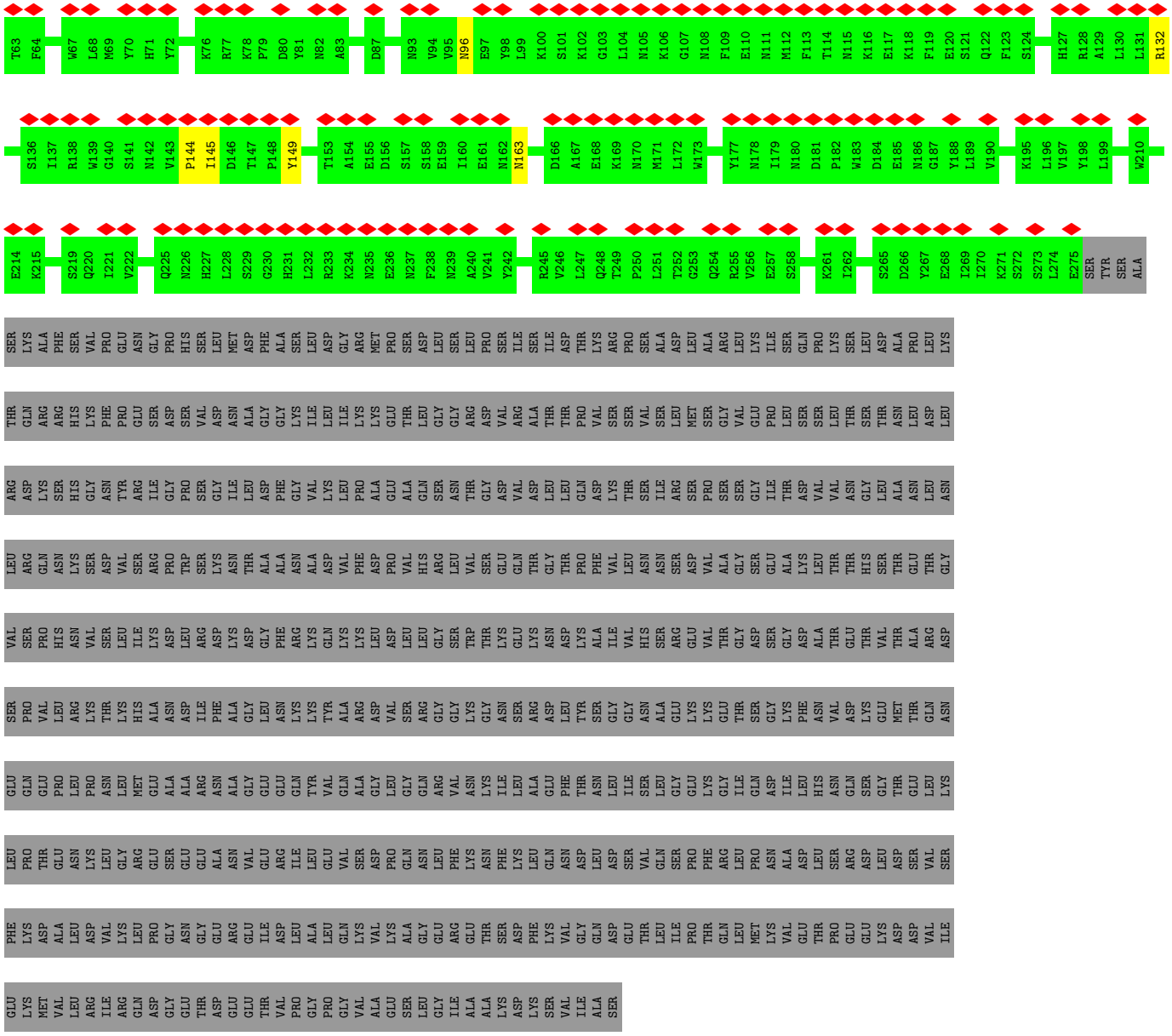


• Molecule 2: Large structural phosphoprotein



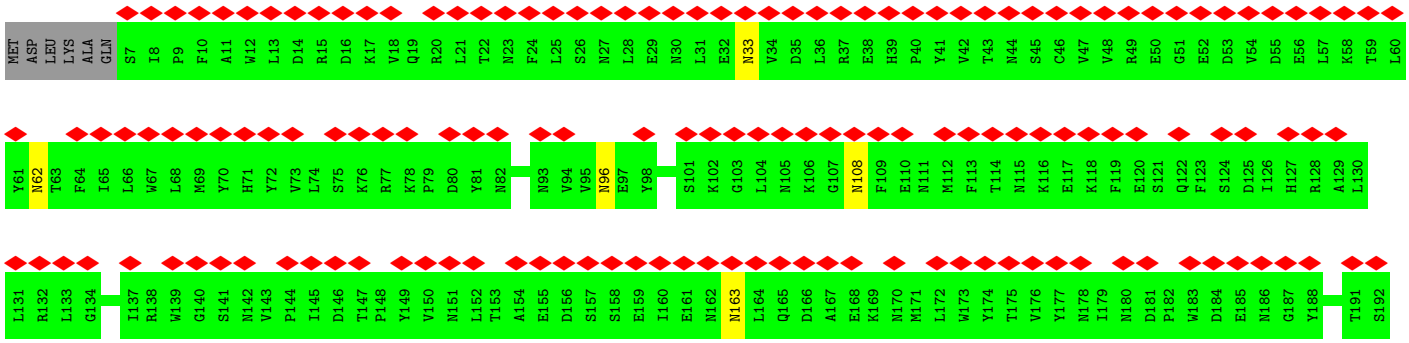
• Molecule 2: Large structural phosphoprotein

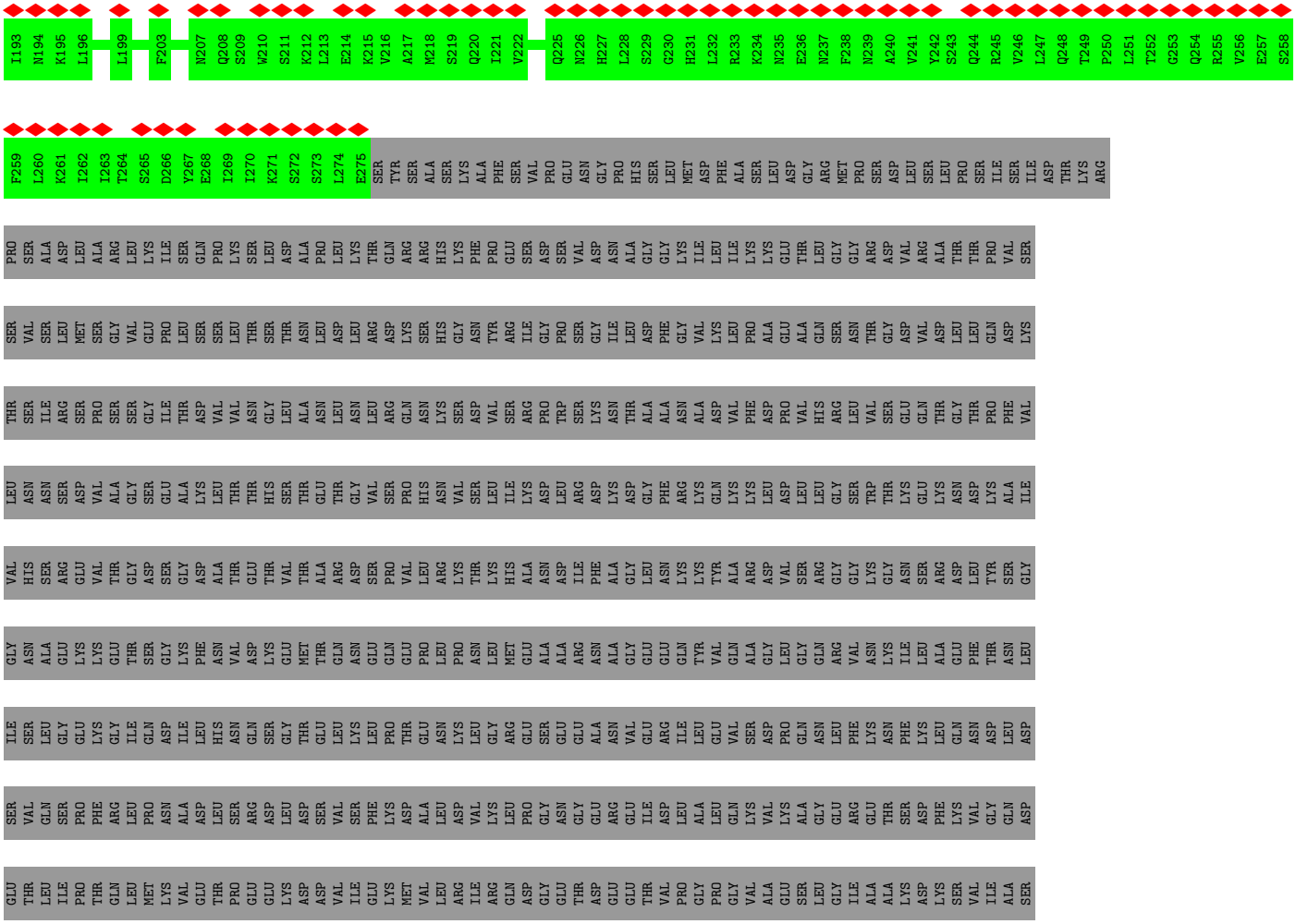




• Molecule 2: Large structural phosphoprotein

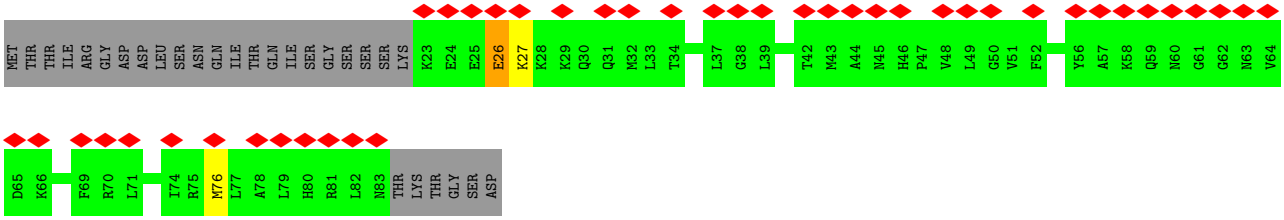
Chain p:





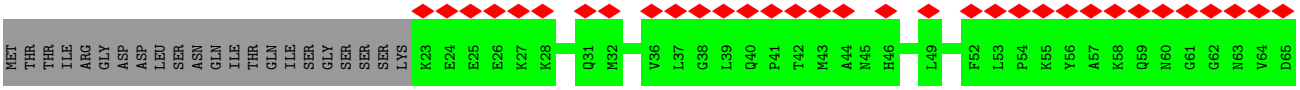
• Molecule 3: Small capsomere-interacting protein

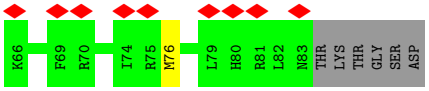
Chain J:



• Molecule 3: Small capsomere-interacting protein

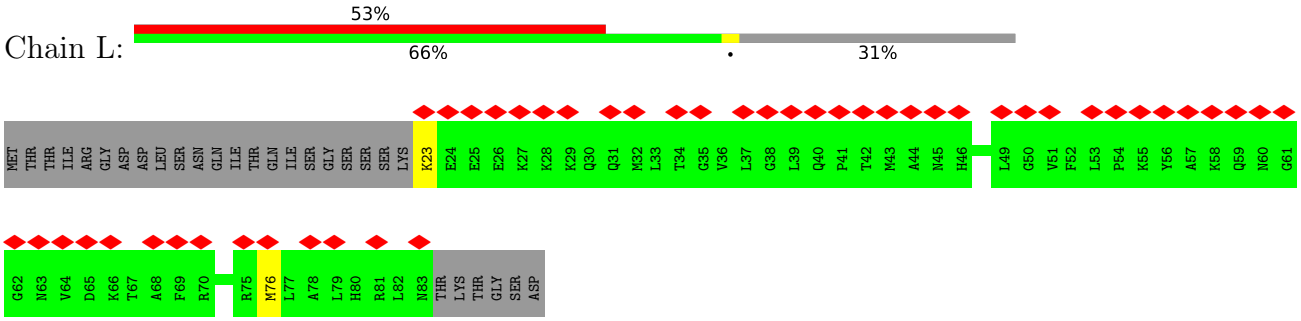
Chain K:





• Molecule 3: Small capsomere-interacting protein

Chain L:



• Molecule 3: Small capsomere-interacting protein

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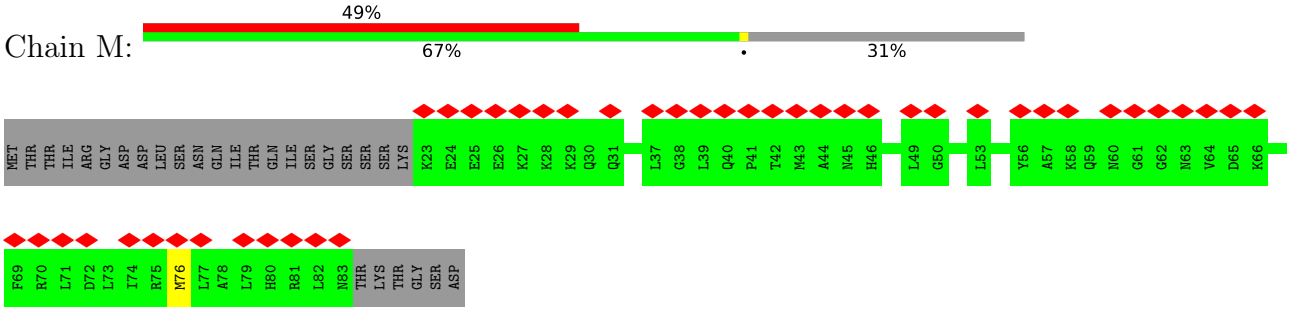
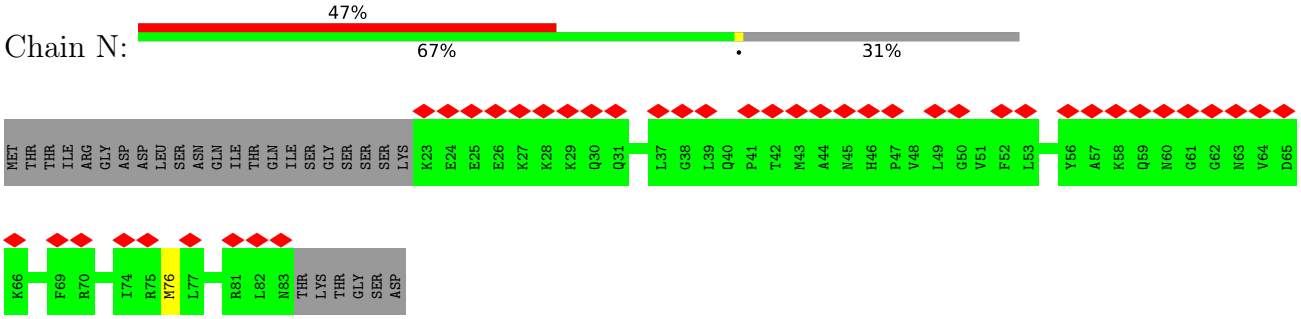


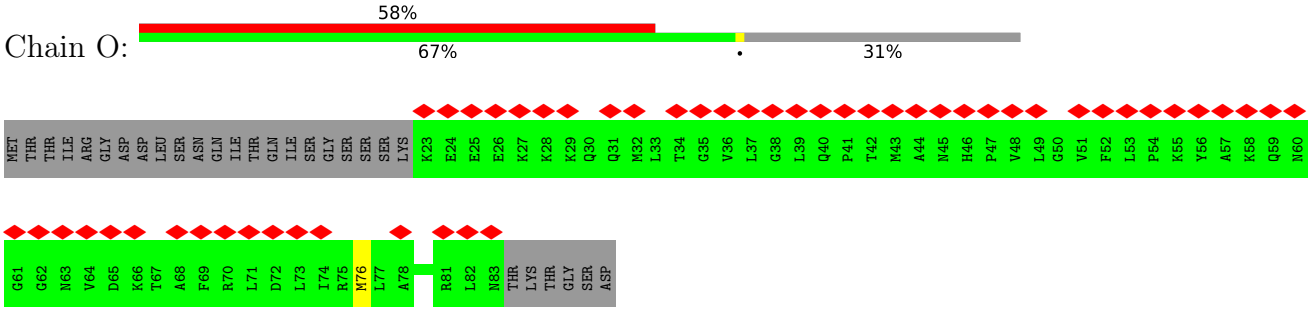
• Molecule 3: Small capsomere-interacting protein

Chain N:



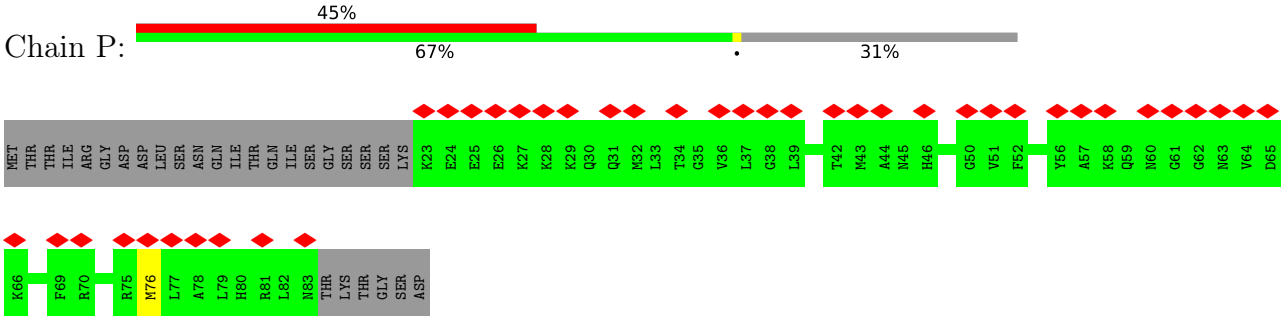
• Molecule 3: Small capsomere-interacting protein

Chain O:



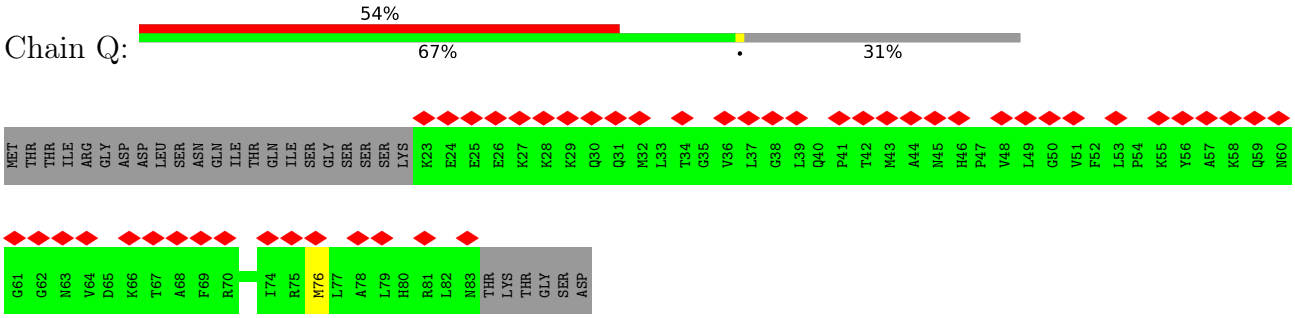
• Molecule 3: Small capsomere-interacting protein

Chain P:



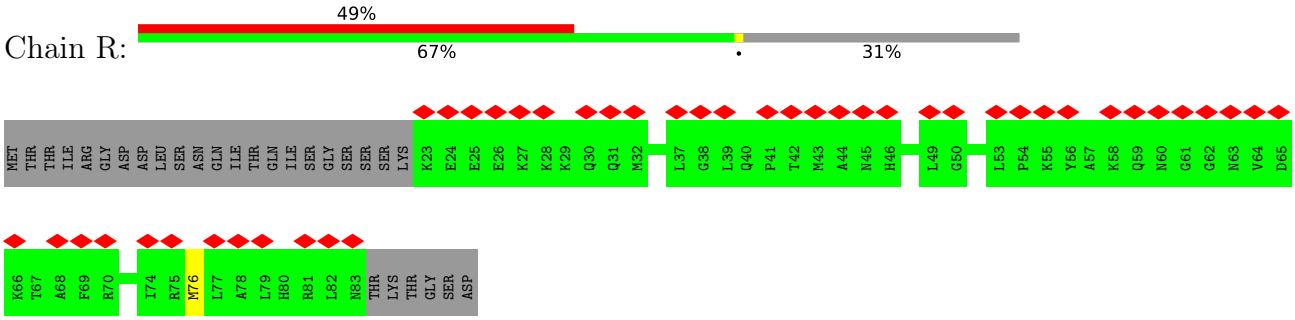
• Molecule 3: Small capsomere-interacting protein

Chain Q:



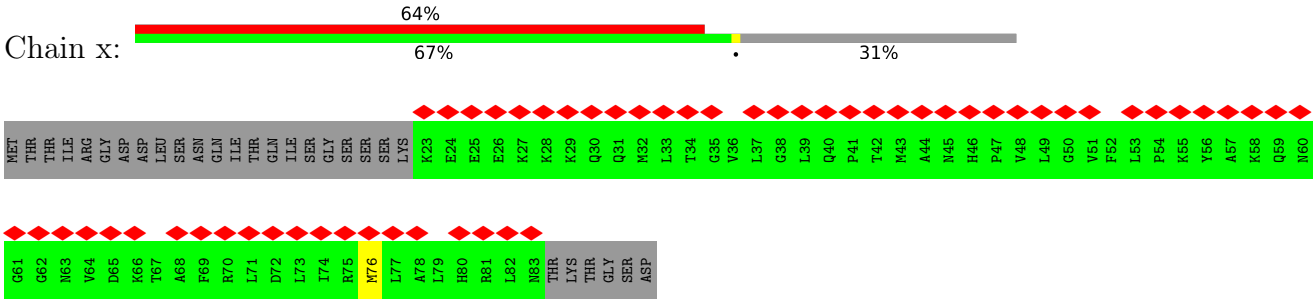
• Molecule 3: Small capsomere-interacting protein

Chain R:



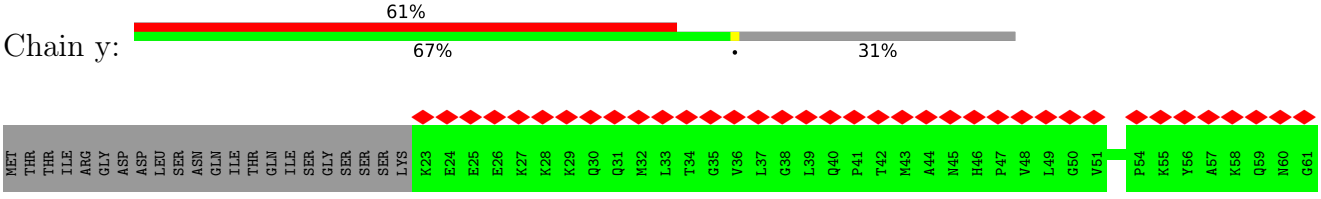
• Molecule 3: Small capsomere-interacting protein

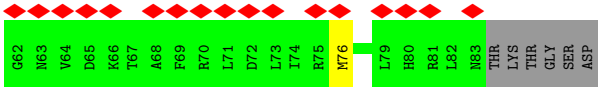
Chain x:



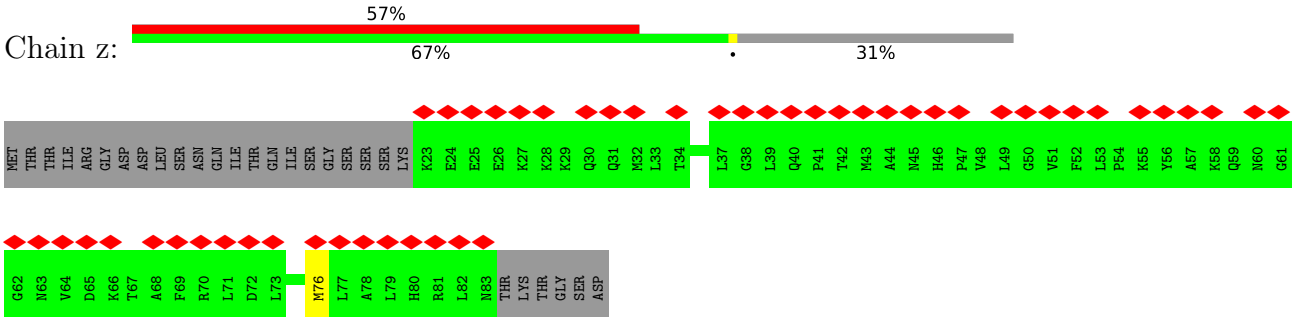
• Molecule 3: Small capsomere-interacting protein

Chain y:

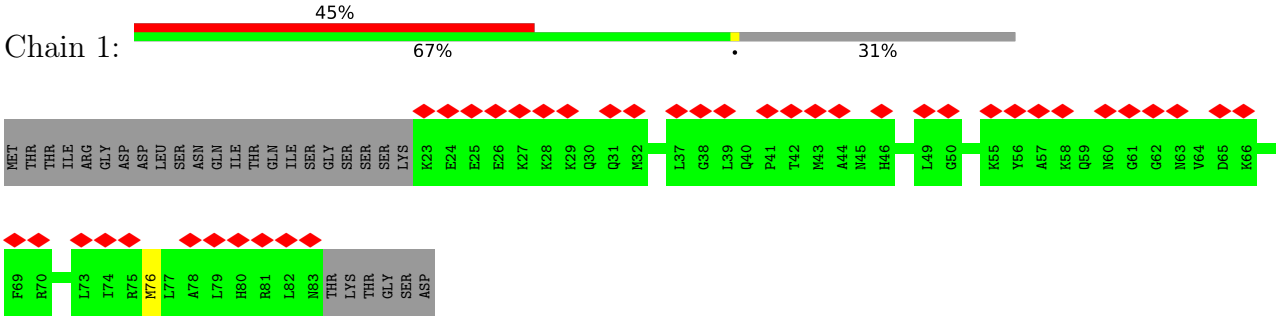




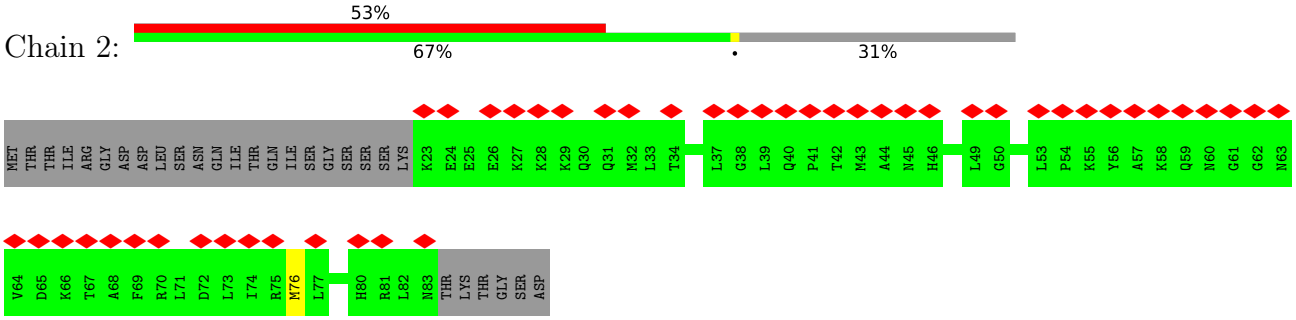
• Molecule 3: Small capsomere-interacting protein



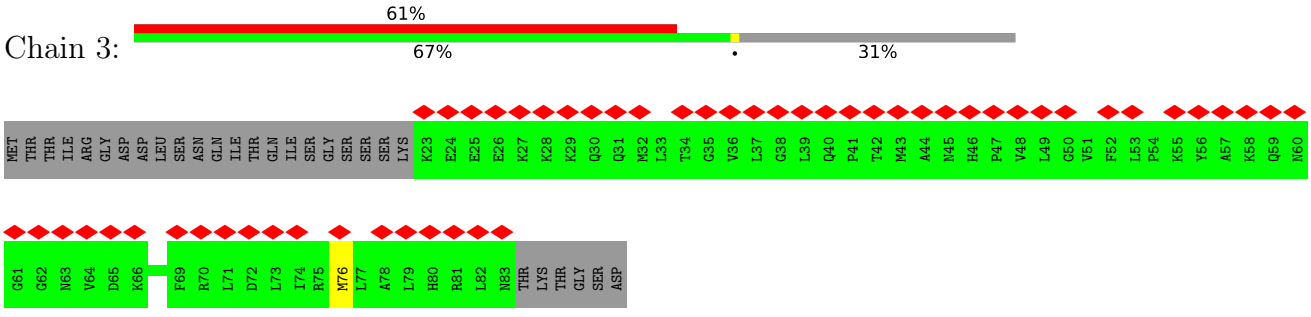
• Molecule 3: Small capsomere-interacting protein



• Molecule 3: Small capsomere-interacting protein

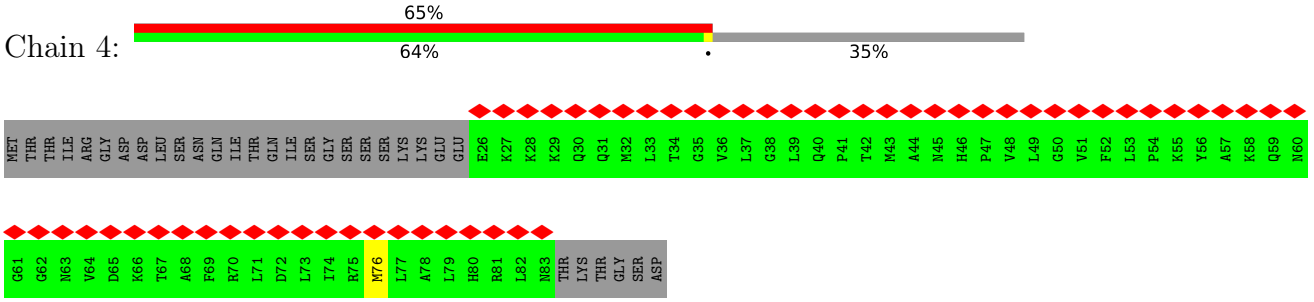


• Molecule 3: Small capsomere-interacting protein



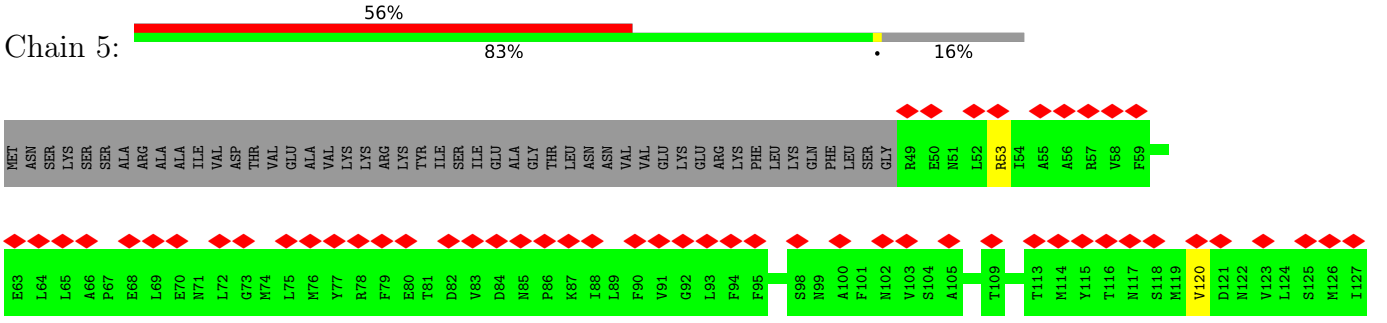
• Molecule 3: Small capsomere-interacting protein

Chain 4:



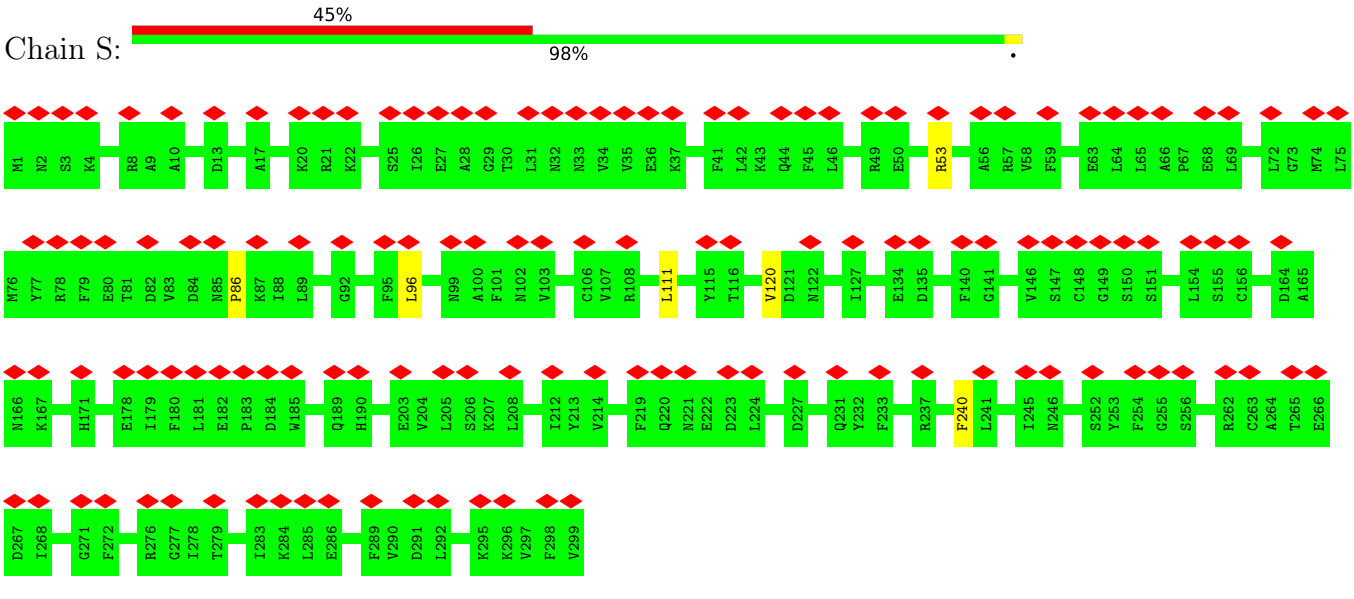
• Molecule 4: Triplex capsid protein 1

Chain 5:



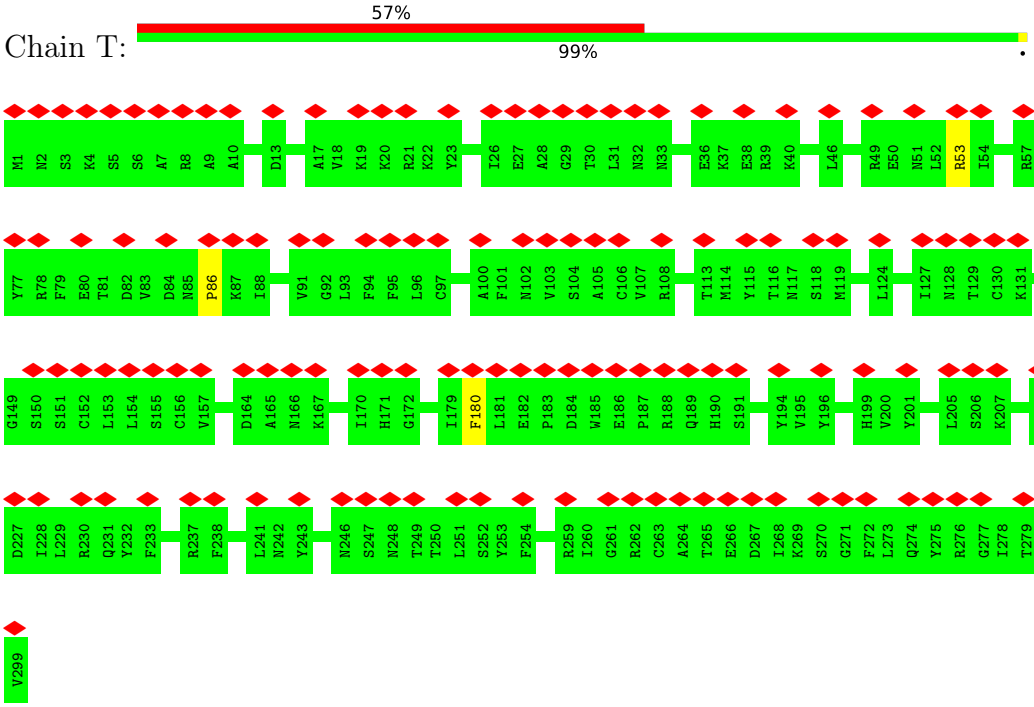
• Molecule 4: Triplex capsid protein 1

Chain S:



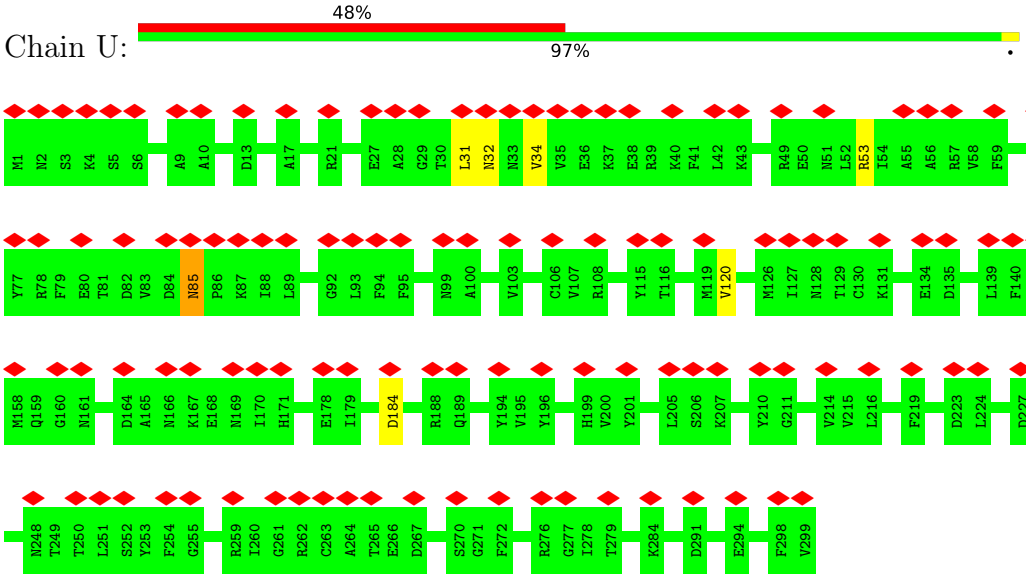
• Molecule 4: Triplex capsid protein 1

Chain T:



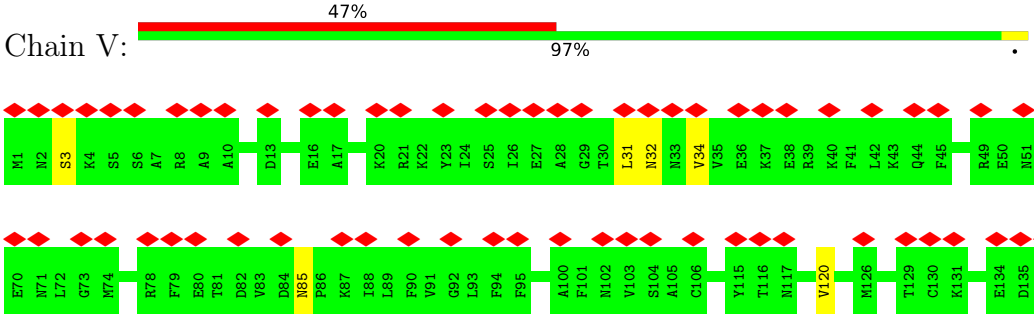
• Molecule 4: Triplex capsid protein 1

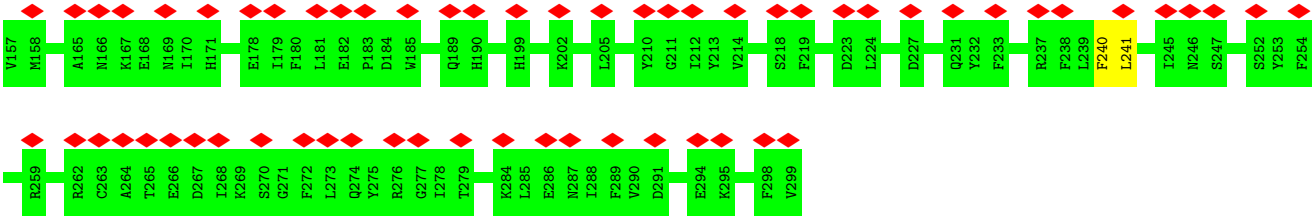
Chain U:



• Molecule 4: Triplex capsid protein 1

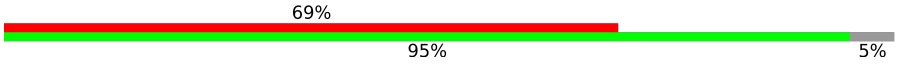
Chain V:

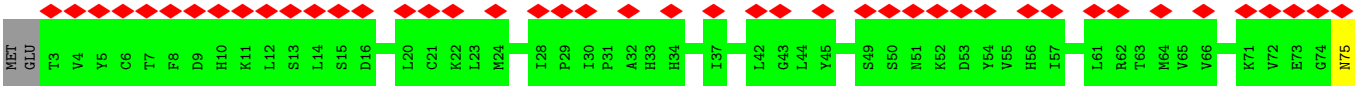


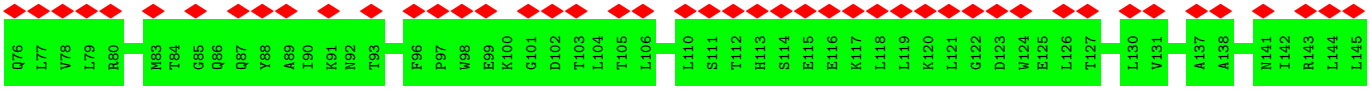


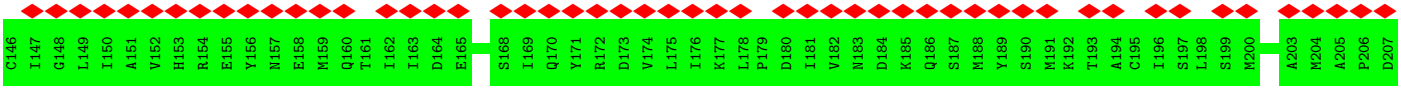
• Molecule 5: Triplex capsid protein 2

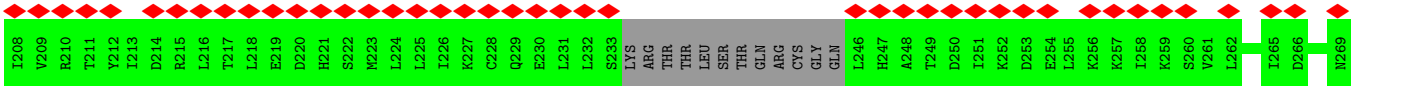
Chain 6:





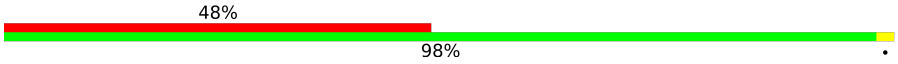


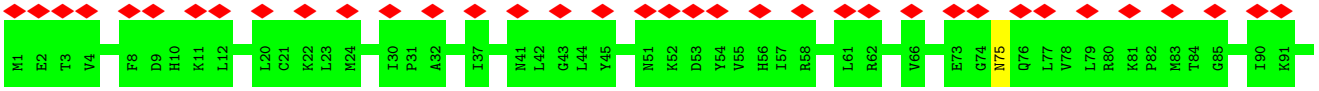


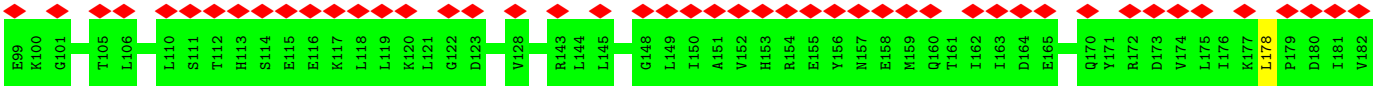


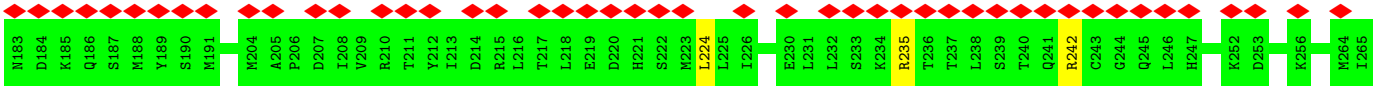
• Molecule 5: Triplex capsid protein 2

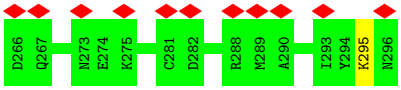
Chain W:





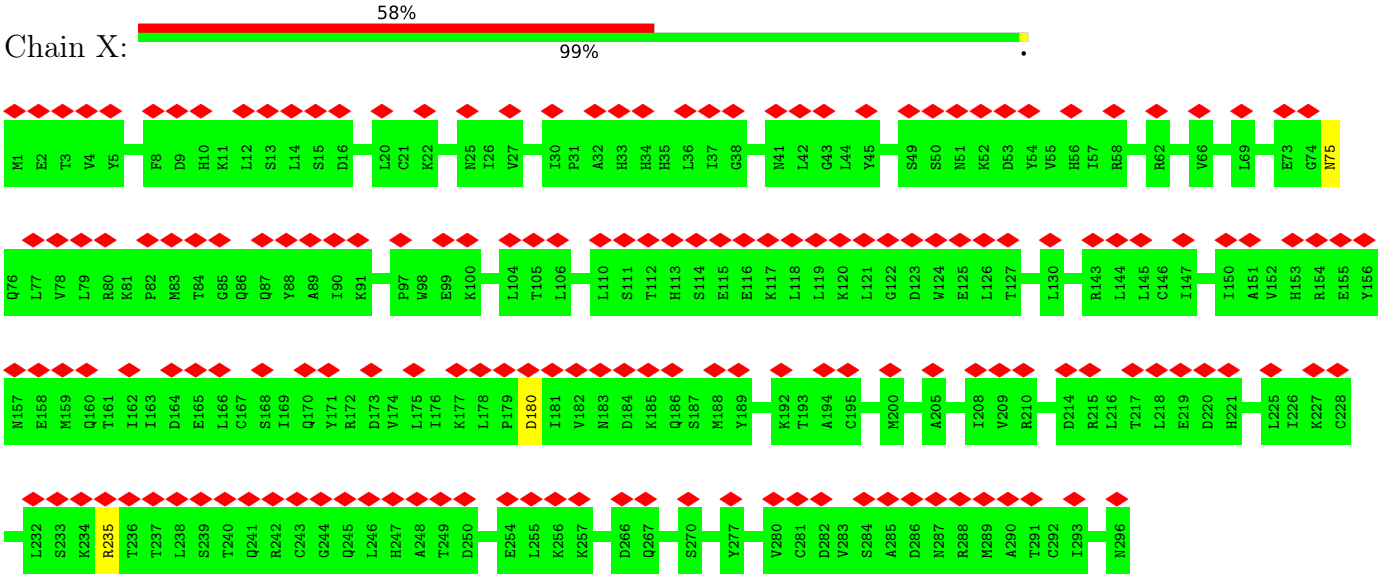






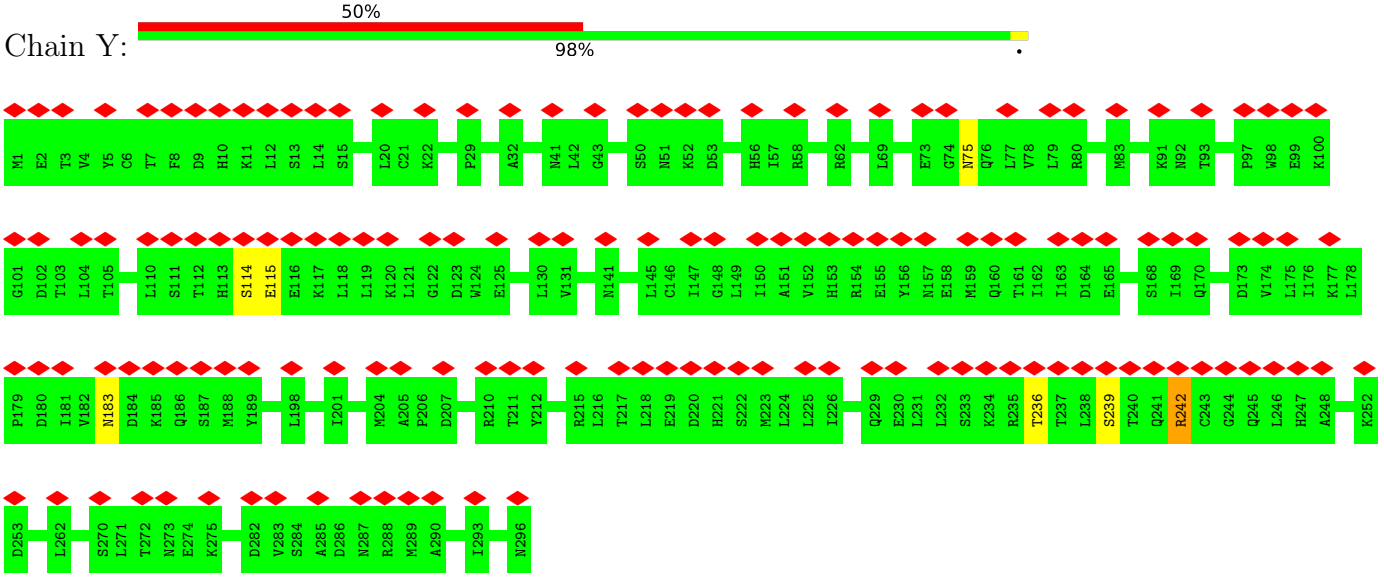
• Molecule 5: Triplex capsid protein 2

Chain X:



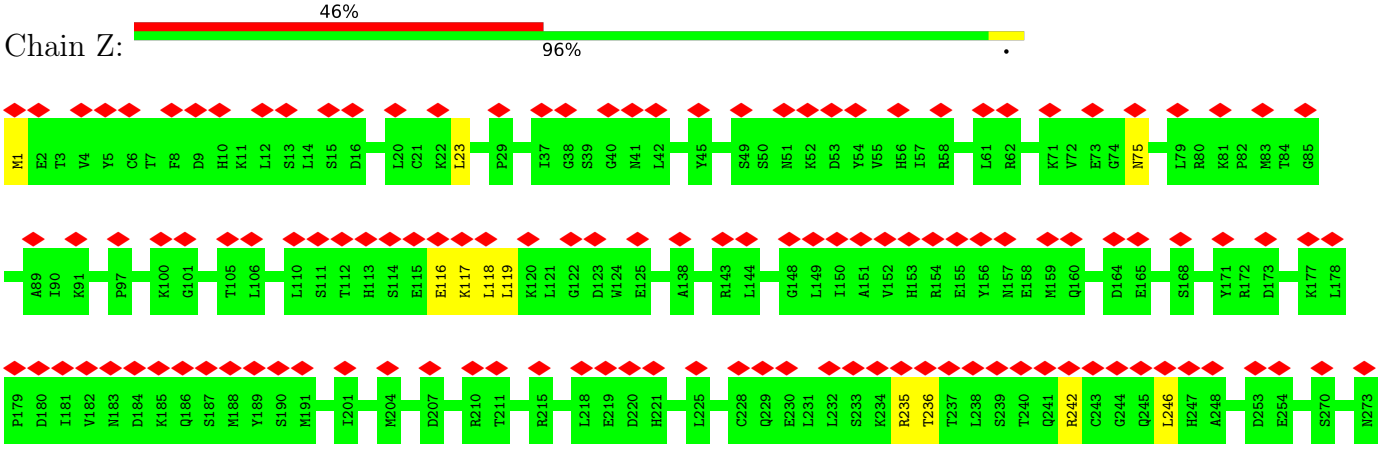
• Molecule 5: Triplex capsid protein 2

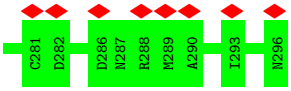
Chain Y:



• Molecule 5: Triplex capsid protein 2

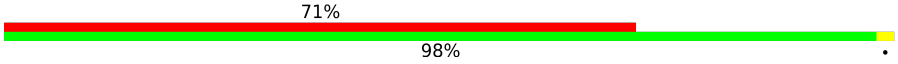
Chain Z:

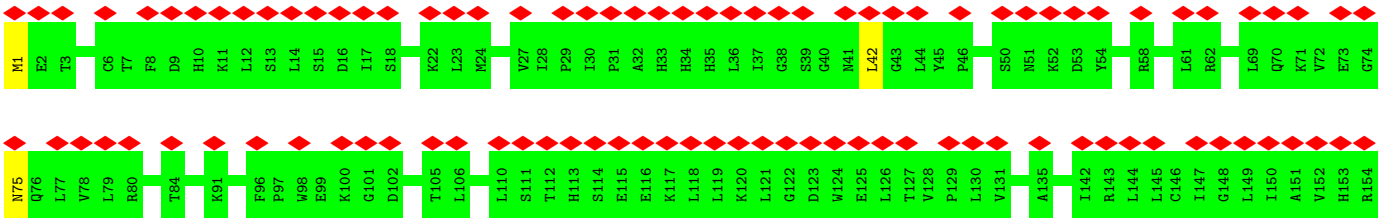




• Molecule 5: Triplex capsid protein 2

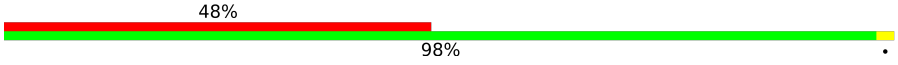
Chain 7:

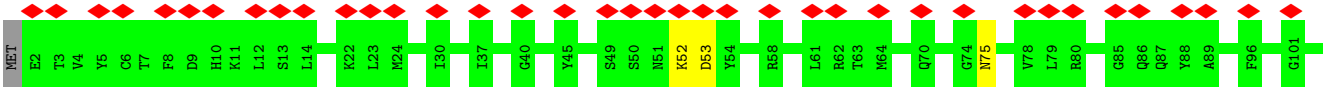


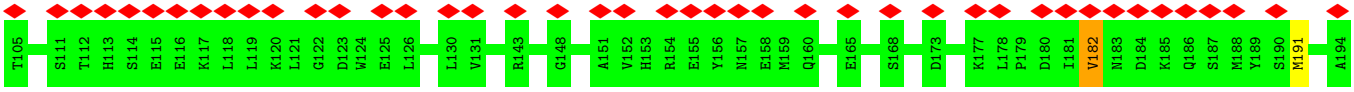


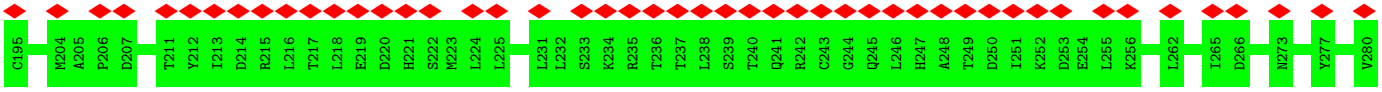
• Molecule 5: Triplex capsid protein 2

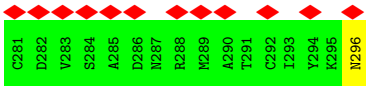
Chain a:





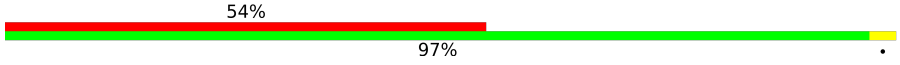


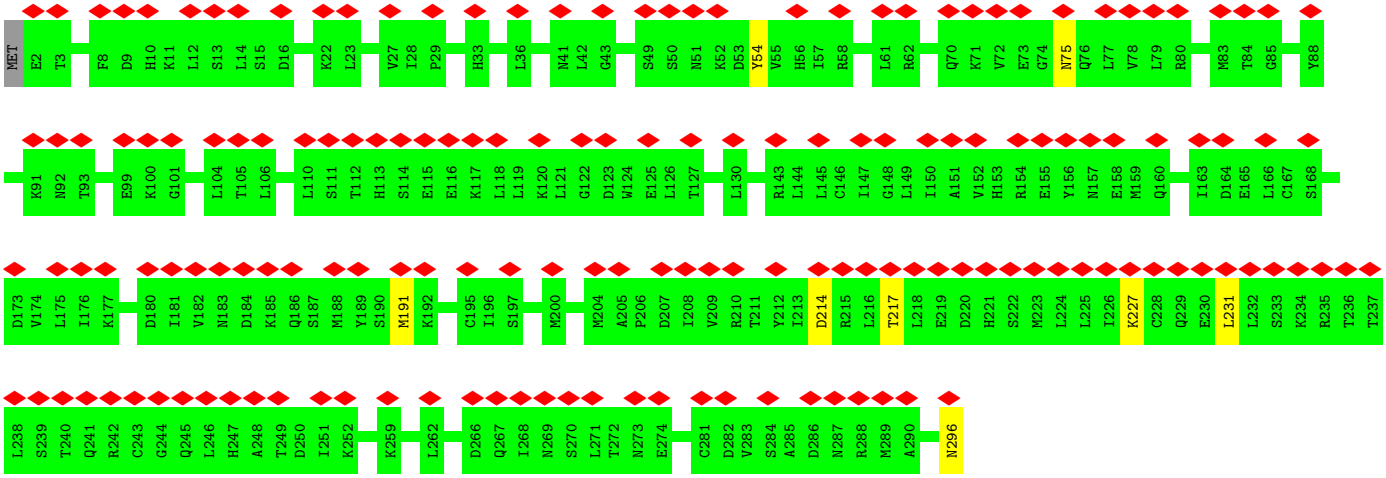




• Molecule 5: Triplex capsid protein 2

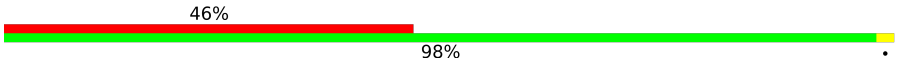
Chain b:





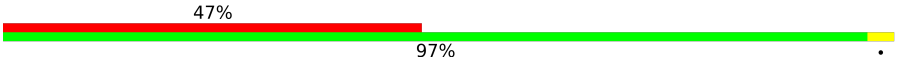
• Molecule 5: Triplex capsid protein 2

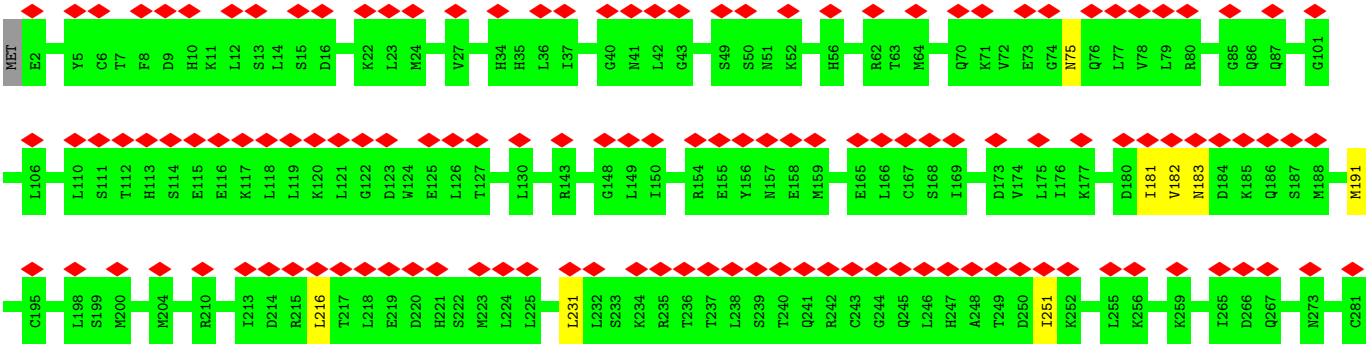
Chain c:

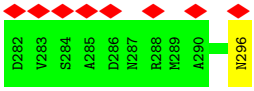


• Molecule 5: Triplex capsid protein 2

Chain d:






D282
V283
S284
A285
D286
N287
R288
M289
A290
N296

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	6443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	23	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	64000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	1388.8, 1388.8, 1388.8	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.17, 2.17, 2.17	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.51	0/10927	0.68	0/14860
1	B	0.46	0/10927	0.66	0/14860
1	C	0.46	0/10793	0.63	0/14676
1	D	0.46	0/10927	0.64	1/14860 (0.0%)
1	E	0.50	0/10927	0.66	0/14860
1	F	0.42	0/10927	0.65	0/14860
1	G	0.42	1/10927 (0.0%)	0.66	0/14860
1	H	0.50	0/10927	0.66	0/14860
1	I	0.47	0/10927	0.64	0/14860
1	q	0.42	0/10550	0.64	0/14349
1	r	0.38	0/10927	0.62	0/14860
1	s	0.39	0/10927	0.64	0/14860
1	t	0.40	0/10927	0.63	0/14860
1	u	0.38	0/10935	0.62	0/14870
1	v	0.38	0/10566	0.62	0/14366
1	w	0.38	0/10161	0.66	1/13814 (0.0%)
2	e	0.32	0/2272	0.54	0/3084
2	f	0.34	0/2272	0.62	0/3084
2	g	0.35	0/2272	0.62	0/3084
2	h	0.31	0/2272	0.56	0/3084
2	i	0.32	0/2272	0.63	0/3084
2	j	0.32	0/2272	0.59	0/3084
2	k	0.33	0/2272	0.58	0/3084
2	l	0.32	0/2272	0.57	1/3084 (0.0%)
2	m	0.36	0/2272	0.60	1/3084 (0.0%)
2	n	0.34	0/2272	0.63	1/3084 (0.0%)
2	o	0.40	0/2272	0.66	0/3084
2	p	0.34	0/2272	0.60	0/3084
3	1	0.29	0/490	0.44	0/656
3	2	0.29	0/490	0.44	0/656
3	3	0.28	0/490	0.44	0/656
3	4	0.29	0/463	0.44	0/621
3	J	0.28	0/490	0.44	0/656
3	K	0.28	0/490	0.44	0/656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	L	0.29	0/490	0.44	0/656
3	M	0.29	0/490	0.44	0/656
3	N	0.29	0/490	0.44	0/656
3	O	0.29	0/490	0.44	0/656
3	P	0.29	0/490	0.44	0/656
3	Q	0.28	0/490	0.44	0/656
3	R	0.29	0/490	0.44	0/656
3	x	0.29	0/490	0.44	0/656
3	y	0.29	0/490	0.44	0/656
3	z	0.29	0/490	0.44	0/656
4	5	0.39	0/2062	0.67	0/2793
4	S	0.49	0/2440	0.67	0/3297
4	T	0.48	0/2440	0.70	0/3297
4	U	0.41	0/2440	0.67	0/3297
4	V	0.41	0/2440	0.66	0/3297
5	6	0.39	0/2262	0.67	0/3069
5	7	0.33	0/2374	0.66	0/3219
5	W	0.42	0/2374	0.68	0/3219
5	X	0.38	0/2374	0.62	0/3219
5	Y	0.39	0/2374	0.68	0/3219
5	Z	0.41	0/2374	0.72	0/3219
5	a	0.44	0/2366	0.73	0/3209
5	b	0.44	0/2366	0.73	0/3209
5	c	0.52	0/2366	0.77	0/3209
5	d	0.41	0/2366	0.75	0/3209
All	All	0.42	1/243697 (0.0%)	0.64	5/330985 (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
2	o	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1115	GLU	C-N	-5.30	1.21	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	w	563	LEU	C-N-CD	-8.35	102.23	120.60
2	l	181	ASP	N-CA-C	5.66	126.28	111.00
2	m	154	ALA	N-CA-C	5.37	125.51	111.00
2	n	179	ILE	N-CA-C	-5.11	97.21	111.00
1	D	255	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	o	7	SER	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1341/1345 (100%)	1238 (92%)	102 (8%)	1 (0%)	51	86
1	B	1341/1345 (100%)	1251 (93%)	87 (6%)	3 (0%)	47	81
1	C	1321/1345 (98%)	1239 (94%)	80 (6%)	2 (0%)	47	81
1	D	1341/1345 (100%)	1248 (93%)	89 (7%)	4 (0%)	41	77
1	E	1341/1345 (100%)	1243 (93%)	94 (7%)	4 (0%)	41	77
1	F	1341/1345 (100%)	1243 (93%)	96 (7%)	2 (0%)	51	86
1	G	1341/1345 (100%)	1253 (93%)	83 (6%)	5 (0%)	34	72
1	H	1341/1345 (100%)	1253 (93%)	84 (6%)	4 (0%)	41	77
1	I	1341/1345 (100%)	1242 (93%)	98 (7%)	1 (0%)	51	86
1	q	1292/1345 (96%)	1190 (92%)	99 (8%)	3 (0%)	47	81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	r	1341/1345 (100%)	1235 (92%)	103 (8%)	3 (0%)	47 81
1	s	1341/1345 (100%)	1246 (93%)	93 (7%)	2 (0%)	51 86
1	t	1341/1345 (100%)	1240 (92%)	98 (7%)	3 (0%)	47 81
1	u	1342/1345 (100%)	1234 (92%)	106 (8%)	2 (0%)	51 86
1	v	1299/1345 (97%)	1204 (93%)	89 (7%)	6 (0%)	29 69
1	w	1240/1345 (92%)	1141 (92%)	98 (8%)	1 (0%)	51 86
2	e	267/858 (31%)	254 (95%)	13 (5%)	0	100 100
2	f	267/858 (31%)	248 (93%)	16 (6%)	3 (1%)	14 52
2	g	267/858 (31%)	255 (96%)	9 (3%)	3 (1%)	14 52
2	h	267/858 (31%)	248 (93%)	19 (7%)	0	100 100
2	i	267/858 (31%)	245 (92%)	17 (6%)	5 (2%)	8 38
2	j	267/858 (31%)	249 (93%)	16 (6%)	2 (1%)	22 63
2	k	267/858 (31%)	249 (93%)	17 (6%)	1 (0%)	34 72
2	l	267/858 (31%)	247 (92%)	19 (7%)	1 (0%)	34 72
2	m	267/858 (31%)	248 (93%)	18 (7%)	1 (0%)	34 72
2	n	267/858 (31%)	244 (91%)	18 (7%)	5 (2%)	8 38
2	o	267/858 (31%)	247 (92%)	16 (6%)	4 (2%)	10 46
2	p	267/858 (31%)	249 (93%)	18 (7%)	0	100 100
3	1	59/89 (66%)	52 (88%)	7 (12%)	0	100 100
3	2	59/89 (66%)	52 (88%)	7 (12%)	0	100 100
3	3	59/89 (66%)	52 (88%)	7 (12%)	0	100 100
3	4	56/89 (63%)	49 (88%)	7 (12%)	0	100 100
3	J	59/89 (66%)	51 (86%)	7 (12%)	1 (2%)	9 42
3	K	59/89 (66%)	52 (88%)	7 (12%)	0	100 100
3	L	59/89 (66%)	52 (88%)	7 (12%)	0	100 100
3	M	59/89 (66%)	52 (88%)	7 (12%)	0	100 100
3	N	59/89 (66%)	52 (88%)	7 (12%)	0	100 100
3	O	59/89 (66%)	52 (88%)	7 (12%)	0	100 100
3	P	59/89 (66%)	52 (88%)	7 (12%)	0	100 100
3	Q	59/89 (66%)	52 (88%)	7 (12%)	0	100 100
3	R	59/89 (66%)	52 (88%)	7 (12%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	x	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	y	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	z	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
4	5	249/299 (83%)	226 (91%)	23 (9%)	0	100	100
4	S	297/299 (99%)	269 (91%)	27 (9%)	1 (0%)	41	77
4	T	297/299 (99%)	275 (93%)	21 (7%)	1 (0%)	41	77
4	U	297/299 (99%)	267 (90%)	29 (10%)	1 (0%)	41	77
4	V	297/299 (99%)	268 (90%)	27 (9%)	2 (1%)	22	63
5	6	278/296 (94%)	260 (94%)	18 (6%)	0	100	100
5	7	294/296 (99%)	259 (88%)	32 (11%)	3 (1%)	15	55
5	W	294/296 (99%)	277 (94%)	17 (6%)	0	100	100
5	X	294/296 (99%)	273 (93%)	20 (7%)	1 (0%)	41	77
5	Y	294/296 (99%)	269 (92%)	22 (8%)	3 (1%)	15	55
5	Z	294/296 (99%)	274 (93%)	19 (6%)	1 (0%)	41	77
5	a	293/296 (99%)	262 (89%)	28 (10%)	3 (1%)	15	55
5	b	293/296 (99%)	268 (92%)	24 (8%)	1 (0%)	41	77
5	c	293/296 (99%)	259 (88%)	33 (11%)	1 (0%)	41	77
5	d	293/296 (99%)	258 (88%)	30 (10%)	5 (2%)	9	42
All	All	29747/37695 (79%)	27475 (92%)	2177 (7%)	95 (0%)	44	77

5 of 95 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1218/1220 (100%)	1202 (99%)	16 (1%)	69	81
1	B	1218/1220 (100%)	1201 (99%)	17 (1%)	67	80
1	C	1204/1220 (99%)	1191 (99%)	13 (1%)	73	84
1	D	1218/1220 (100%)	1197 (98%)	21 (2%)	60	78
1	E	1218/1220 (100%)	1200 (98%)	18 (2%)	65	80
1	F	1218/1220 (100%)	1198 (98%)	20 (2%)	62	79
1	G	1218/1220 (100%)	1199 (98%)	19 (2%)	62	79
1	H	1218/1220 (100%)	1197 (98%)	21 (2%)	60	78
1	I	1218/1220 (100%)	1204 (99%)	14 (1%)	73	84
1	q	1180/1220 (97%)	1168 (99%)	12 (1%)	76	86
1	r	1218/1220 (100%)	1204 (99%)	14 (1%)	73	84
1	s	1218/1220 (100%)	1202 (99%)	16 (1%)	69	81
1	t	1218/1220 (100%)	1207 (99%)	11 (1%)	78	87
1	u	1219/1220 (100%)	1205 (99%)	14 (1%)	73	84
1	v	1180/1220 (97%)	1170 (99%)	10 (1%)	81	89
1	w	1133/1220 (93%)	1123 (99%)	10 (1%)	78	87
2	e	253/761 (33%)	247 (98%)	6 (2%)	49	69
2	f	253/761 (33%)	253 (100%)	0	100	100
2	g	253/761 (33%)	246 (97%)	7 (3%)	43	65
2	h	253/761 (33%)	249 (98%)	4 (2%)	62	79
2	i	253/761 (33%)	245 (97%)	8 (3%)	39	61
2	j	253/761 (33%)	246 (97%)	7 (3%)	43	65
2	k	253/761 (33%)	246 (97%)	7 (3%)	43	65
2	l	253/761 (33%)	246 (97%)	7 (3%)	43	65
2	m	253/761 (33%)	249 (98%)	4 (2%)	62	79
2	n	253/761 (33%)	247 (98%)	6 (2%)	49	69
2	o	253/761 (33%)	247 (98%)	6 (2%)	49	69
2	p	253/761 (33%)	248 (98%)	5 (2%)	55	74
3	1	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	2	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	3	52/77 (68%)	51 (98%)	1 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4	49/77 (64%)	48 (98%)	1 (2%)	55	74
3	J	52/77 (68%)	49 (94%)	3 (6%)	20	45
3	K	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	L	52/77 (68%)	50 (96%)	2 (4%)	33	57
3	M	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	N	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	O	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	P	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	Q	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	R	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	x	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	y	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	z	52/77 (68%)	51 (98%)	1 (2%)	57	75
4	5	232/273 (85%)	230 (99%)	2 (1%)	78	87
4	S	273/273 (100%)	268 (98%)	5 (2%)	59	77
4	T	273/273 (100%)	271 (99%)	2 (1%)	84	90
4	U	273/273 (100%)	265 (97%)	8 (3%)	42	64
4	V	273/273 (100%)	266 (97%)	7 (3%)	46	66
5	6	261/274 (95%)	260 (100%)	1 (0%)	91	94
5	7	274/274 (100%)	270 (98%)	4 (2%)	65	80
5	W	274/274 (100%)	268 (98%)	6 (2%)	52	71
5	X	274/274 (100%)	272 (99%)	2 (1%)	84	90
5	Y	274/274 (100%)	269 (98%)	5 (2%)	59	77
5	Z	274/274 (100%)	264 (96%)	10 (4%)	35	59
5	a	273/274 (100%)	269 (98%)	4 (2%)	65	80
5	b	273/274 (100%)	266 (97%)	7 (3%)	46	66
5	c	273/274 (100%)	268 (98%)	5 (2%)	59	77
5	d	273/274 (100%)	269 (98%)	4 (2%)	65	80
All	All	27226/33989 (80%)	26822 (98%)	404 (2%)	66	80

5 of 404 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	v	772	ASN
2	l	33	ASN
5	c	296	ASN
1	w	231	ASN
2	h	62	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 534 such sidechains are listed below:

Mol	Chain	Res	Type
3	3	59	GLN
5	6	170	GLN
3	2	60	ASN
5	c	113	HIS
1	q	438	GLN

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 monosaccharides 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.

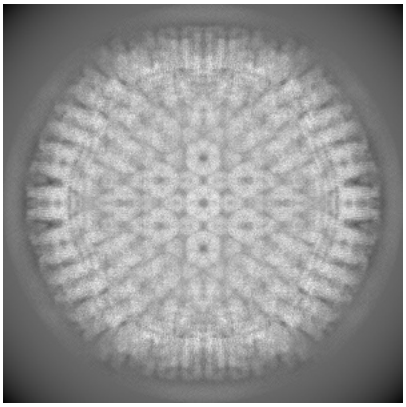
6 Map visualisation

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

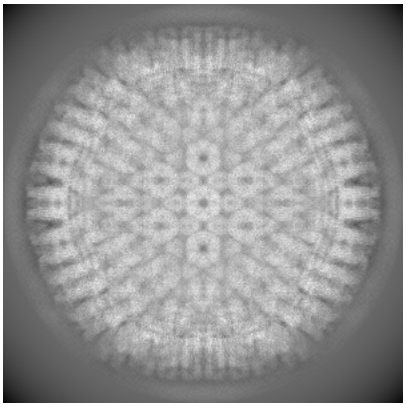
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

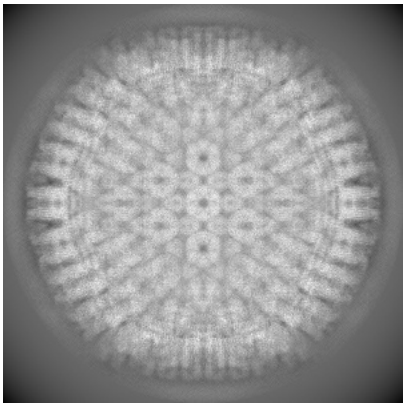
6.1.1 Primary map



X



Y

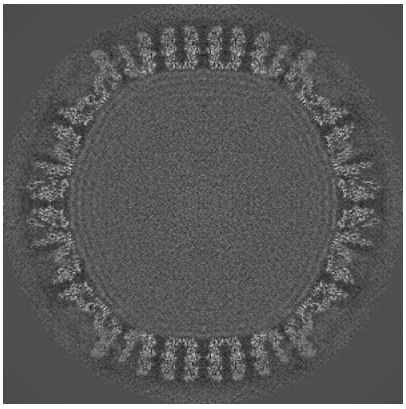


Z

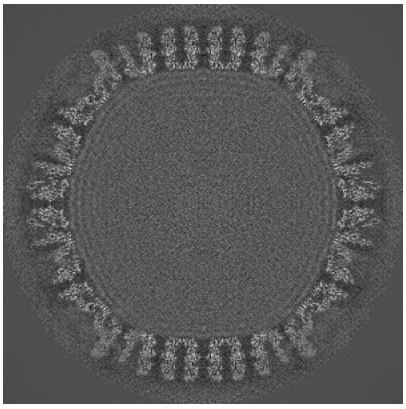
The images above show the map projected in three orthogonal directions.

6.2 Central slices

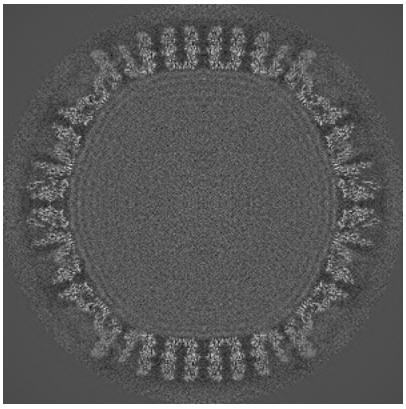
6.2.1 Primary map



X Index: 320



Y Index: 320

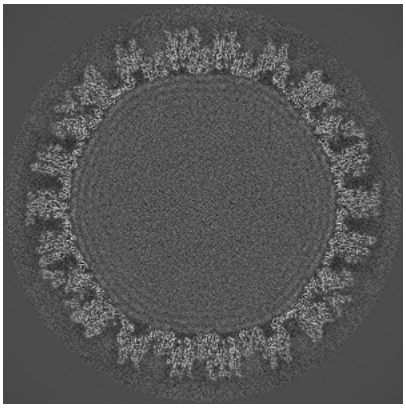


Z Index: 320

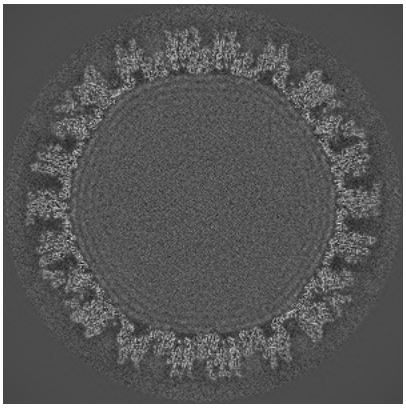
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

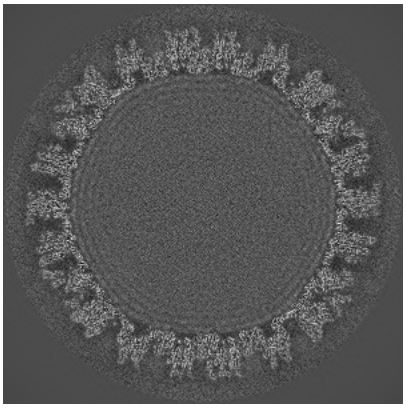
6.3.1 Primary map



X Index: 266



Y Index: 266



Z Index: 266

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

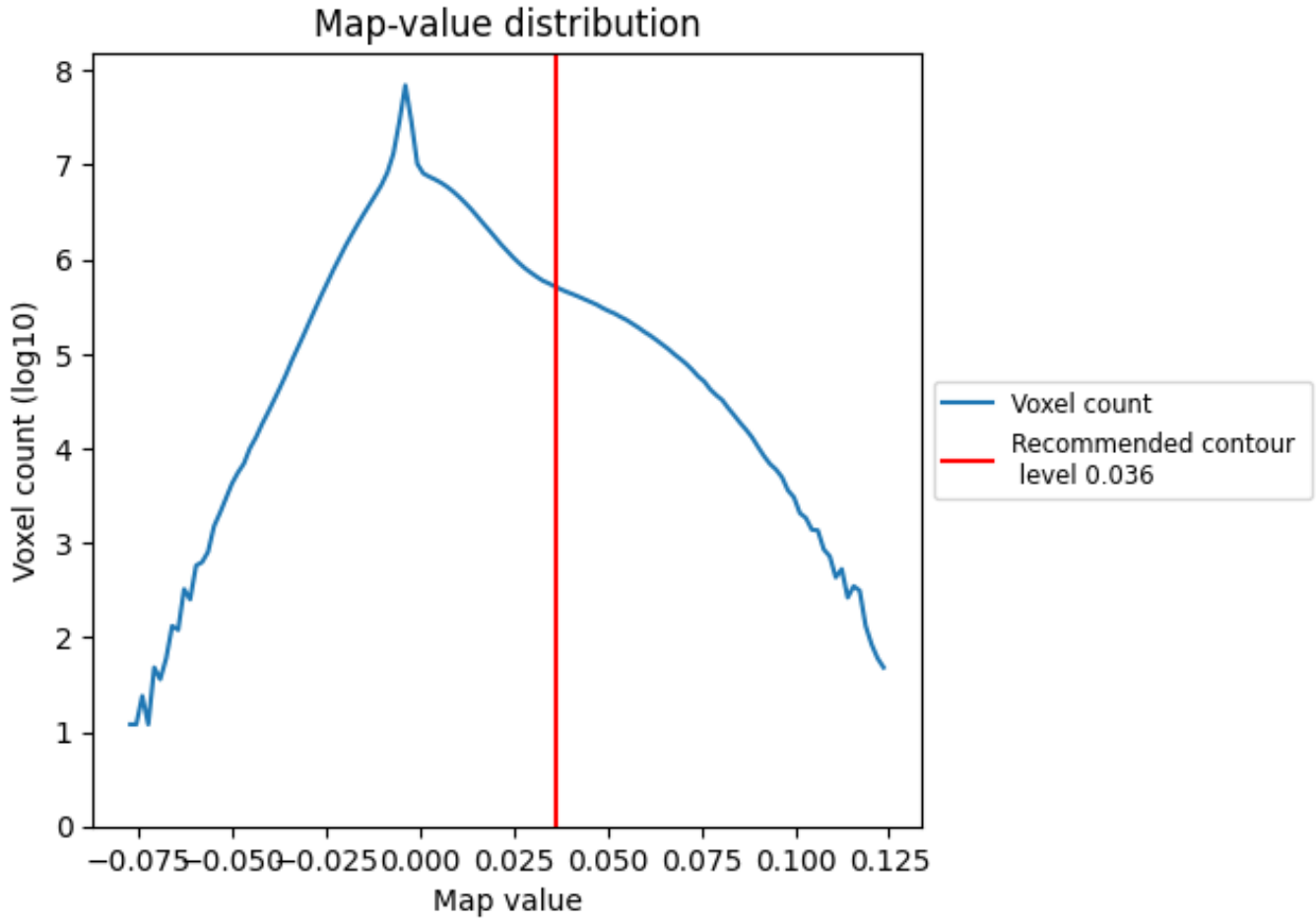
6.5 Mask visualisation (i)

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

7 Map analysis

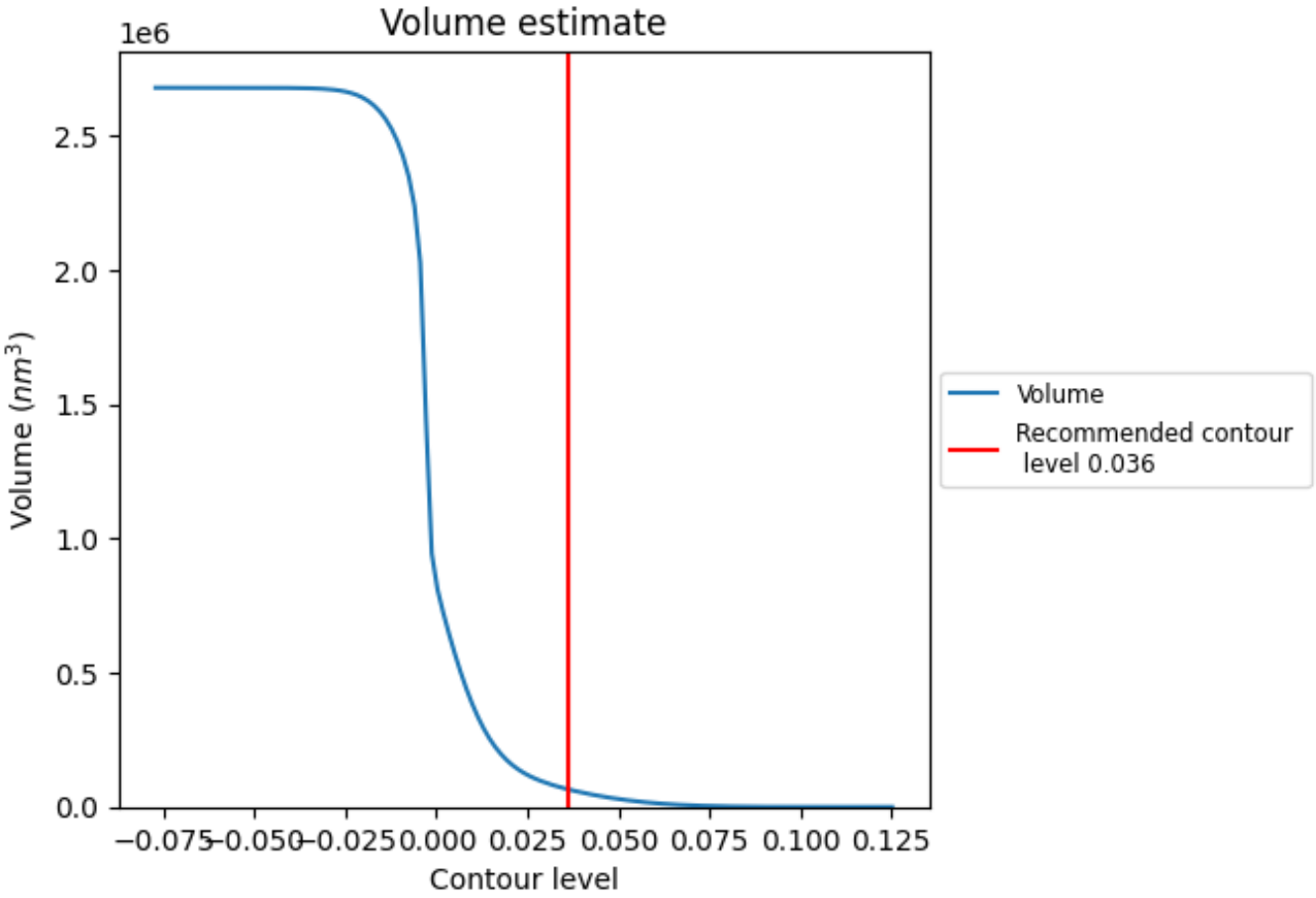
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

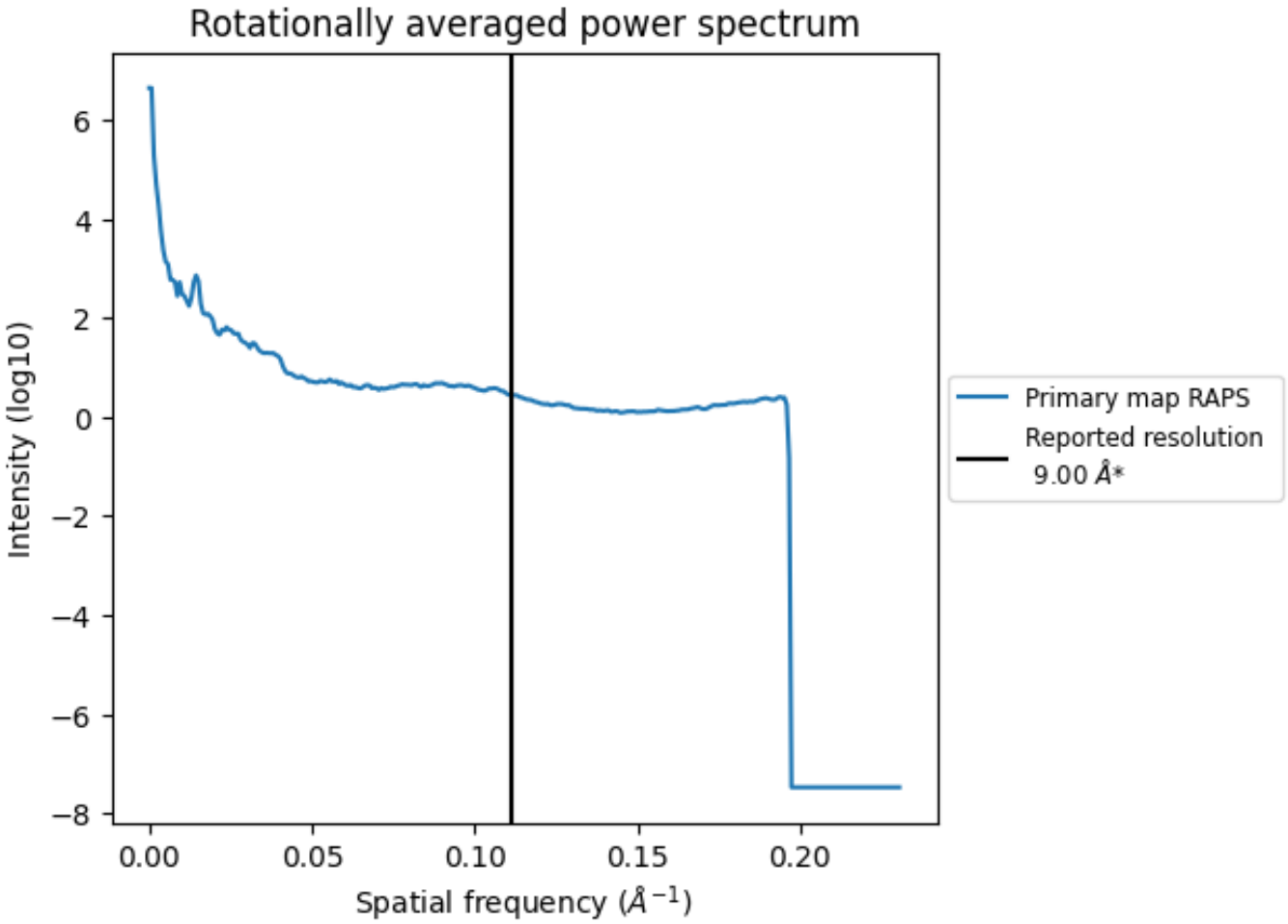
7.2 Volume estimate (i)



The volume at the recommended contour level is 66298 nm^3; this corresponds to an approximate mass of 59889 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.111 Å^{-1}

8 Fourier-Shell correlation

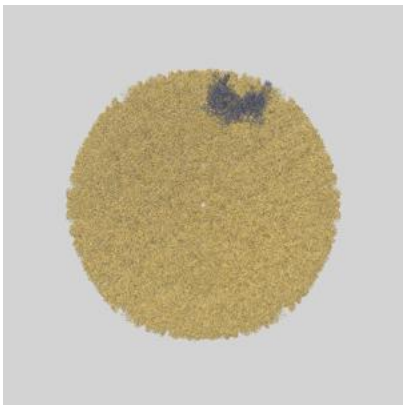
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

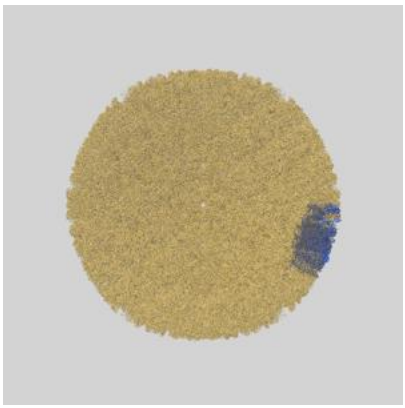
This section contains information regarding the fit between EMDB map EMD-20557 and PDB model 6Q1F. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

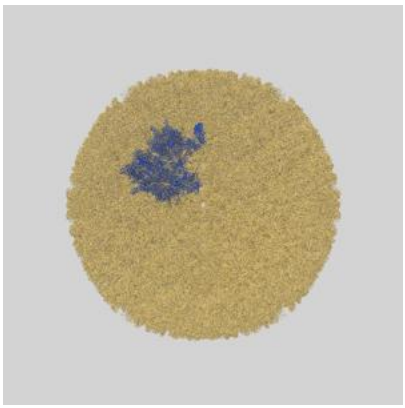
9.1.1 Map-model overlay



X

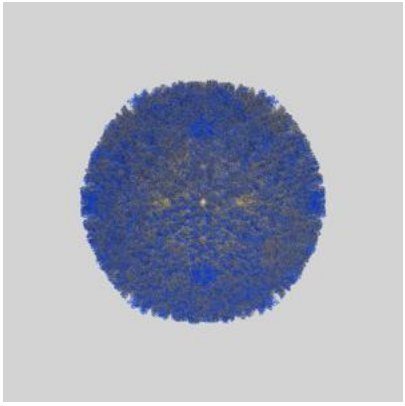


Y

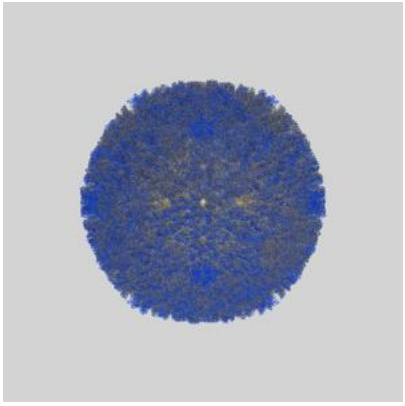


Z

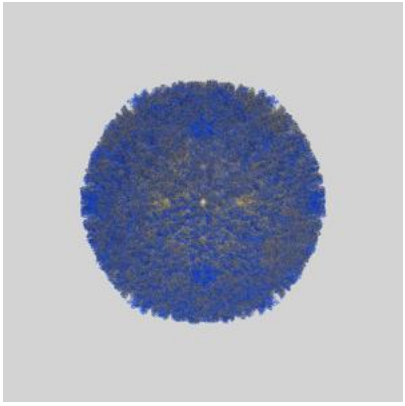
9.1.2 Map-model assembly overlay



X



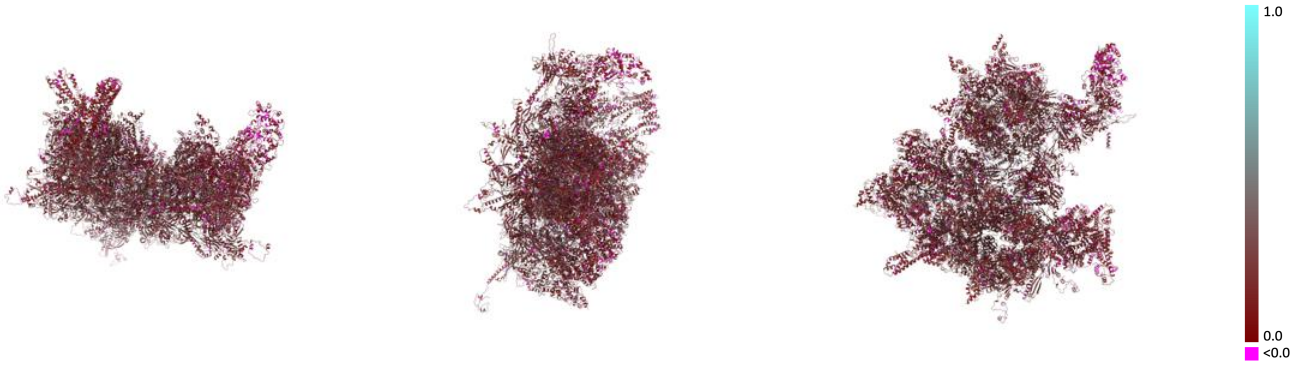
Y



Z

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

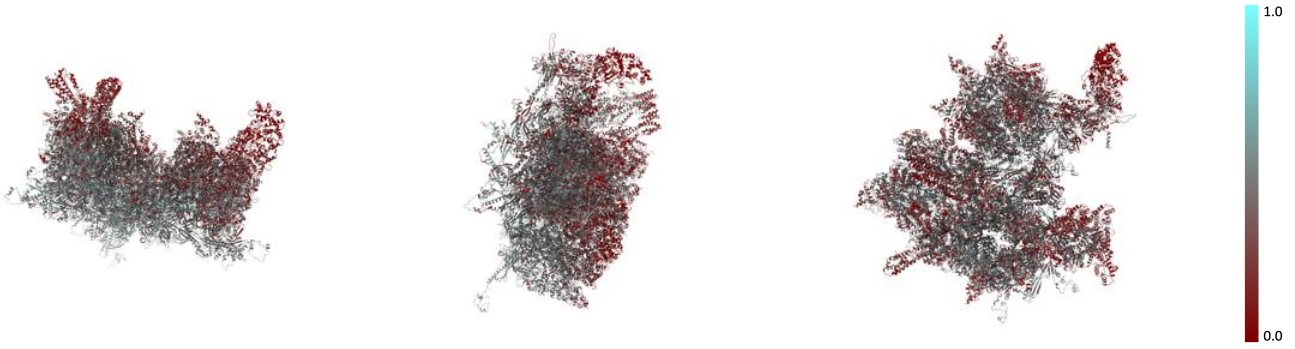
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

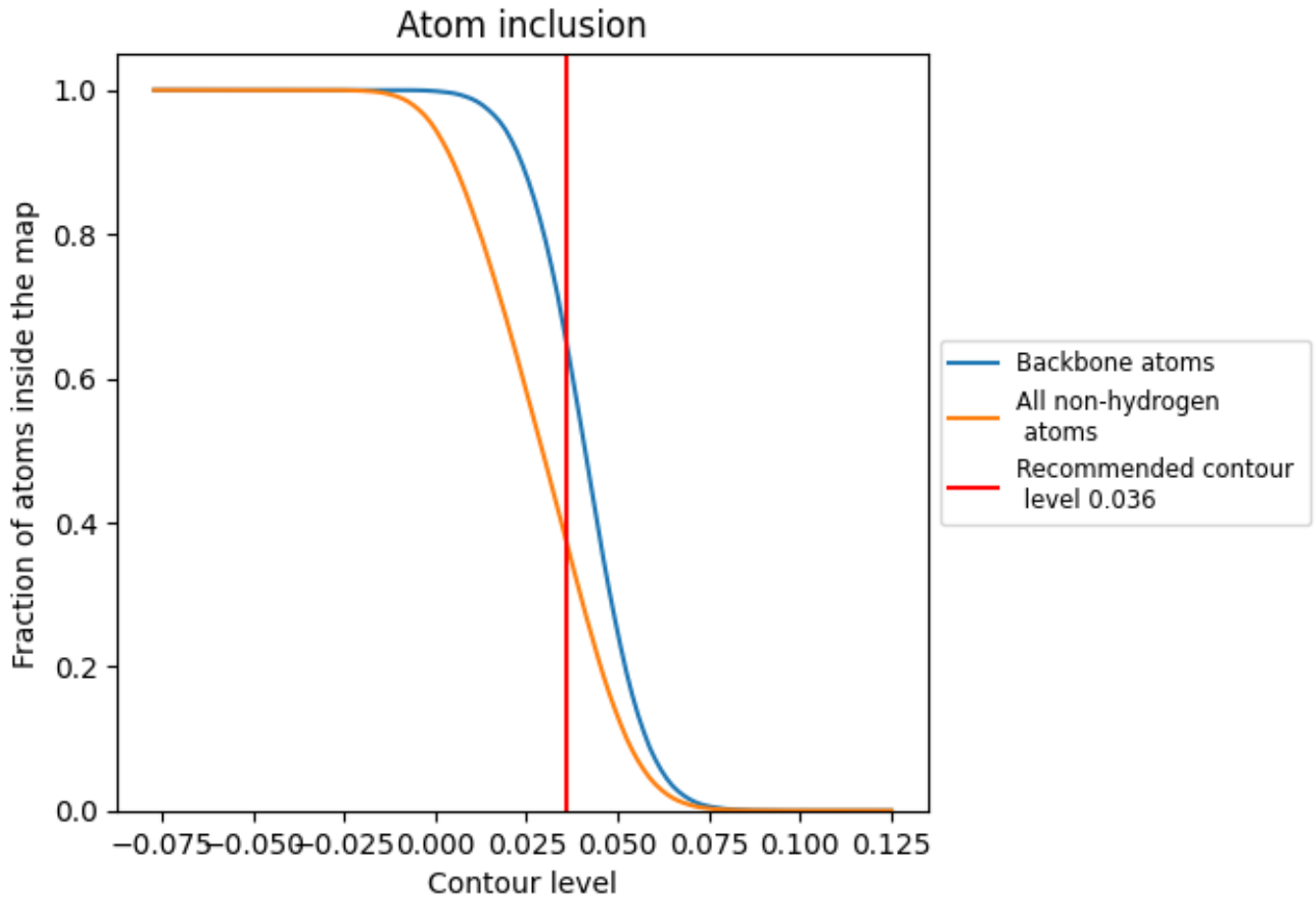
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.036).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 37% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3730	0.2130
1	0.3130	0.1980
2	0.2626	0.1960
3	0.1555	0.1720
4	0.0022	0.1250
5	0.3020	0.2000
6	0.2609	0.1820
7	0.2514	0.1770
A	0.4445	0.2310
B	0.4324	0.2250
C	0.4356	0.2330
D	0.4517	0.2340
E	0.4519	0.2330
F	0.4256	0.2240
G	0.4414	0.2260
H	0.4618	0.2370
I	0.4432	0.2290
J	0.2857	0.1930
K	0.2752	0.2050
L	0.2458	0.2050
M	0.2899	0.1910
N	0.2605	0.2000
O	0.2164	0.2160
P	0.2899	0.1820
Q	0.2479	0.1880
R	0.2794	0.1850
S	0.4238	0.2310
T	0.3592	0.2160
U	0.4064	0.2300
V	0.4195	0.2280
W	0.3782	0.2090
X	0.3296	0.2030
Y	0.3682	0.2050
Z	0.3843	0.2100
a	0.3795	0.2150

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Chain	Atom inclusion	Q-score
b	0.3542	0.2050
c	0.3908	0.2110
d	0.3852	0.2110
e	0.1902	0.1650
f	0.1627	0.1710
g	0.2108	0.1730
h	0.1068	0.1560
i	0.1962	0.1750
j	0.1237	0.1680
k	0.2246	0.1540
l	0.1049	0.1590
m	0.2479	0.1690
n	0.2658	0.1640
o	0.2993	0.1730
p	0.2172	0.1740
q	0.3608	0.2130
r	0.3995	0.2230
s	0.4047	0.2190
t	0.4223	0.2250
u	0.4019	0.2170
v	0.3810	0.2120
w	0.1815	0.1650
x	0.1408	0.1800
y	0.1681	0.1790
z	0.2248	0.1960