wwPDB EM Validation Summary Report

Oct 27, 2024 – 12:58 AM EDT

PDB ID	:	6NHJ
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:

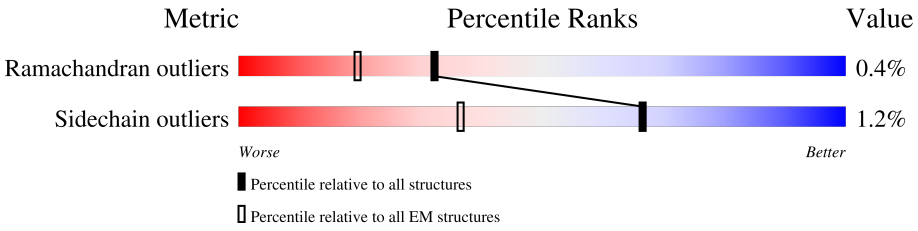
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1353	28% 98%
1	B	1353	27% 96%
1	C	1353	30% 95%
1	D	1353	30% 96%
1	E	1353	28% 98%
1	F	1353	28% 96%
1	G	1353	32% 98%
1	H	1353	34% 98%
1	I	1353	33% 97%

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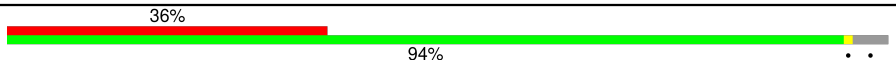
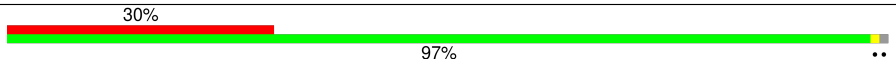
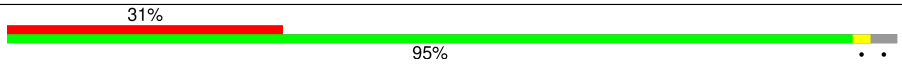
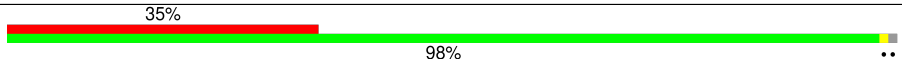
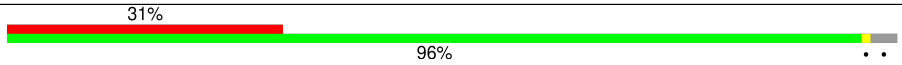
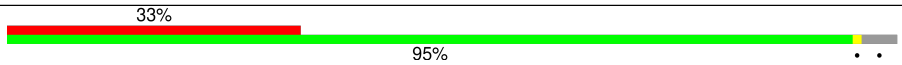
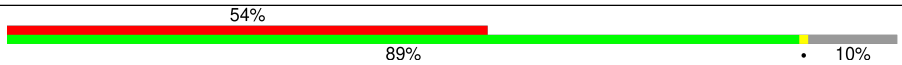
Mol	Chain	Length	Quality of chain
1	k	1353	
1	l	1353	
1	m	1353	
1	n	1353	
1	o	1353	
1	p	1353	
1	q	1353	
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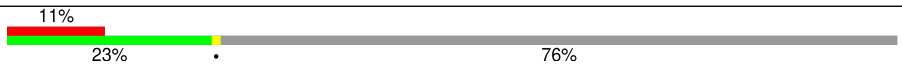
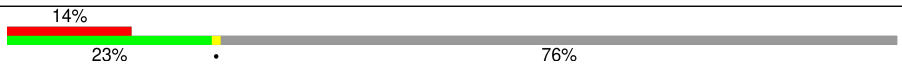
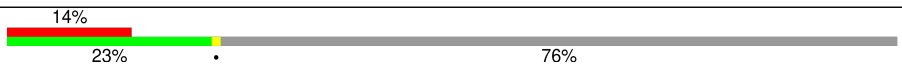
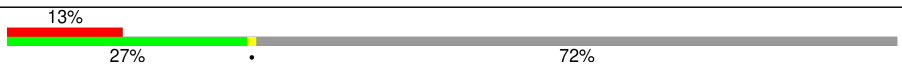
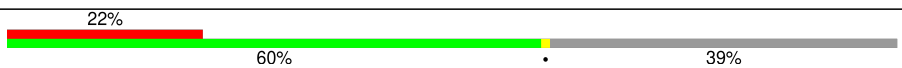
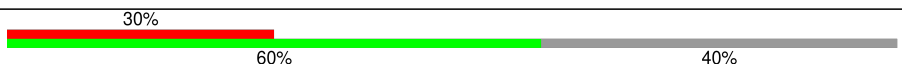
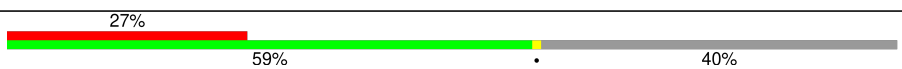
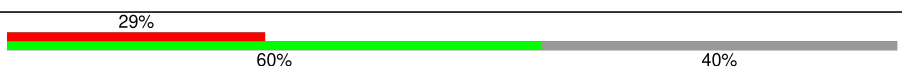
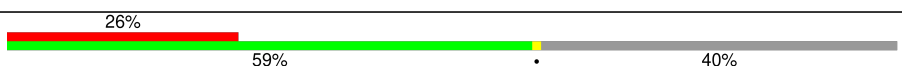
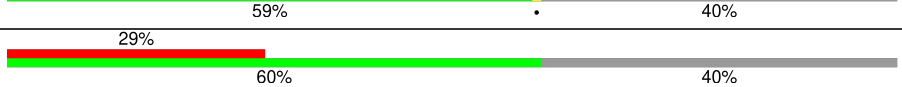
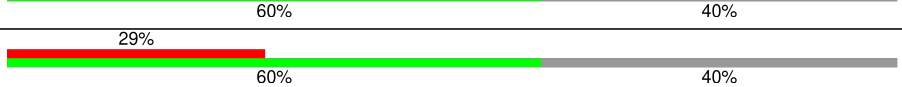
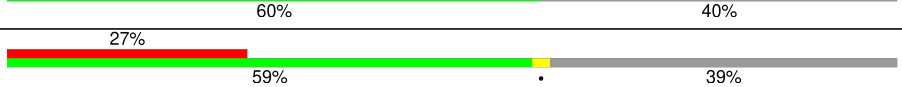
2	3	718	
2	e	718	
2	f	718	
2	g	718	
2	h	718	
2	i	718	
2	j	718	
3	J	98	
3	K	98	
3	L	98	
3	M	98	
3	N	98	
3	O	98	
3	P	98	
3	Q	98	
3	R	98	
3	r	98	

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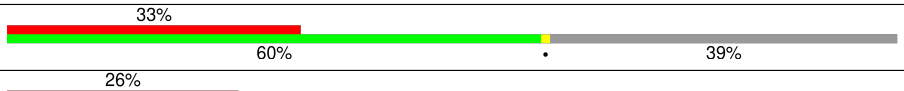
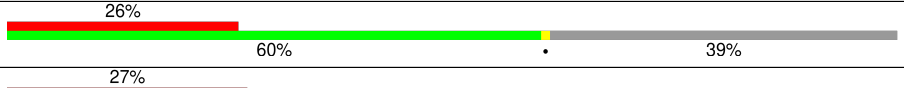
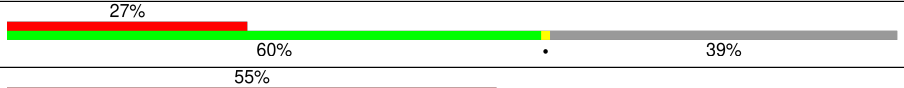
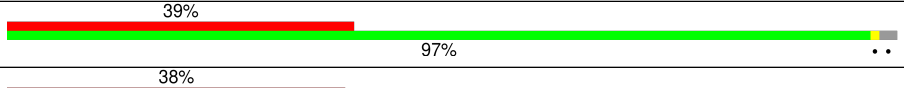
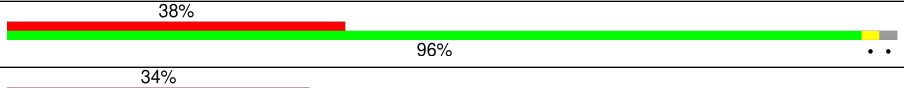
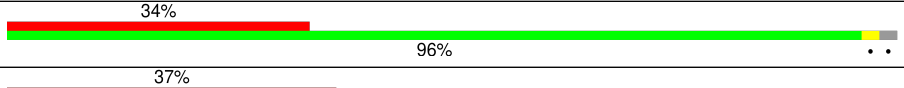
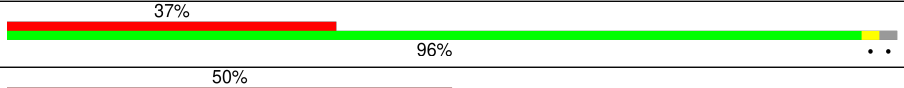
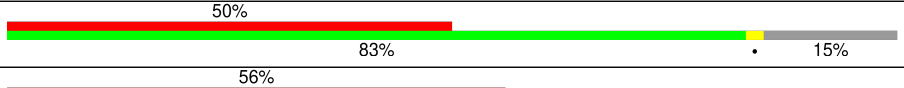
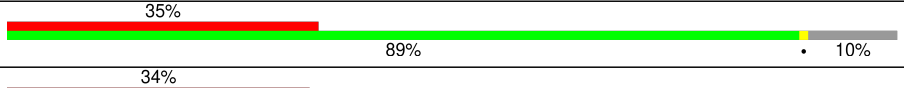
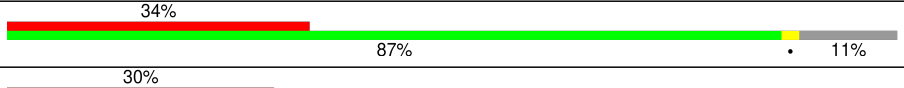
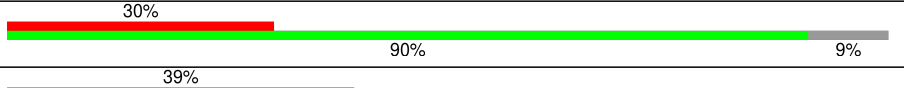
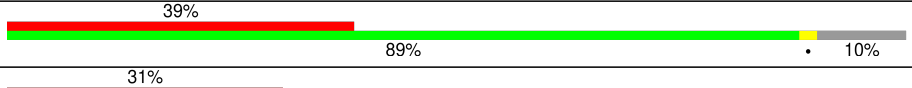
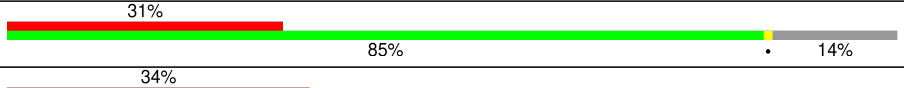
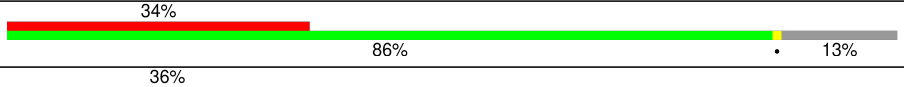
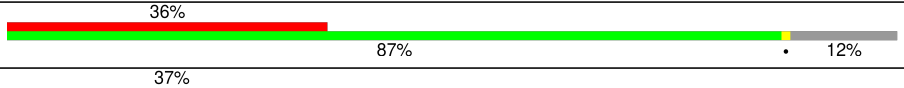
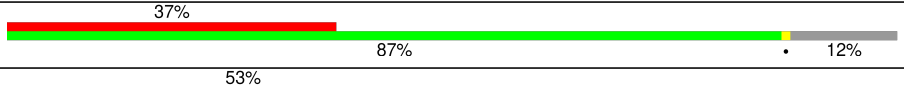
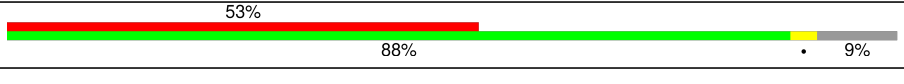
Mol	Chain	Length	Quality of chain
3	s	98	
3	t	98	
3	u	98	
3	v	98	
3	w	98	
3	x	98	
4	S	294	
4	T	294	
4	U	294	
4	V	294	
4	y	294	
5	1	311	
5	W	311	
5	X	311	
5	Y	311	
5	Z	311	
5	a	311	
5	b	311	
5	c	311	
5	d	311	
5	z	311	

2 Entry composition (i)

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

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

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

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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		

Continued on next page...

Continued from previous page...

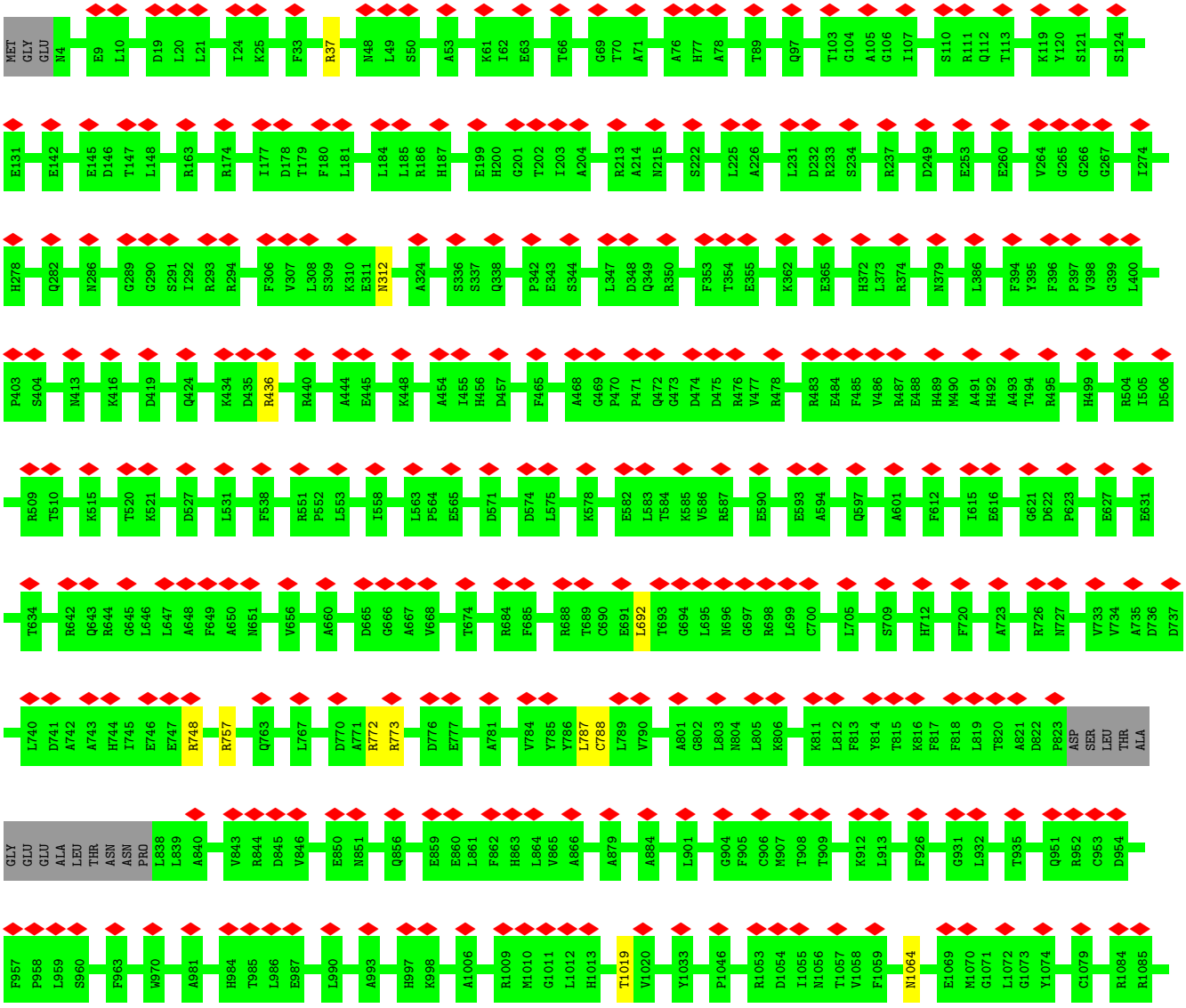
Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	274	Total	C	N	O	S	0	0
			2141	1349	371	401	20		
5	d	274	Total	C	N	O	S	0	0
			2140	1351	370	399	20		

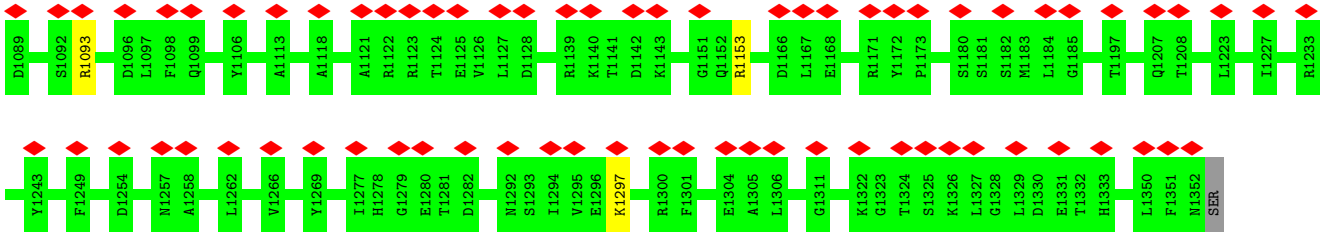
3 Residue-property plots (i)

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

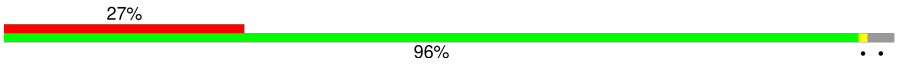
Chain A:

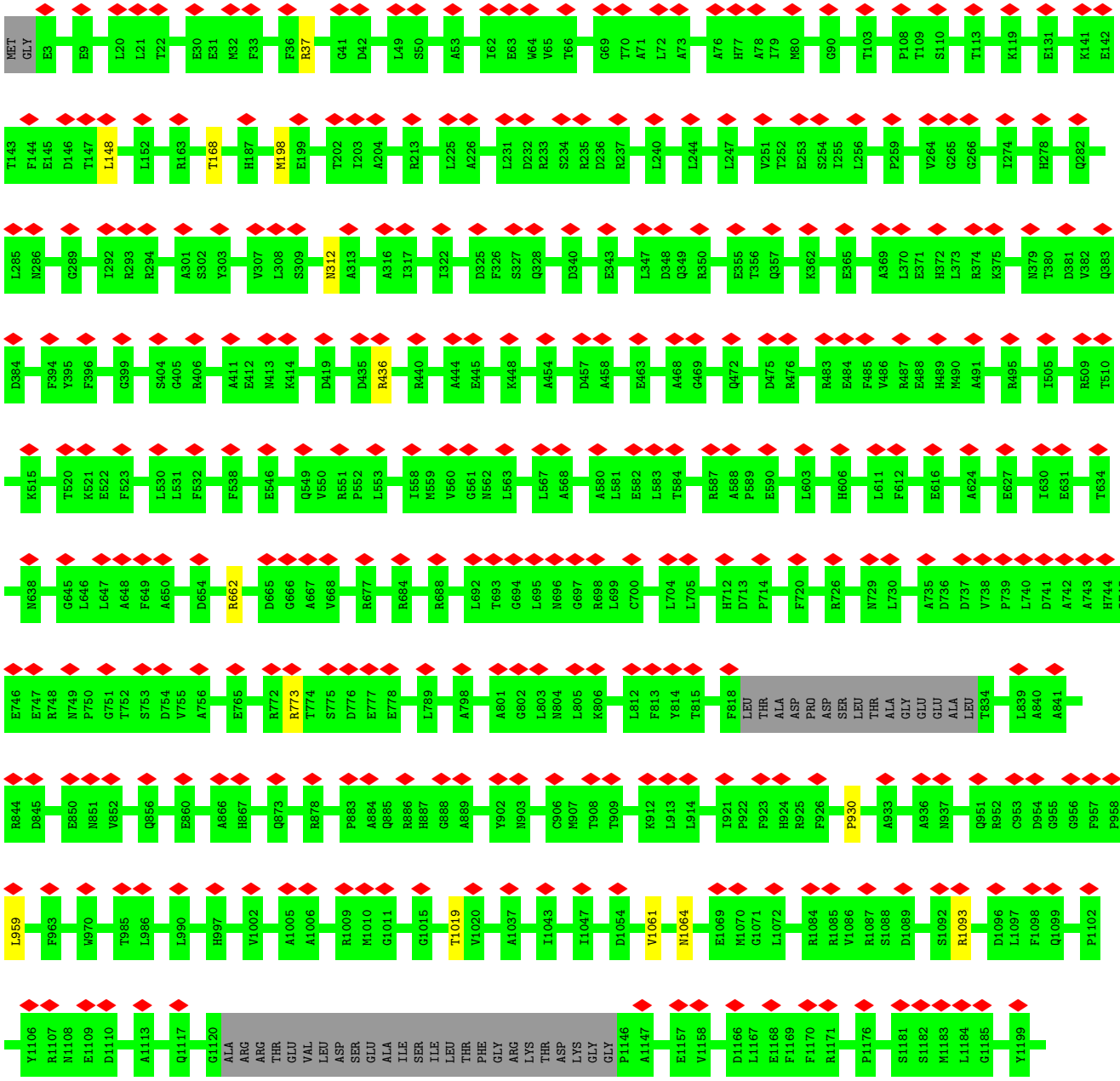


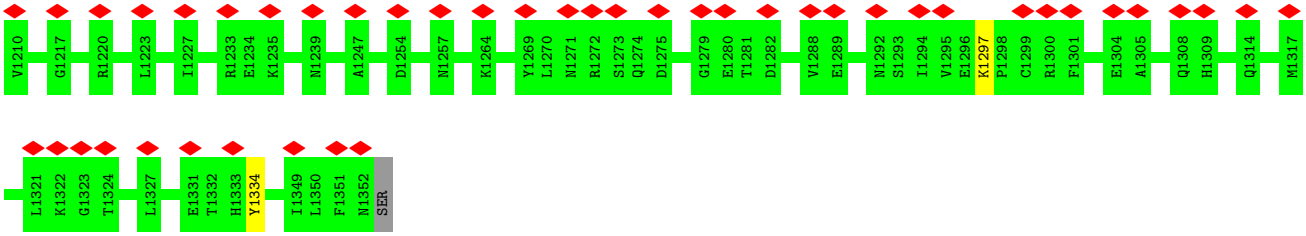


- Molecule 1: Major capsid protein

Chain B:

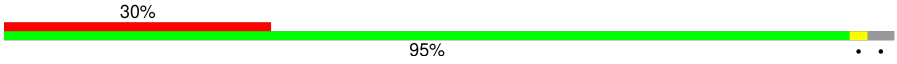


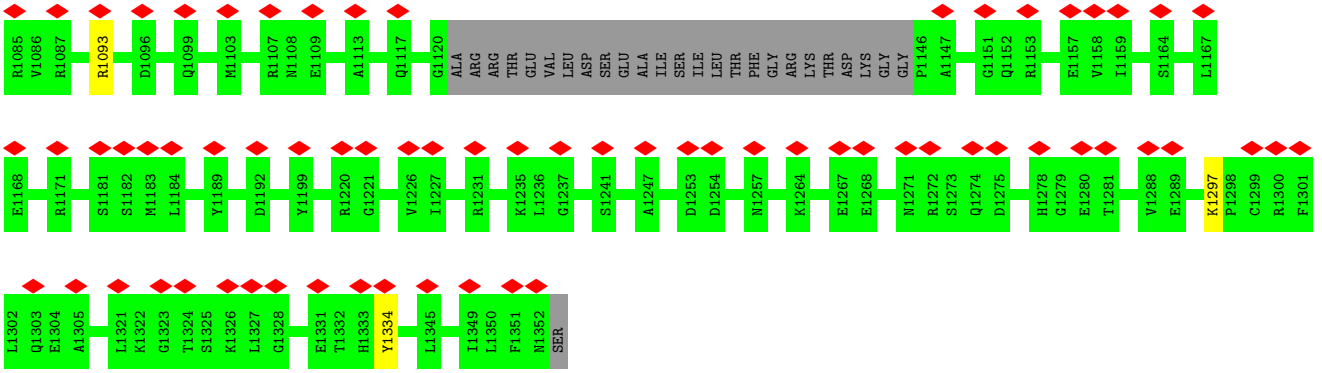




• Molecule 1: Major capsid protein

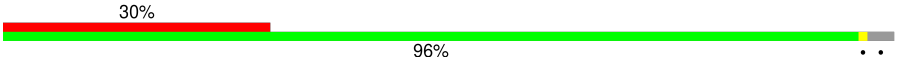
Chain C:

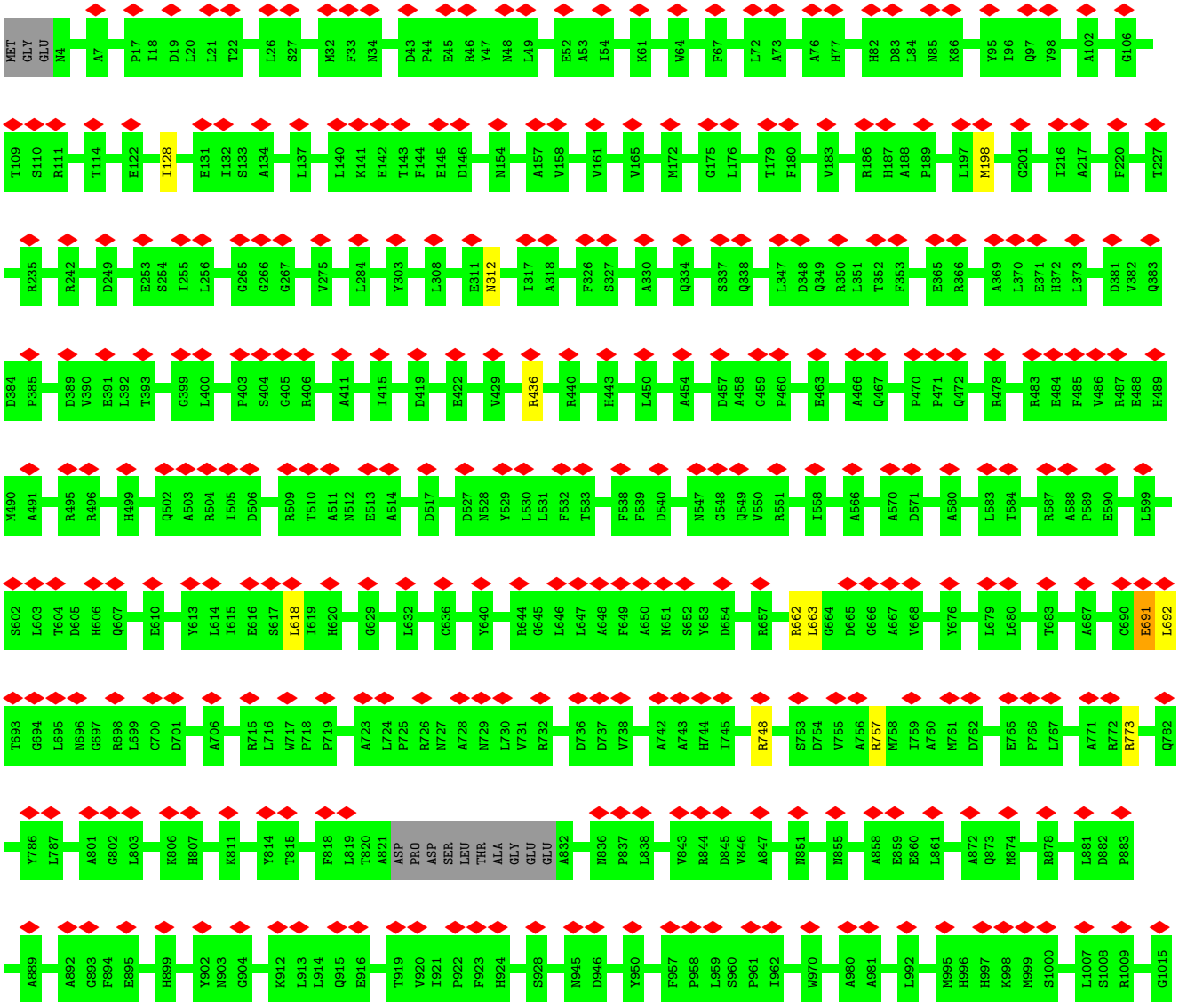




• Molecule 1: Major capsid protein

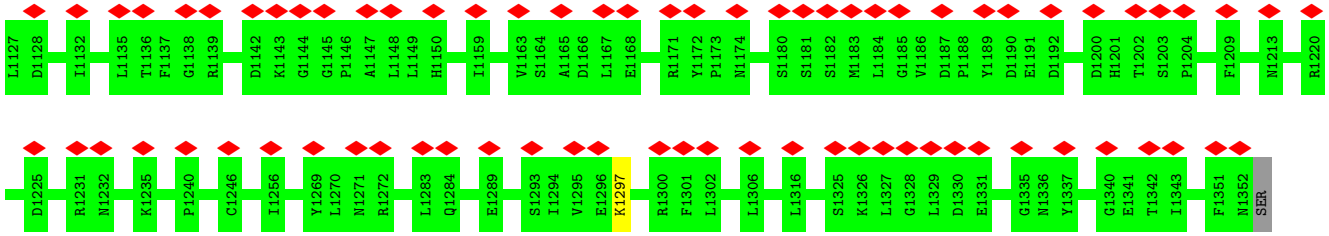
Chain D:





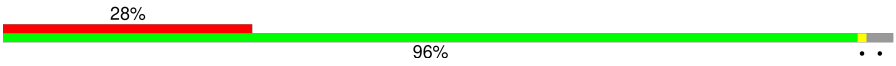
• Molecule 1: Major capsid protein

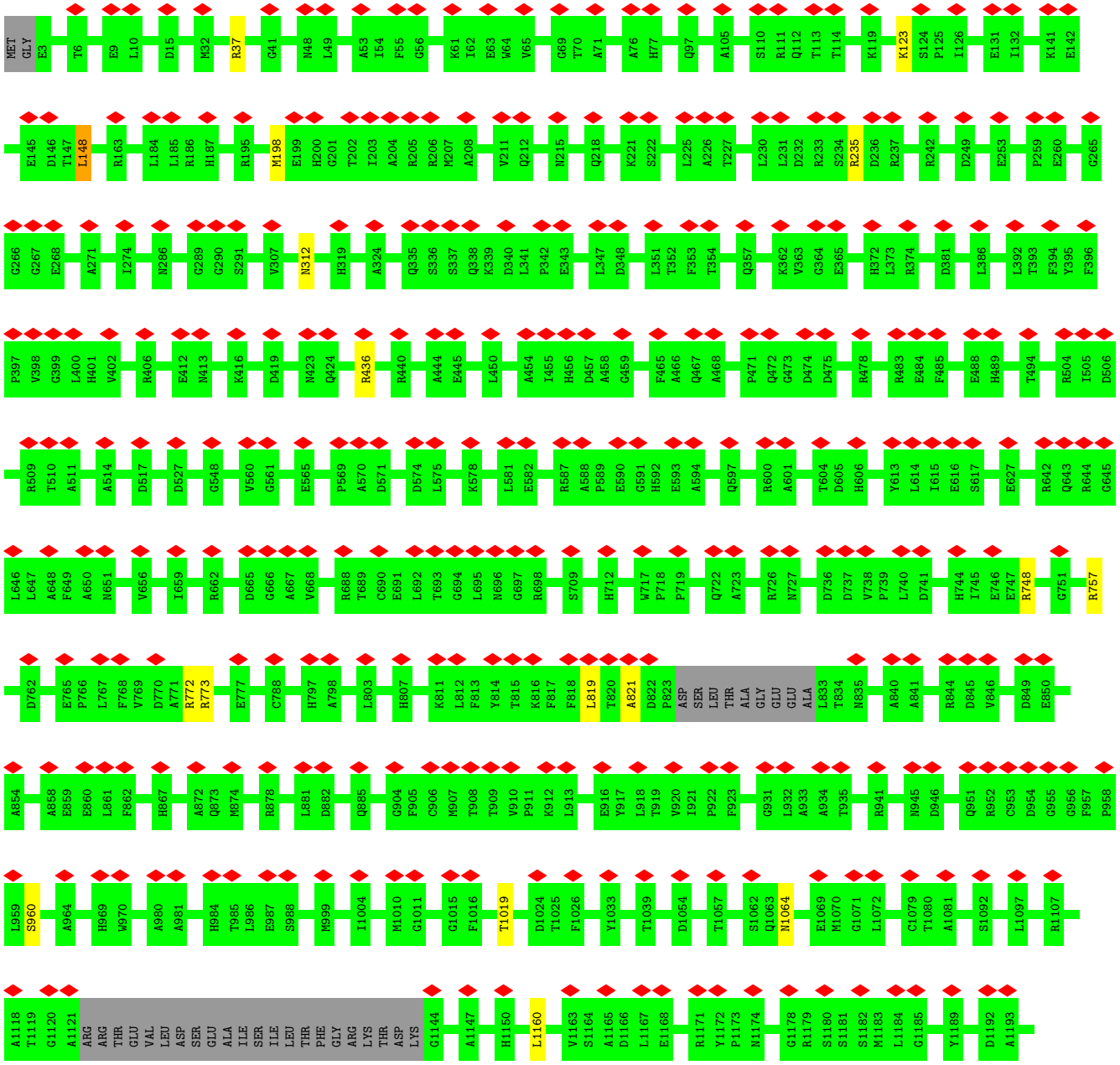
Chain E:

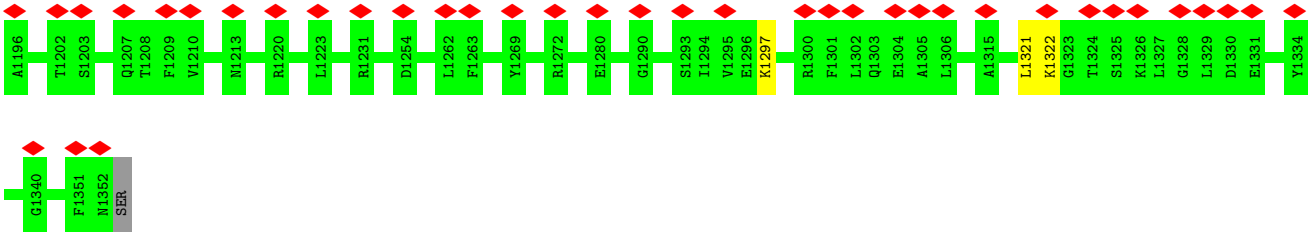


• Molecule 1: Major capsid protein

Chain F:

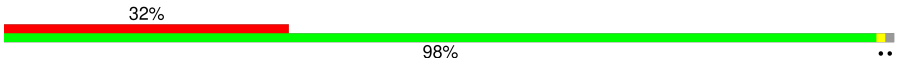


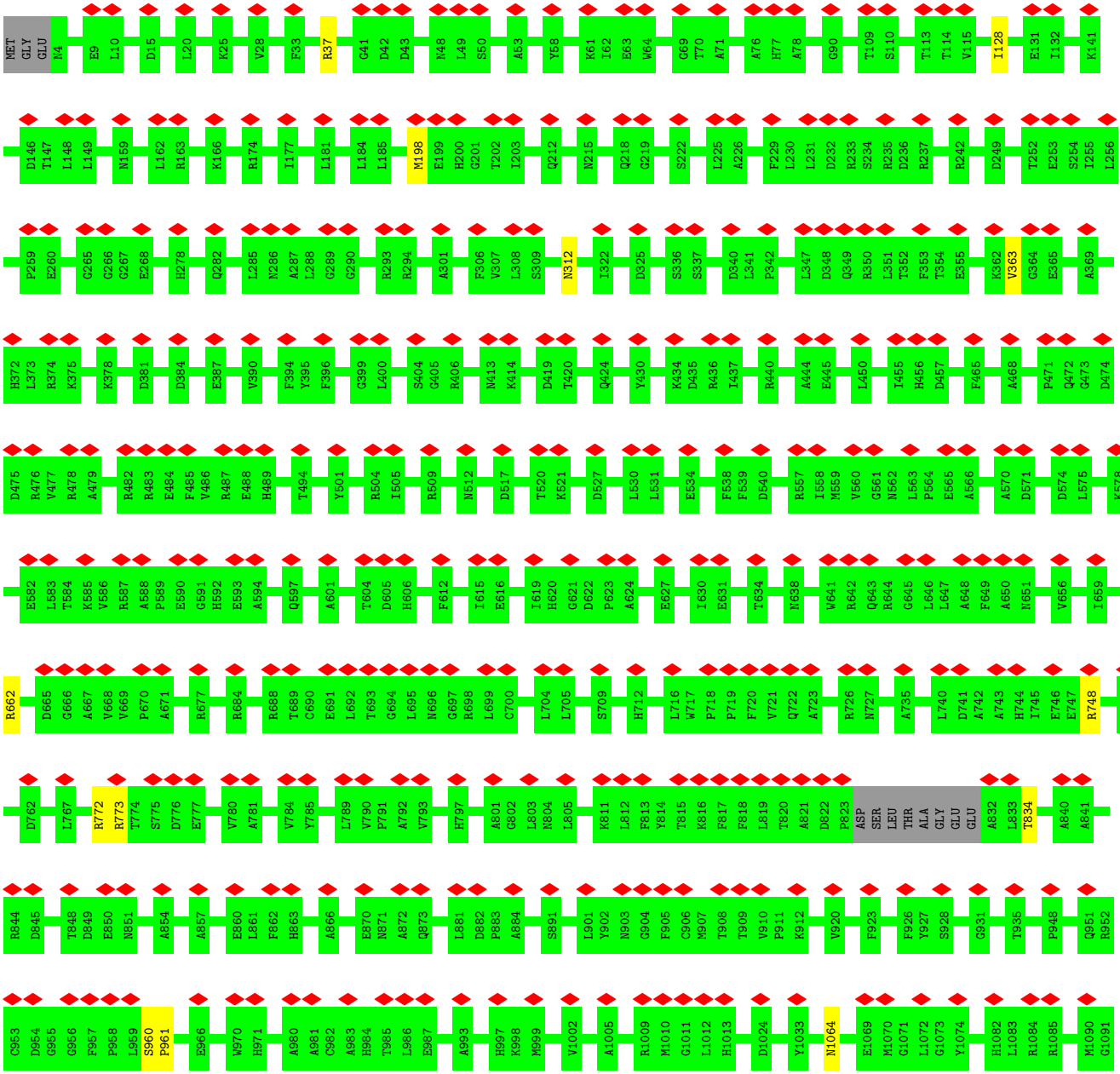


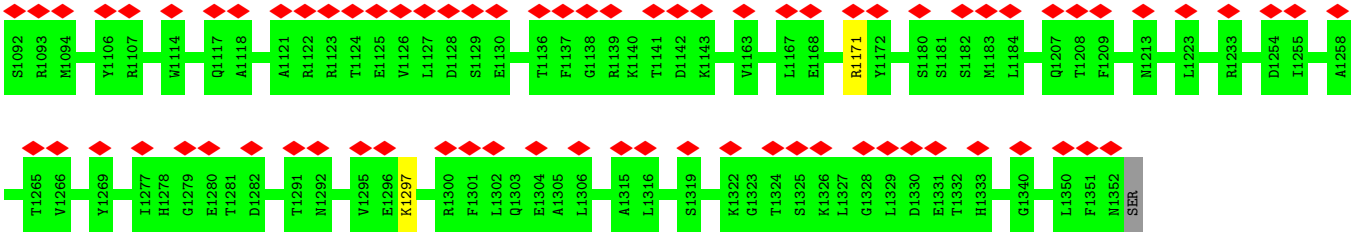


• Molecule 1: Major capsid protein

Chain G:

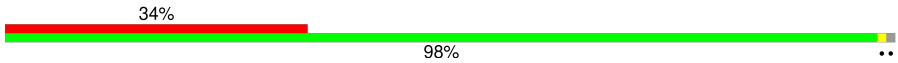


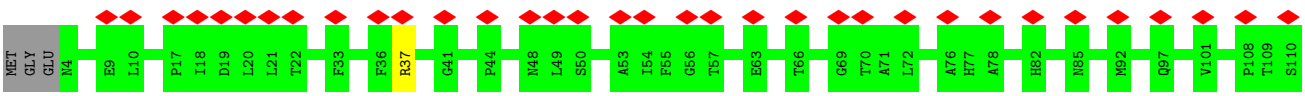


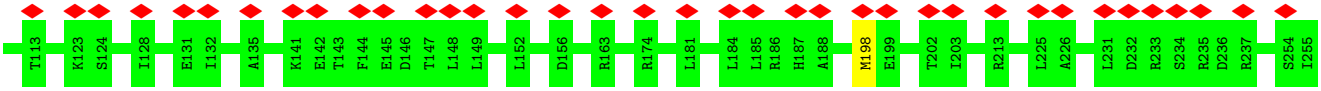


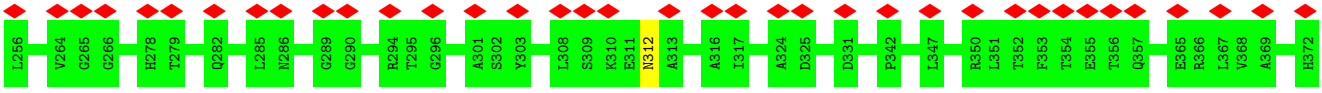
• Molecule 1: Major capsid protein

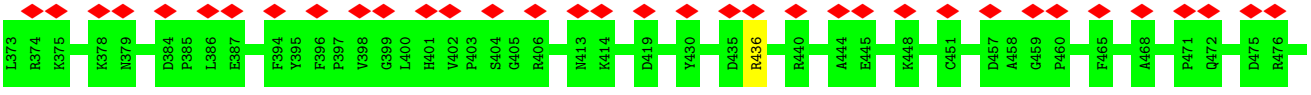
Chain H:

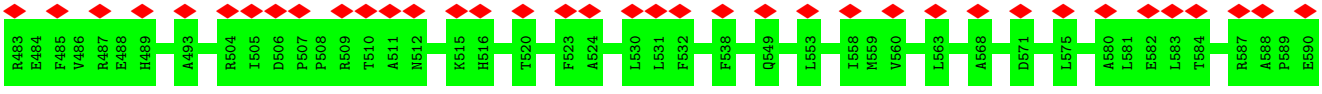


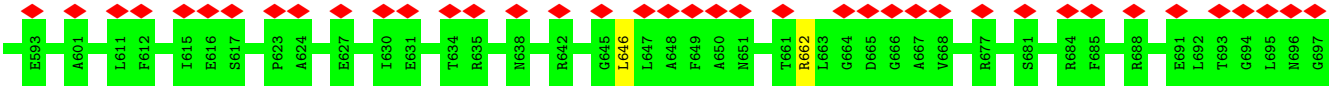


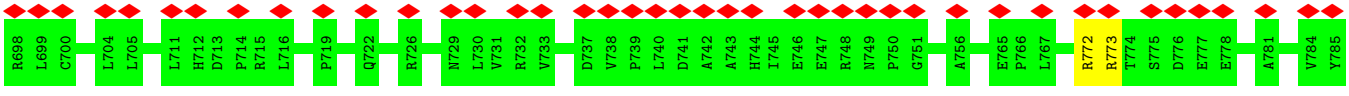


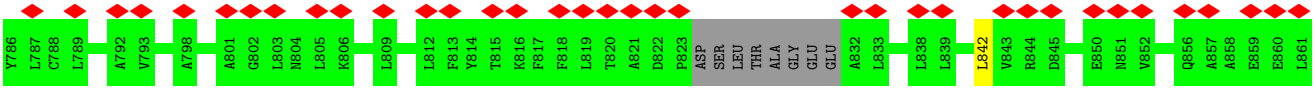


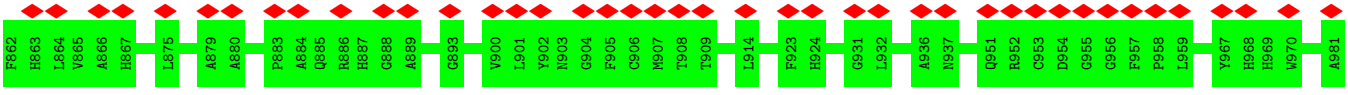


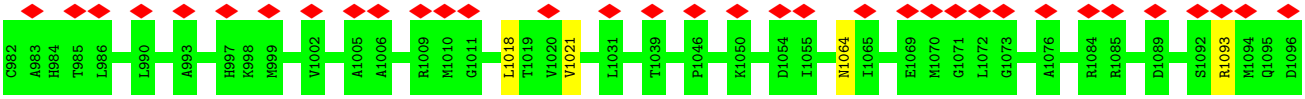


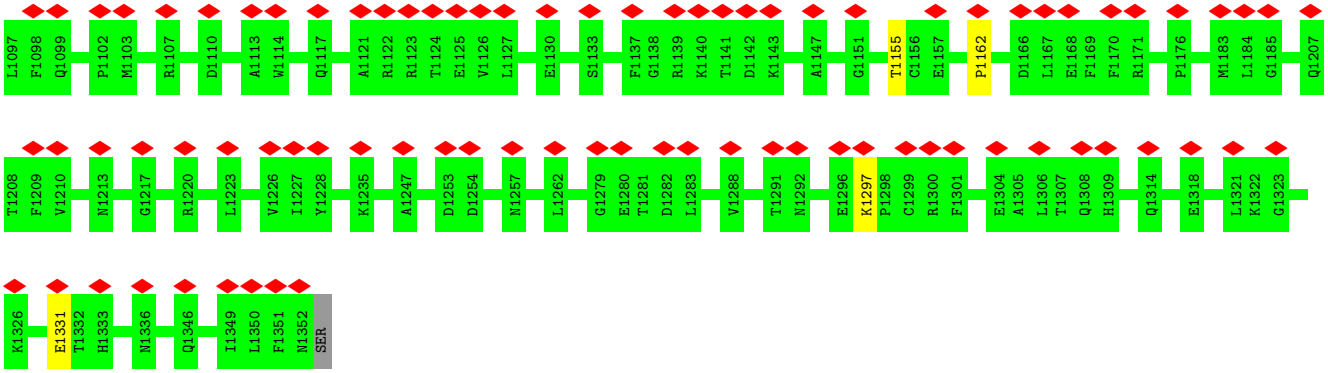






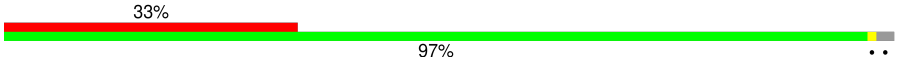


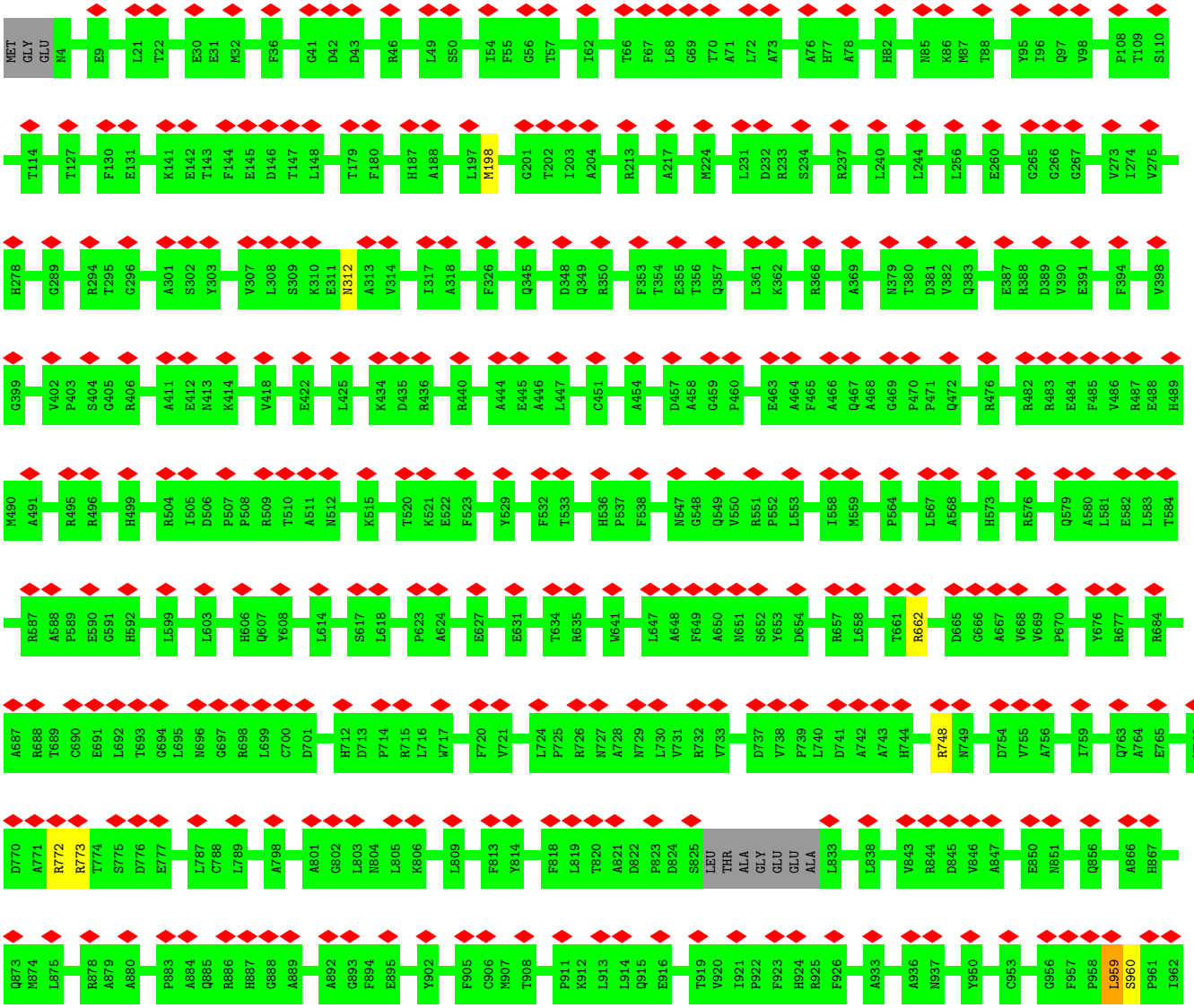


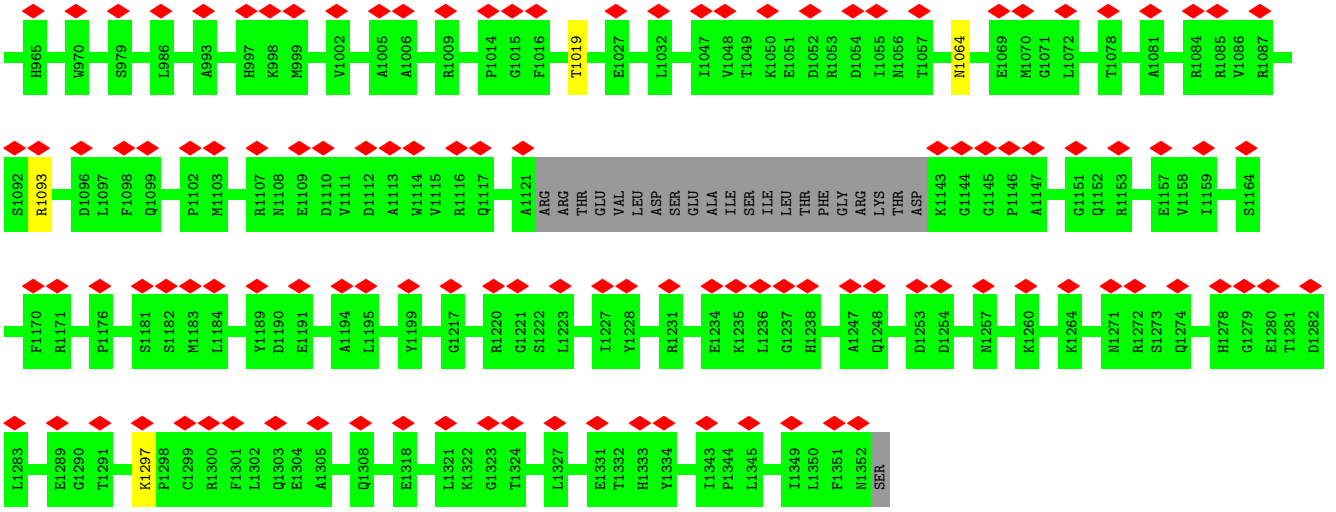


• Molecule 1: Major capsid protein

Chain I:

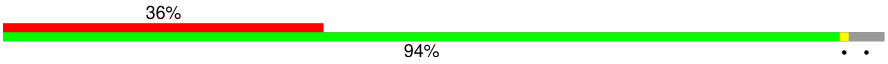


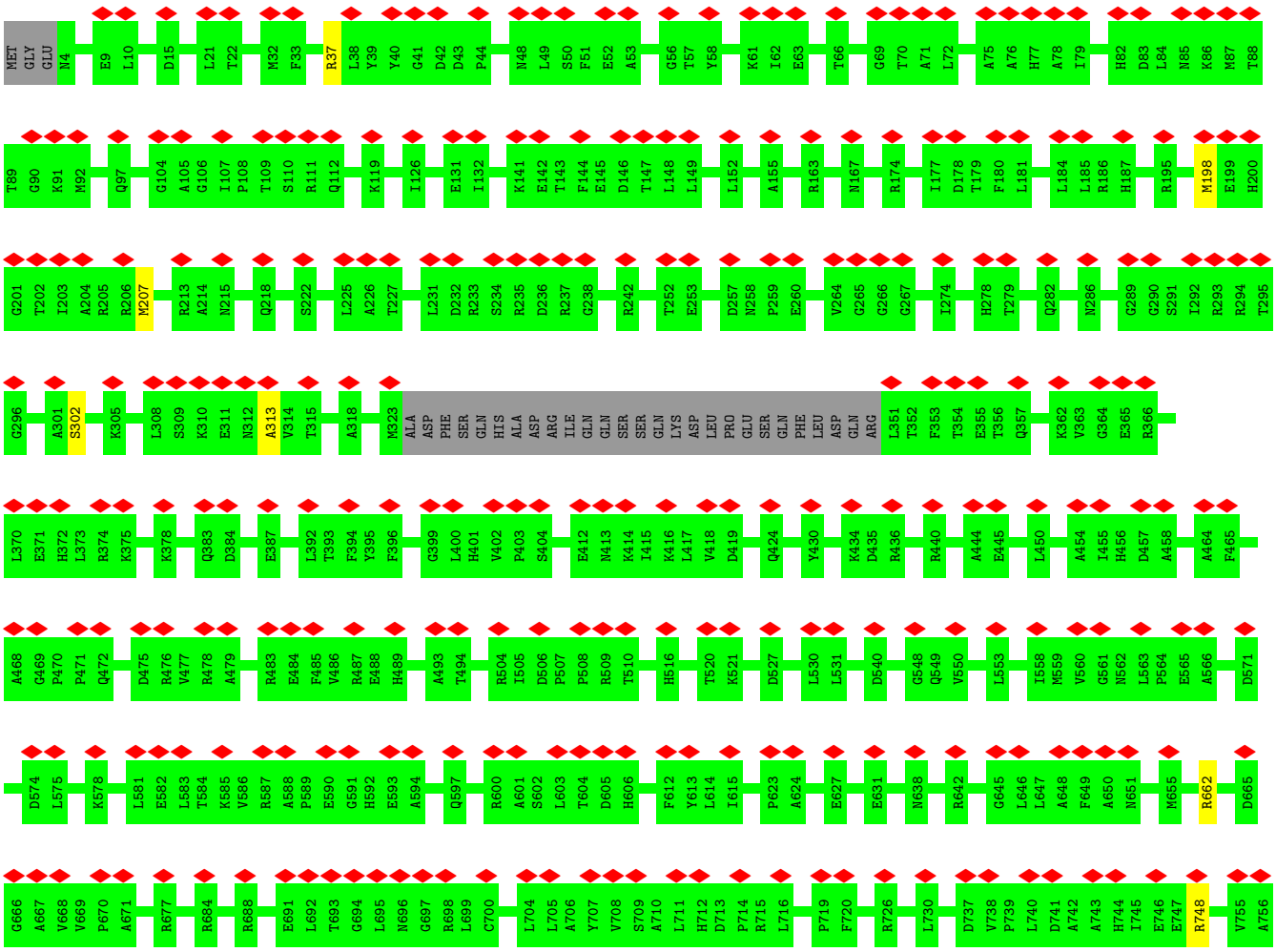


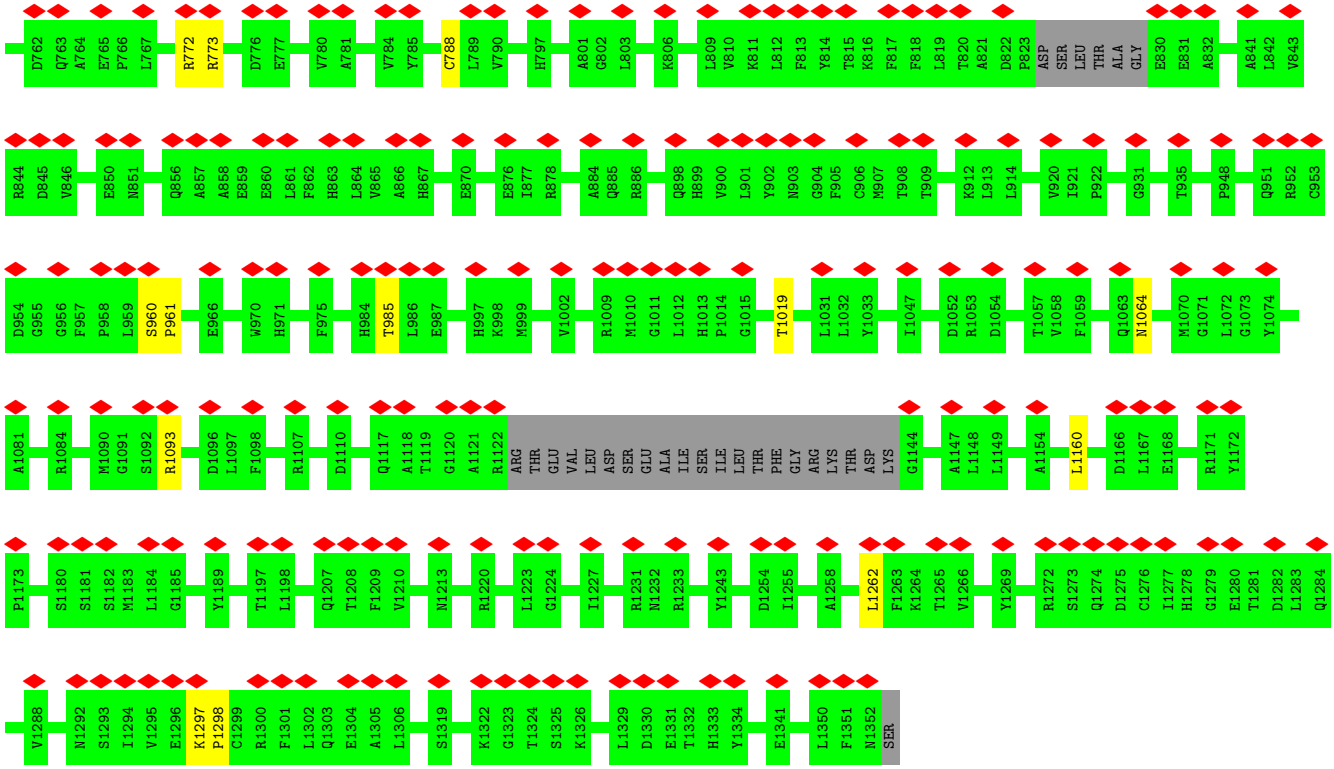


- Molecule 1: Major capsid protein

Chain k:

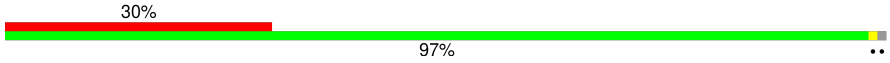


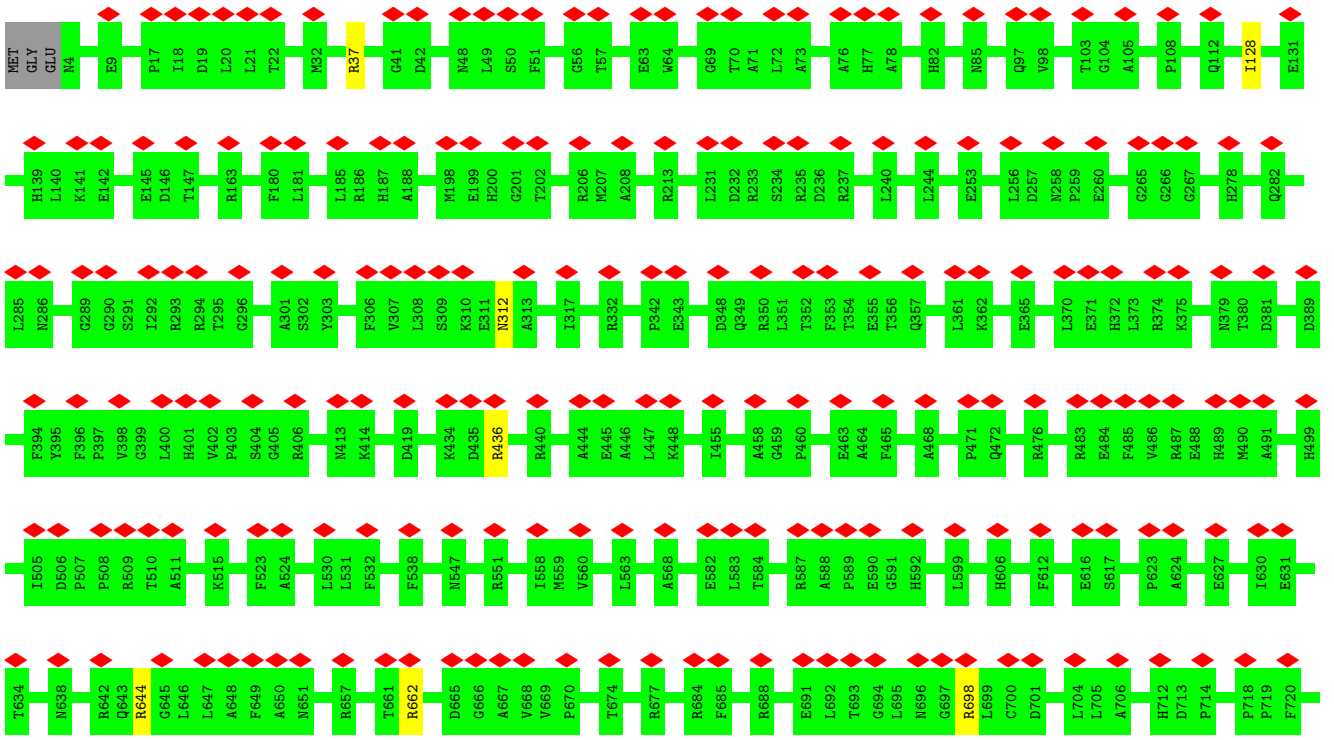


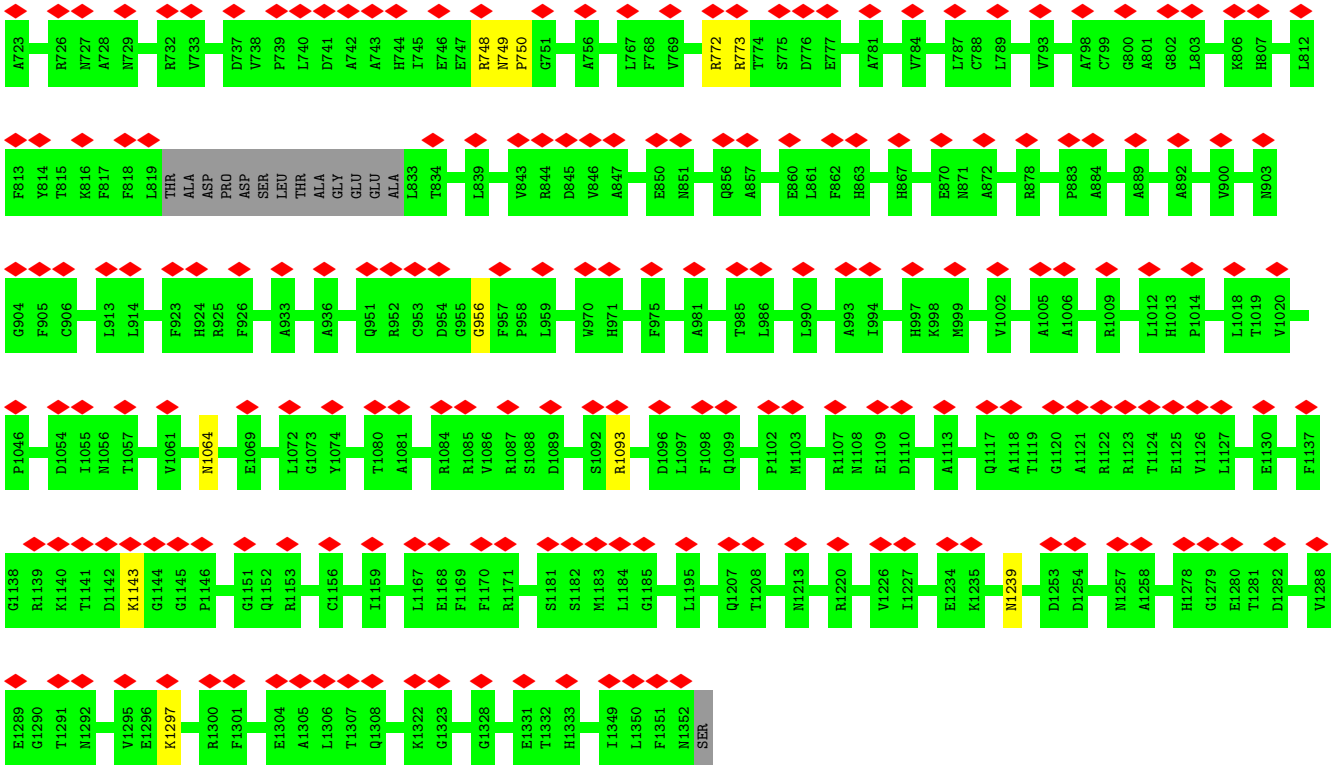


- Molecule 1: Major capsid protein

Chain l:

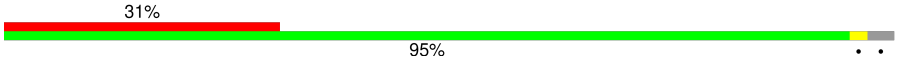


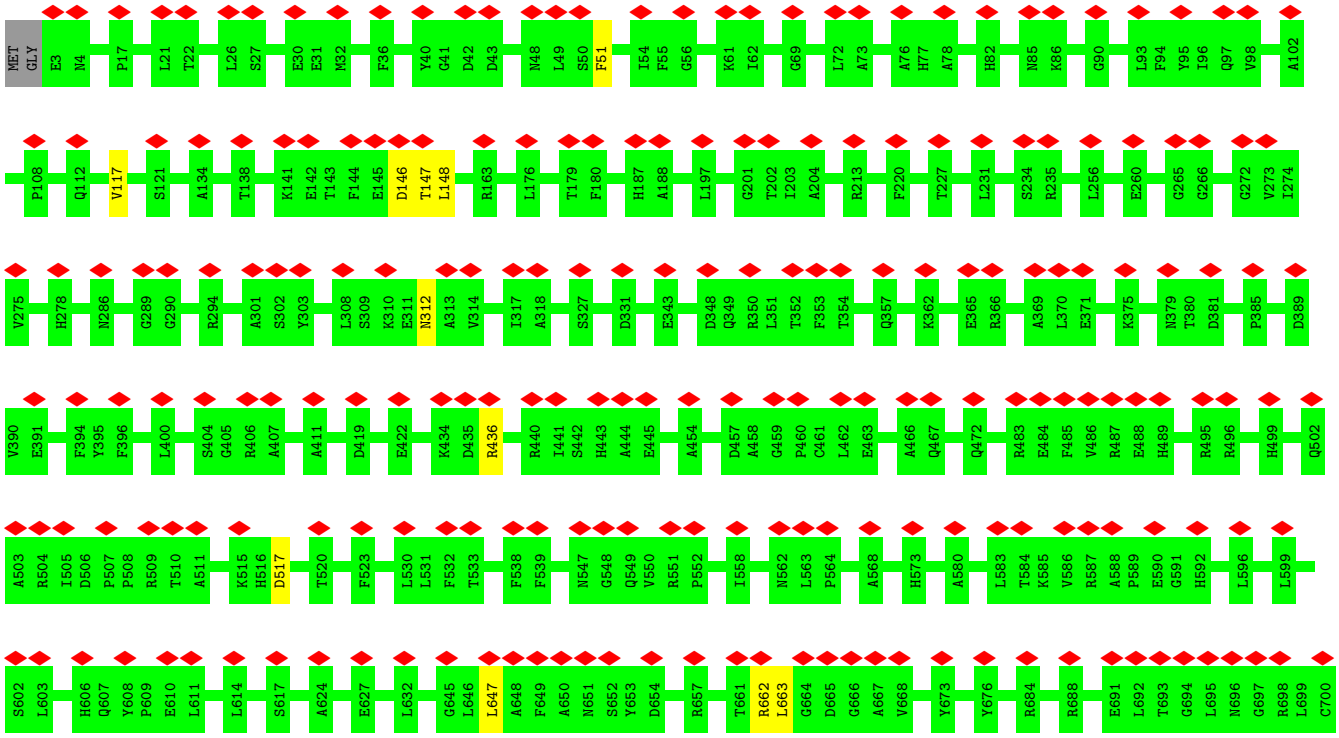


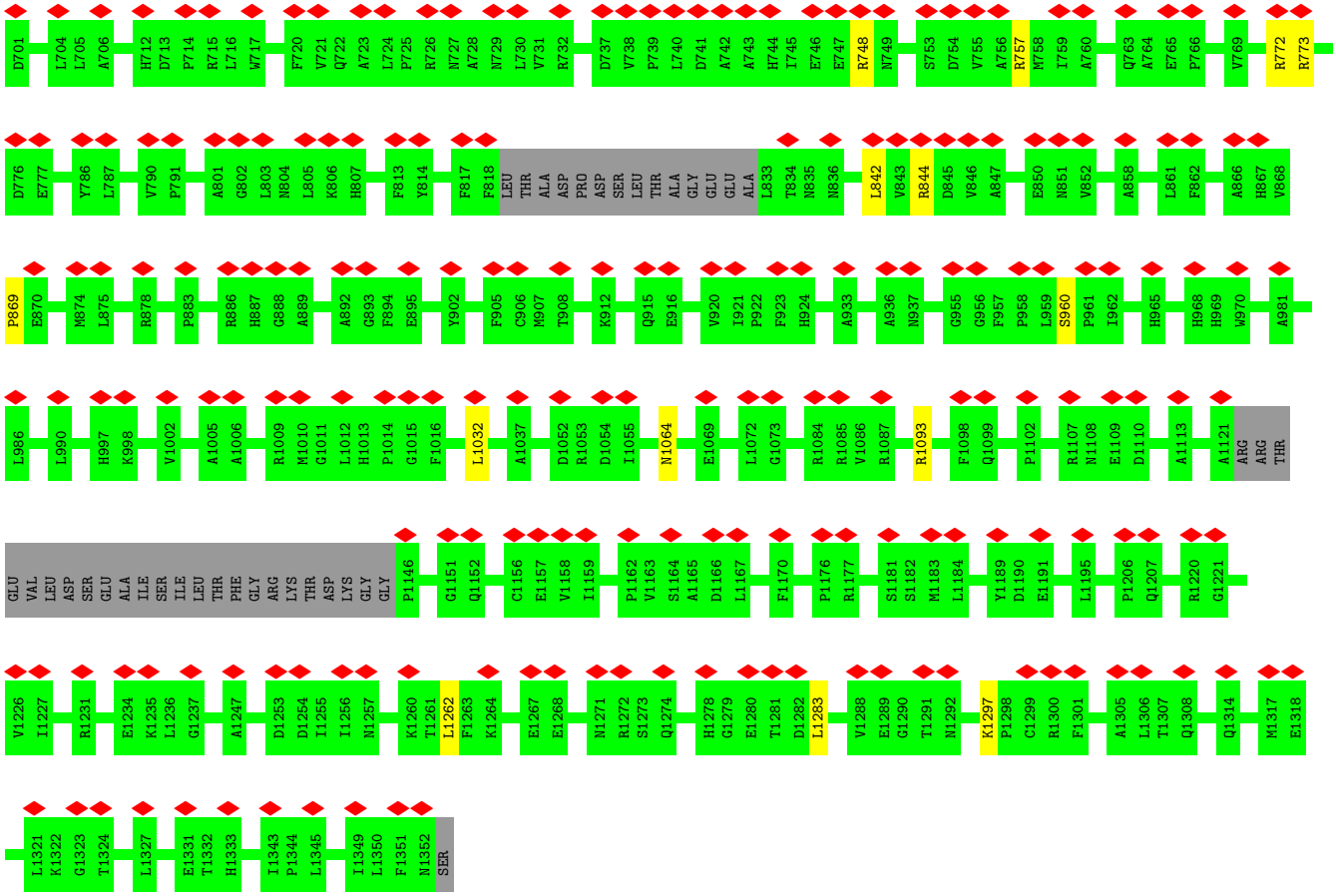


• Molecule 1: Major capsid protein

Chain m:

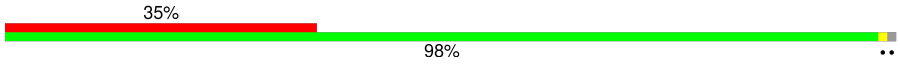


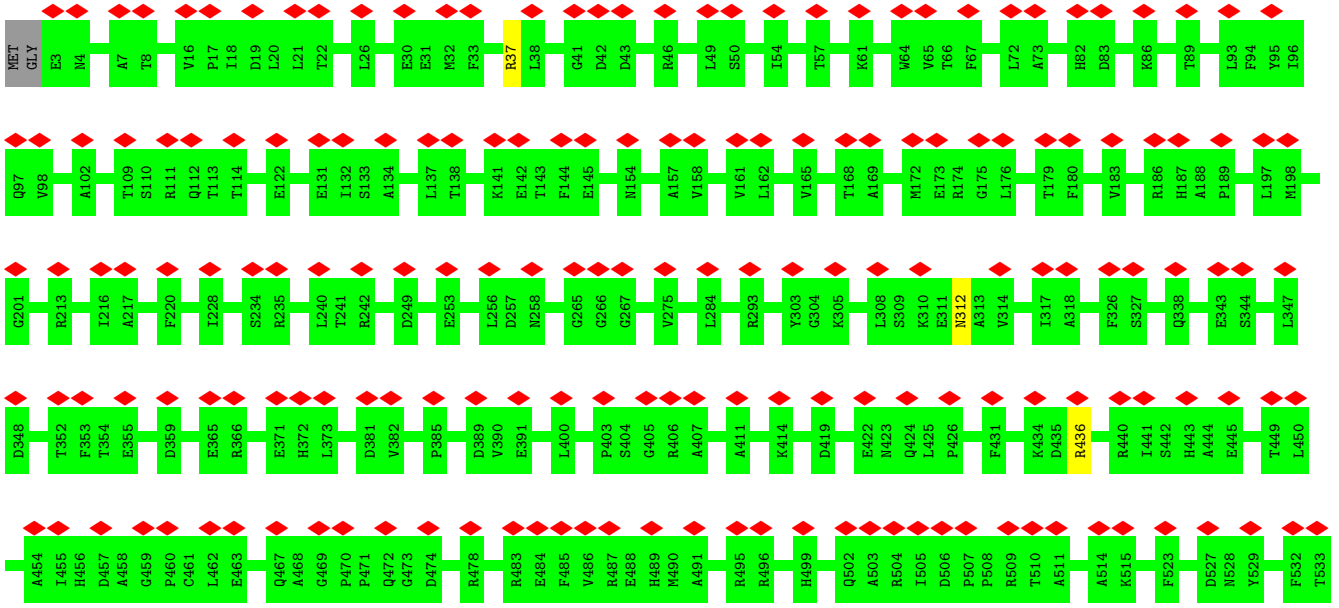


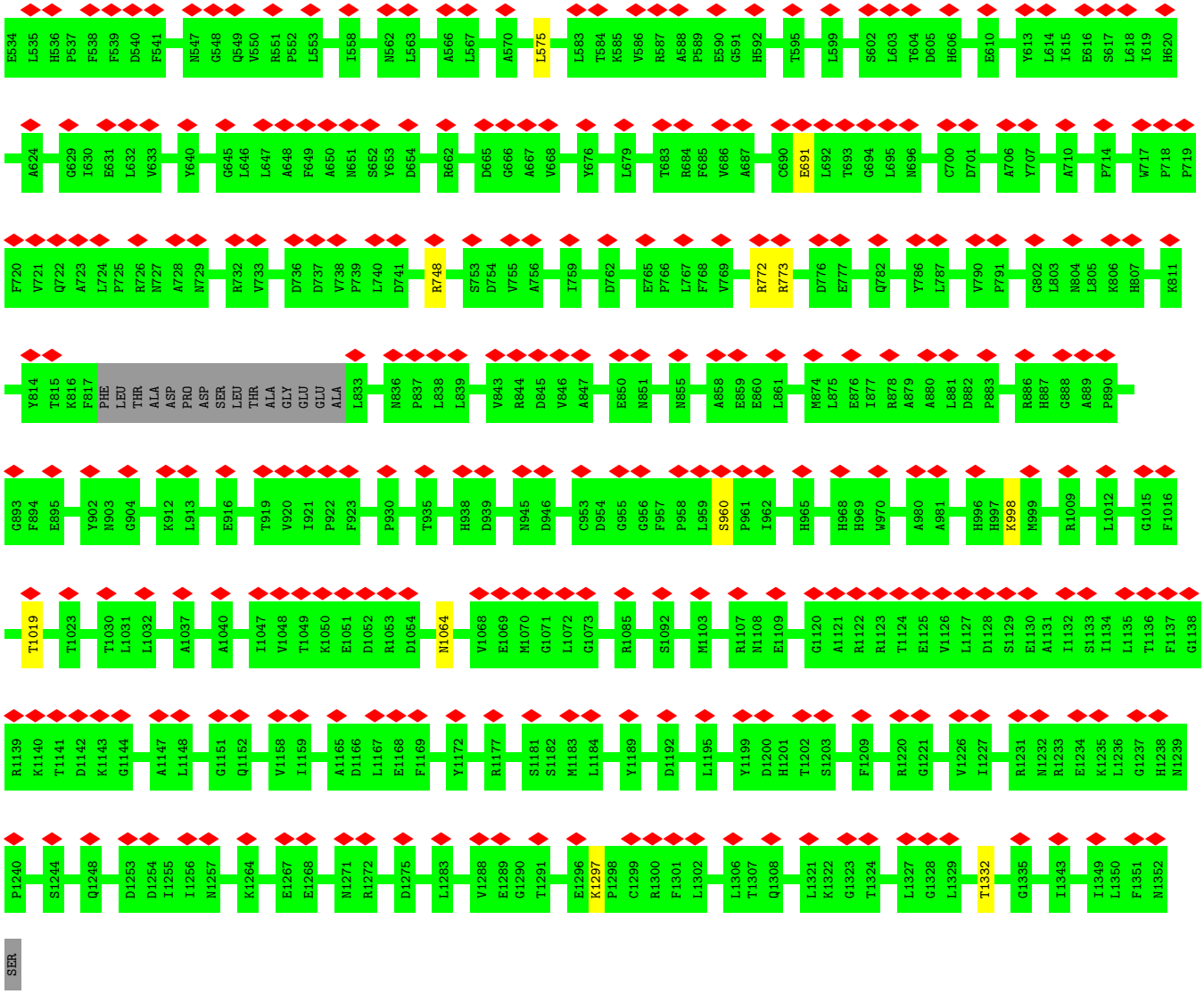


• Molecule 1: Major capsid protein

Chain n:

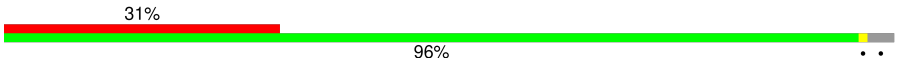


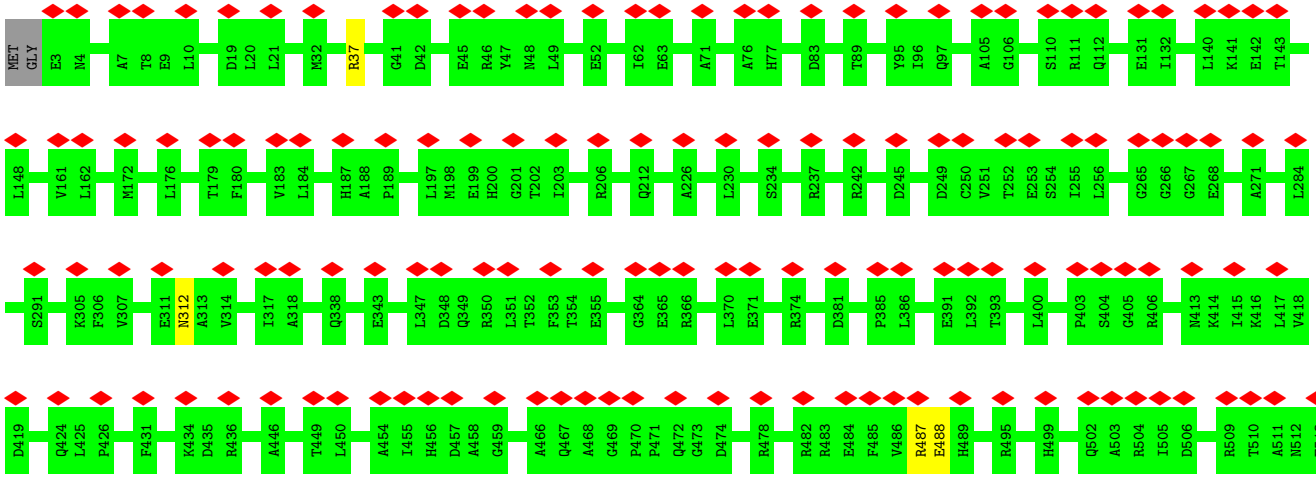


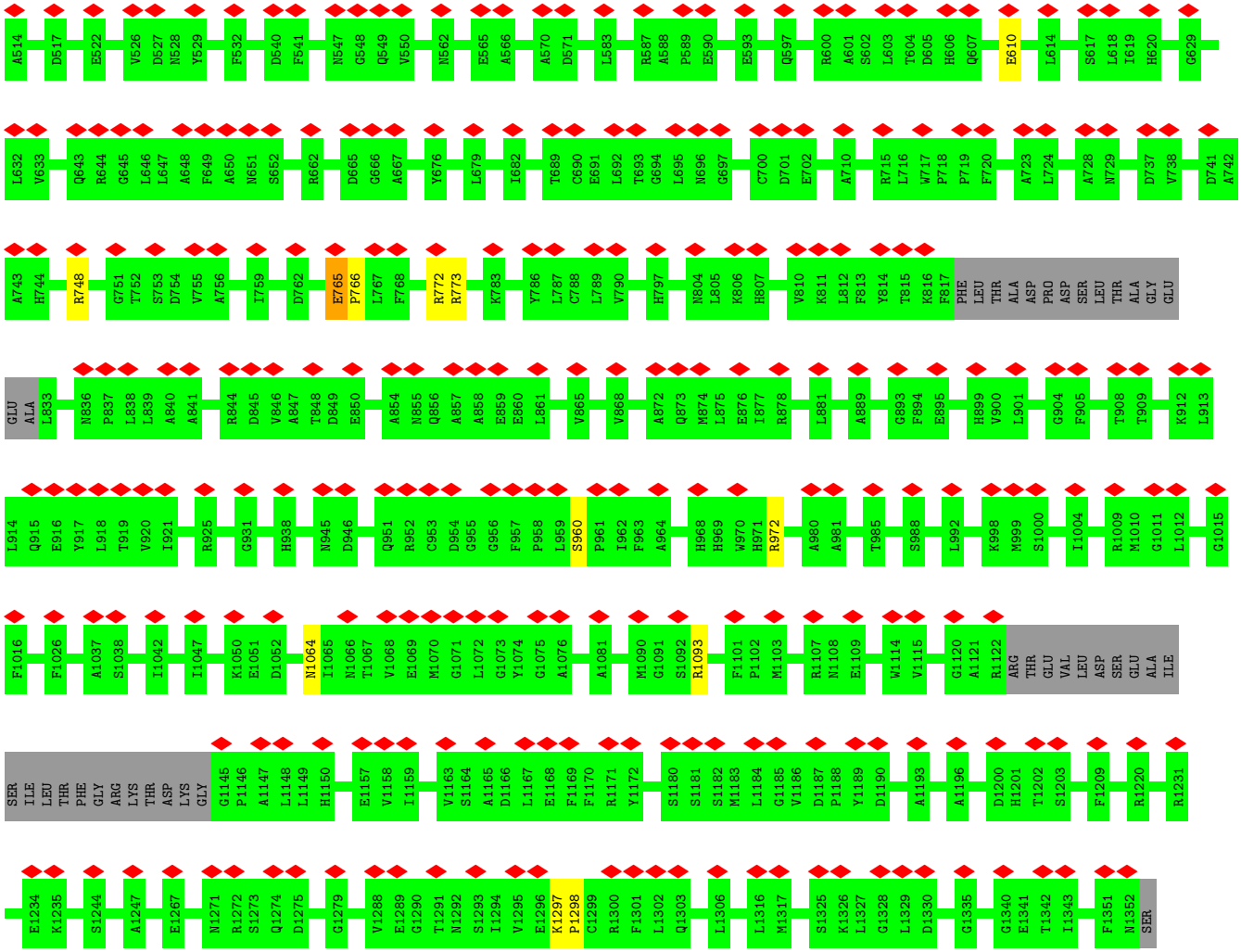


- Molecule 1: Major capsid protein

Chain o:

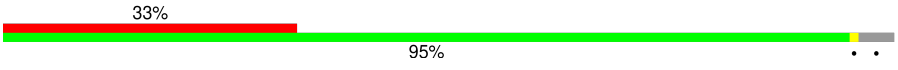


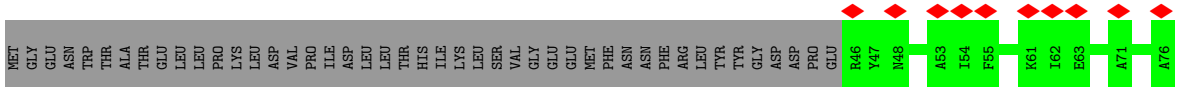


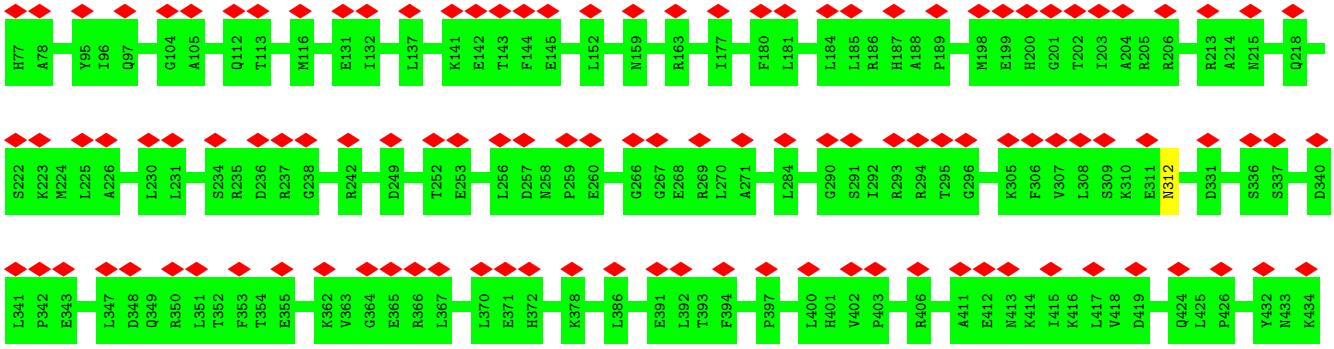


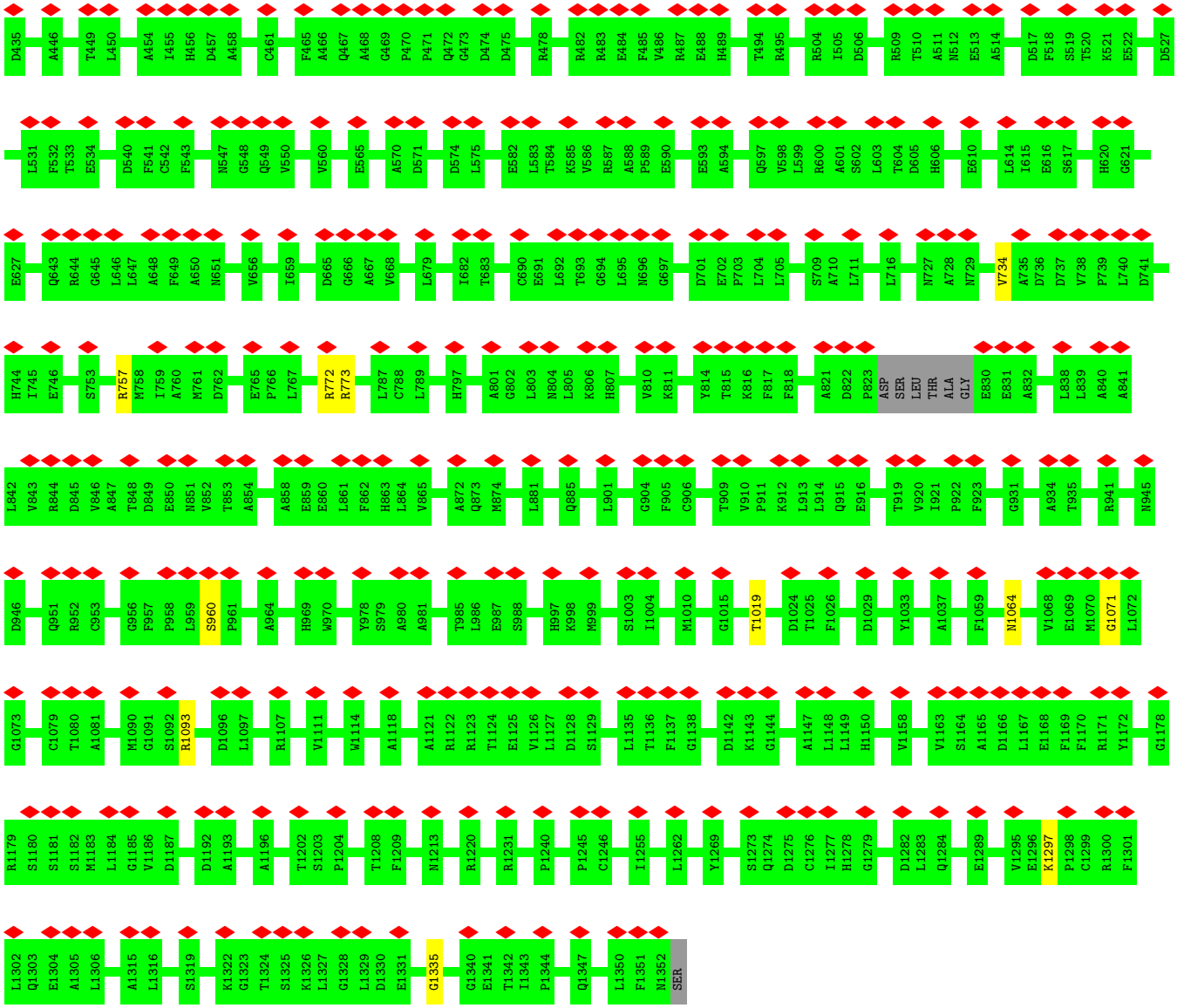
• Molecule 1: Major capsid protein

Chain p:



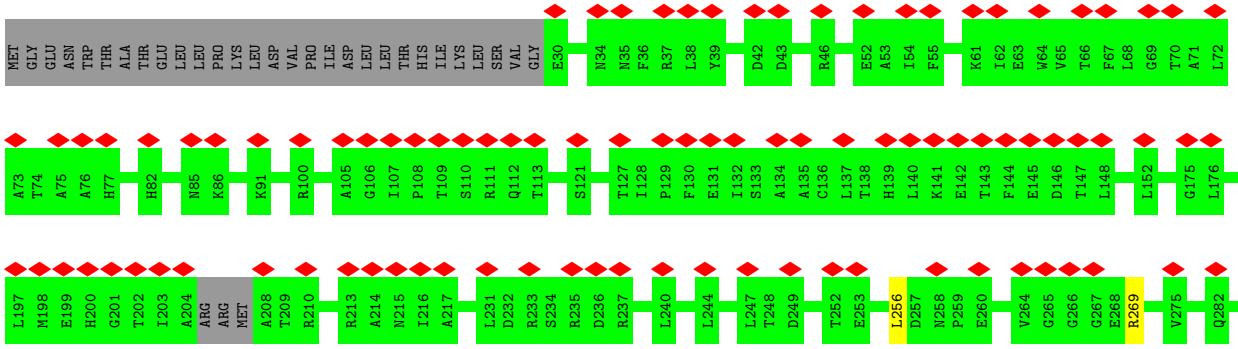


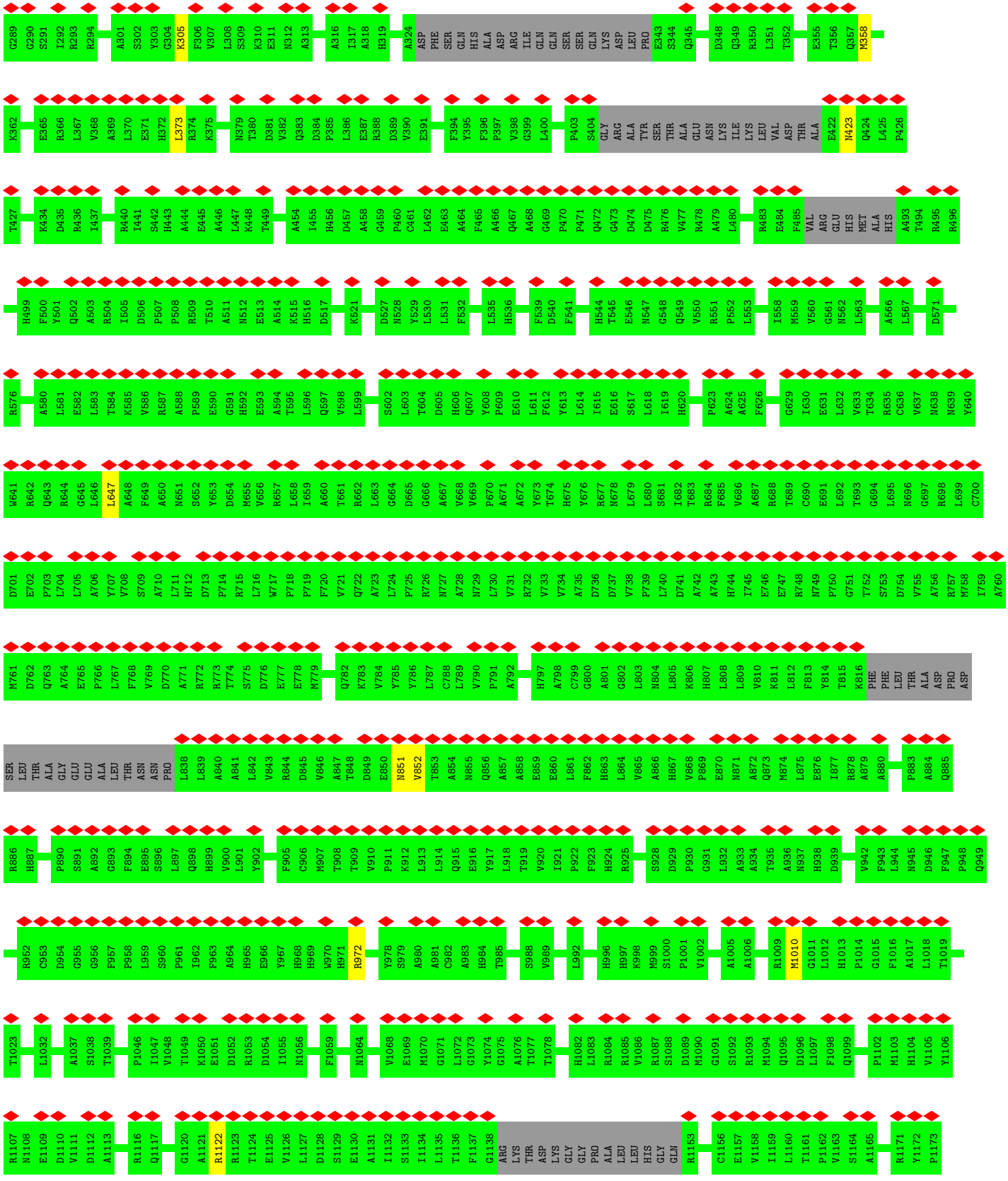




• Molecule 1: Major capsid protein

Chain q:

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K362 E365 R366 L367 V368 A369 L370 E371 H372 L373 R374 K375 N379 T380 D381 V382 Q383 D384 P385 L386 E387 R388 D389 V390 E391 F394 Y395 F396 P397 V398 G399 L400 P403 S404 GLY ARG ALA TYR SER THR ALA GLU ASN LYS ILE LYS LEU VAL ASP THR ALA E422 N423 Q424 L425 P426
T427 K434 D435 R436 I437 R440 I441 S442 H443 A444 E445 A446 L447 K448 T449 A454 I455 H456 D457 A458 G459 P460 C461 L462 E463 A464 F465 A466 Q467 A468 G469 P470 P471 Q472 G473 D474 D475 R476 V477 R478 A479 L480 R483 E484 F485 VAL ARG GLU HIS MET ALA HIS A493 T494 R495 R496
H499 F500 Y501 Q502 A503 R504 I505 D506 P507 P508 R509 T510 A511 N512 E513 A514 K515 H516 D517 K521 D527 N528 Y529 L530 L531 F532 L535 H536 F539 D540 F541 H544 T545 E546 N547 G548 Q549 V550 R551 P552 L553 I558 M559 V560 G561 N562 L563 A566 L567 D571
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W641 R642 Q643 R644 G645 L646 L647 A648 F649 A650 N651 S652 Y653 D654 M655 V656 R657 L658 I659 A660 T661 R662 L663 G664 D665 G666 A667 V668 V669 P670 A671 A672 Y673 T674 H675 Y676 R677 N678 L679 L680 S681 I682 T683 R684 F685 V686 A687 R688 T689 C690 E691 L692 T693 G694 L695 N696 G697 R698 L699 C700
D701 E702 P703 L704 L705 A706 Y707 V708 S709 A710 L711 H712 D713 P714 R715 L716 W717 P718 P719 F720 V721 Q722 A723 L724 P725 R726 N727 A728 N729 L730 V731 R732 V733 V734 A735 D736 D737 V738 P739 L740 D741 A742 A743 H744 I745 E746 E747 R748 N749 P750 G751 T752 S753 D754 V755 A756 R757 M758 I759 A760
M761 D762 Q763 A764 E765 P766 L767 F768 V769 D770 A771 R772 R773 T774 S775 D776 E777 E778 M779 Q782 K783 V784 Y785 Y786 L787 C788 L789 V790 P791 A792 H797 A798 C799 G800 A801 G802 L803 N804 L805 K806 H807 L808 L809 V810 K811 L812 F813 Y814 T815 K816 PHE PHE LEU THR ALA ASP PRO ASP
SER LEU THR ALA GLY GLU GLU ALA LEU THR ASN ASN PRO L838 L839 A840 A841 L842 V843 R844 D845 V846 A847 T848 D849 E850 N851 V852 T853 A854 N855 Q856 A857 A858 E859 E860 L861 F862 H863 L864 V865 A866 H867 V868 P869 E870 N871 A872 Q873 M874 L875 E876 I877 R878 A879 A880 P883 A884 Q885
R886 H887 P890 S891 A892 G893 F894 E895 S896 L897 Q898 H899 V900 L901 Y902 F905 C906 M907 T908 T909 V910 P911 K912 L913 L914 Q915 E916 Y917 L918 T919 V920 I921 P922 F923 H924 R925 S928 D929 P930 G931 L932 A933 A934 T935 A936 N937 H938 D939 V942 F943 L944 N945 D946 F947 P948 Q949
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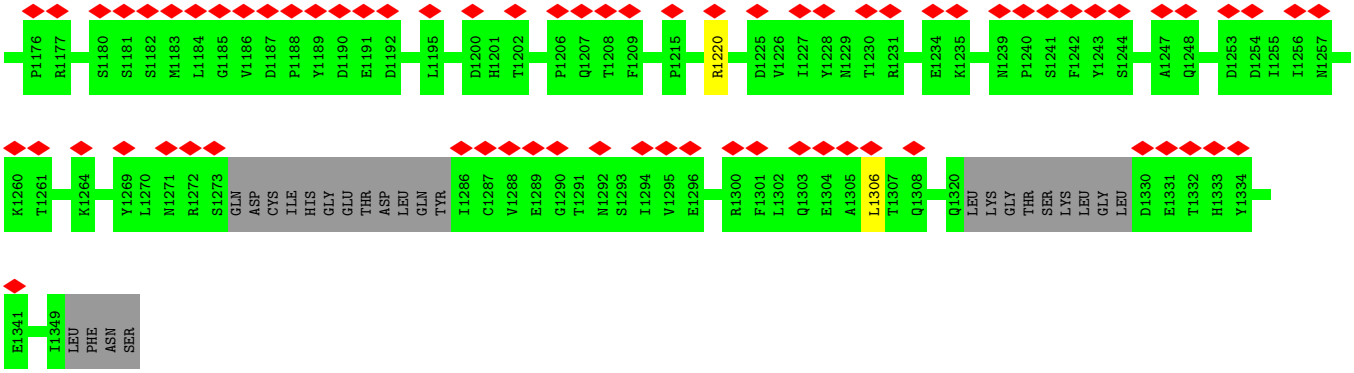
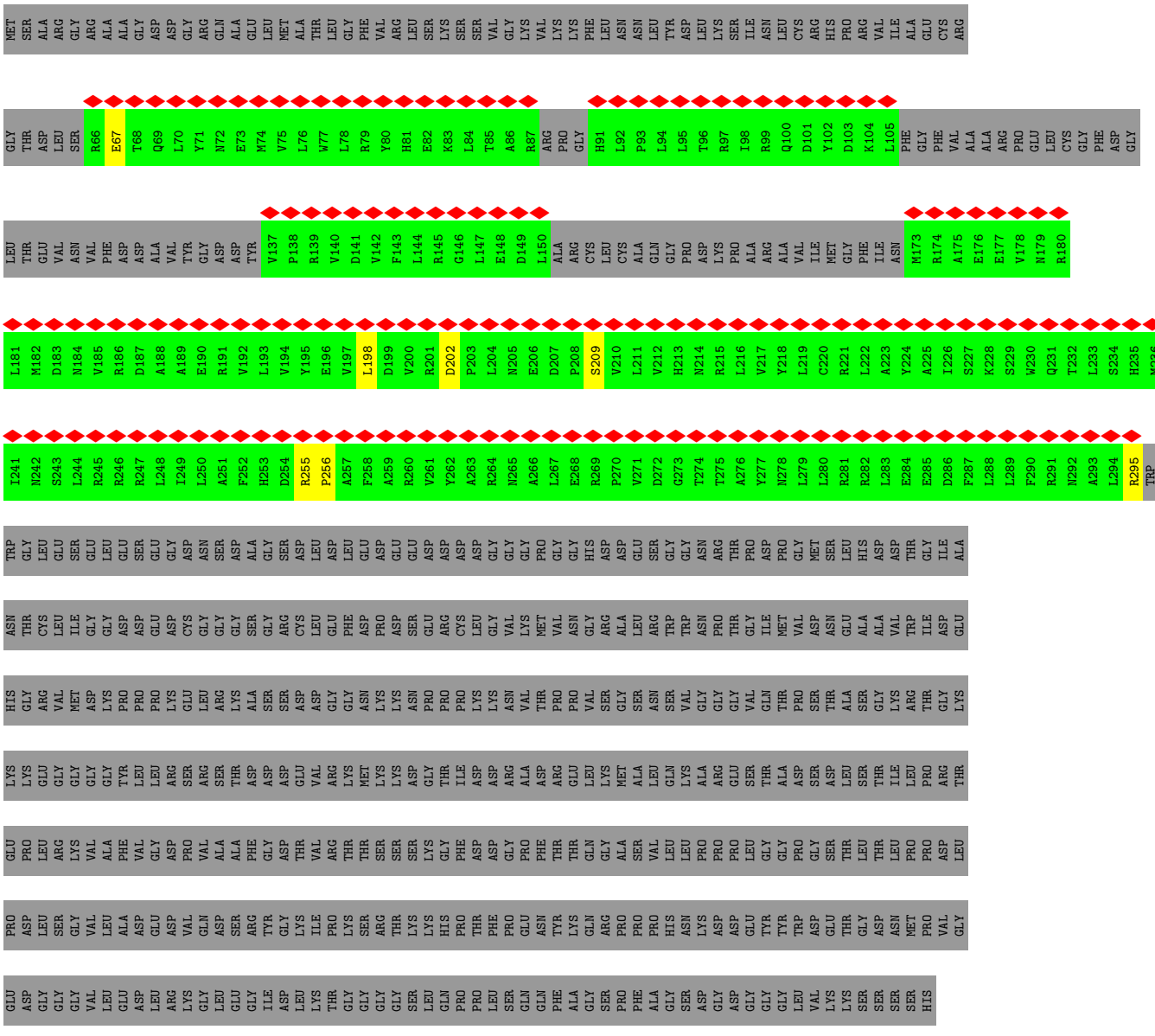


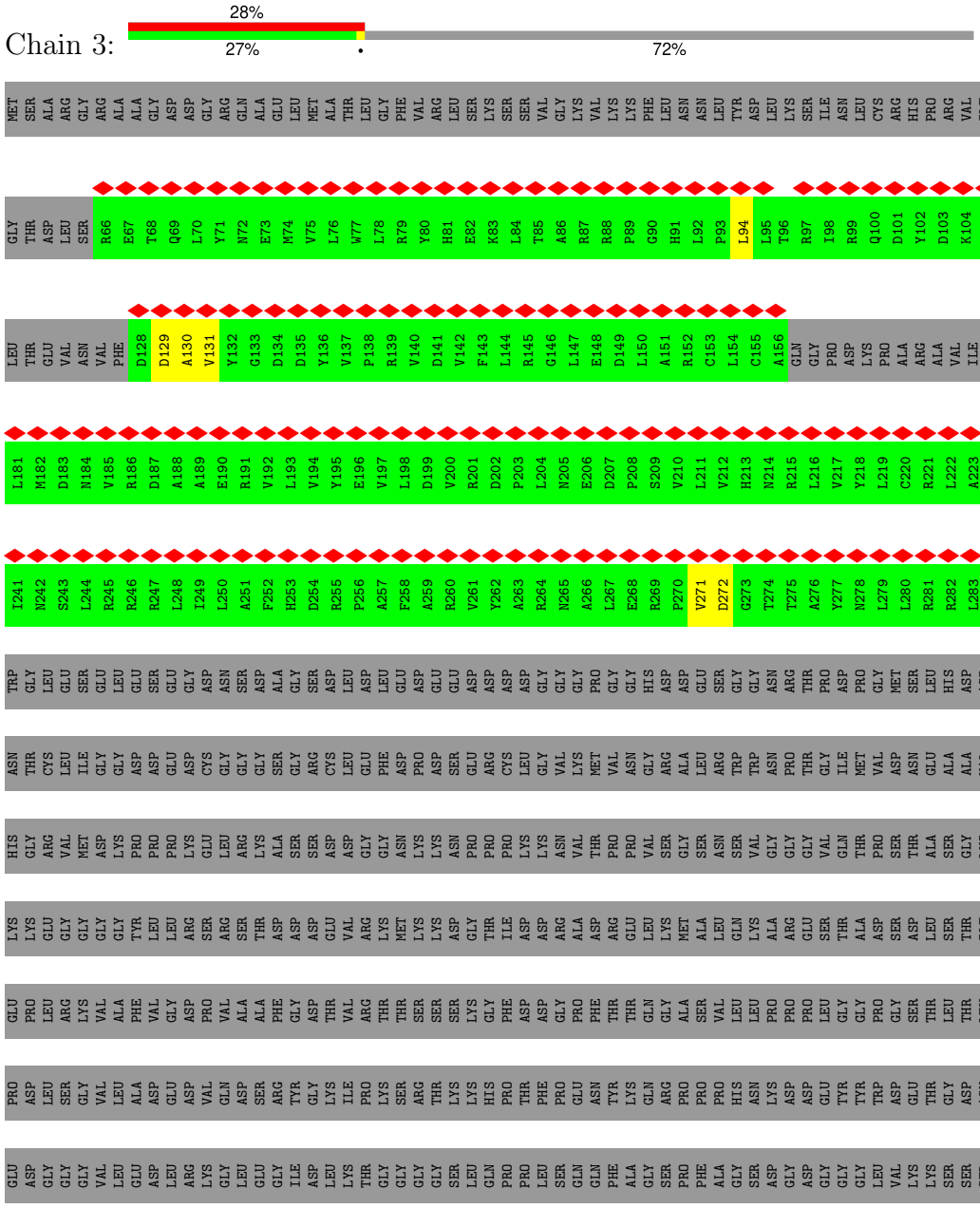
• Molecule 2: Tegument protein

Chain 2:



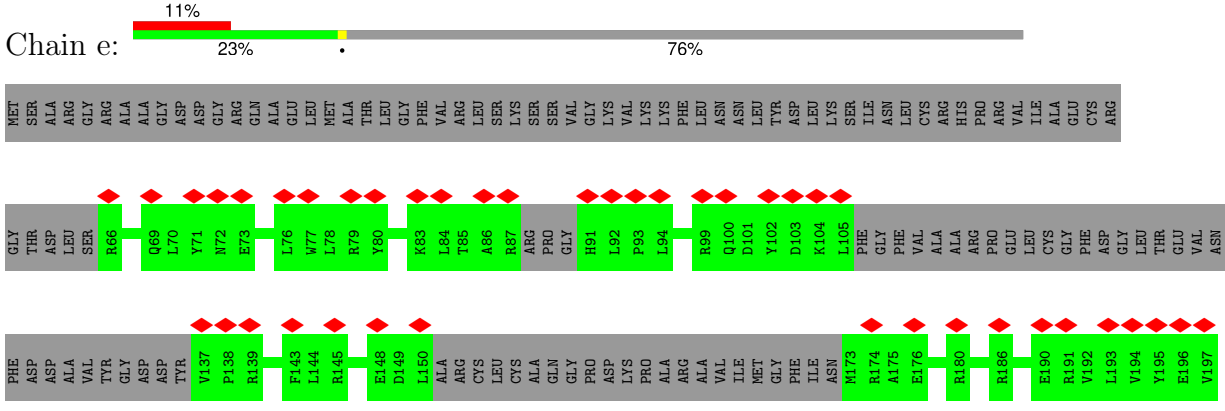
• Molecule 2: Tegument protein

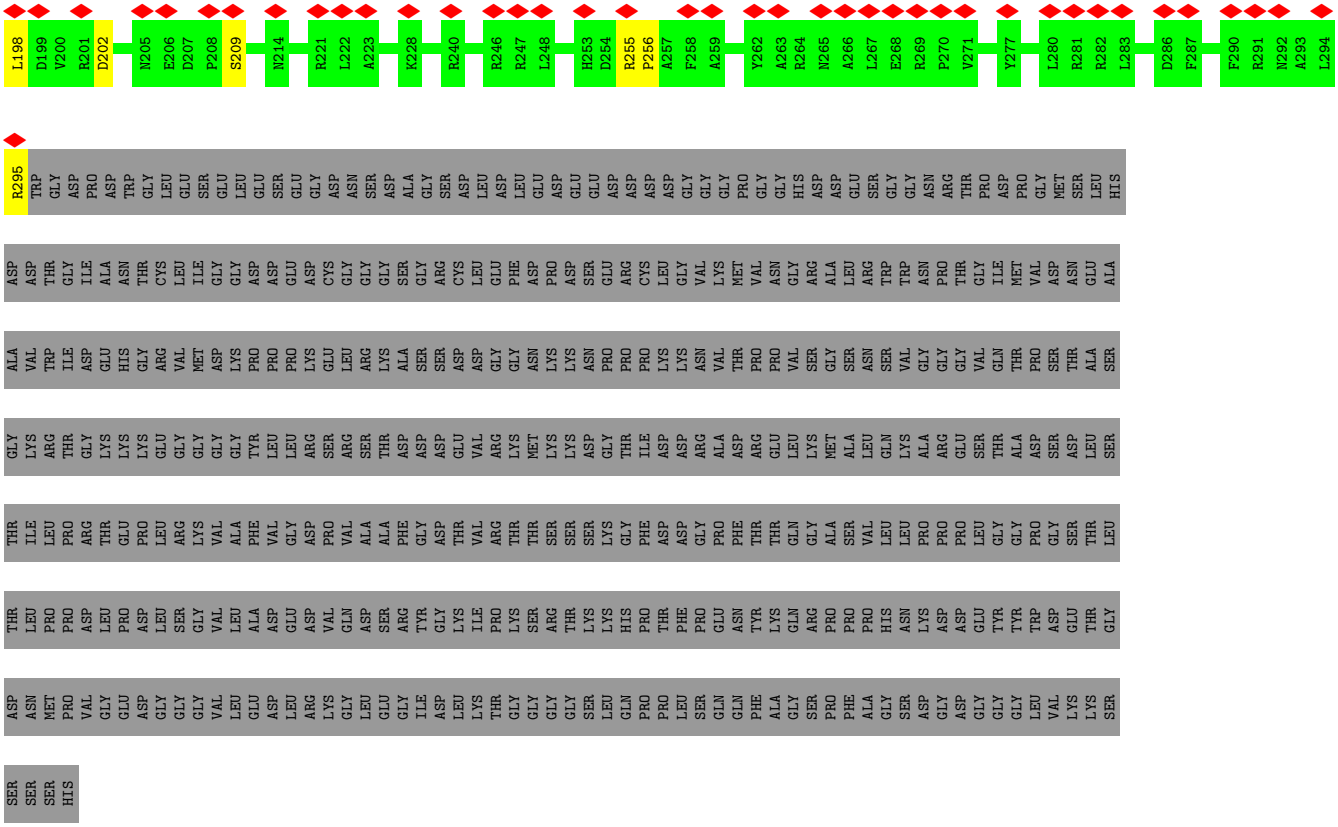
Chain 3:



• Molecule 2: Tegument protein

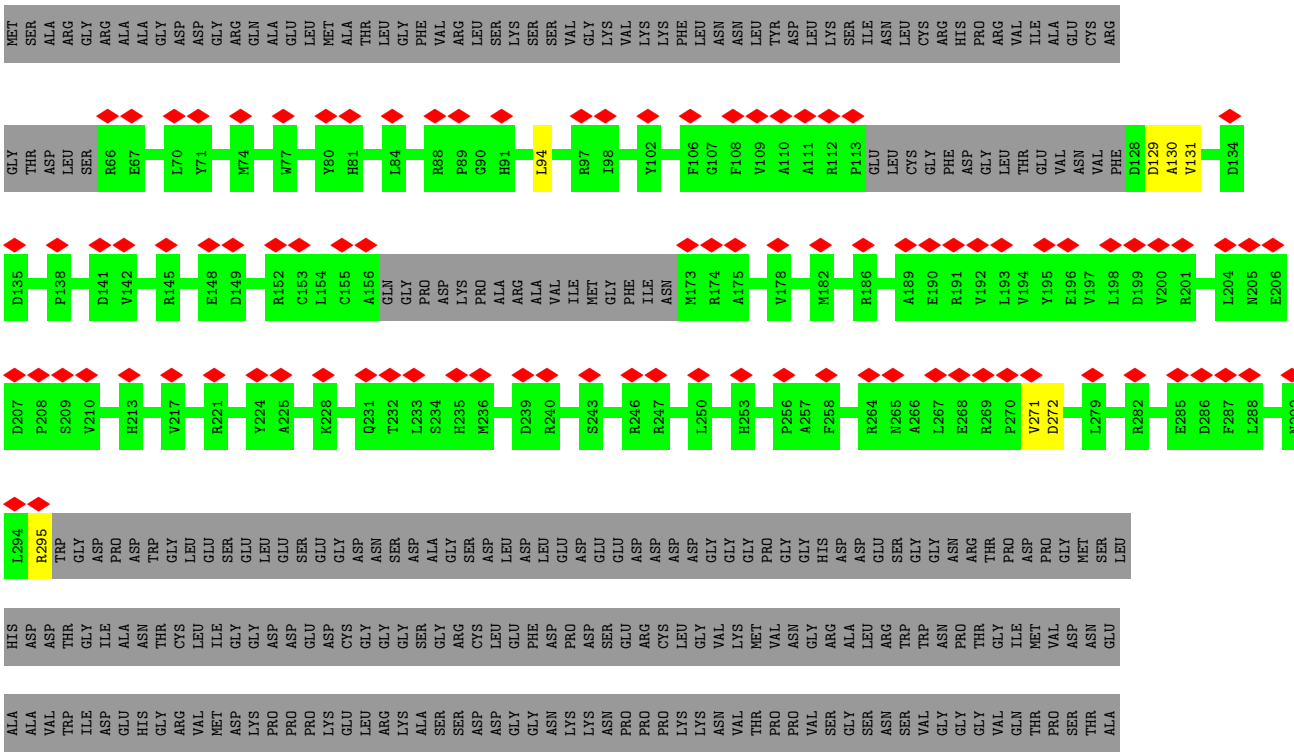
Chain e:

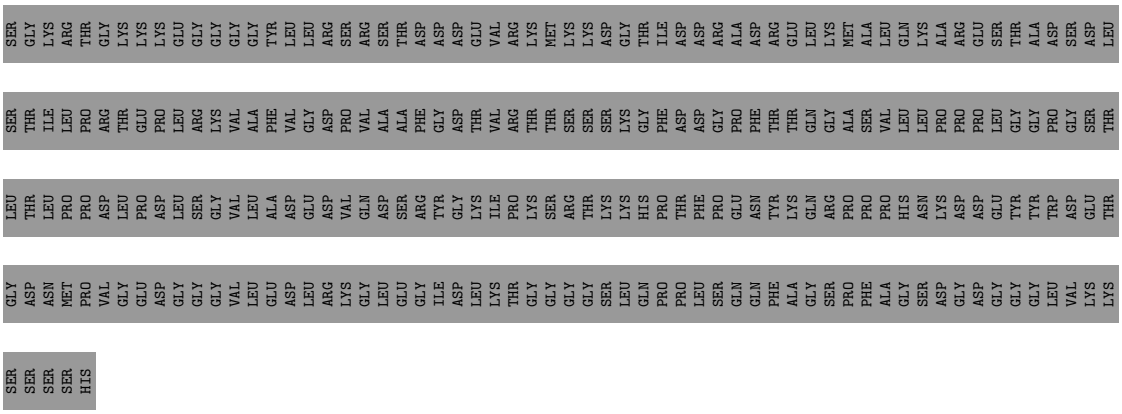




• Molecule 2: Tegument protein

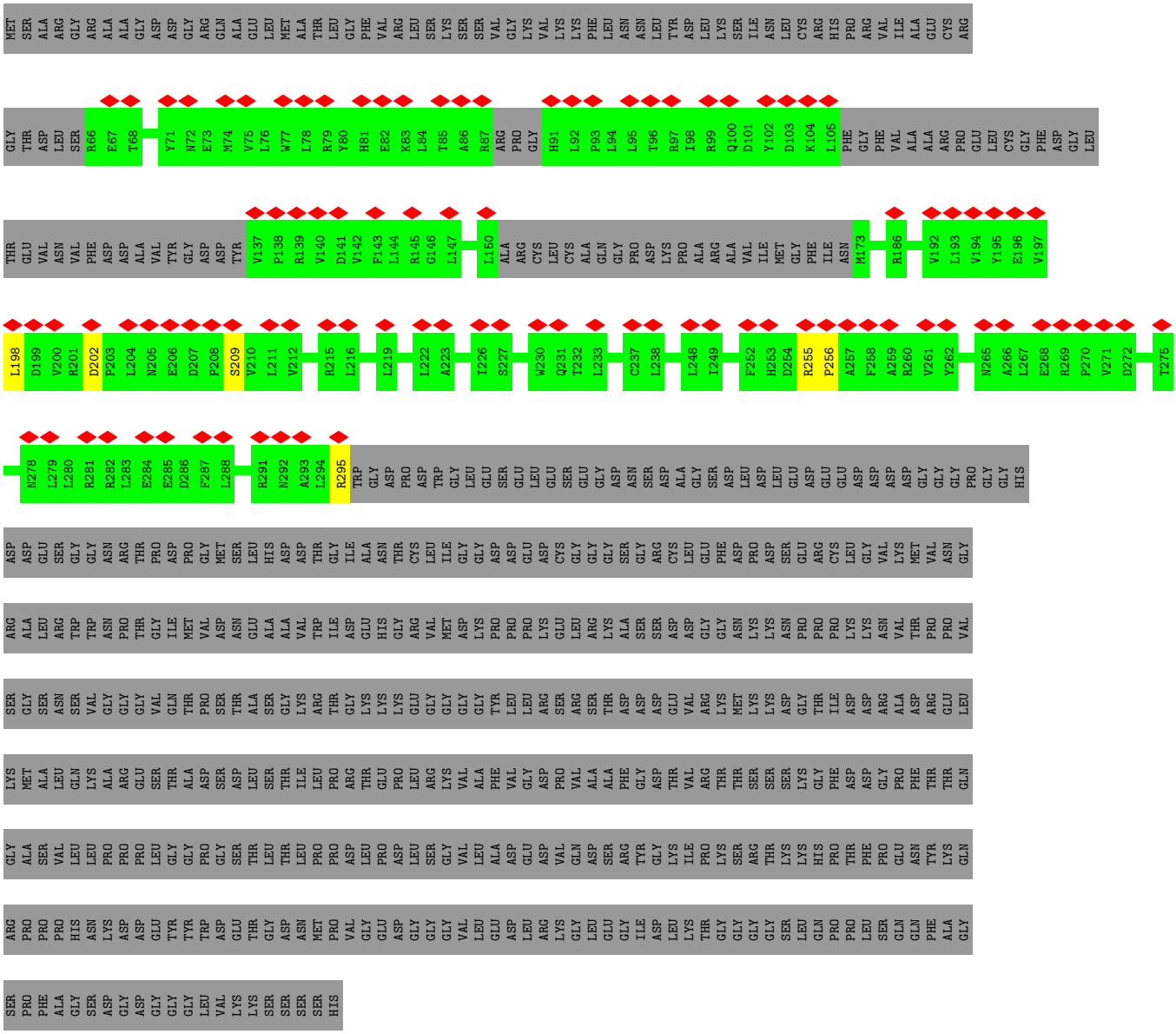
Chain h:





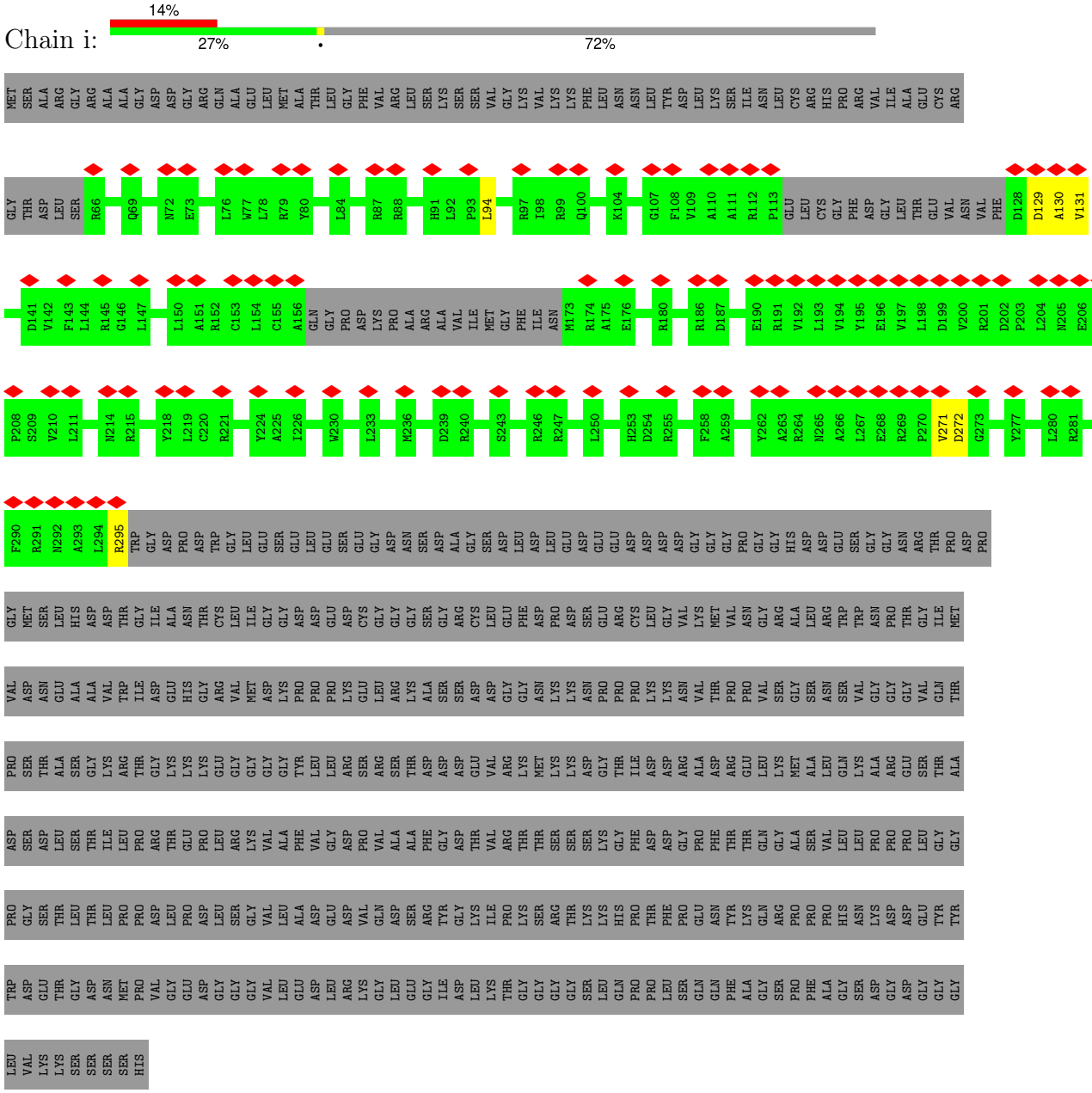
• Molecule 2: Tegument protein

Chain f:



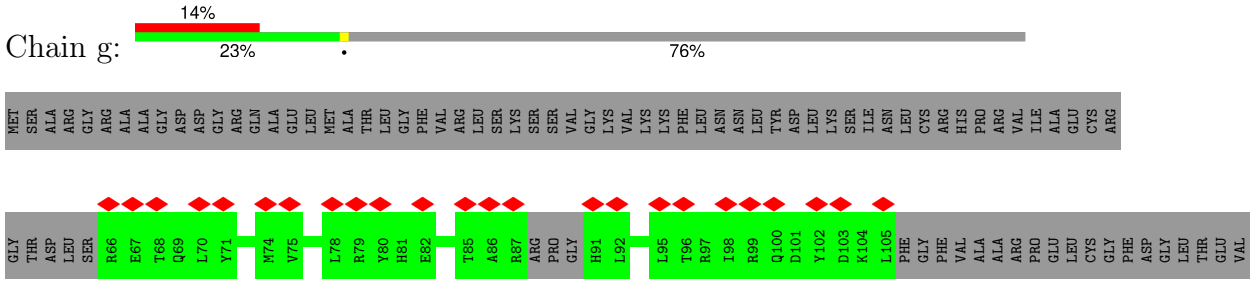
• Molecule 2: Tegument protein

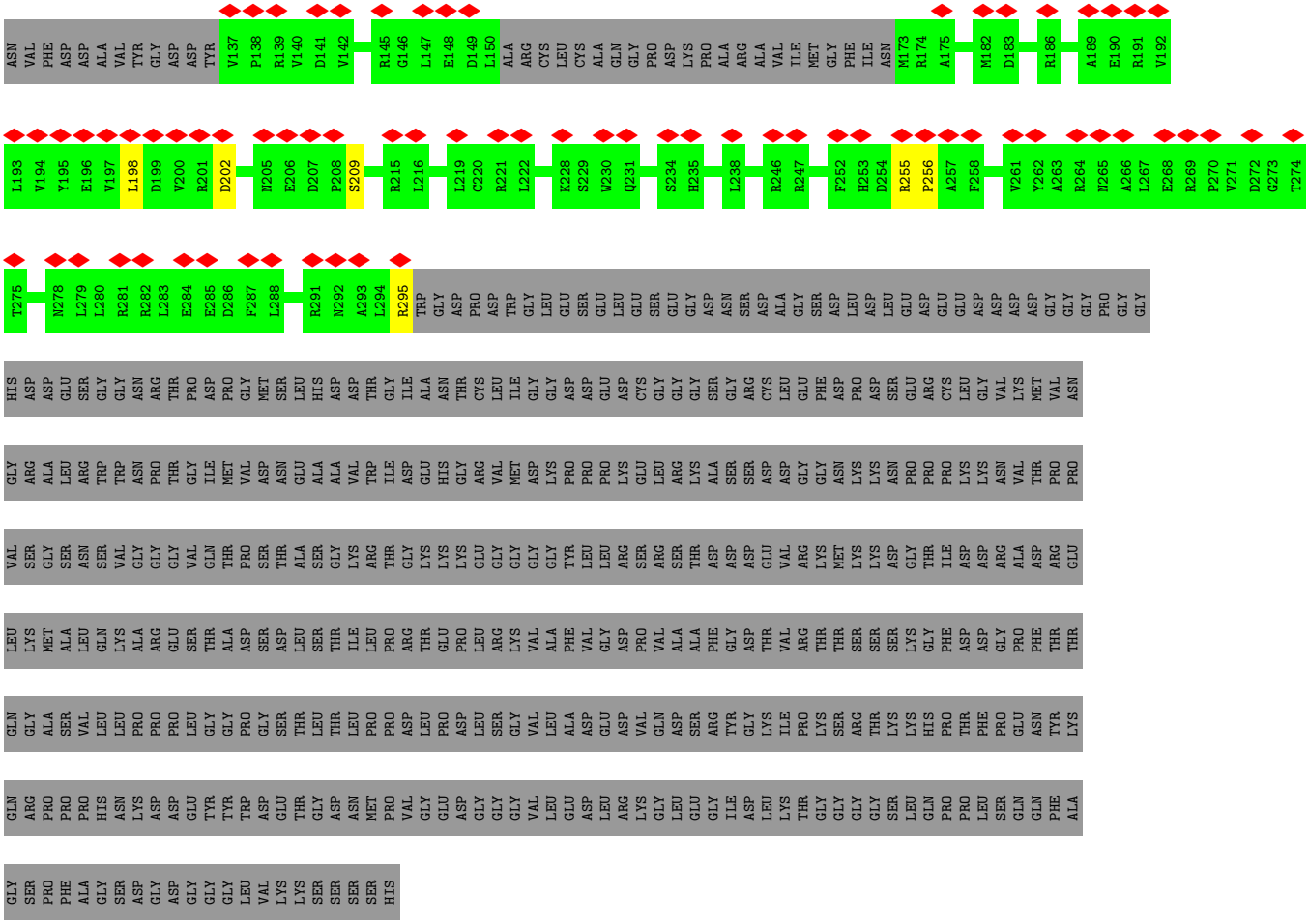
Chain i:



• Molecule 2: Tegument protein

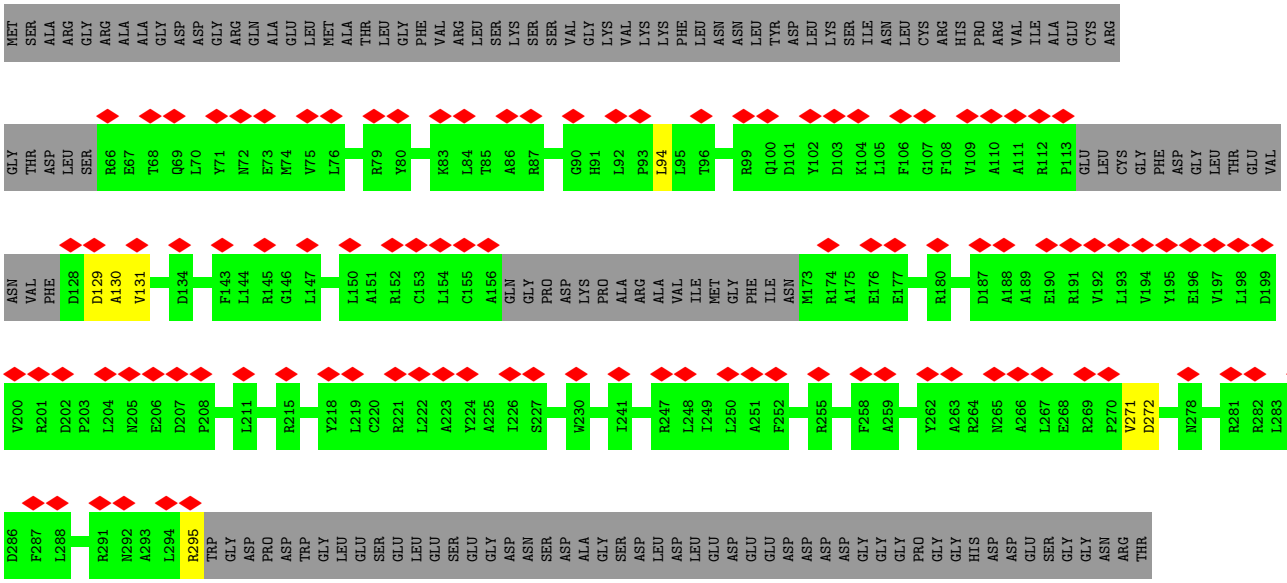
Chain g:





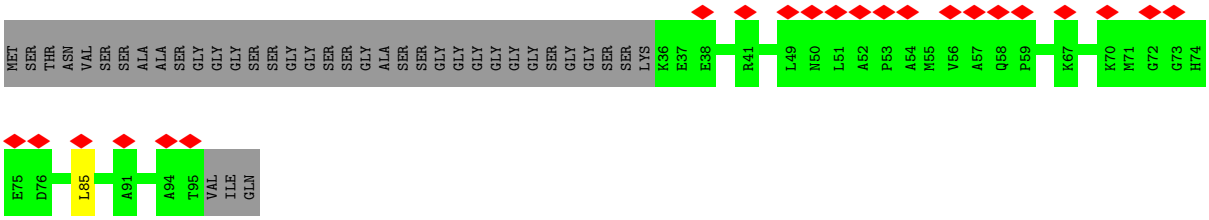
• Molecule 2: Tegument protein

Chain j:



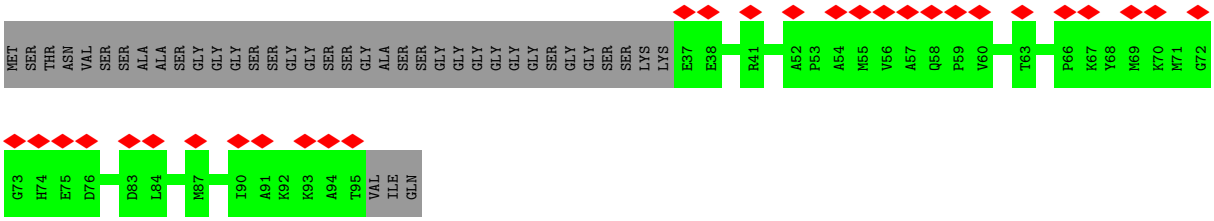
• Molecule 3: Small capsomere-interacting protein

Chain J:



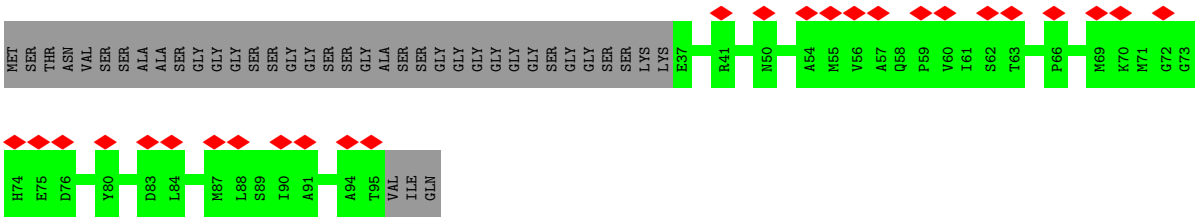
• Molecule 3: Small capsomere-interacting protein

Chain K:



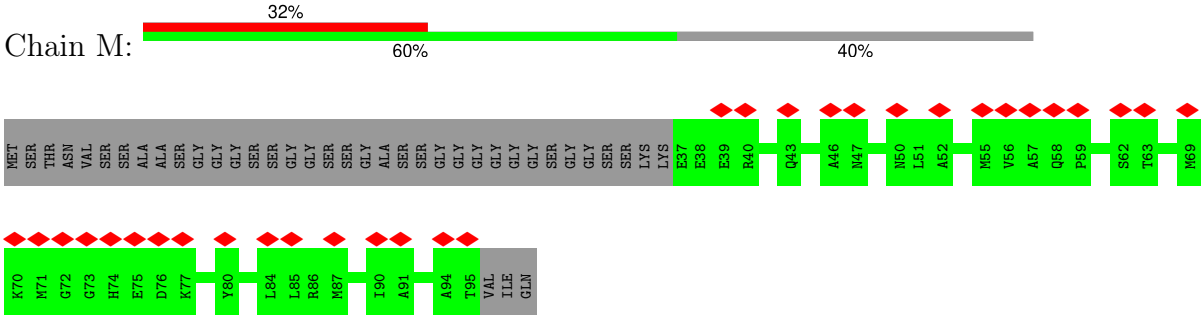
• Molecule 3: Small capsomere-interacting protein

Chain L:



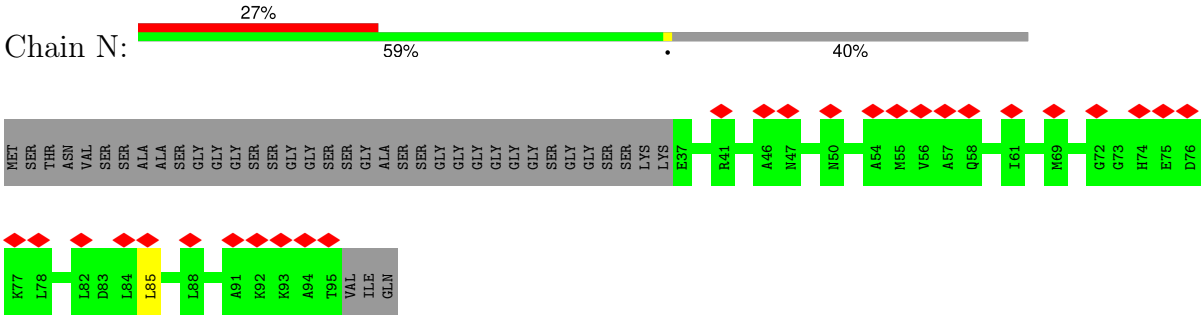
• Molecule 3: Small capsomere-interacting protein

Chain M:



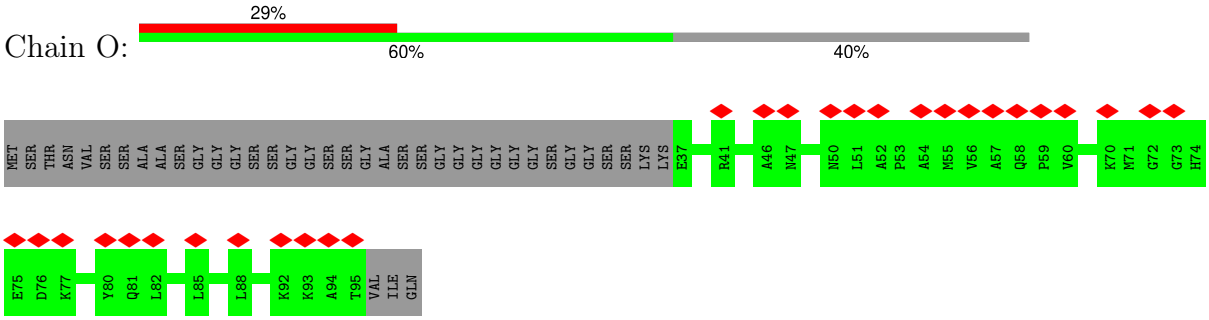
• Molecule 3: Small capsomere-interacting protein

Chain N:



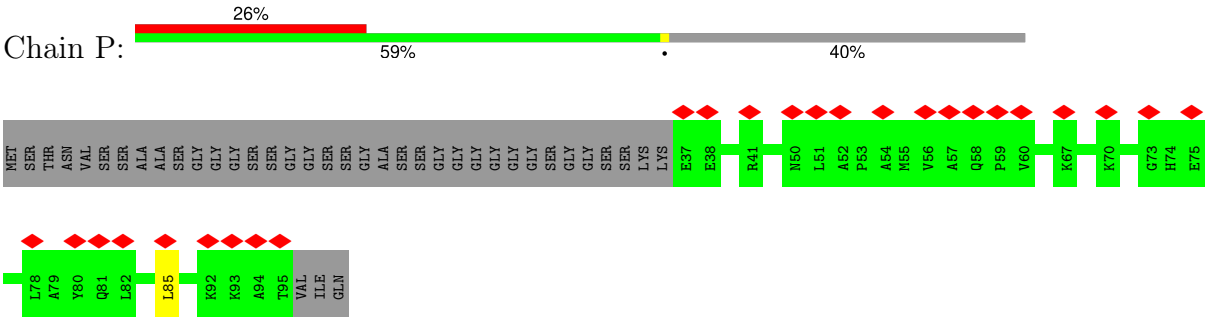
• Molecule 3: Small capsomere-interacting protein

Chain O:



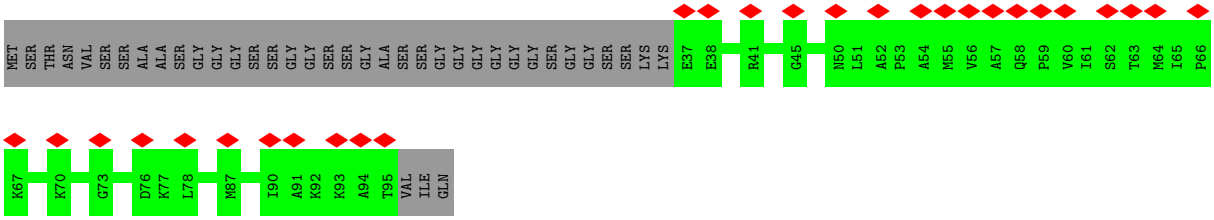
• Molecule 3: Small capsomere-interacting protein

Chain P:



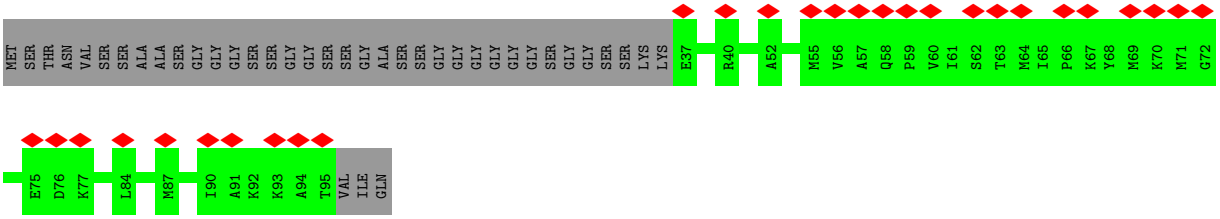
• Molecule 3: Small capsomere-interacting protein

Chain Q:



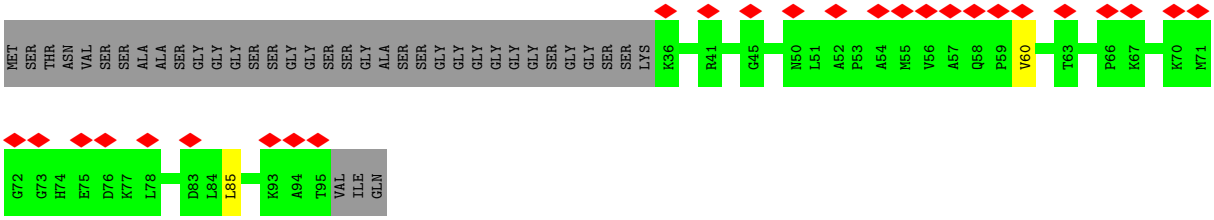
• Molecule 3: Small capsomere-interacting protein

Chain R:



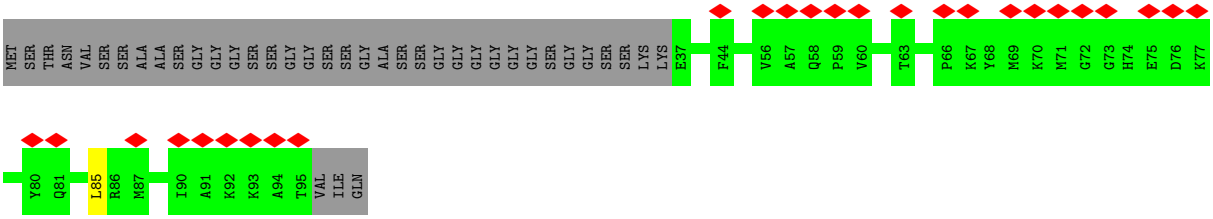
• Molecule 3: Small capsomere-interacting protein

Chain r:



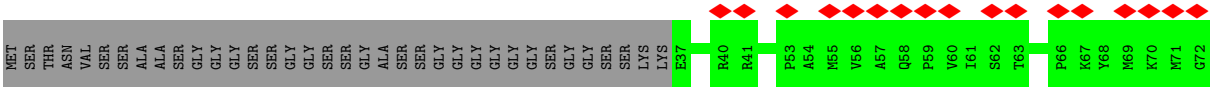
• Molecule 3: Small capsomere-interacting protein

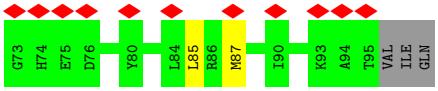
Chain s:



• Molecule 3: Small capsomere-interacting protein

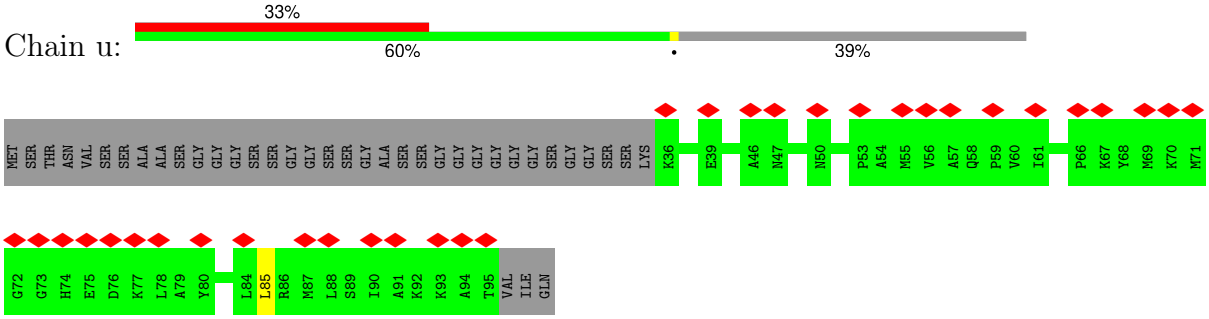
Chain t:





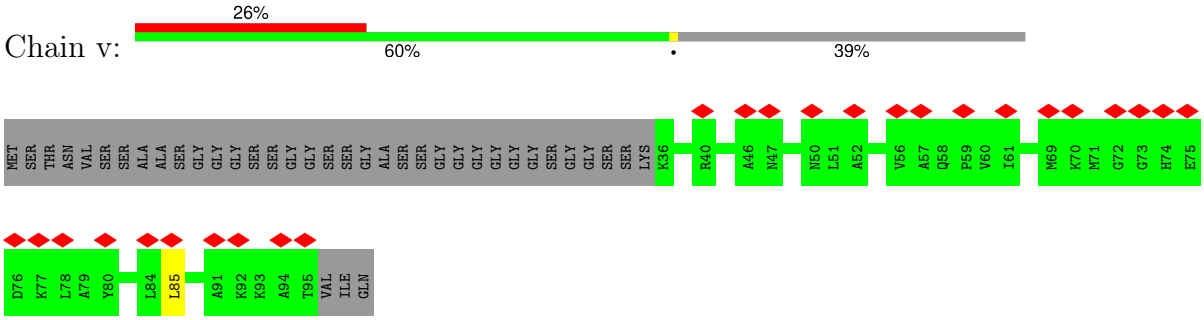
• Molecule 3: Small capsomere-interacting protein

Chain u:



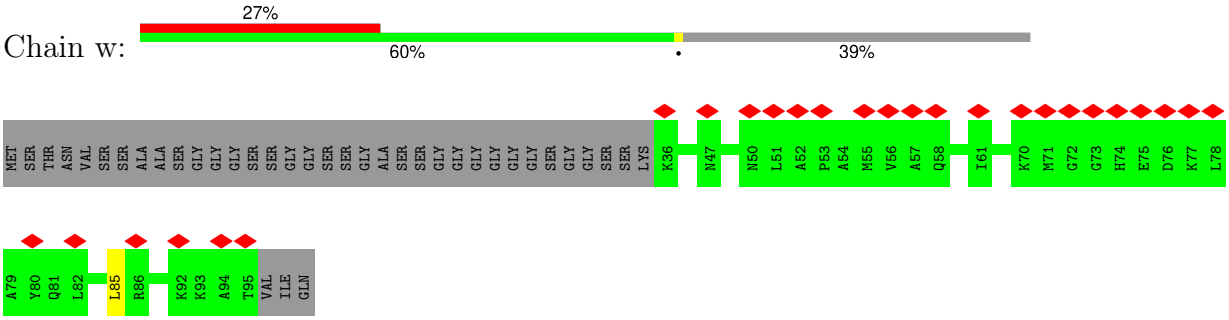
• Molecule 3: Small capsomere-interacting protein

Chain v:



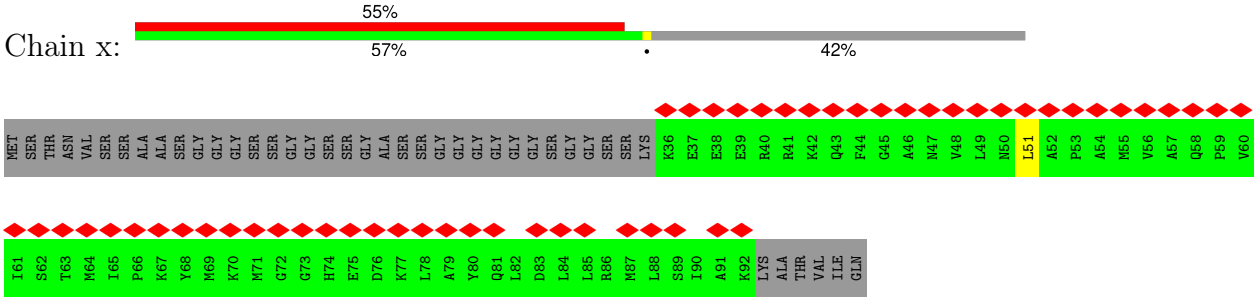
• Molecule 3: Small capsomere-interacting protein

Chain w:



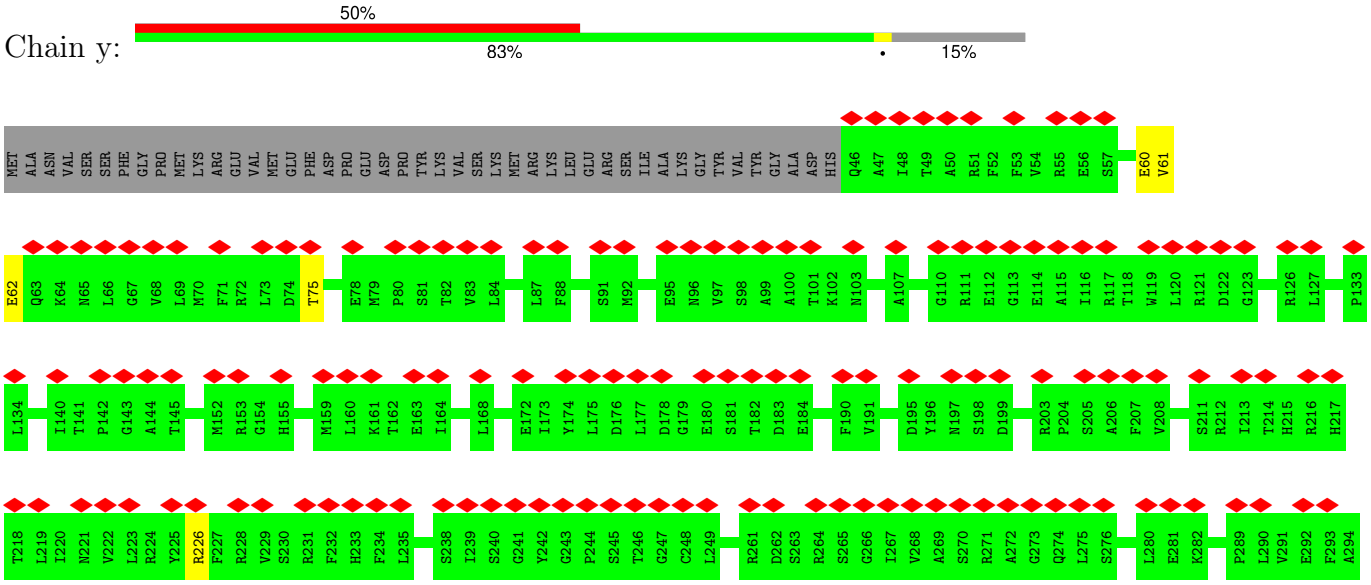
• Molecule 3: Small capsomere-interacting protein

Chain x:



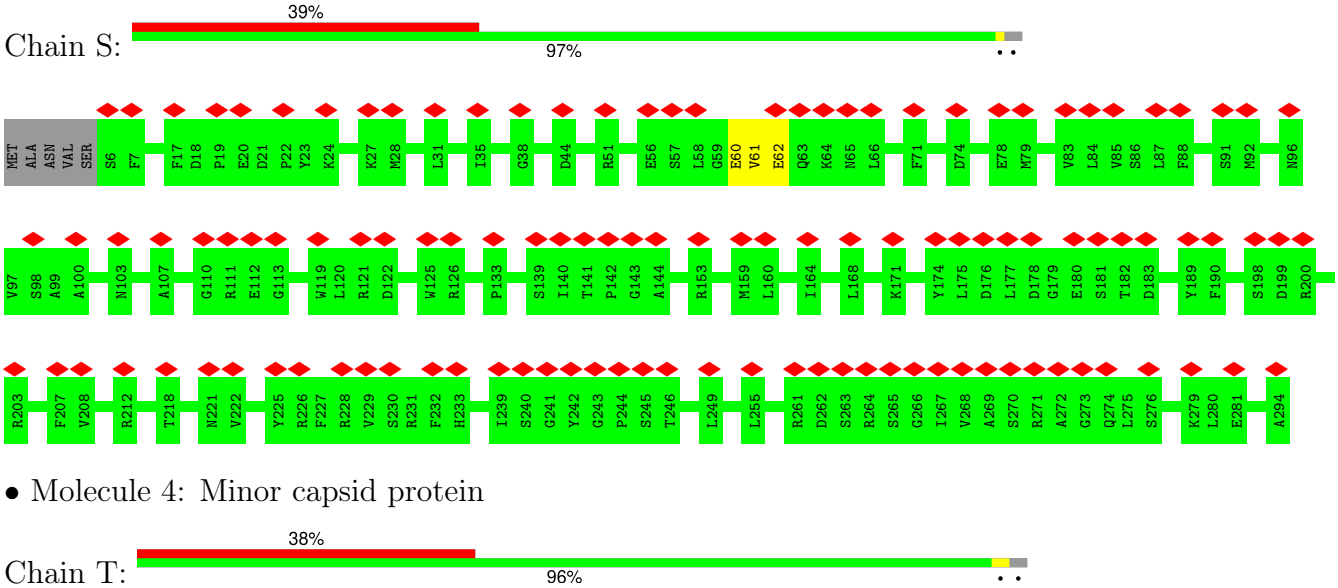
• Molecule 4: Minor capsid protein

Chain y:



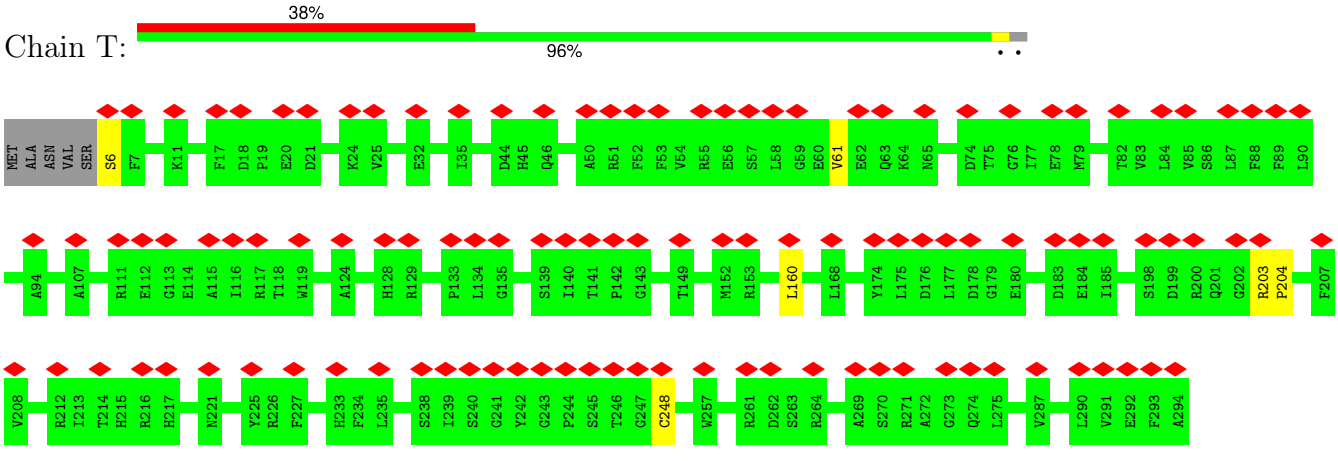
• Molecule 4: Minor capsid protein

Chain S:



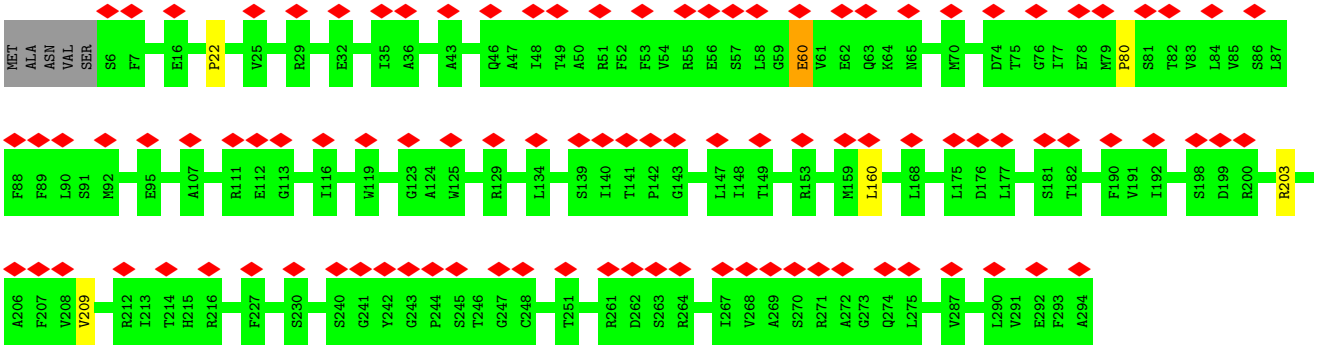
• Molecule 4: Minor capsid protein

Chain T:



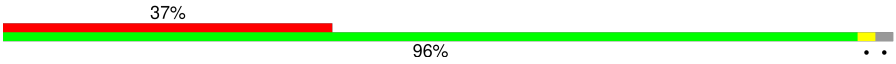
• Molecule 4: Minor capsid protein

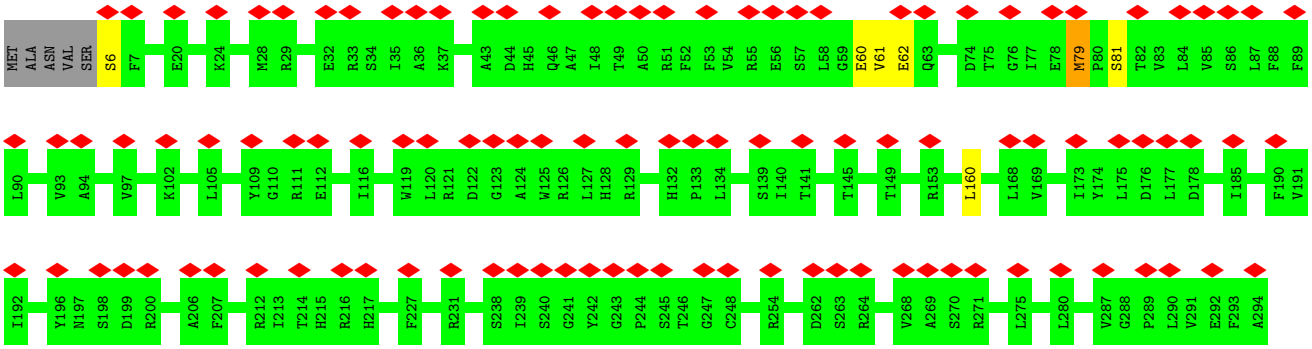
Chain U:



• Molecule 4: Minor capsid protein

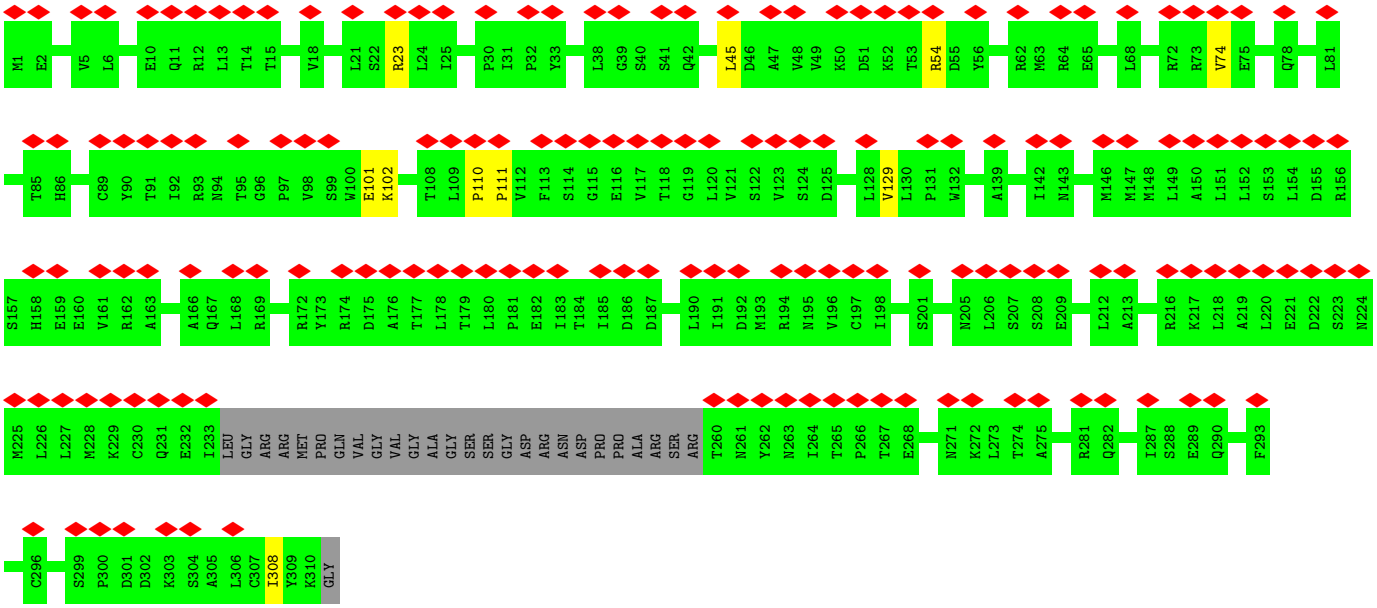
Chain V:





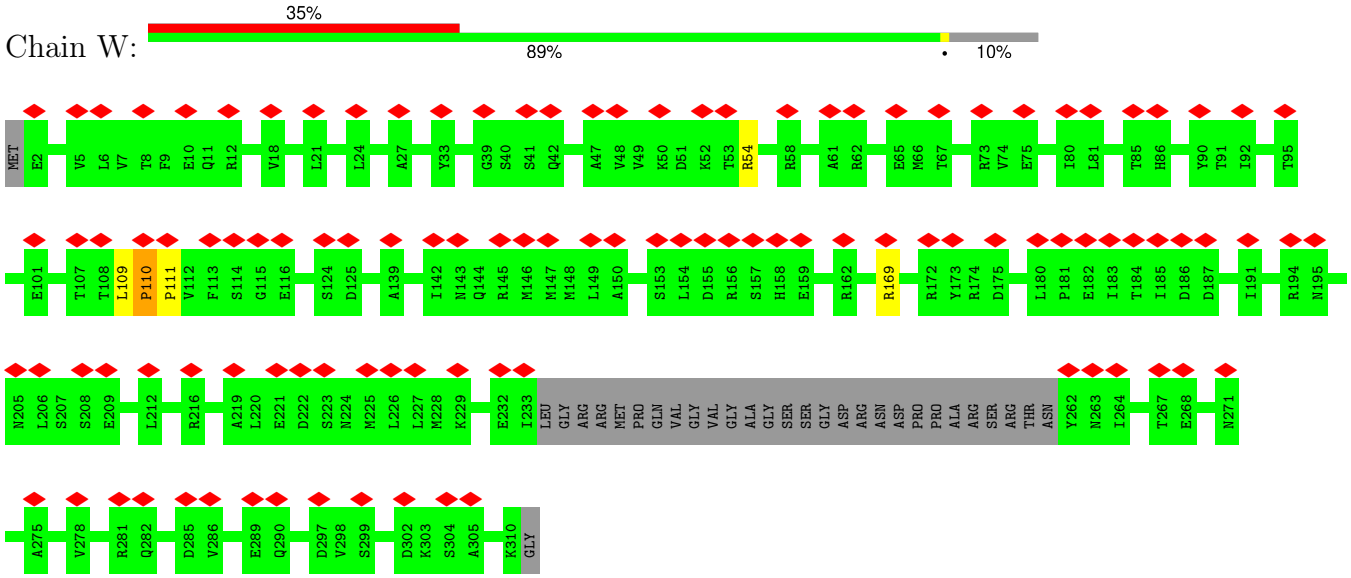
• Molecule 5: Triplex capsid protein 2

Chain z:



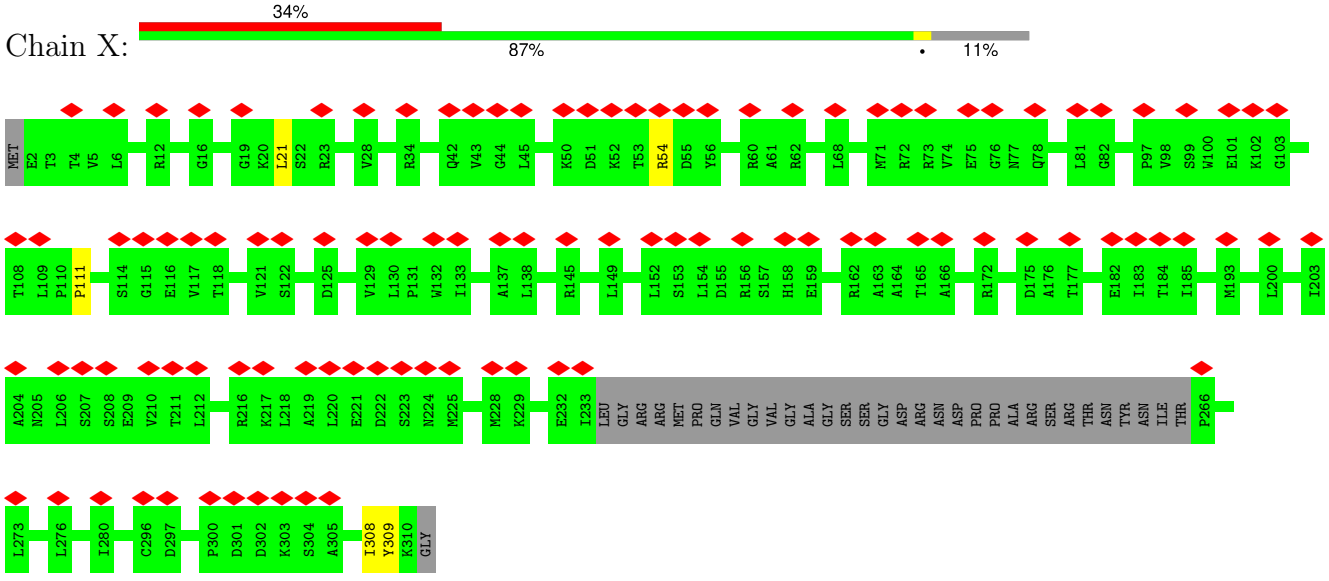
• Molecule 5: Triplex capsid protein 2

Chain W:



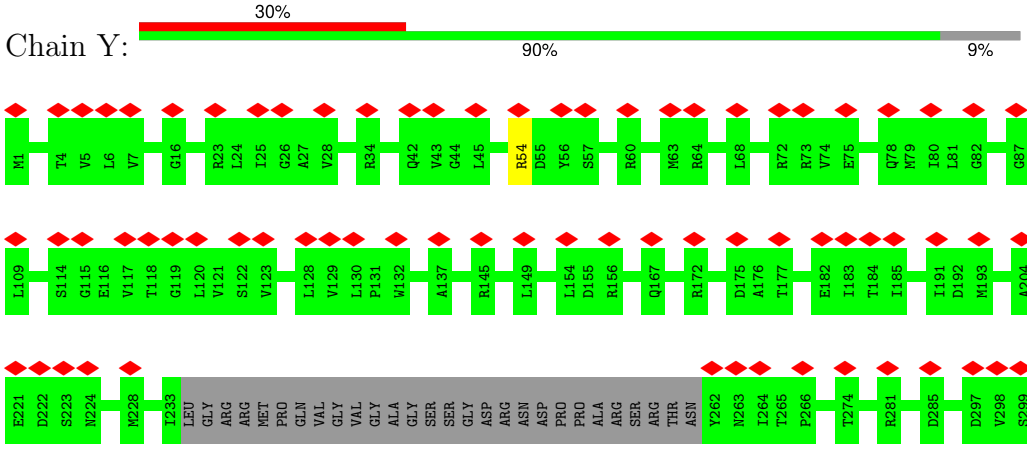
• Molecule 5: Triplex capsid protein 2

Chain X:



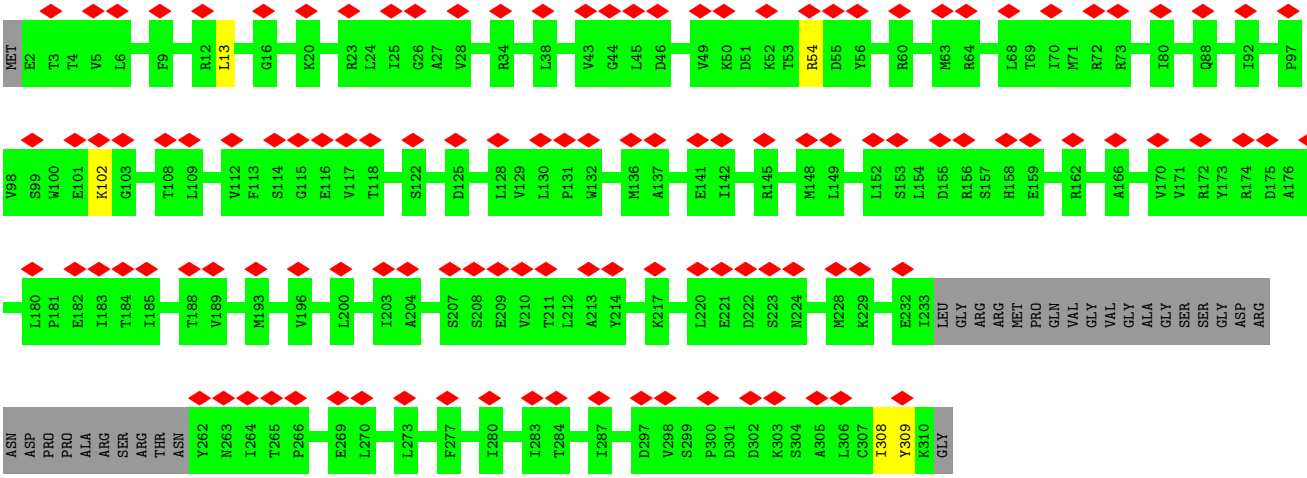
• Molecule 5: Triplex capsid protein 2

Chain Y:



• Molecule 5: Triplex capsid protein 2

Chain Z:



• Molecule 5: Triplex capsid protein 2

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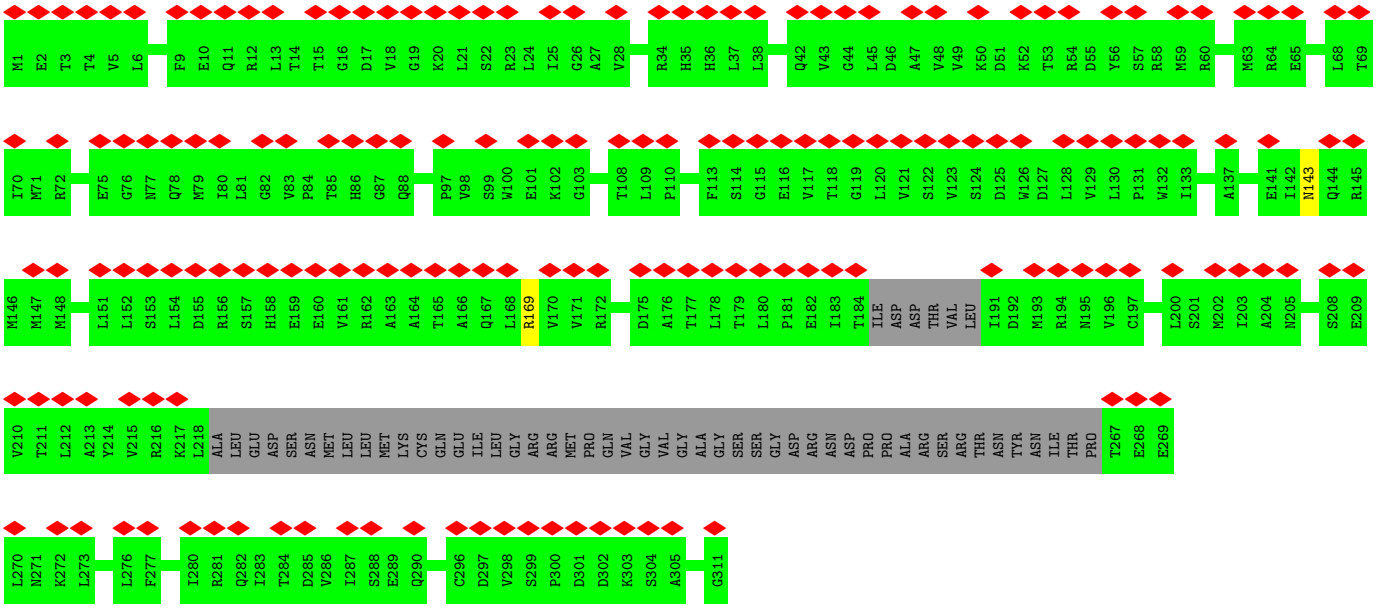
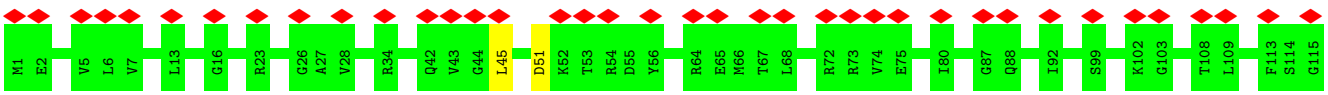
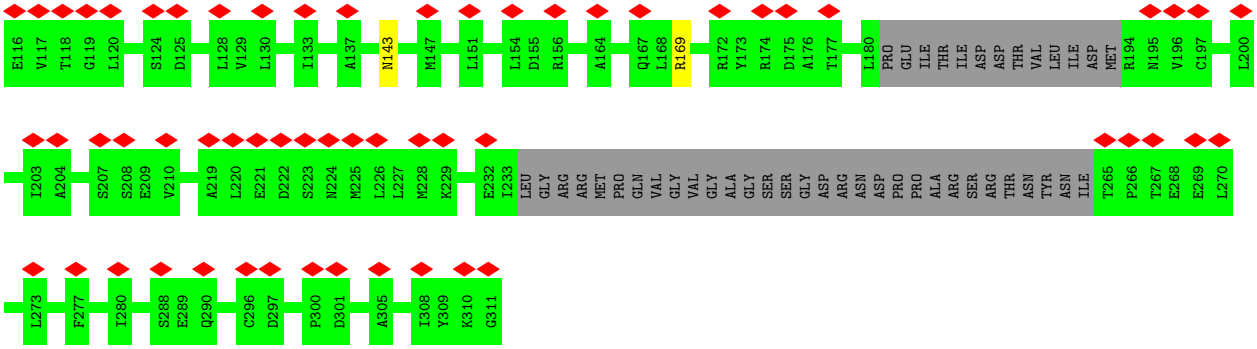


• Molecule 5: Triplex capsid protein 2

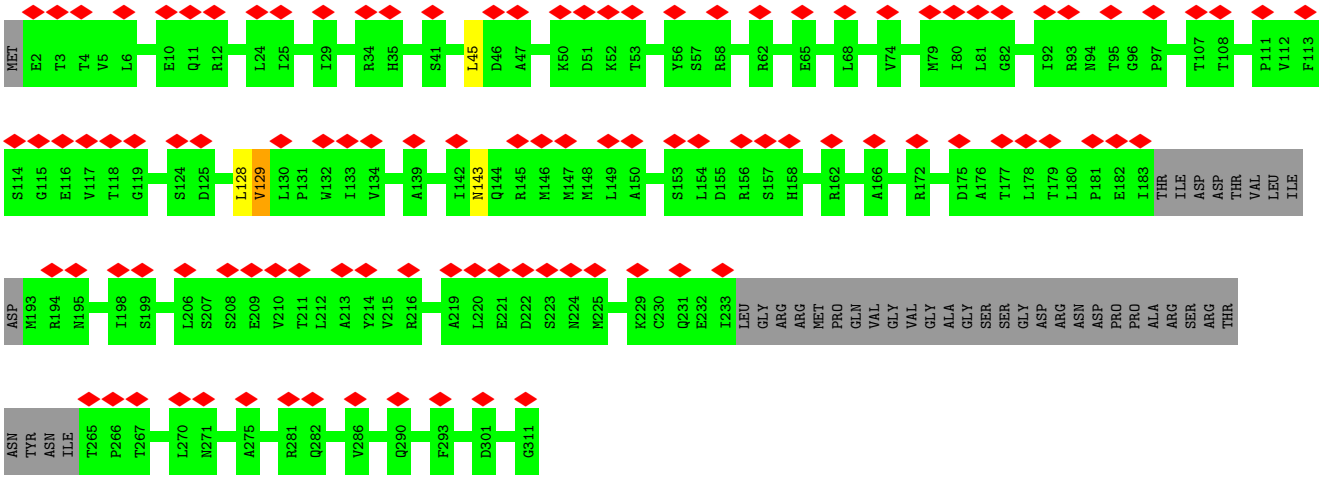
Chain a:





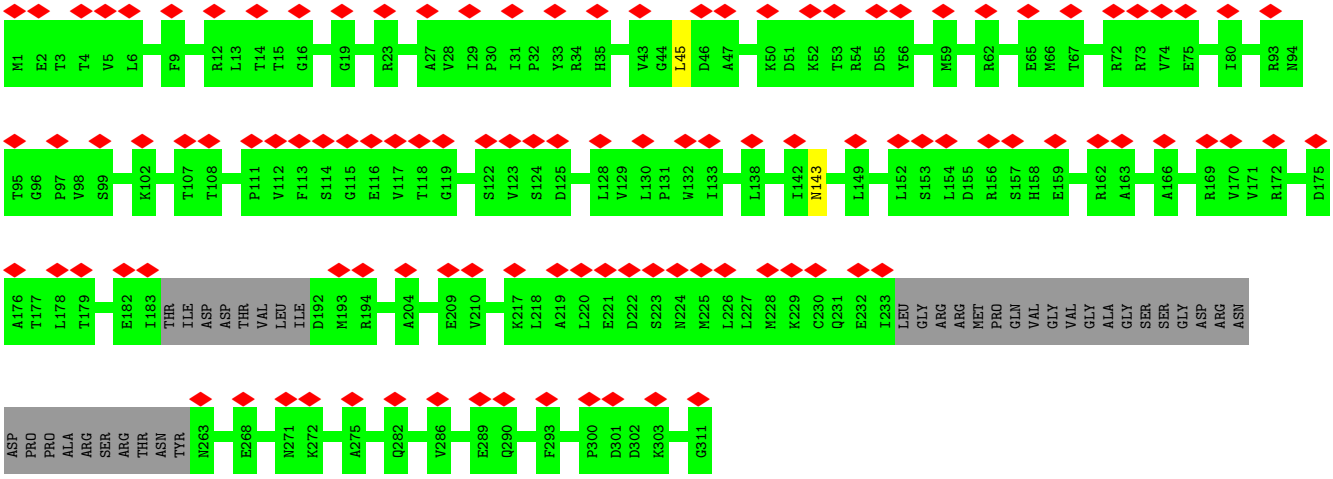
• Molecule 5: Triplex capsid protein 2

Chain b:



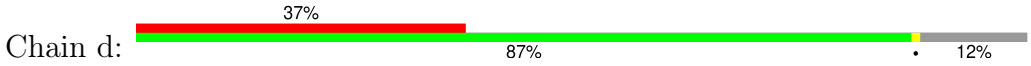
• Molecule 5: Triplex capsid protein 2

Chain c:



• Molecule 5: Triplex capsid protein 2

Chain d: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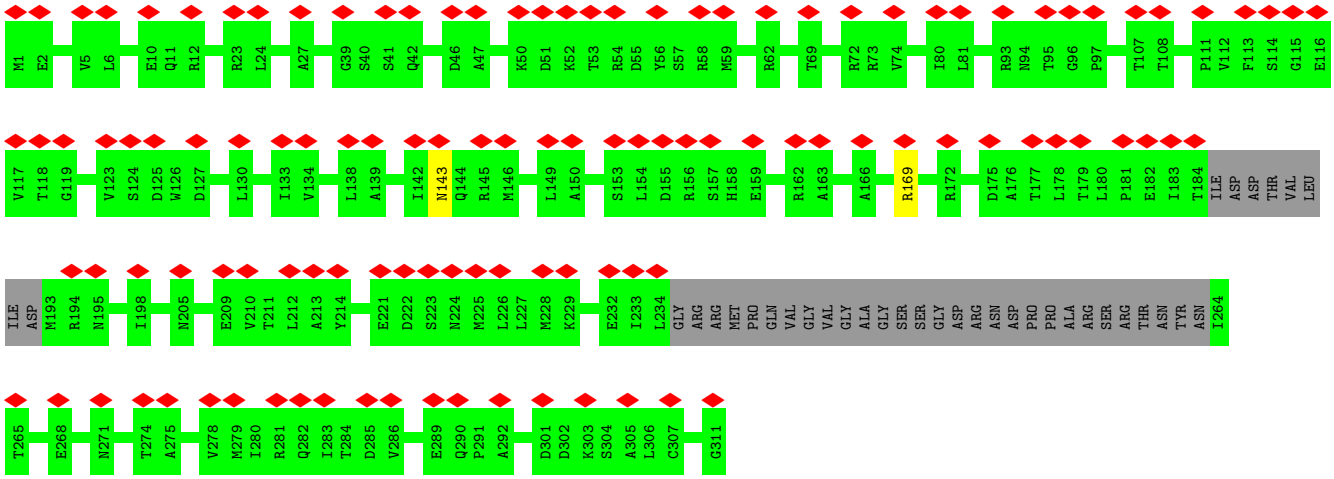
87%
12%


M1 E2 V5 L6 E10 Q11 R12 R23 L24 A27 G39 S40 S41 Q42 D46 A47 K50 D51 K52 T53 R54 D55 Y56 S57 R58 M59 R62 T69 R72 R73 V74 I80 L81 R93 N94 T95 G96 P97 T107 T108 P111 V112 F113 S114 G115 E116
V117 T118 G119 V123 S124 D125 W126 D127 L130 I133 V134 L138 A139 I142 N143 Q144 R145 M146 L149 A150 S153 L154 D155 R156 S157 H158 E159 R162 A163 A166 R169 R172 D175 A176 T177 L178 T179 L180 P181 E182 I183 T184 ILE ASP ASP THR VAL LEU
ILE ASP M193 R194 N195 I198 N205 E209 V210 T211 L212 A213 Y214 E221 D222 S223 N224 M225 L226 L227 M228 K229 E232 I233 L234 GLY ARG ARG MET PRO GLN VAL GLY VAL GLY ALA GLY SER SER GLY ASP ARG ASN ASP PRO PRO ALA ARG SER ARG THR ASN TYR ASN I264
T265 E268 N271 T274 A275 V278 M279 I280 R281 Q282 I283 T284 D285 V286 E289 Q290 P291 A292 D301 D302 K303 S304 A305 L306 C307 G311

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	1729.2799, 1729.2799, 1729.2799	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.351, 1.351, 1.351	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	0.40	0/10779	0.63	0/14662
1	B	0.42	0/10591	0.63	0/14408
1	C	0.47	0/10590	0.66	0/14407
1	D	0.46	0/10615	0.66	0/14442
1	E	0.35	0/10735	0.61	0/14602
1	F	0.40	0/10648	0.63	0/14488
1	G	0.47	0/10823	0.67	0/14724
1	H	0.41	0/10823	0.64	0/14724
1	I	0.38	0/10662	0.62	0/14506
1	k	0.40	0/10445	0.64	0/14213
1	l	0.40	0/10790	0.65	2/14677 (0.0%)
1	m	0.41	0/10604	0.65	0/14426
1	n	0.36	0/10779	0.65	0/14662
1	o	0.39	0/10607	0.64	0/14430
1	p	0.38	0/10485	0.64	0/14261
1	q	0.35	0/9837	0.64	3/13377 (0.0%)
2	2	0.39	1/1493 (0.1%)	0.65	2/2016 (0.1%)
2	3	0.34	0/1696	0.59	0/2294
2	e	0.40	1/1493 (0.1%)	0.65	2/2016 (0.1%)
2	f	0.39	1/1493 (0.1%)	0.65	2/2016 (0.1%)
2	g	0.39	1/1493 (0.1%)	0.65	2/2016 (0.1%)
2	h	0.34	0/1696	0.59	0/2294
2	i	0.34	0/1696	0.59	0/2294
2	j	0.34	0/1696	0.59	0/2294
3	J	0.32	0/477	0.61	0/637
3	K	0.32	0/468	0.63	0/626
3	L	0.33	0/468	0.60	0/626
3	M	0.43	0/468	0.65	0/626
3	N	0.32	0/468	0.62	0/626
3	O	0.33	0/468	0.65	0/626
3	P	0.36	0/468	0.62	0/626
3	Q	0.33	0/468	0.60	0/626
3	R	0.33	0/468	0.65	0/626
3	r	0.33	0/477	0.68	0/637

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	s	0.32	0/468	0.63	0/626
3	t	0.33	0/468	0.63	0/626
3	u	0.32	0/477	0.62	0/637
3	v	0.32	0/477	0.62	0/637
3	w	0.34	0/477	0.68	0/637
3	x	0.34	0/456	0.70	1/609 (0.2%)
4	S	0.40	0/2357	0.63	0/3185
4	T	0.38	0/2357	0.66	4/3185 (0.1%)
4	U	0.37	0/2357	0.64	0/3185
4	V	0.36	0/2357	0.64	0/3185
4	y	0.42	0/2020	0.71	0/2735
5	1	0.34	0/2037	0.65	0/2761
5	W	0.32	0/2232	0.65	1/3031 (0.0%)
5	X	0.30	0/2196	0.60	0/2980
5	Y	0.34	0/2240	0.66	0/3041
5	Z	0.33	0/2232	0.64	0/3031
5	a	0.35	0/2113	0.62	0/2862
5	b	0.31	0/2138	0.60	0/2897
5	c	0.35	0/2170	0.62	0/2940
5	d	0.36	0/2169	0.61	0/2939
5	z	0.35	1/2255 (0.0%)	0.67	1/3062 (0.0%)
All	All	0.39	5/223320 (0.0%)	0.64	20/303322 (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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	209	SER	C-N	9.91	1.56	1.34
2	2	209	SER	C-N	9.90	1.56	1.34
2	g	209	SER	C-N	9.89	1.56	1.34
2	f	209	SER	C-N	9.88	1.56	1.34
5	z	129	VAL	C-N	-5.37	1.21	1.34

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	e	209	SER	O-C-N	-11.48	104.33	122.70
2	f	209	SER	O-C-N	-11.48	104.34	122.70
2	2	209	SER	O-C-N	-11.47	104.35	122.70
2	g	209	SER	O-C-N	-11.46	104.36	122.70
5	W	110	PRO	C-N-CD	-8.26	102.42	120.60

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)

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	1331/1353 (98%)	1204 (90%)	126 (10%)	1 (0%)	48 83
1	B	1304/1353 (96%)	1209 (93%)	92 (7%)	3 (0%)	44 78
1	C	1304/1353 (96%)	1182 (91%)	119 (9%)	3 (0%)	44 78
1	D	1308/1353 (97%)	1184 (90%)	123 (9%)	1 (0%)	48 83
1	E	1326/1353 (98%)	1186 (89%)	138 (10%)	2 (0%)	44 78
1	F	1313/1353 (97%)	1216 (93%)	92 (7%)	5 (0%)	30 68
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%)	44 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	k	1287/1353 (95%)	1164 (90%)	117 (9%)	6 (0%)	25	64
1	l	1332/1353 (98%)	1211 (91%)	120 (9%)	1 (0%)	48	83
1	m	1306/1353 (96%)	1175 (90%)	125 (10%)	6 (0%)	25	64
1	n	1331/1353 (98%)	1202 (90%)	128 (10%)	1 (0%)	48	83
1	o	1307/1353 (97%)	1173 (90%)	130 (10%)	4 (0%)	37	72
1	p	1297/1353 (96%)	1167 (90%)	127 (10%)	3 (0%)	44	78
1	q	1201/1353 (89%)	1058 (88%)	143 (12%)	0	100	100
2	2	166/718 (23%)	153 (92%)	9 (5%)	4 (2%)	5	27
2	3	194/718 (27%)	177 (91%)	13 (7%)	4 (2%)	5	30
2	e	166/718 (23%)	153 (92%)	10 (6%)	3 (2%)	7	34
2	f	166/718 (23%)	154 (93%)	9 (5%)	3 (2%)	7	34
2	g	166/718 (23%)	154 (93%)	9 (5%)	3 (2%)	7	34
2	h	194/718 (27%)	177 (91%)	13 (7%)	4 (2%)	5	30
2	i	194/718 (27%)	176 (91%)	14 (7%)	4 (2%)	5	30
2	j	194/718 (27%)	176 (91%)	14 (7%)	4 (2%)	5	30
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	S	287/294 (98%)	254 (88%)	30 (10%)	3 (1%)	13 49
4	T	287/294 (98%)	255 (89%)	30 (10%)	2 (1%)	19 56
4	U	287/294 (98%)	256 (89%)	28 (10%)	3 (1%)	13 49
4	V	287/294 (98%)	242 (84%)	40 (14%)	5 (2%)	7 35
4	y	247/294 (84%)	211 (85%)	33 (13%)	3 (1%)	11 44
5	1	251/311 (81%)	233 (93%)	17 (7%)	1 (0%)	30 68
5	W	277/311 (89%)	239 (86%)	36 (13%)	2 (1%)	19 56
5	X	273/311 (88%)	250 (92%)	21 (8%)	2 (1%)	19 56
5	Y	278/311 (89%)	251 (90%)	27 (10%)	0	100 100
5	Z	277/311 (89%)	253 (91%)	23 (8%)	1 (0%)	30 68
5	a	261/311 (84%)	241 (92%)	20 (8%)	0	100 100
5	b	264/311 (85%)	249 (94%)	14 (5%)	1 (0%)	30 68
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%)	19 56
All	All	27383/33540 (82%)	24832 (91%)	2455 (9%)	96 (0%)	32 68

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 (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	1142/1156 (99%)	1128 (99%)	14 (1%)	67 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	1123/1156 (97%)	1110 (99%)	13 (1%)	67 79
1	C	1123/1156 (97%)	1105 (98%)	18 (2%)	58 74
1	D	1125/1156 (97%)	1108 (98%)	17 (2%)	60 75
1	E	1138/1156 (98%)	1131 (99%)	7 (1%)	84 88
1	F	1128/1156 (98%)	1112 (99%)	16 (1%)	62 76
1	G	1147/1156 (99%)	1134 (99%)	13 (1%)	70 80
1	H	1147/1156 (99%)	1132 (99%)	15 (1%)	65 77
1	I	1130/1156 (98%)	1119 (99%)	11 (1%)	73 82
1	k	1105/1156 (96%)	1091 (99%)	14 (1%)	65 77
1	l	1144/1156 (99%)	1129 (99%)	15 (1%)	65 77
1	m	1124/1156 (97%)	1105 (98%)	19 (2%)	56 72
1	n	1143/1156 (99%)	1130 (99%)	13 (1%)	70 80
1	o	1124/1156 (97%)	1111 (99%)	13 (1%)	67 79
1	p	1110/1156 (96%)	1101 (99%)	9 (1%)	79 85
1	q	1042/1156 (90%)	1031 (99%)	11 (1%)	70 80
2	2	159/596 (27%)	157 (99%)	2 (1%)	65 77
2	3	177/596 (30%)	174 (98%)	3 (2%)	56 72
2	e	159/596 (27%)	157 (99%)	2 (1%)	65 77
2	f	159/596 (27%)	157 (99%)	2 (1%)	65 77
2	g	159/596 (27%)	157 (99%)	2 (1%)	65 77
2	h	177/596 (30%)	174 (98%)	3 (2%)	56 72
2	i	177/596 (30%)	174 (98%)	3 (2%)	56 72
2	j	177/596 (30%)	174 (98%)	3 (2%)	56 72
3	J	50/71 (70%)	49 (98%)	1 (2%)	50 68
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%)	50 68
3	O	49/71 (69%)	49 (100%)	0	100 100
3	P	49/71 (69%)	48 (98%)	1 (2%)	50 68
3	Q	49/71 (69%)	49 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	R	49/71 (69%)	49 (100%)	0	100	100
3	r	50/71 (70%)	48 (96%)	2 (4%)	27	48
3	s	49/71 (69%)	48 (98%)	1 (2%)	50	68
3	t	49/71 (69%)	47 (96%)	2 (4%)	26	47
3	u	50/71 (70%)	49 (98%)	1 (2%)	50	68
3	v	50/71 (70%)	49 (98%)	1 (2%)	50	68
3	w	50/71 (70%)	49 (98%)	1 (2%)	50	68
3	x	48/71 (68%)	48 (100%)	0	100	100
4	S	251/255 (98%)	251 (100%)	0	100	100
4	T	251/255 (98%)	251 (100%)	0	100	100
4	U	251/255 (98%)	247 (98%)	4 (2%)	58	74
4	V	251/255 (98%)	248 (99%)	3 (1%)	67	79
4	y	216/255 (85%)	214 (99%)	2 (1%)	75	83
5	1	229/275 (83%)	228 (100%)	1 (0%)	89	91
5	W	253/275 (92%)	250 (99%)	3 (1%)	67	79
5	X	249/275 (90%)	246 (99%)	3 (1%)	67	79
5	Y	254/275 (92%)	253 (100%)	1 (0%)	89	91
5	Z	253/275 (92%)	249 (98%)	4 (2%)	58	74
5	a	238/275 (86%)	234 (98%)	4 (2%)	56	72
5	b	241/275 (88%)	237 (98%)	4 (2%)	56	72
5	c	245/275 (89%)	243 (99%)	2 (1%)	79	85
5	d	245/275 (89%)	243 (99%)	2 (1%)	79	85
5	z	256/275 (93%)	250 (98%)	6 (2%)	45	64
All	All	23810/28425 (84%)	23522 (99%)	288 (1%)	66	79

5 of 288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	i	272	ASP
5	d	143	ASN
3	J	85	LEU
5	z	54	ARG
1	G	1297	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 406 such sidechains are listed below:

Mol	Chain	Res	Type
1	l	1333	HIS
1	o	77	HIS
5	b	78	GLN
1	m	312	ASN
1	m	1303	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 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.

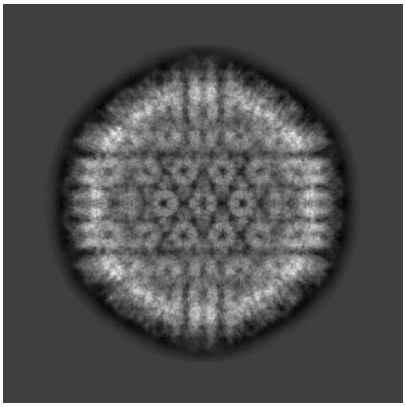
6 Map visualisation

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.

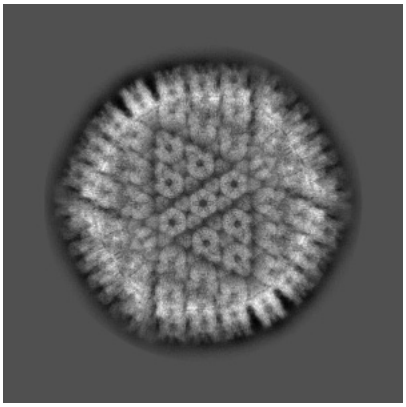
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

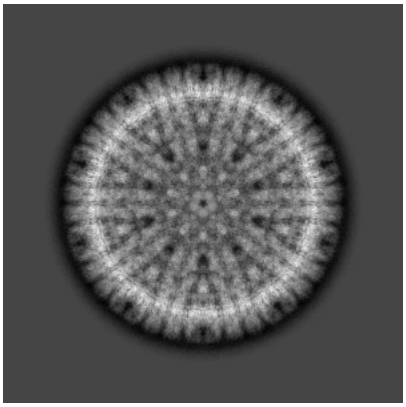
6.1.1 Primary map



X



Y

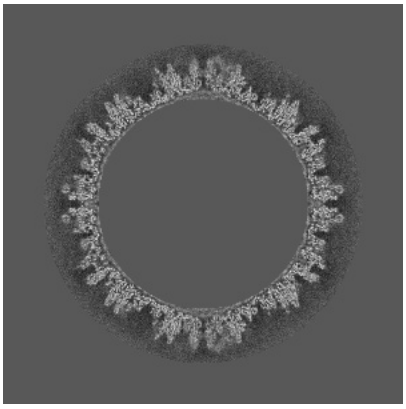


Z

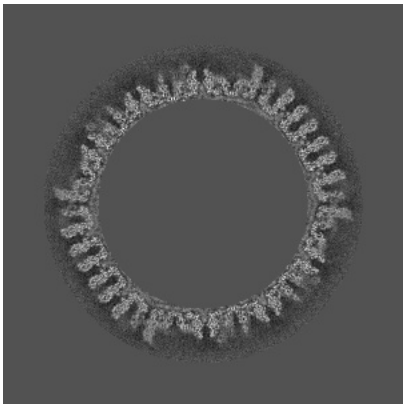
The images above show the map projected in three orthogonal directions.

6.2 Central slices

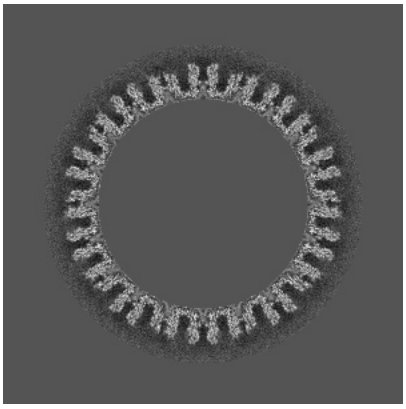
6.2.1 Primary map



X Index: 640



Y Index: 640

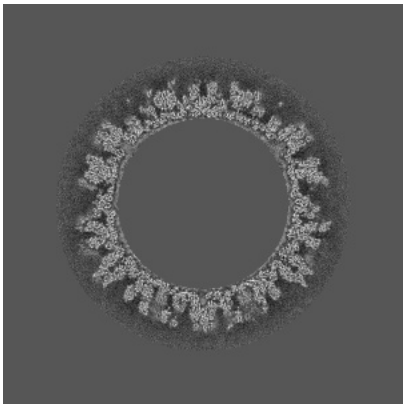


Z Index: 640

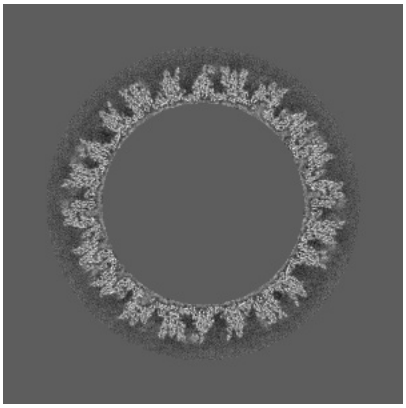
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

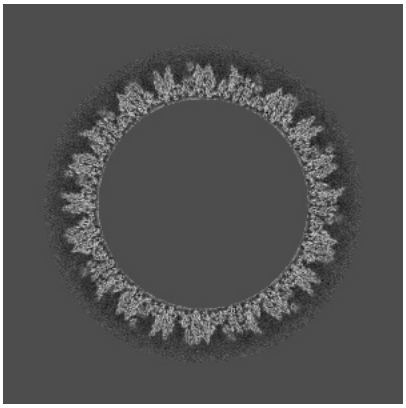
6.3.1 Primary map



X Index: 445



Y Index: 731

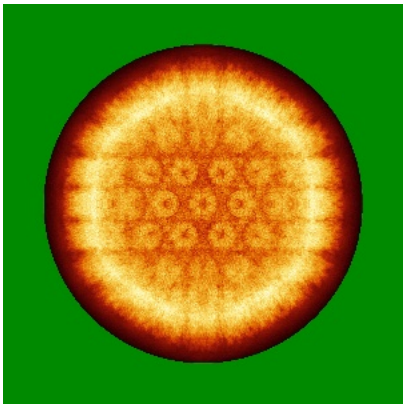


Z Index: 618

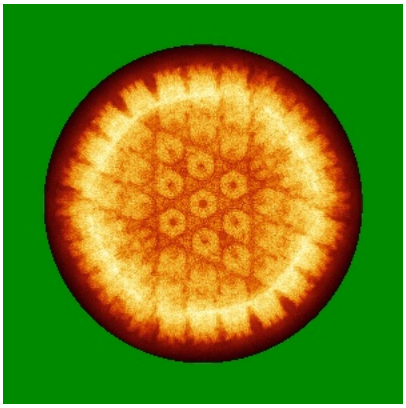
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

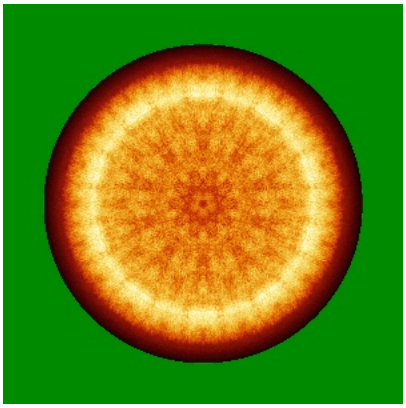
6.4.1 Primary map



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

X Y Z

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.

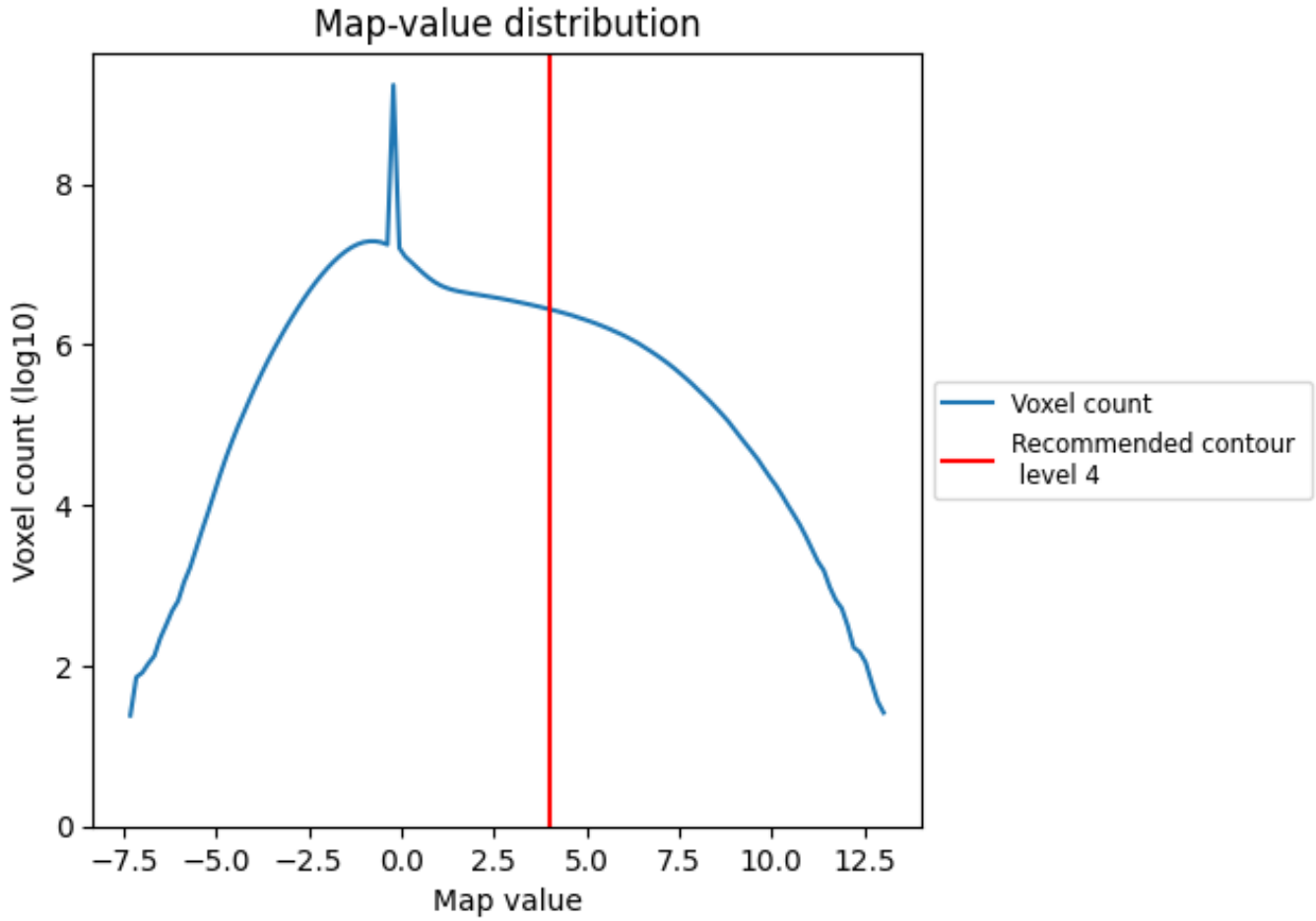
6.6 Mask visualisation (i)

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

7 Map analysis

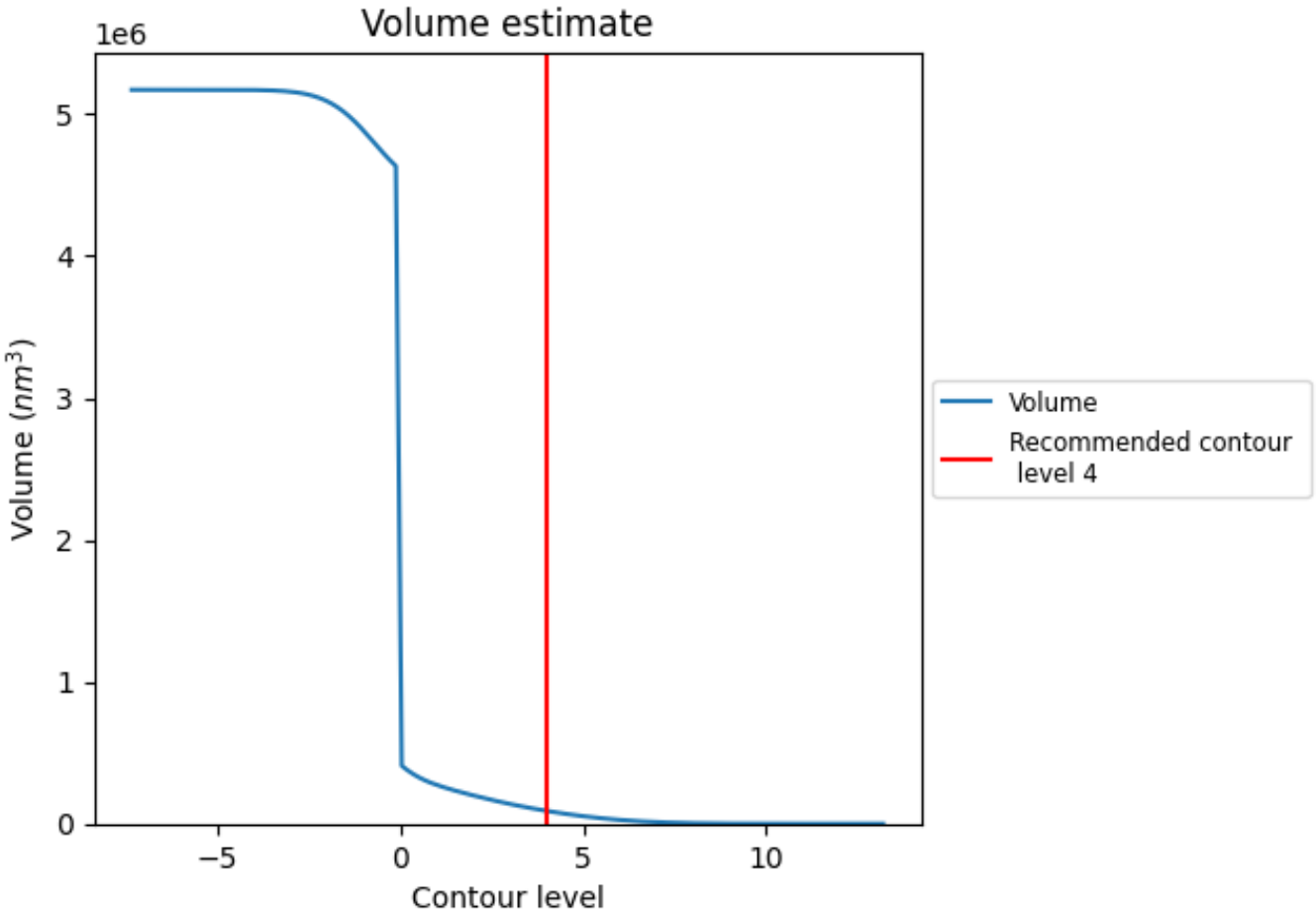
This section contains the results of statistical analysis of the map.

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.

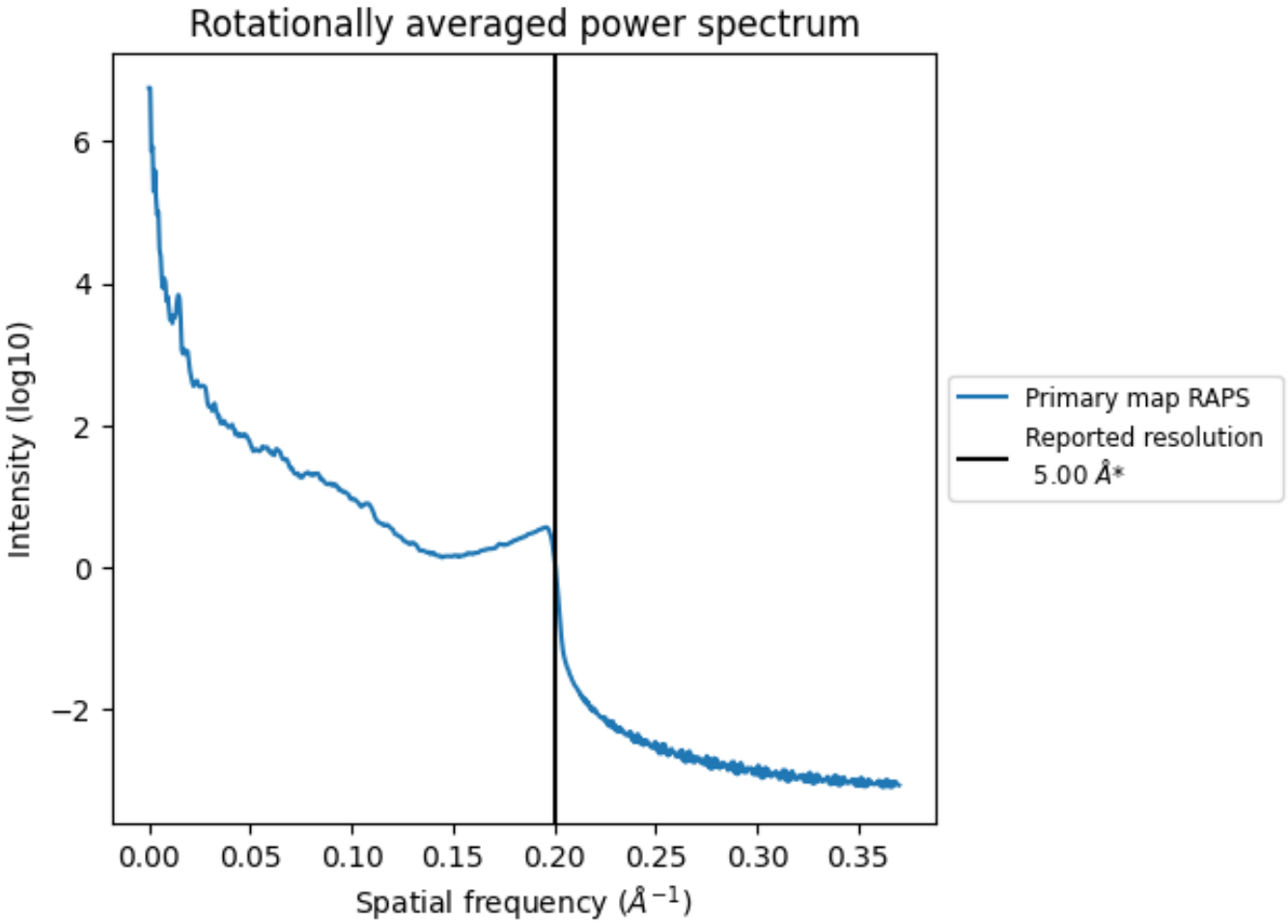
7.2 Volume estimate (i)



The volume at the recommended contour level is 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 (i)



*Reported resolution corresponds to spatial frequency of 0.200 Å^{-1}

8 Fourier-Shell correlation

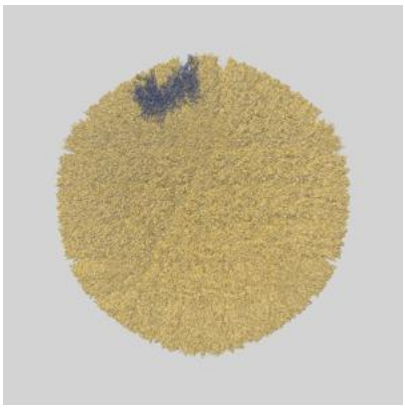
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

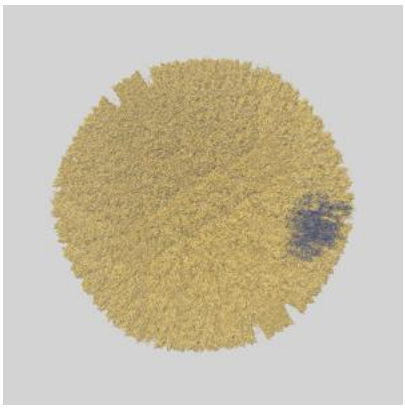
This section contains information regarding the fit between EMDB map EMD-9366 and PDB model 6NHJ. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

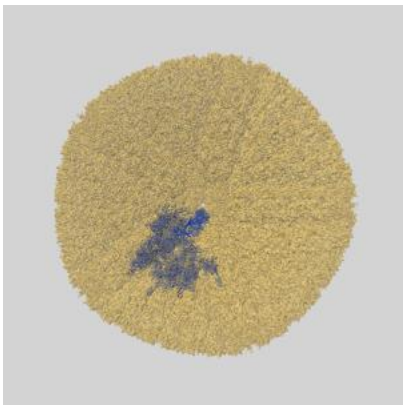
9.1.1 Map-model overlay



X

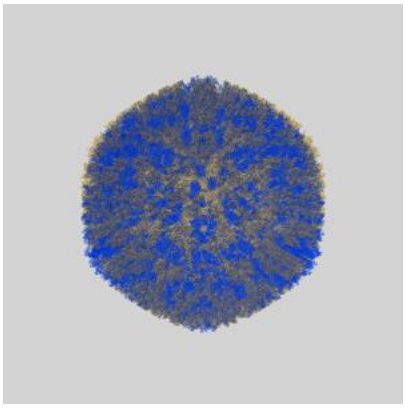


Y

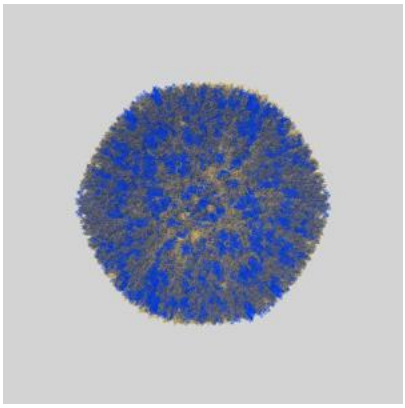


Z

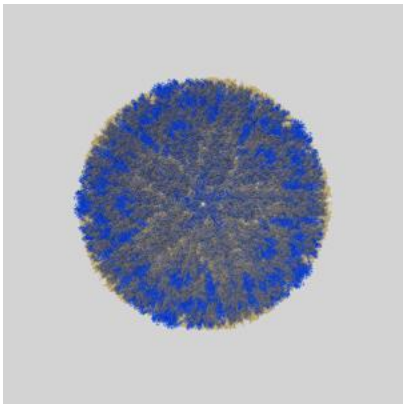
9.1.2 Map-model assembly overlay



X



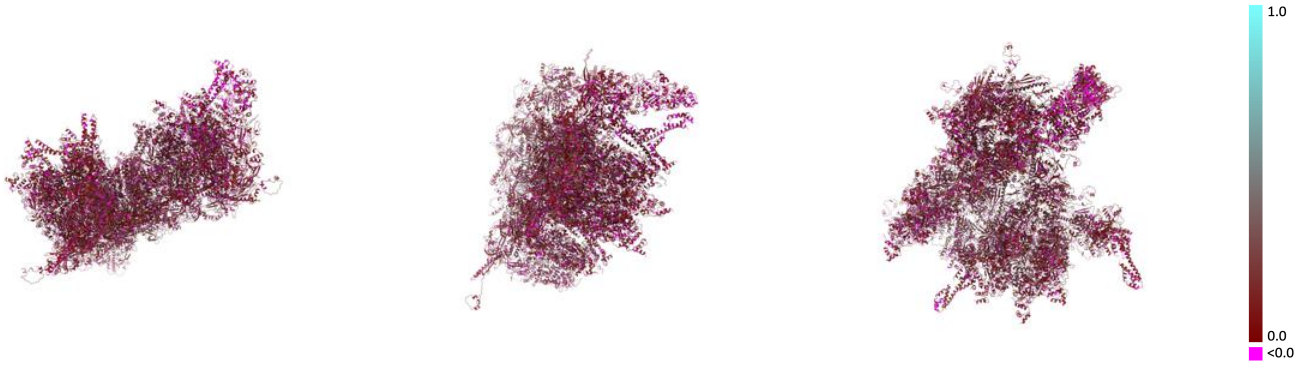
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 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.

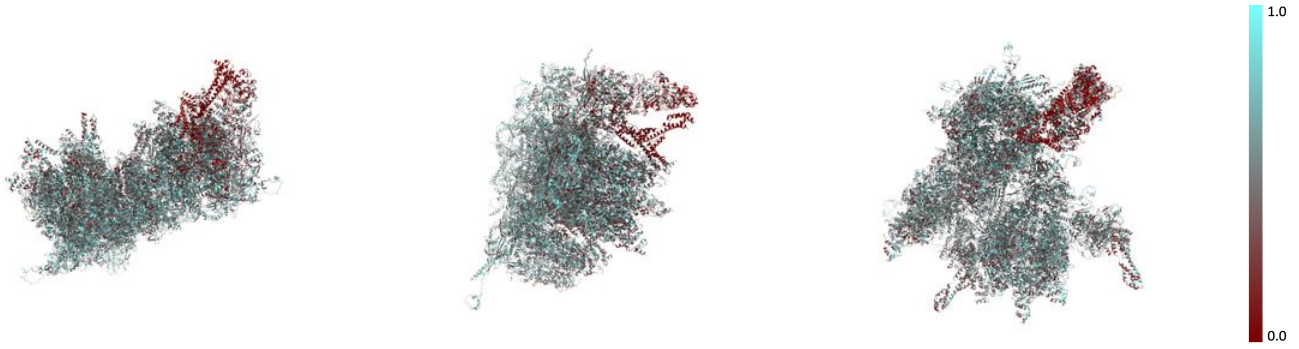
9.2 Q-score mapped to coordinate model



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.

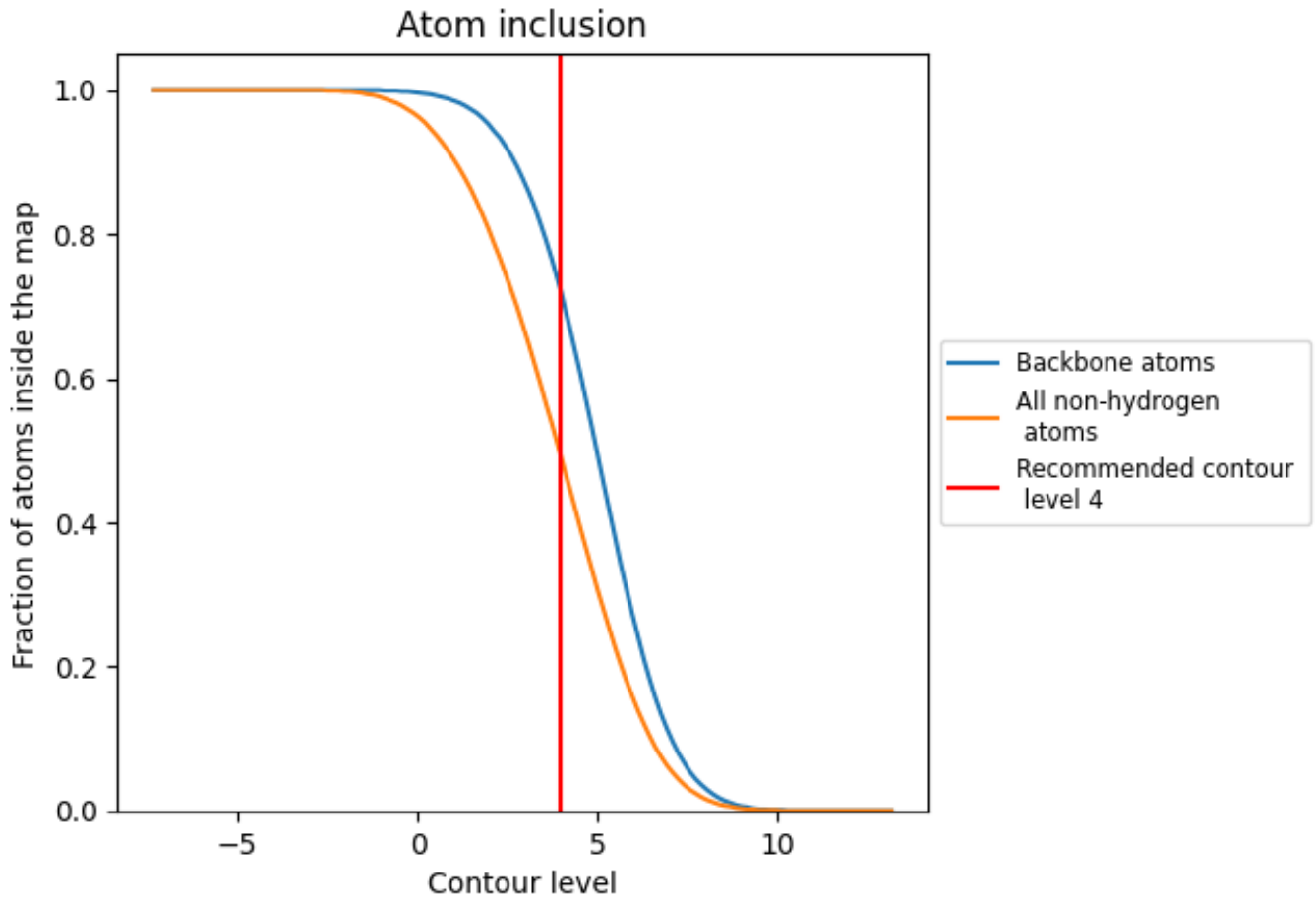
9.3 Atom inclusion mapped to coordinate model



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 (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