wwPDB EM Validation Summary Report (i)

Oct 15, 2024 – 11:37 AM JST

PDB ID	:	7FJ3
EMDB ID	:	EMD-31612
Title	:	Cryo-EM structure of PRV A-capid
Authors	:	Zheng, Q.; Li, S.; Zha, Z.; Sun, H.
Deposited on	:	2021-08-02
Resolution	:	4.53 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:

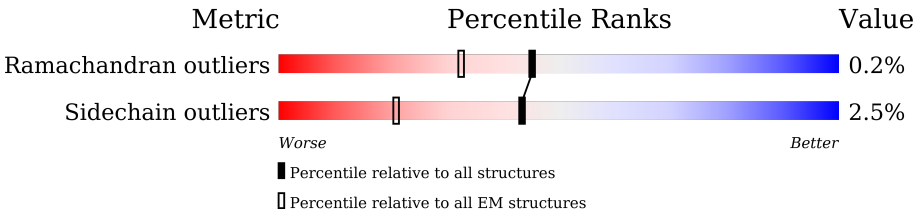
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.53 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	0	1330	54% 98% .
1	A	1330	51% 97% ..
1	S	1330	51% 97% .
1	U	1330	51% 98% .
1	a	1330	51% 97% .
1	e	1330	56% 85% 15%
1	f	1330	51% 98% .
1	g	1330	53% 98% .
1	l	1330	51% 98% .

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Mol	Chain	Length	Quality of chain
1	m	1330	50% 99%
1	n	1330	50% 98%
1	p	1330	53% 98%
1	q	1330	52% 99%
1	u	1330	52% 98%
1	w	1330	52% 98%
1	y	1330	52% 98%
2	1	296	54% 94% 6%
2	2	296	54% 93% 6%
2	3	296	53% 94% 6%
2	j	296	79% 90% 10%
2	k	296	80% 94% 6%
2	o	296	56% 100%
2	s	296	50% 94% 6%
2	v	296	55% 97%
2	x	296	60% 100%
2	z	296	62% 100%
3	B	368	94%
3	C	368	94%
3	D	368	94%
3	T	368	51% 75% 14% 11%
3	W	368	94%
3	d	368	96%
3	h	368	48% 75% 14% 11%
3	i	368	76% 75% 14% 11%

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Mol	Chain	Length	Quality of chain
3	r	368	46% 75% 13% • 11%
3	t	368	49% 75% 14% • 11%
4	E	103	56% 74% 15% 12%
4	F	103	49% 74% 15% 12%
4	G	103	48% 74% 15% 12%
4	H	103	40% 74% 15% 12%
4	I	103	50% 74% 15% 12%
4	J	103	59% 74% 15% 12%
4	K	103	53% 74% 15% 12%
4	L	103	49% 74% 15% 12%
4	M	103	45% 74% 15% 12%
4	N	103	51% 74% 15% 12%
4	O	103	37% 74% 15% 12%
4	P	103	47% 74% 15% 12%
4	Q	103	50% 74% 15% 12%
4	R	103	53% 74% 15% 12%
4	V	103	59% 74% 15% 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 205888 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	0	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	A	1308	Total	C	N	O	S	0	0
			10112	6393	1820	1837	62		
1	S	1289	Total	C	N	O	S	0	0
			9975	6307	1797	1812	59		
1	U	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	a	1289	Total	C	N	O	S	0	0
			9974	6311	1797	1805	61		
1	e	1126	Total	C	N	O	S	0	0
			8722	5528	1561	1579	54		
1	f	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	g	1310	Total	C	N	O	S	0	0
			10125	6401	1823	1840	61		
1	l	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	m	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	n	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	p	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	q	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	u	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	w	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		
1	y	1311	Total	C	N	O	S	0	0
			10129	6403	1824	1841	61		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	2	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	3	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	j	267	Total	C	N	O	S	0	0
			2009	1269	365	364	11		
2	k	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	o	296	Total	C	N	O	S	0	0
			2229	1403	414	401	11		
2	s	277	Total	C	N	O	S	0	0
			2088	1318	382	377	11		
2	v	289	Total	C	N	O	S	0	0
			2189	1380	404	394	11		
2	x	296	Total	C	N	O	S	0	0
			2229	1403	414	401	11		
2	z	296	Total	C	N	O	S	0	0
			2229	1403	414	401	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	23	Total	C	N	O	S	0	0
			152	96	25	29	2		
3	C	23	Total	C	N	O	S	0	0
			152	96	25	29	2		
3	D	23	Total	C	N	O	S	0	0
			152	96	25	29	2		
3	T	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		
3	W	23	Total	C	N	O	S	0	0
			152	96	25	29	2		
3	d	16	Total	C	N	O	S	0	0
			108	69	18	19	2		
3	h	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		
3	i	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		
3	r	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		
3	t	327	Total	C	N	O	S	0	0
			2538	1582	494	450	12		

- Molecule 4 is a protein called Small capsomere-interacting protein.

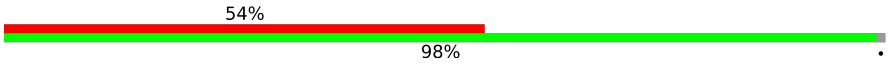
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	F	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	G	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	H	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	I	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	J	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	K	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	L	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	M	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	N	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	O	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	P	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	Q	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	R	91	Total	C	N	O	S	0	0
			722	453	139	128	2		
4	V	91	Total	C	N	O	S	0	0
			722	453	139	128	2		

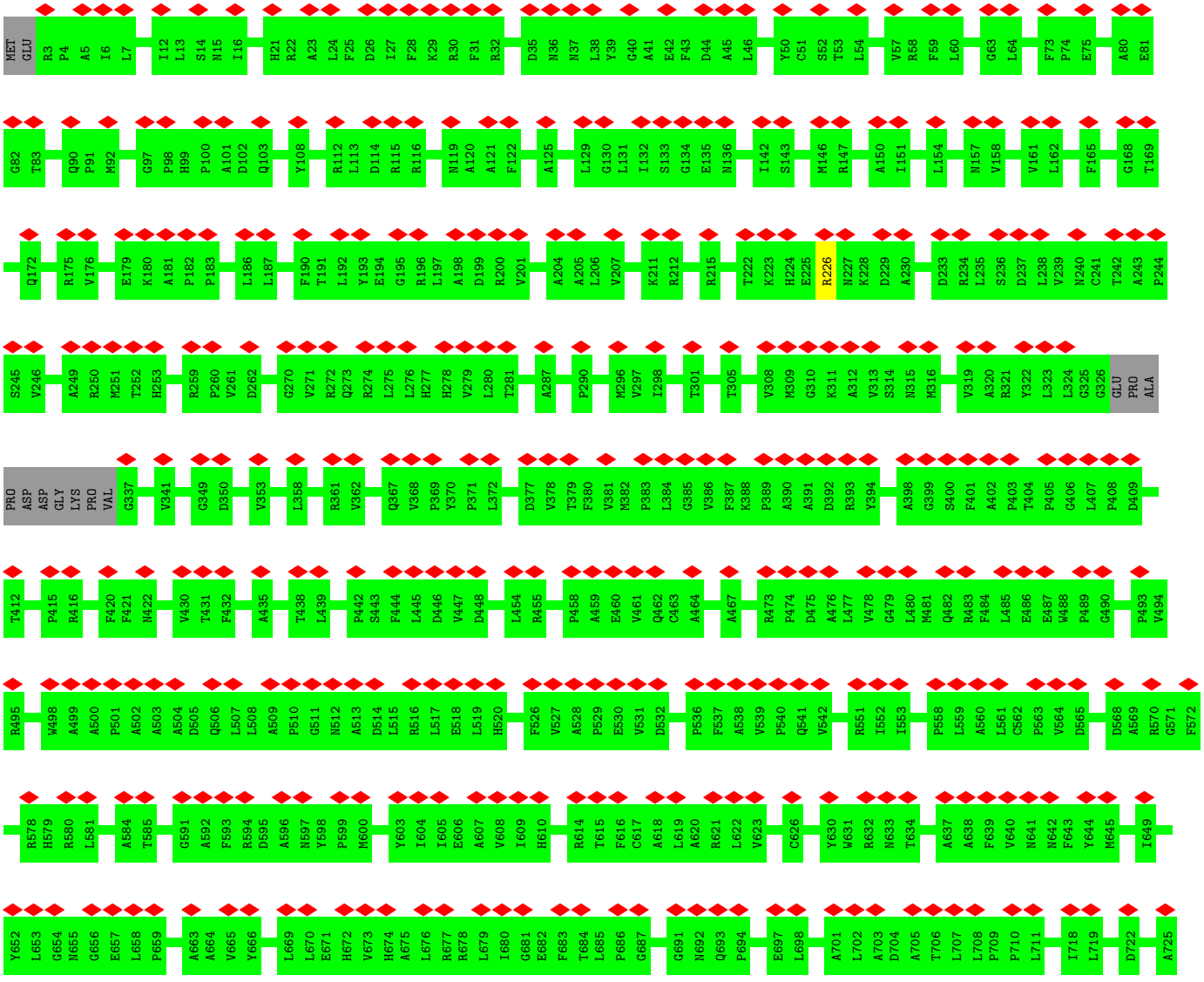
3 Residue-property plots (i)

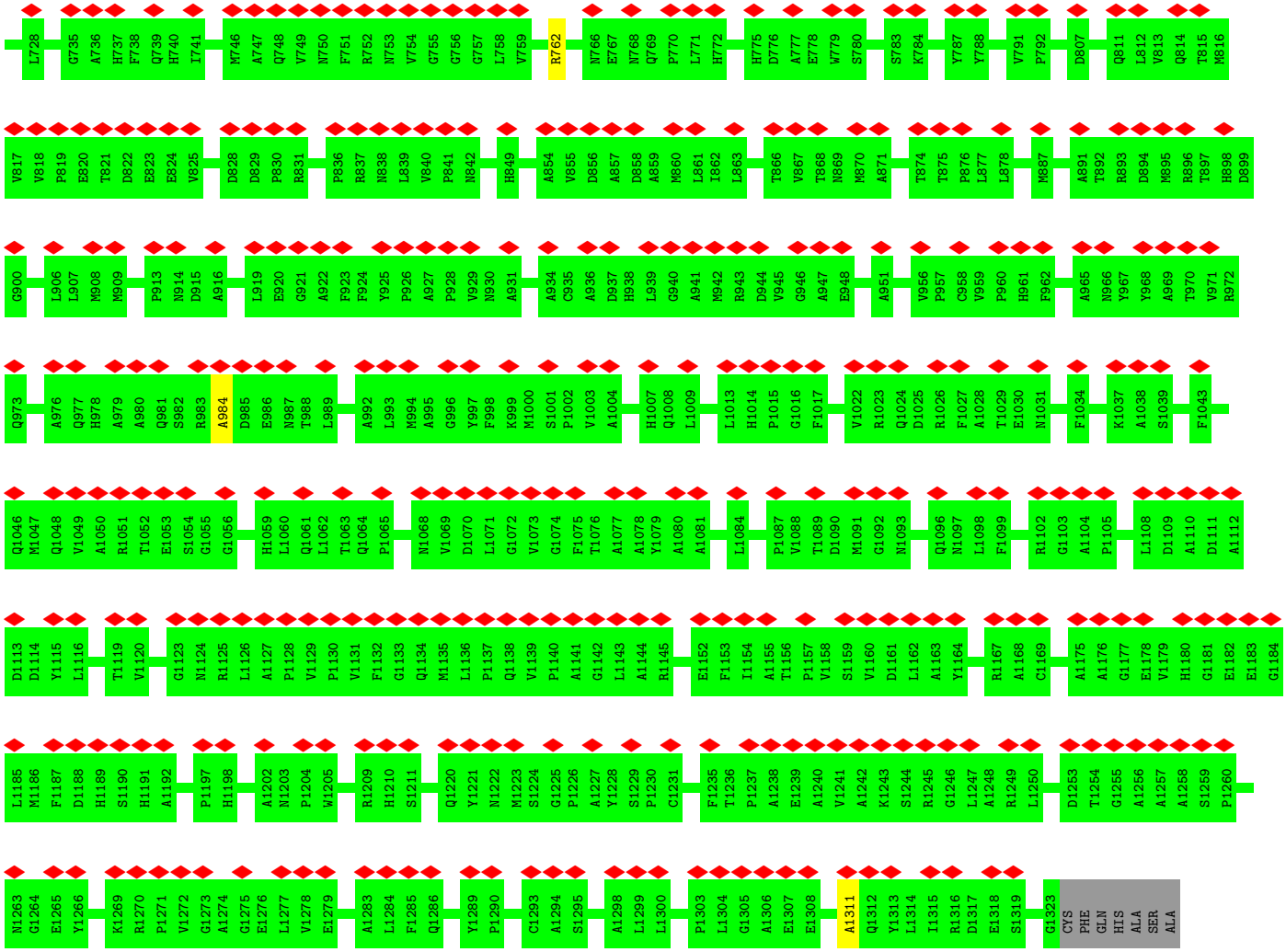
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 0:

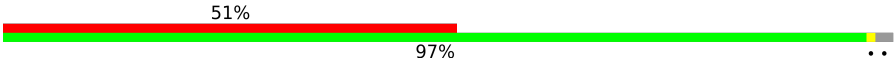


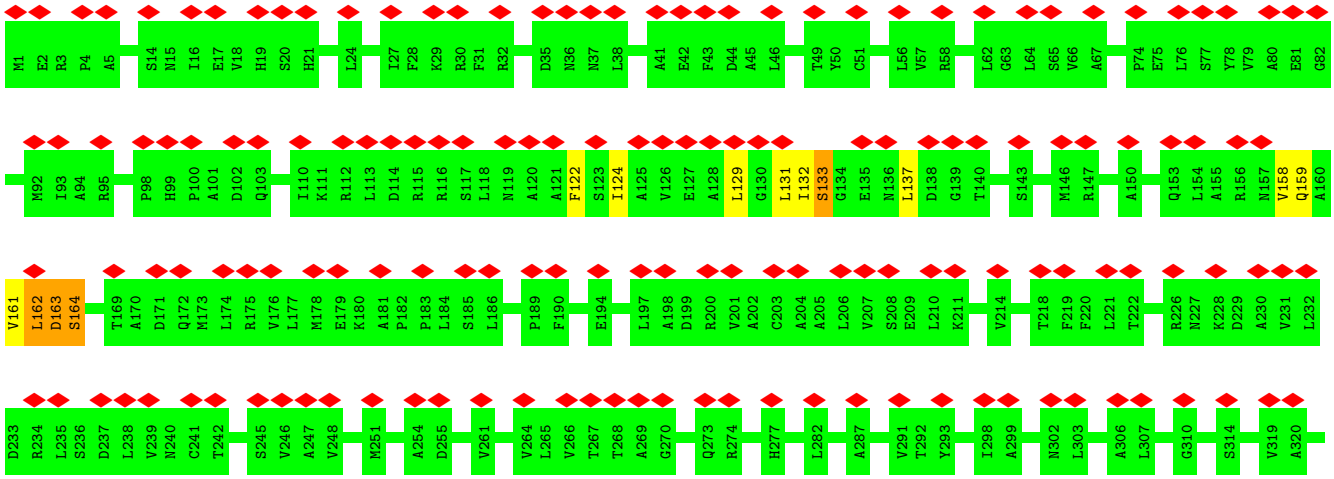


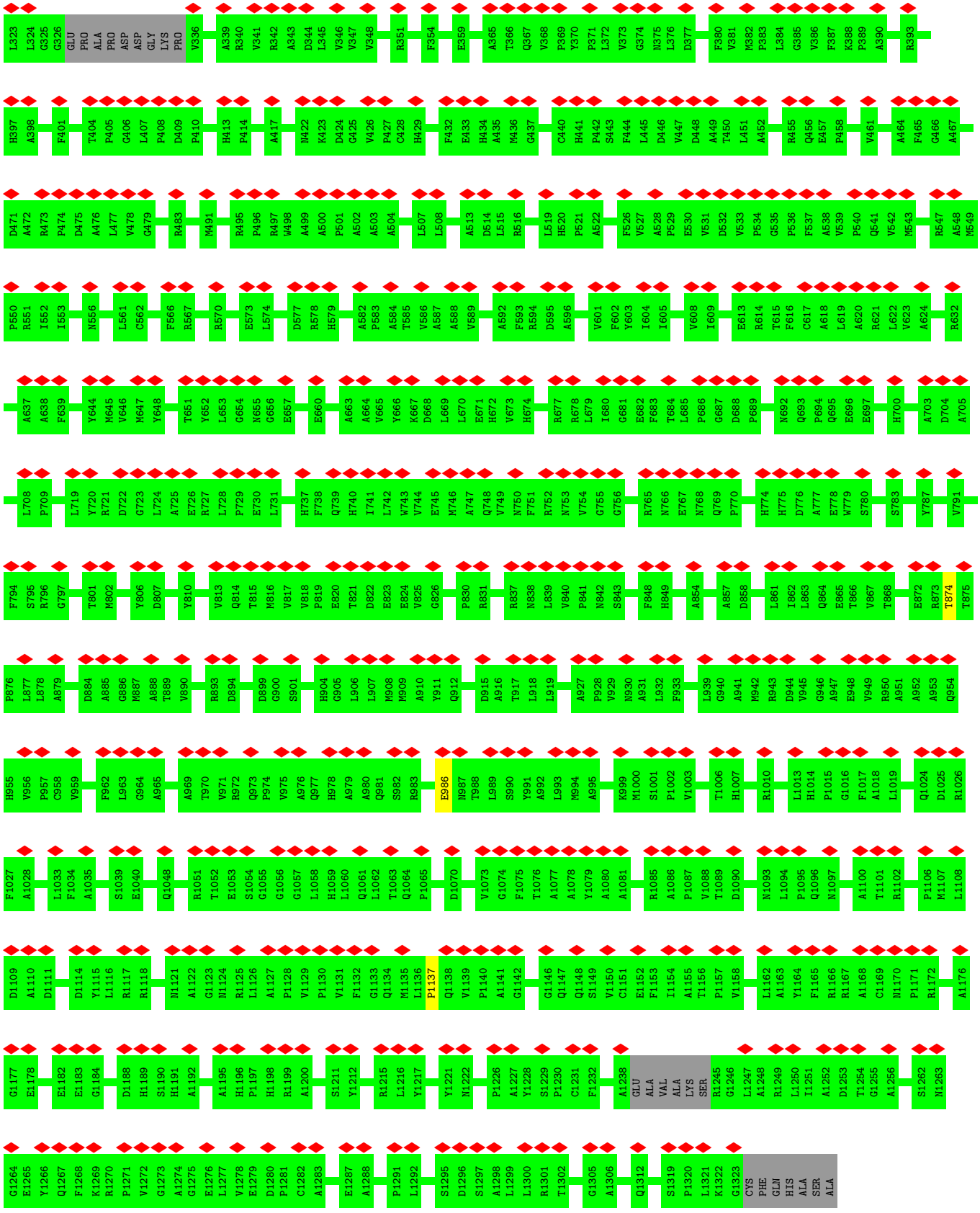


• Molecule 1: Major capsid protein

Chain A:

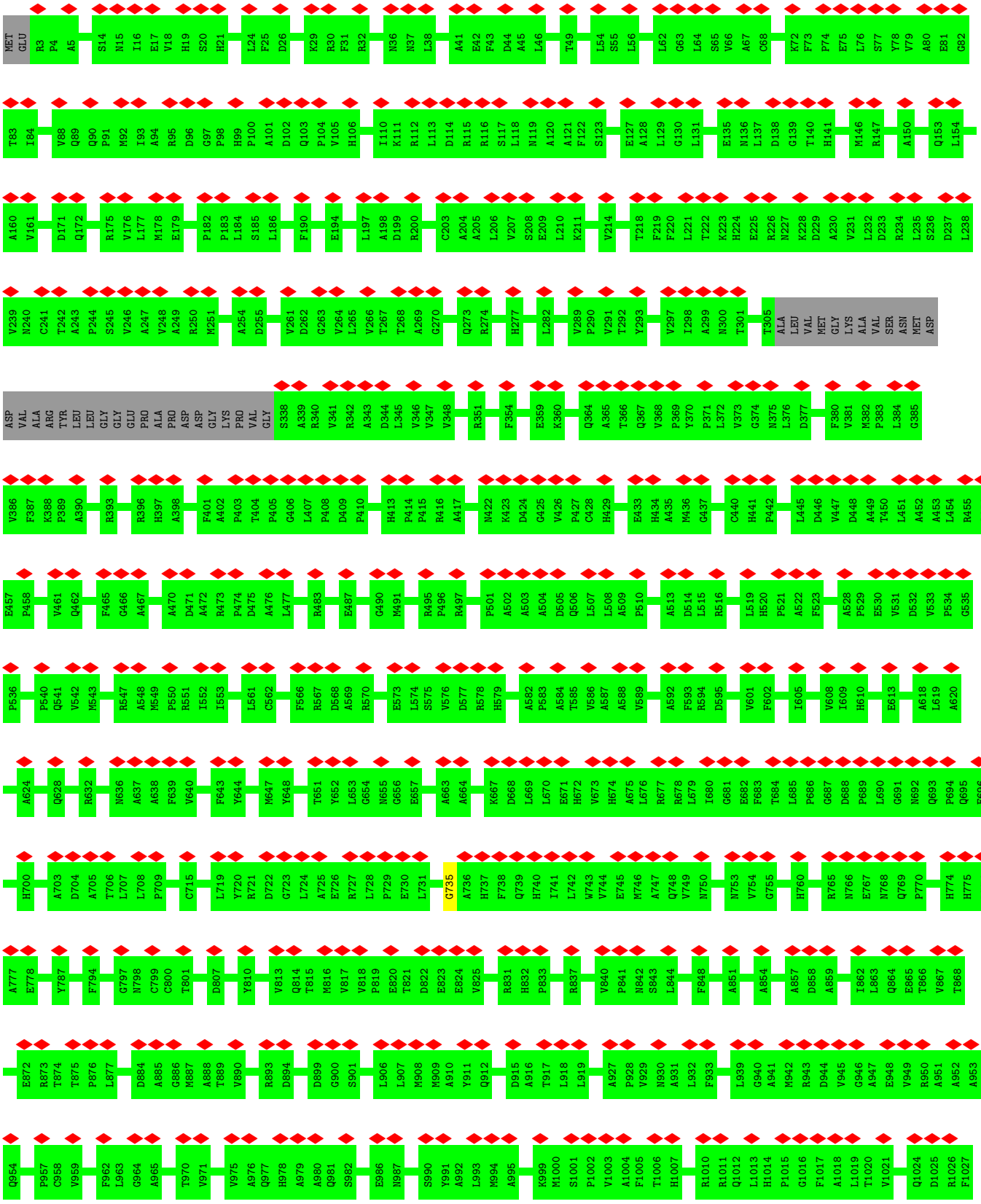


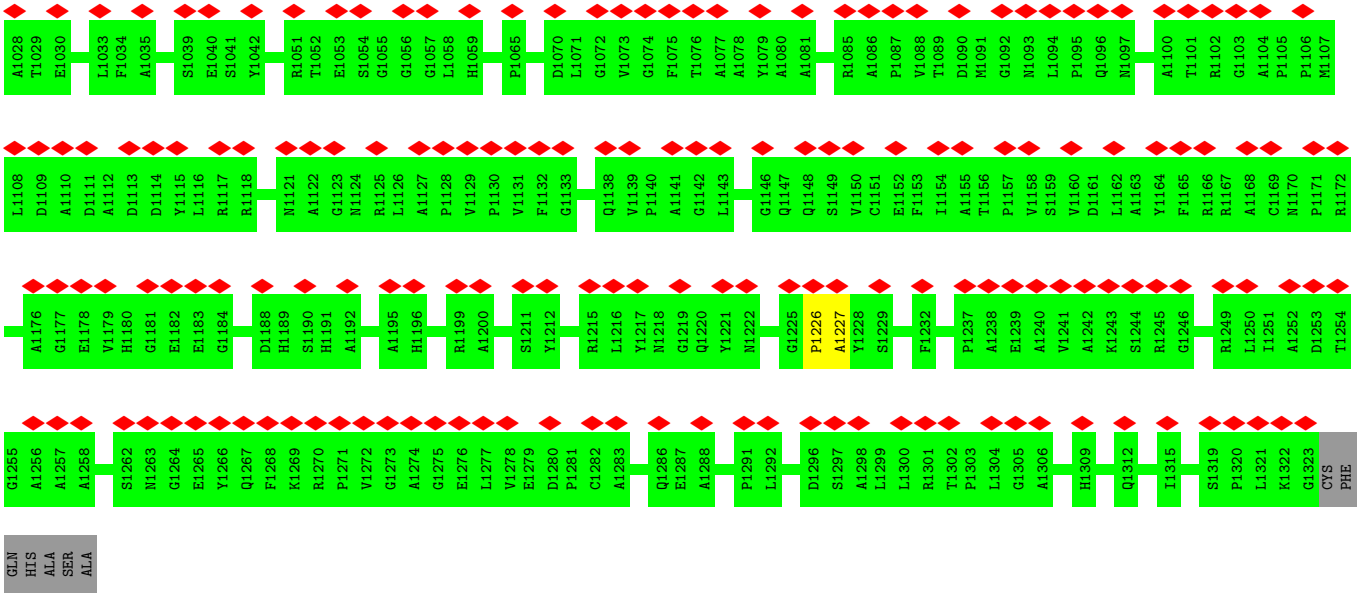




• Molecule 1: Major capsid protein

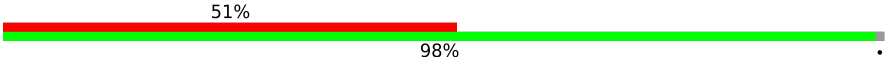
Chain S: 51% 97%

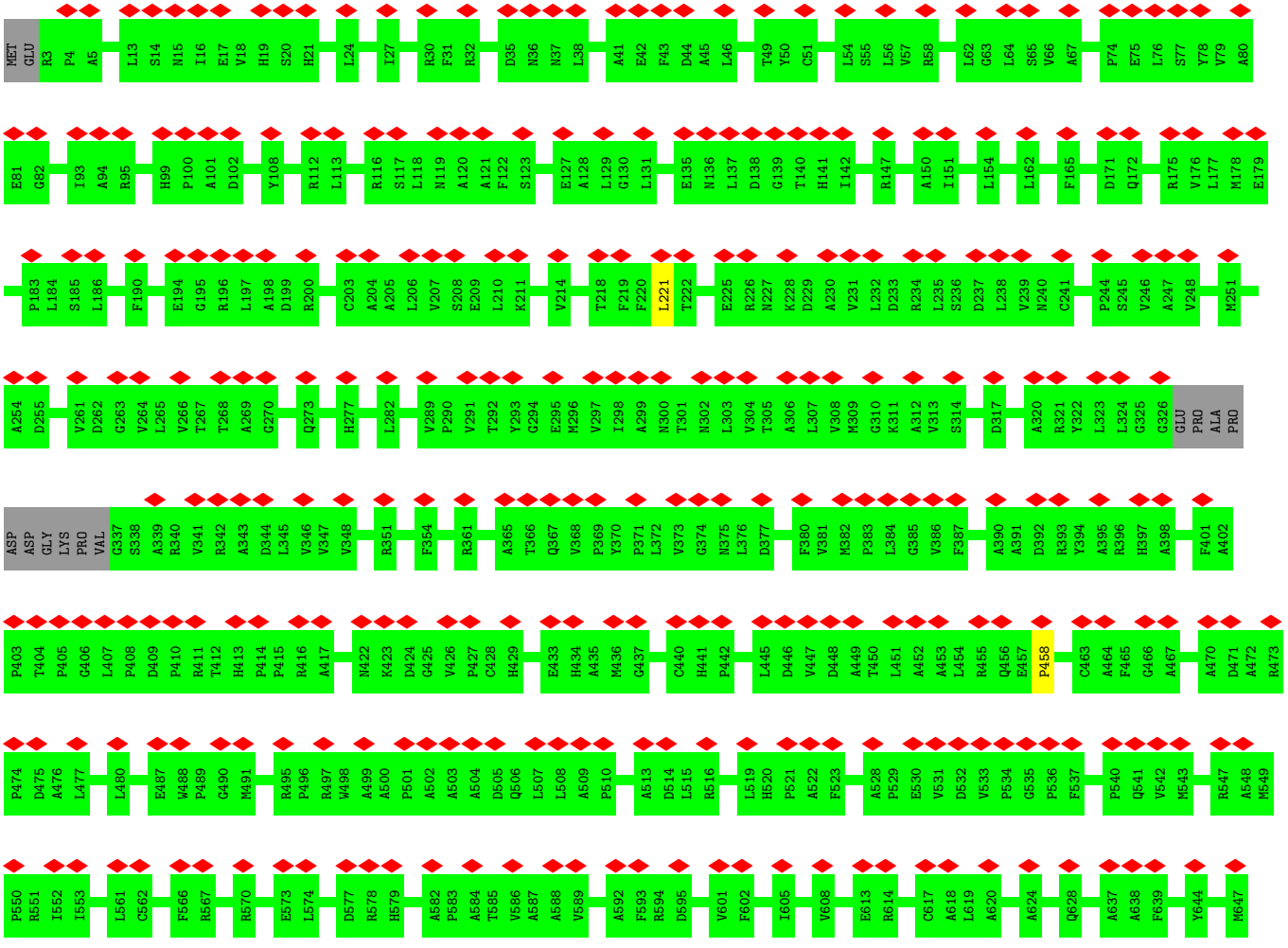

MET GLU R3 P4 A5 S14 N15 I16 E17 V18 H19 S20 H21 L24 F25 D26 K29 R30 F31 R32 N36 N37 L38 A41 E42 F43 D44 A45 L46 T49 L54 S55 L56 L62 G63 L64 S65 V66 A67 C68 K72 F73 P74 E75 L76 S77 Y78 V79 A80 E81 G82
T83 I84 V88 Q89 Q90 P91 M92 I93 A94 R95 D96 G97 P98 H99 P100 A101 D102 Q103 P104 V105 H106 T110 K111 R112 L113 D114 R115 R116 S117 L118 N119 A120 A121 F122 S123 E127 A128 L129 G130 L131 E135 N136 L137 D138 G139 T140 H141 M146 R147 A150 Q153 L154
A160 V161 D171 Q172 R175 V176 L177 M178 E179 P182 P183 L184 S185 L186 F190 E194 L197 A198 D199 R200 C203 A204 A205 L206 V207 S208 E209 L210 K211 V214 T218 F219 F220 L221 T222 K223 H224 E225 R226 N227 K228 D229 A230 V231 L232 D233 R234 L235 S236 D237 L238
V239 N240 C241 T242 A243 P244 S245 V246 A247 V248 A249 R250 M251 A254 D255 V261 D262 G263 V264 L265 V266 T267 T268 A269 G270 Q273 R274 H277 L282 V289 P290 V291 T292 Y293 V297 I298 A299 N300 T301 T305 ALA LEU VAL MET GLY LYS ALA VAL SER ASN MET ASP
ASP VAL ALA ARG TYR LEU LEU GLY GLY GLU PRO ALA PRO ASP ASP GLY LYS PRO VAL GLY S338 A339 R340 V341 R342 A343 D344 L345 V346 V347 V348 R351 F354 E359 K360 Q364 A365 T366 Q367 V368 P369 Y370 P371 L372 V373 G374 N375 L376 D377 F380 V381 M382 P383 L384 G385
V386 P387 K388 P389 A390 R393 R396 H397 A398 F401 A402 P403 T404 P405 G406 L407 P408 D409 P410 H413 P414 P415 R416 A417 N422 K423 D424 G425 V426 P427 C428 H429 E433 H434 A435 M436 G437 C440 H441 P442 L445 D446 V447 D448 A449 T450 L451 A452 A453 L454 R455 Q456
E457 P458 V461 Q462 F465 G466 A467 A470 D471 A472 R473 P474 D475 A476 L477 R483 E487 G490 M491 R495 P496 R497 P501 A502 A503 A504 D505 Q506 L507 L508 A509 P510 A513 D514 L515 R516 L519 H520 P521 A522 F523 A528 P529 E530 V531 D532 V533 P534 G535
P536 P540 Q541 V542 M543 R547 A548 M549 P550 R551 I552 I553 L561 C562 F566 R567 D568 A569 R570 E573 L574 S575 V576 D577 R578 H579 A582 P583 A584 T585 V586 A587 A588 V589 A592 F593 R594 D595 V601 F602 I605 V608 I609 H610 E613 A618 L619 A620
A624 Q628 R632 W636 A637 A638 F639 V640 F643 Y644 M647 Y648 T651 Y652 L653 G654 N655 G656 E657 A663 A664 K667 D668 L669 L670 E671 H672 V673 H674 A675 L676 R677 R678 L679 I680 G681 E682 F683 T684 L685 P686 G687 D688 P689 L690 G691 W692 Q693 P694 Q695 E696
H700 A703 D704 A705 T706 L707 L708 P709 C715 L719 Y720 R721 D722 G723 L724 A725 E726 R727 L728 P729 E730 L731 G735 A736 H737 F738 Q739 H740 I741 L742 W743 V744 E745 M746 A747 Q748 V749 N750 N753 V754 G755 H760 R765 N766 E767 N768 Q769 P770 H774 H775 D776
A777 E778 V787 F794 G797 N798 C799 C800 T801 D807 Y810 V813 Q814 T815 M816 V817 V818 P819 E820 T821 D822 E823 E824 V825 R831 H832 P833 R837 V840 P841 N842 S843 L844 F848 A851 A854 A857 D858 A859 I862 L863 Q864 E865 T866 V867 T868
E872 R873 T874 T875 P876 L877 D884 A885 G886 M887 A888 T889 V890 R893 D894 D899 G900 S901 L906 L907 M908 M909 A910 Y911 Q912 D915 A916 T917 L918 L919 A927 P928 V929 N930 A931 L932 F933 L939 G940 A941 M942 R943 D944 V945 G946 A947 E948 V949 R950 A951 A952 A953
Q954 P957 C958 V959 F962 L963 G964 A965 T970 V971 V975 A976 Q977 H978 A979 A980 Q981 S982 E986 N987 S990 Y991 A992 L993 M994 A995 K999 M1000 S1001 P1002 V1003 A1004 F1005 T1006 H1007 R1010 R1011 Q1012 L1013 H1014 P1015 G1016 F1017 A1018 L1019 T1020 V1021 Q1024 D1025 R1026 F1027



• Molecule 1: Major capsid protein

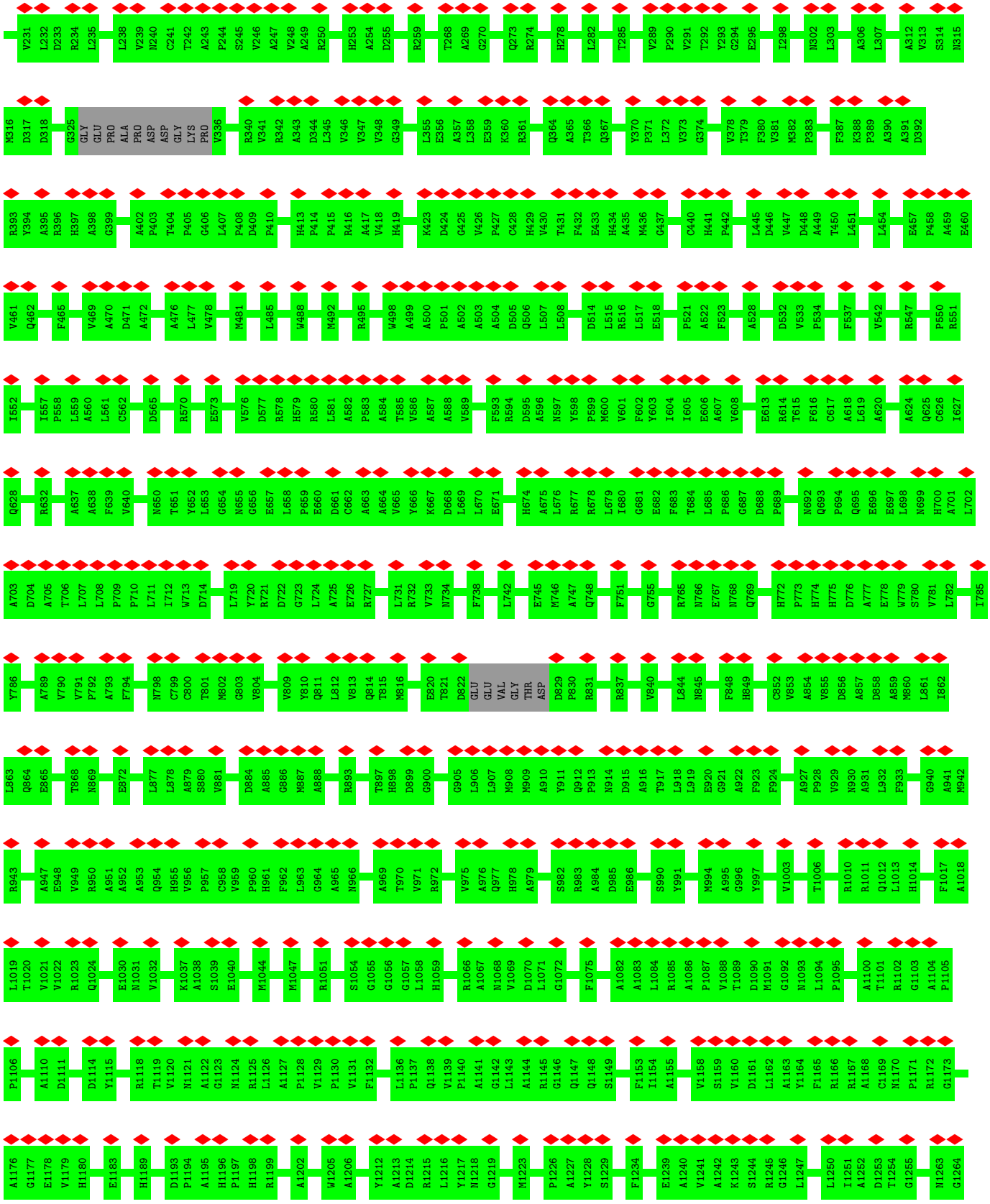
Chain U:





• Molecule 1: Major capsid protein

Chain a:


V231 L232 D233 R234 L235 L238 V239 N240 C241 T242 A243 P244 S245 V246 A247 V248 A249 R250 H253 A254 D255 R259 T268 A269 G270 Q273 R274 H278 L282 T285 V289 P290 V291 T292 Y293 G294 E295 I298 N302 L303 A306 L307 A312 V313 S314 N315
M316 D317 D318 G325 GLY GLU PRO ALA PRO ASP ASP GLY LYS PRO V336 R340 V341 R342 A343 D344 L345 V346 V347 V348 G349 L355 E356 A357 L358 E359 K360 R361 Q364 A365 T366 Q367 Y370 P371 L372 V373 G374 V378 T379 F380 V381 H382 P383 F387 K388 P389 A390 A391 D392
R393 Y394 A395 R396 H397 A398 G399 A402 P403 T404 P405 G406 L407 P408 D409 P410 H413 P414 P415 R416 A417 V418 H419 K423 D424 G425 V426 P427 C428 H429 V430 T431 F432 E433 H434 A435 M436 G437 C440 H441 P442 L445 D446 V447 D448 A449 T450 L451 L454 E457 P458 A459 E460
V461 Q462 F465 V469 A470 D471 A472 A476 L477 V478 M481 L485 W488 M492 R495 W498 A499 A500 P501 A502 A503 A504 D505 Q506 L507 L508 D514 L515 R516 L517 E518 P521 A522 F523 A528 D532 V533 P534 F537 V542 R547 P550 R551
I552 I557 P558 L559 A560 L561 C562 D565 R570 E573 V576 D577 R578 H579 R580 L581 A582 P583 A584 T585 V586 A587 A588 V589 F593 R594 D595 A596 N597 Y598 P599 M600 V601 F602 Y603 I604 I605 E606 A607 V608 E613 R614 T615 F616 C617 A618 L619 A620 A624 Q625 C626 I627
Q628 R632 A637 A638 F639 V640 N650 T651 Y652 L653 G654 N655 G656 E657 L658 P659 E660 D661 C662 A663 A664 V665 Y666 K667 D668 L669 L670 E671 H674 A675 L676 R677 R678 L679 I680 G681 E682 F683 T684 L685 P686 G687 D688 P689 N692 Q693 P694 Q695 E696 E697 L698 N699 H700 A701 L702
A703 D704 A705 T706 L707 L708 P709 P710 L711 I712 W713 D714 L719 Y720 R721 D722 G723 L724 A725 E726 R727 L731 R732 V733 N734 F738 L742 E745 M746 A747 Q748 F751 G755 R765 N766 E767 N768 Q769 H772 P773 H774 H775 D776 A777 E778 W779 S780 V781 L782 I785
Y786 A789 V790 V791 P792 A793 F794 N798 C799 C800 T801 M802 G803 V804 V809 Y810 Q811 L812 V813 Q814 T815 M816 E820 T821 D822 GLU GLU VAL GLY THR ASP D829 P830 R831 R837 V840 L844 N845 F848 H849 C852 V853 A854 V855 D856 A857 D858 A859 M860 L861 I862
L863 Q864 E865 T868 N869 E872 L877 L878 A879 S880 V881 D884 A885 G886 M887 A888 R893 T897 H898 D899 G900 G905 L906 L907 M908 M909 A910 Y911 Q912 P913 N914 D915 A916 T917 L918 L919 E920 G921 A922 F923 F924 A927 P928 V929 N930 A931 L932 F933 G940 A941 M942
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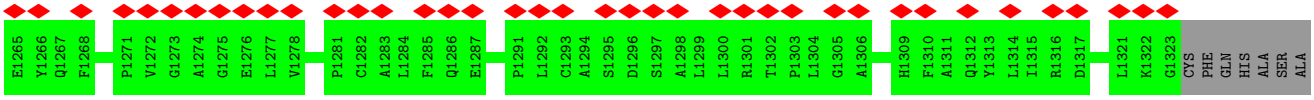
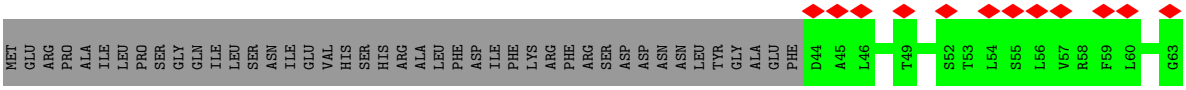
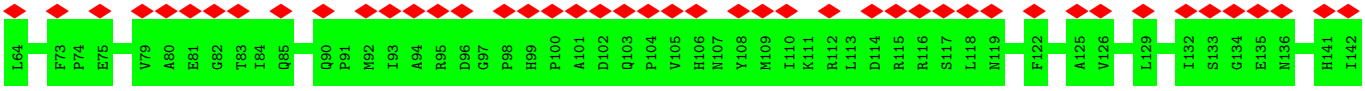
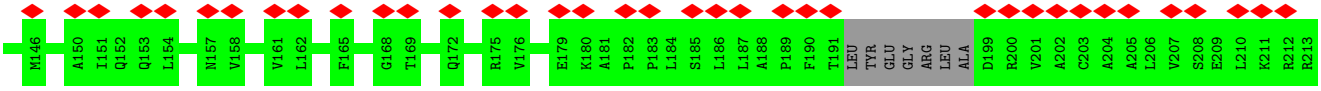


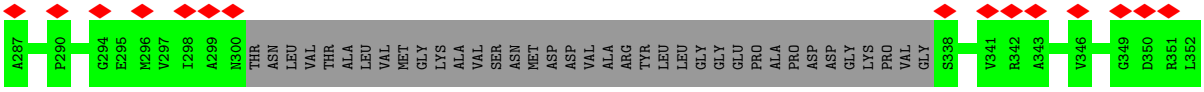
• Molecule 1: Major capsid protein

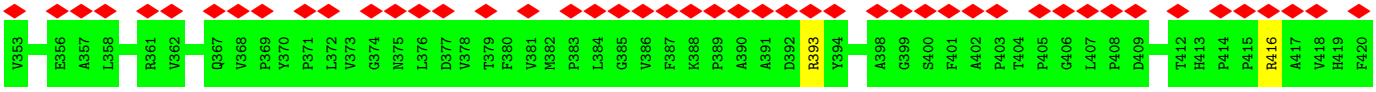
Chain e:

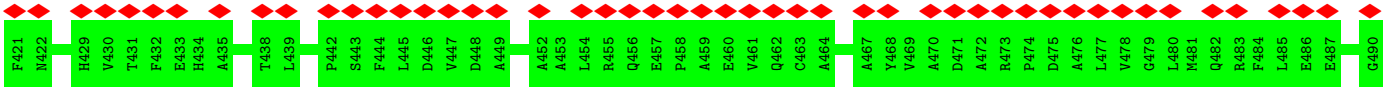


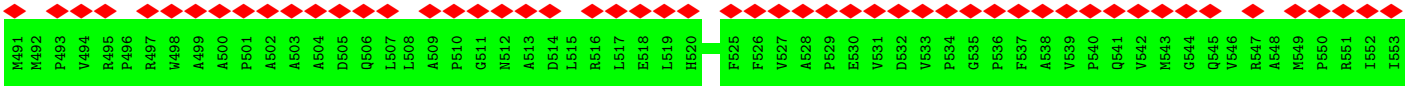


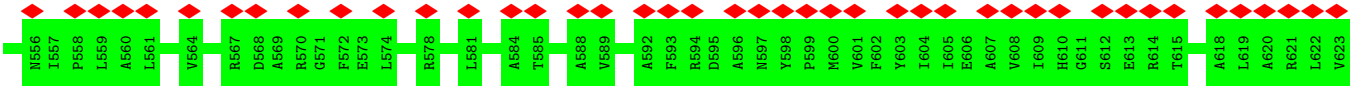


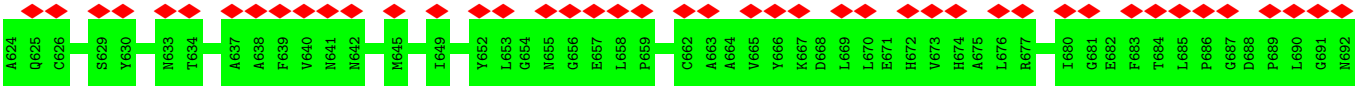


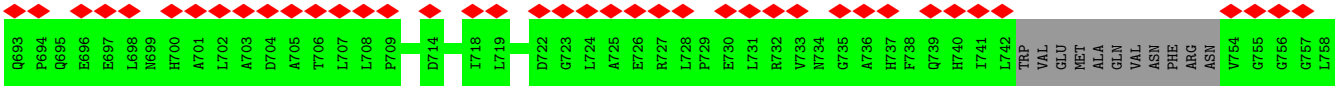


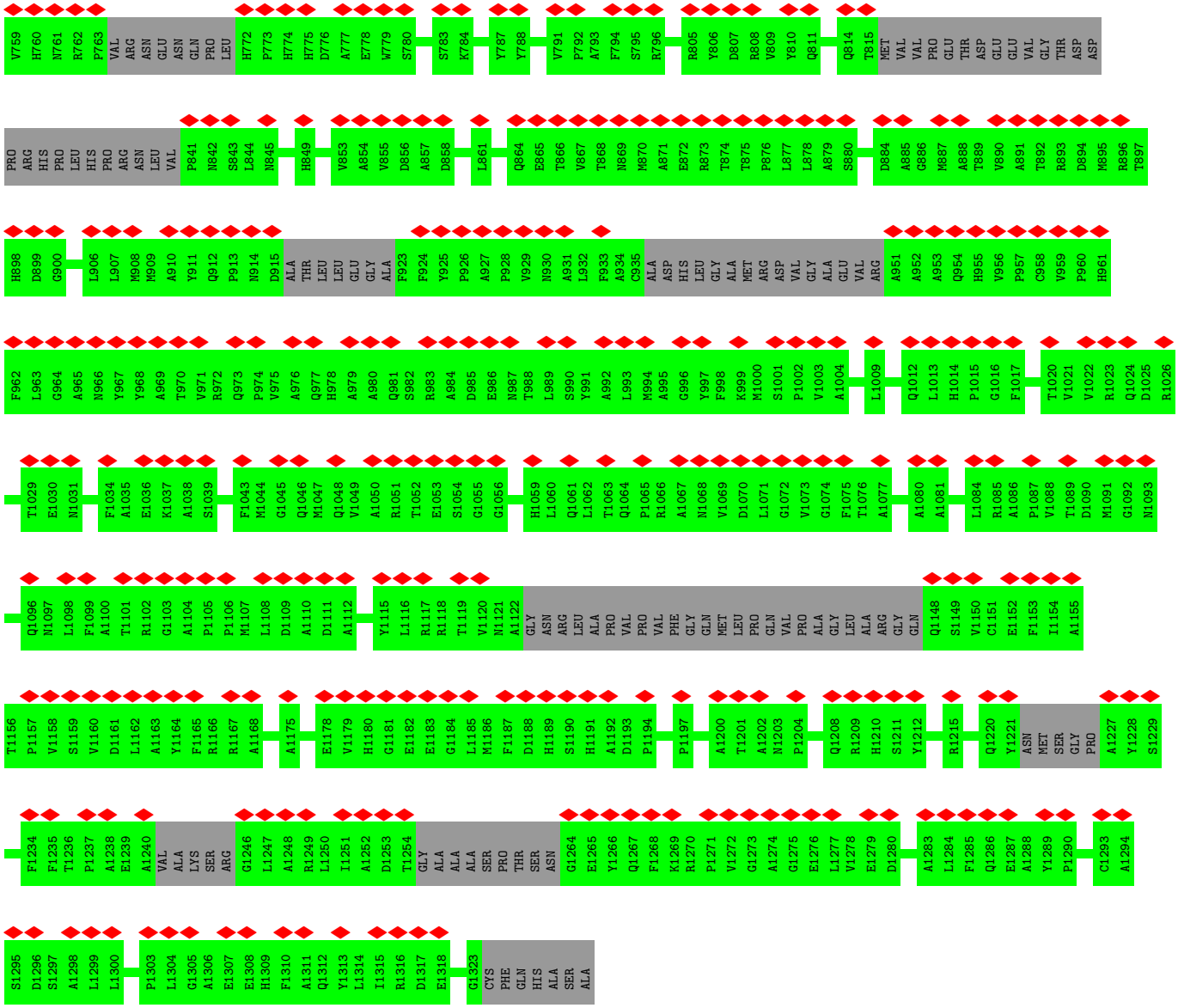






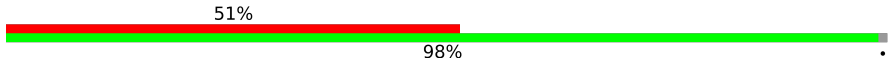


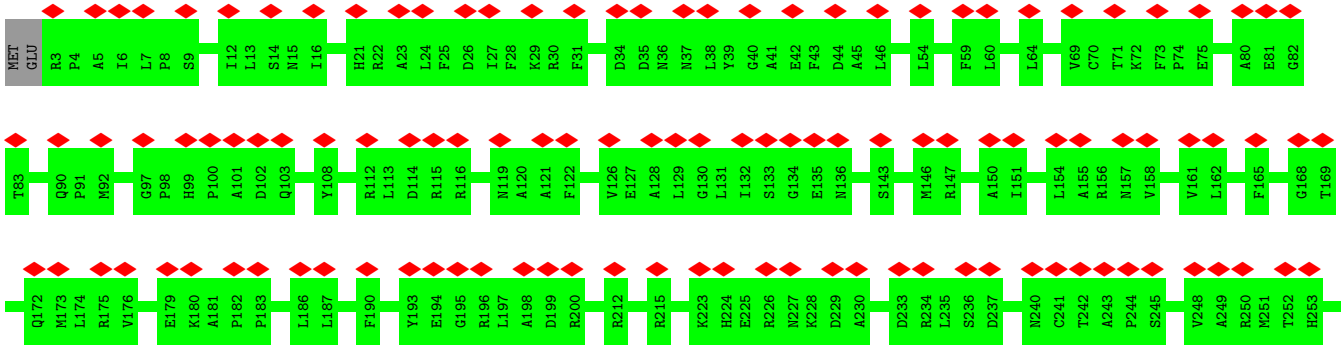


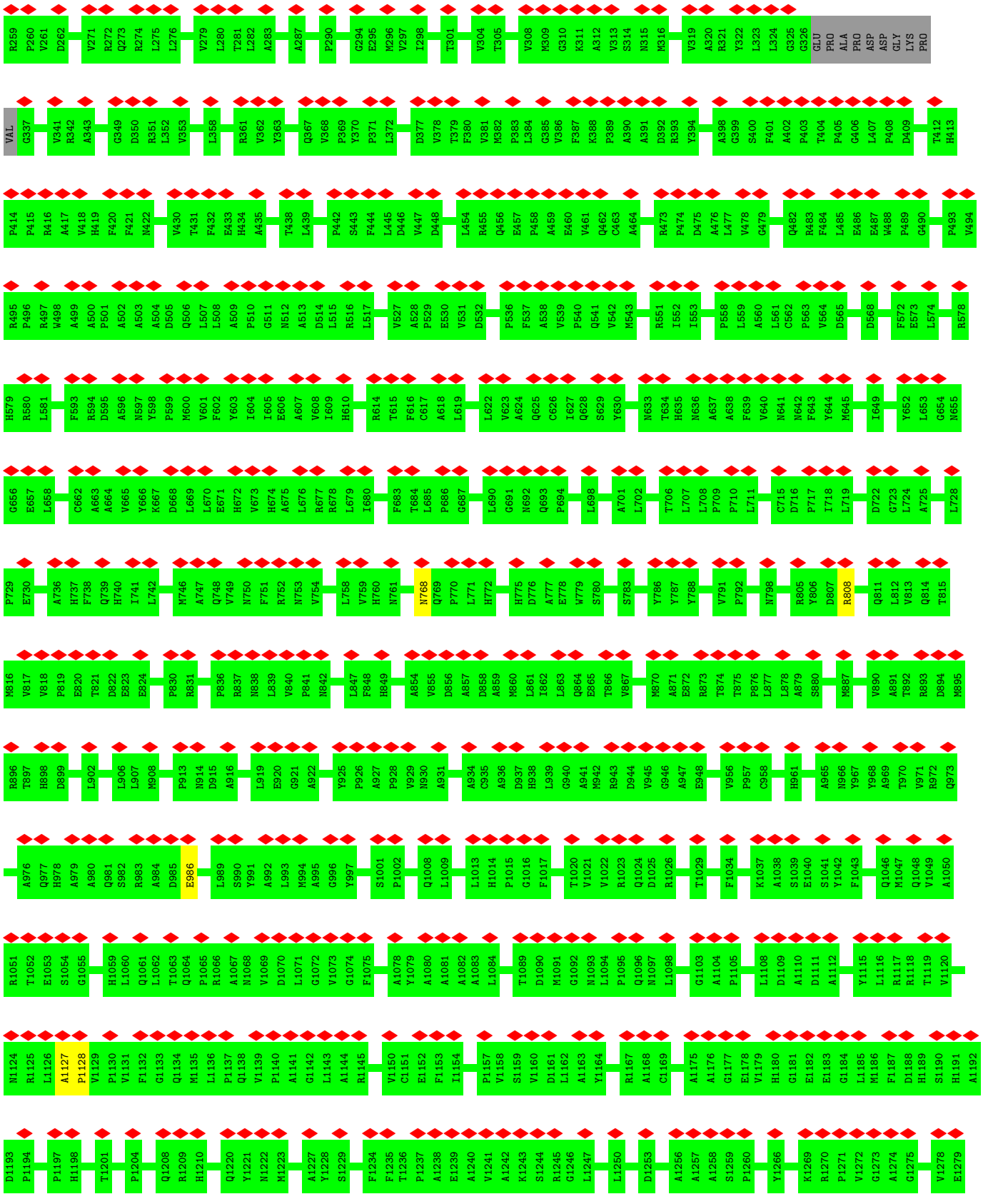


• Molecule 1: Major capsid protein

Chain f:



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VAL G337 V341 R342 A343 G349 D350 R351 L352 V353 L358 R361 V362 Y363 Q367 V368 P369 Y370 P371 L372 D377 V378 T379 F380 V381 M382 P383 L384 G385 V386 F387 K388 P389 A390 A391 D392 R393 Y394 A398 G399 S400 F401 A402 P403 T404 P405 G406 L407 P408 D409 T412 H413
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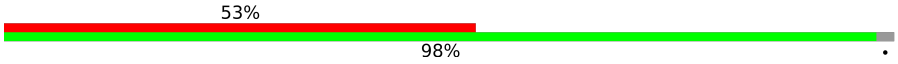
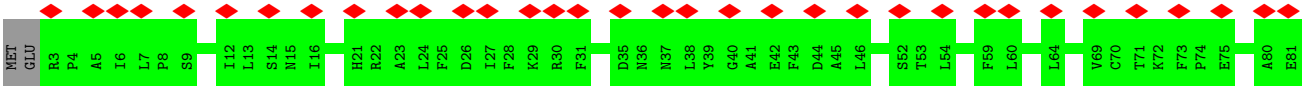
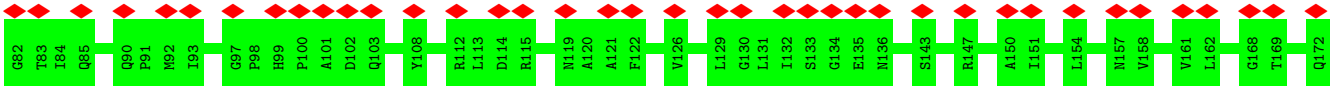
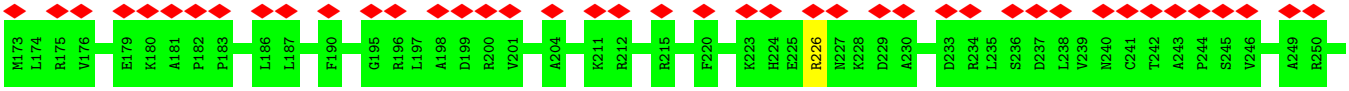
• Molecule 1: Major capsid protein

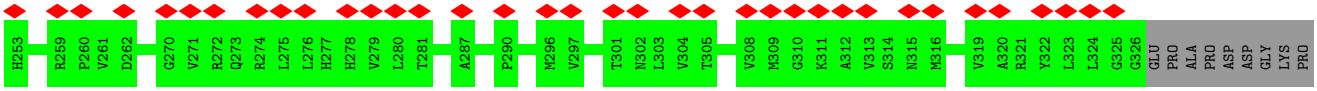
Chain g:

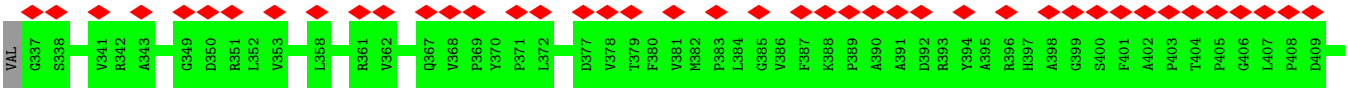


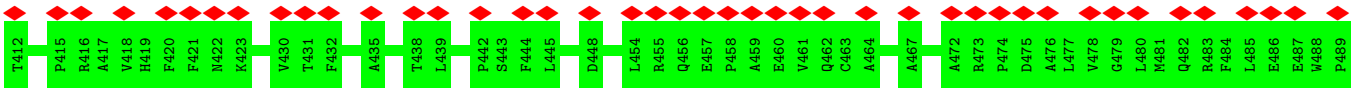


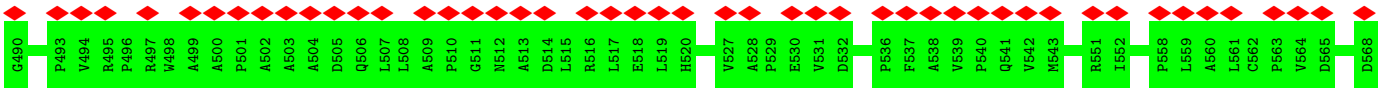


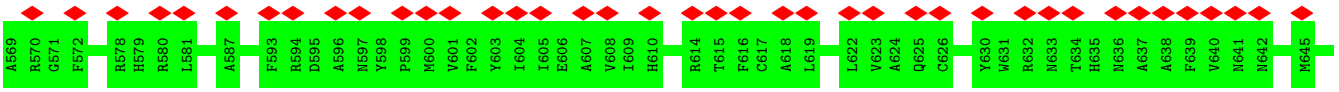


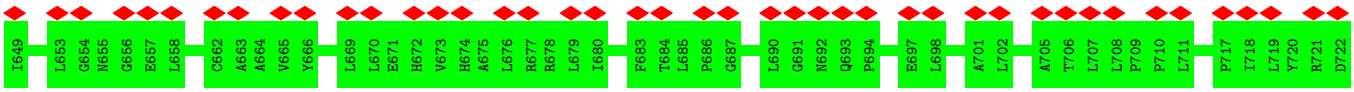


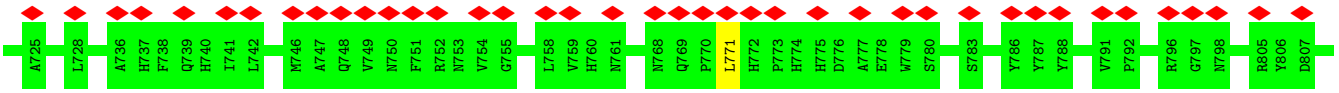


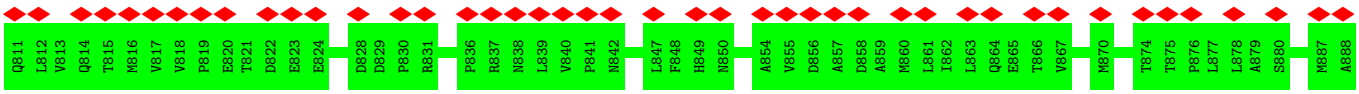


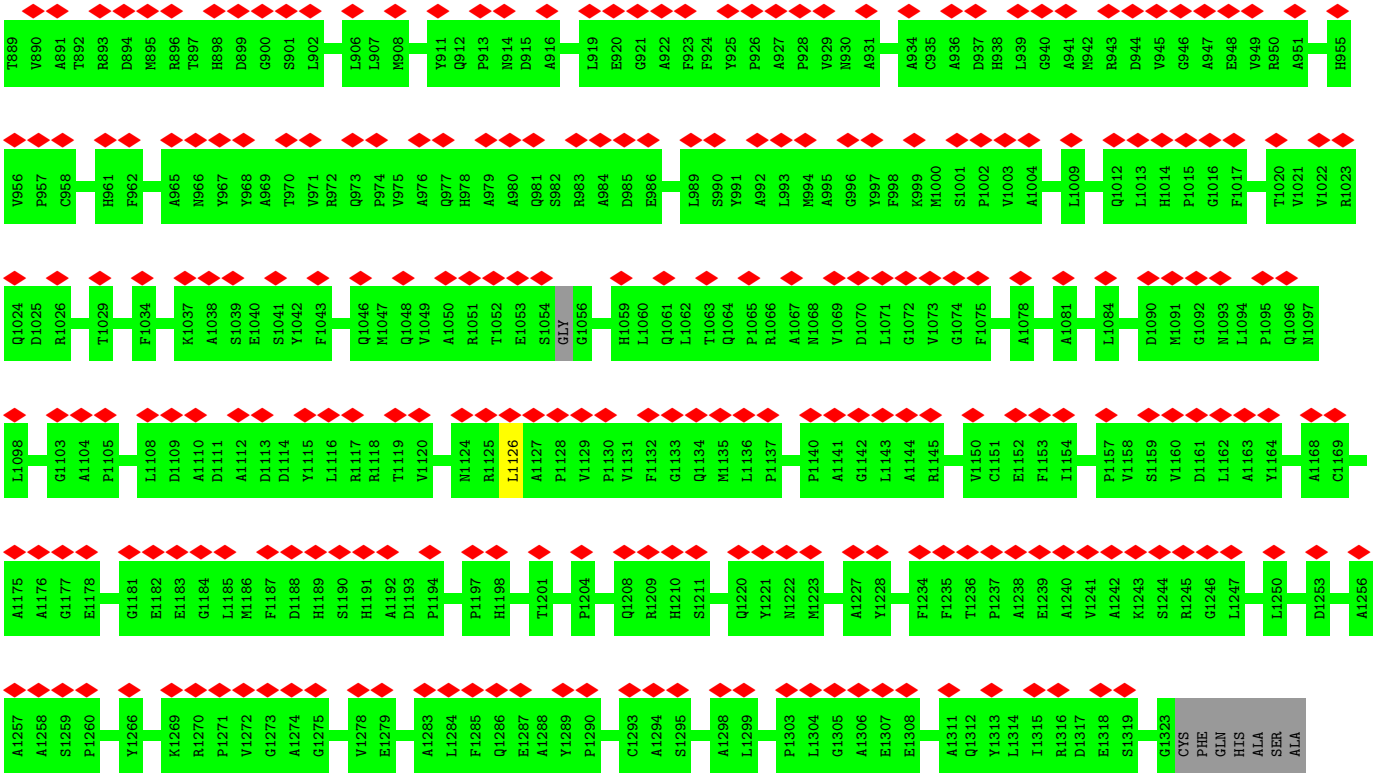






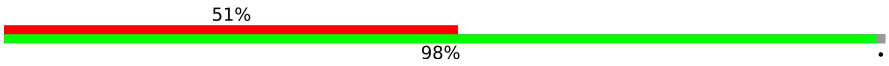


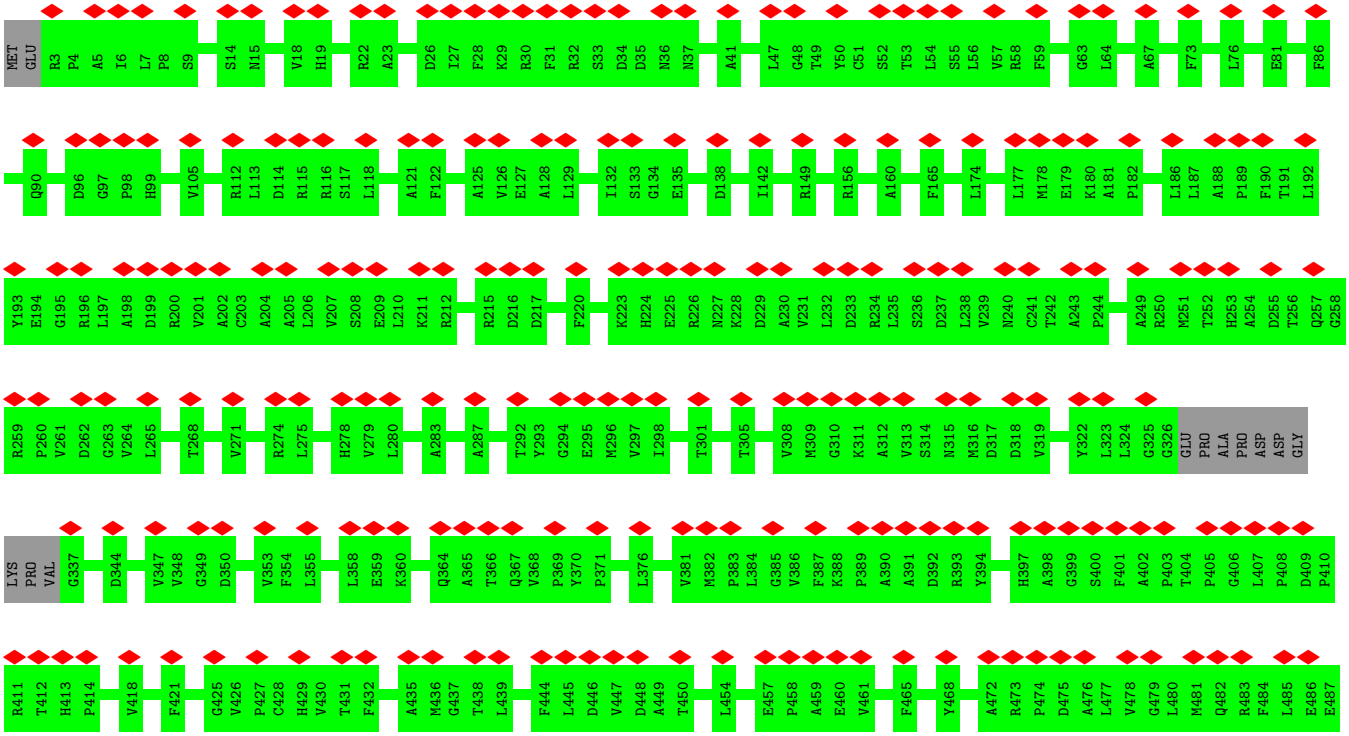


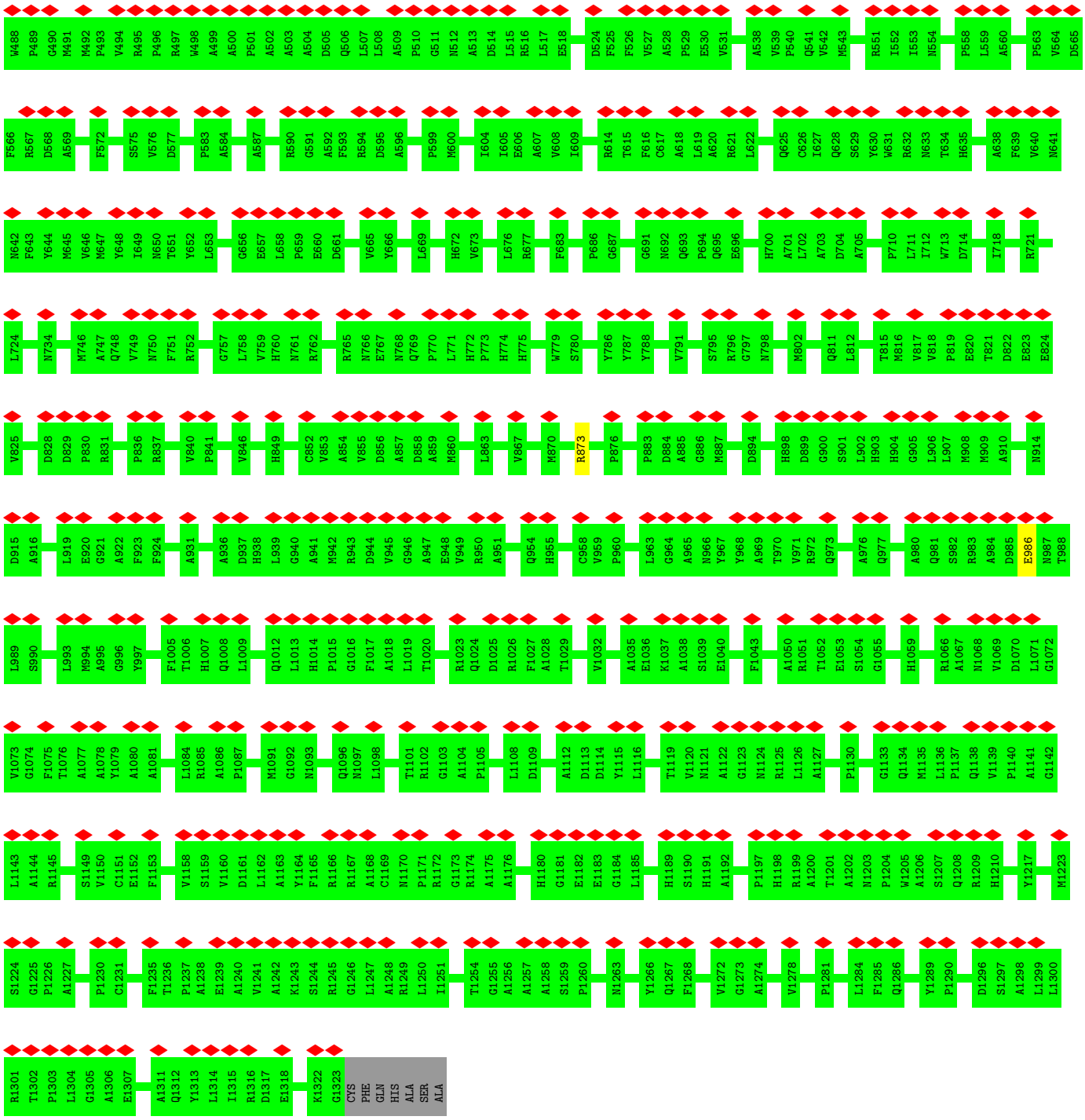


- Molecule 1: Major capsid protein

Chain l:

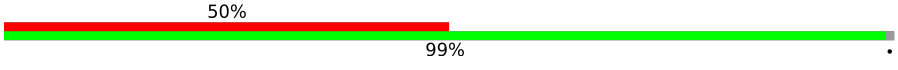


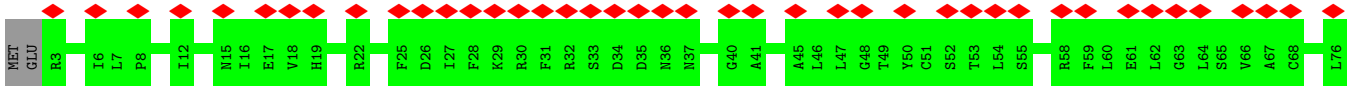


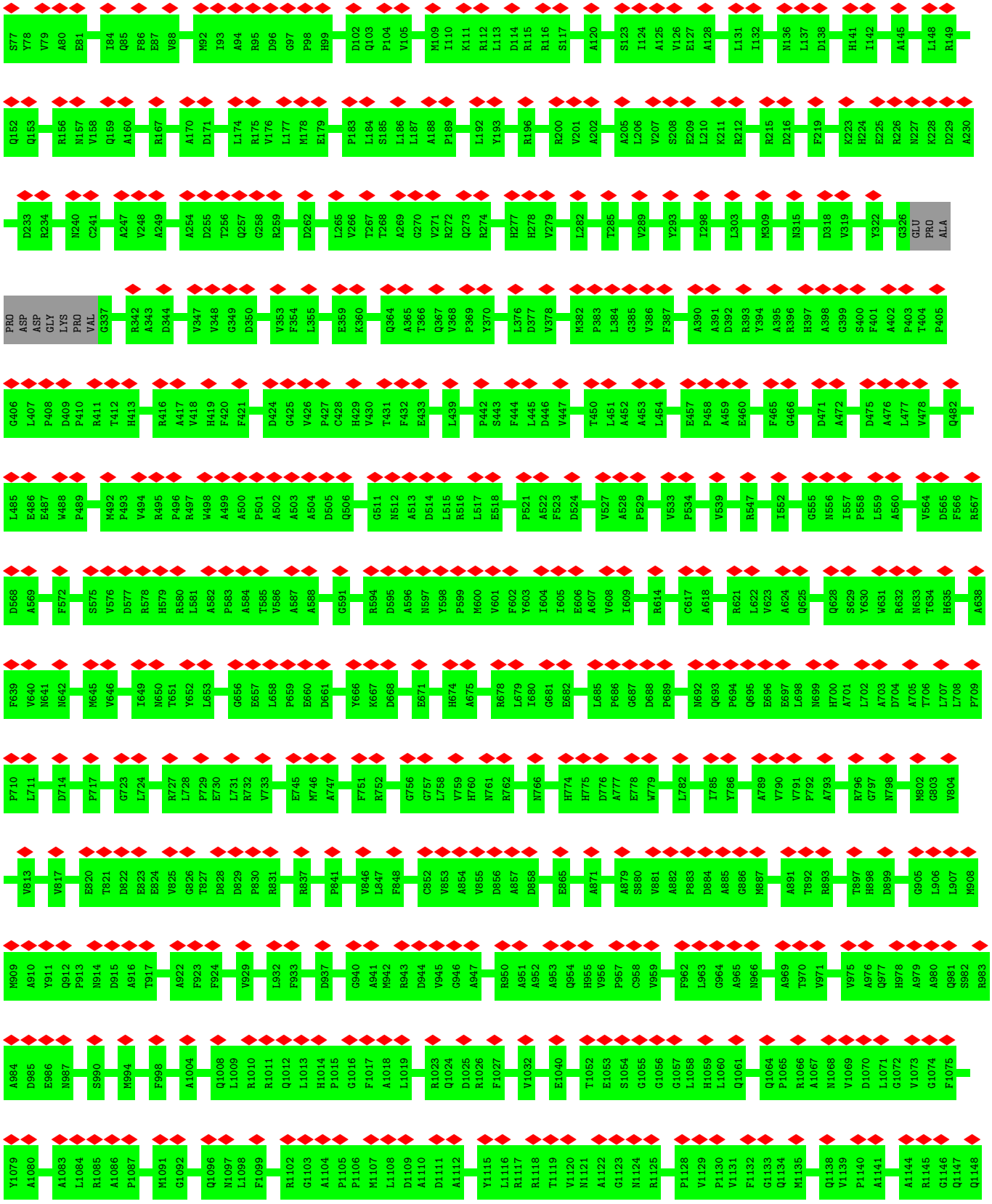


• Molecule 1: Major capsid protein

Chain m:



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D102 Q103 P104 V105
M109 I110 K111 R112 L113 D114 R115 R116 S117
A120
S123 I124 A125 V126 E127 A128
L131 I132
N136 L137 D138
H141 I142
A145
L148 R149
Q152 Q153
R156 N157 V158 Q159 A160
R167
A170 D171
L174 R175 V176 L177 M178 E179
P183 L184 S185 L186 L187 A188 P189
L192 Y193
R196
R200 V201 A202
A205 L206 V207 S208 E209 L210 K211 R212
R215 D216
F219
K223 H224 E225 R226 N227 K228 D229 A230
D233 R234
N240 C241
A247 V248 A249
A254 D255 T256 Q257 G258 R259
D262
L265 V266 T267 T268 A269 G270 V271 R272 Q273 R274
H277 H278 V279
L282
T285
V289
Y293
I298
L303
M309
N315
D318 V319
Y322
G326 GLU PRO ALA
PRO ASP ASP GLY LYS PRO VAL G337
R342 A343 D344
V347 V348 G349 D350
V353 F354 L355
E359 K360
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L376 D377 V378
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L439
P442 S443 F444 L445 D446 V447
T450 L451 A452 A453 L454
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F465 G466
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E865
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T897 H898 D899
G905 L906 L907 M908
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V929
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D937
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F962 L963 G964 A965 N966
A969 T970 V971
V975 A976 Q977 H978 A979 A980 Q981 S982 R983
A984 D985 E986 N987
S990
M994
F998
A1004
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V1032
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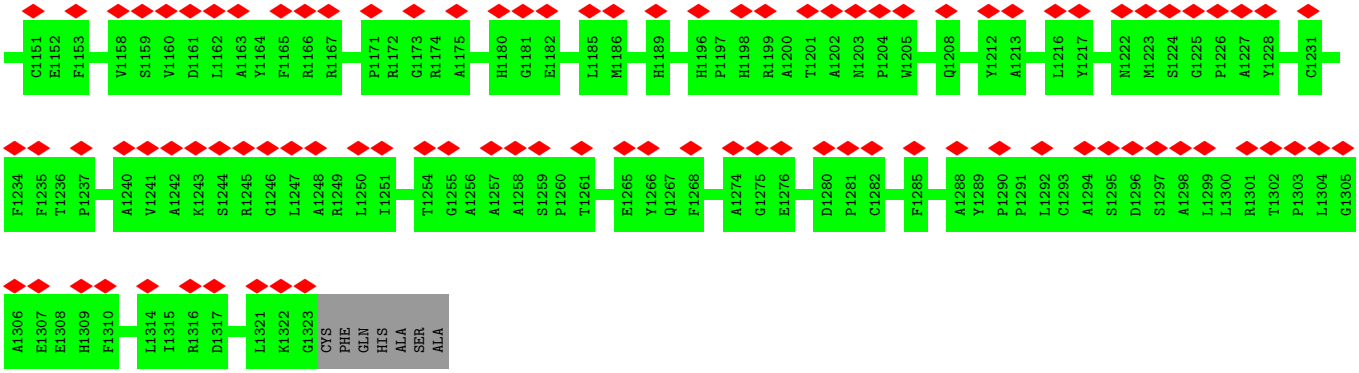
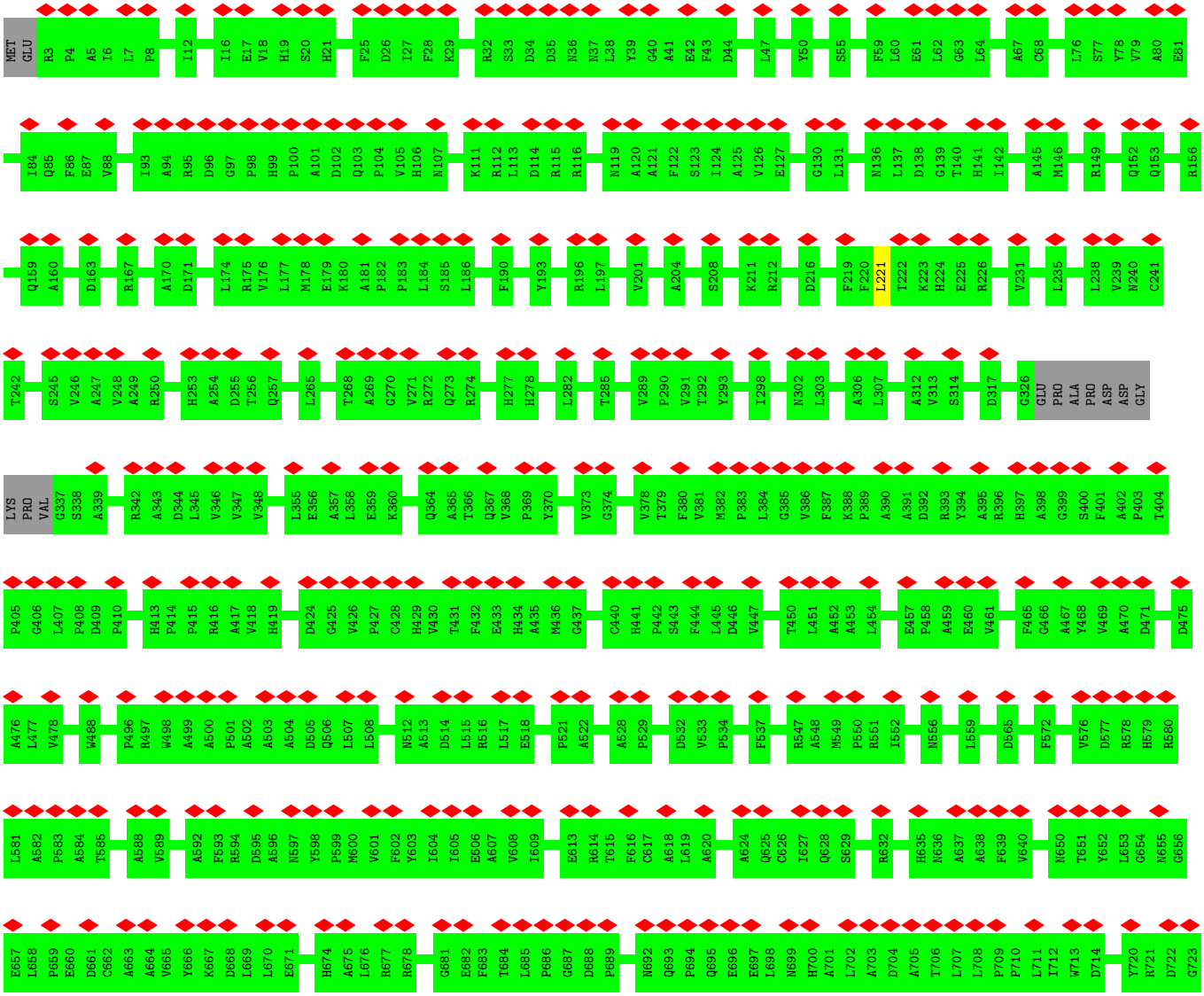
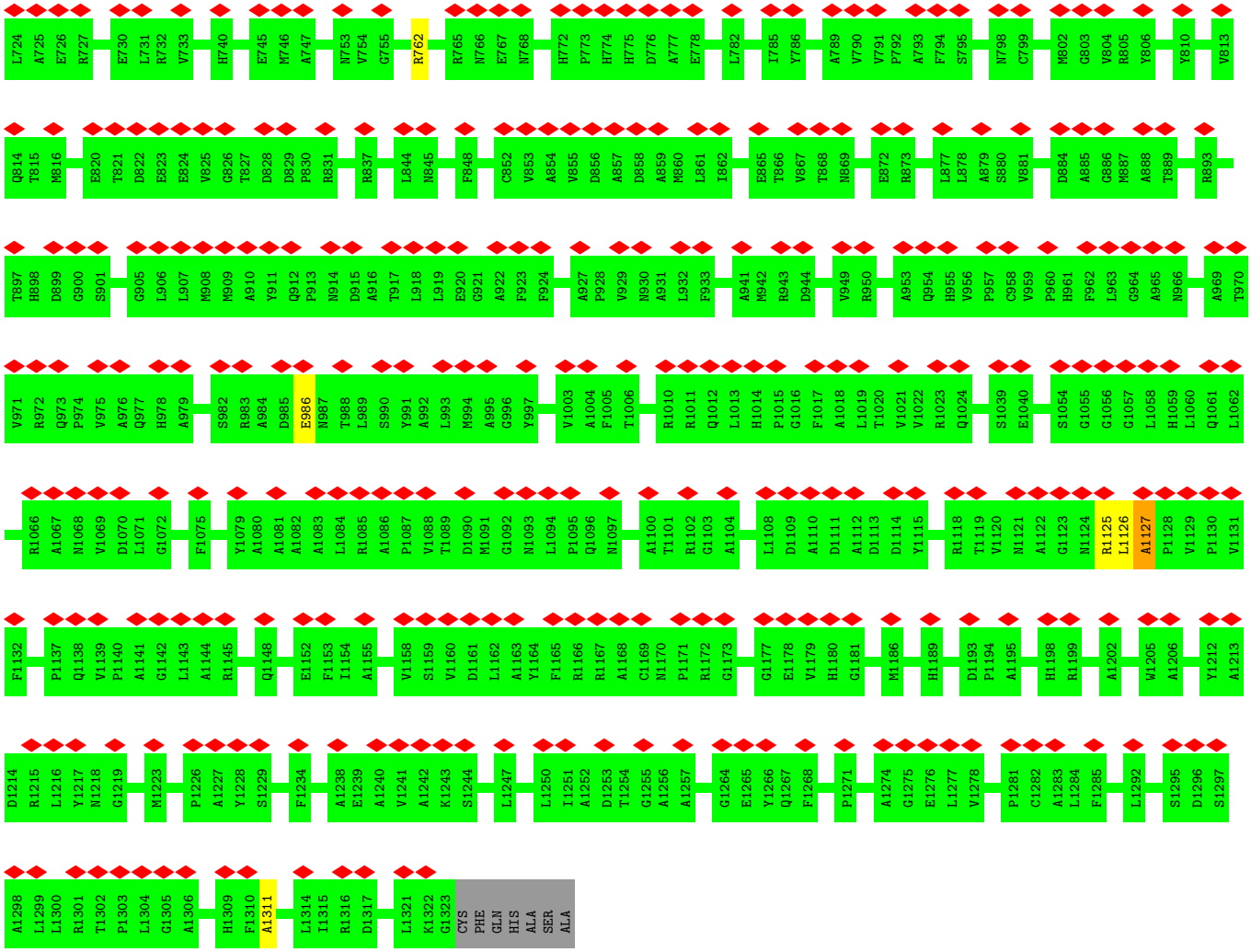


• Molecule 1: Major capsid protein





• Molecule 1: Major capsid protein

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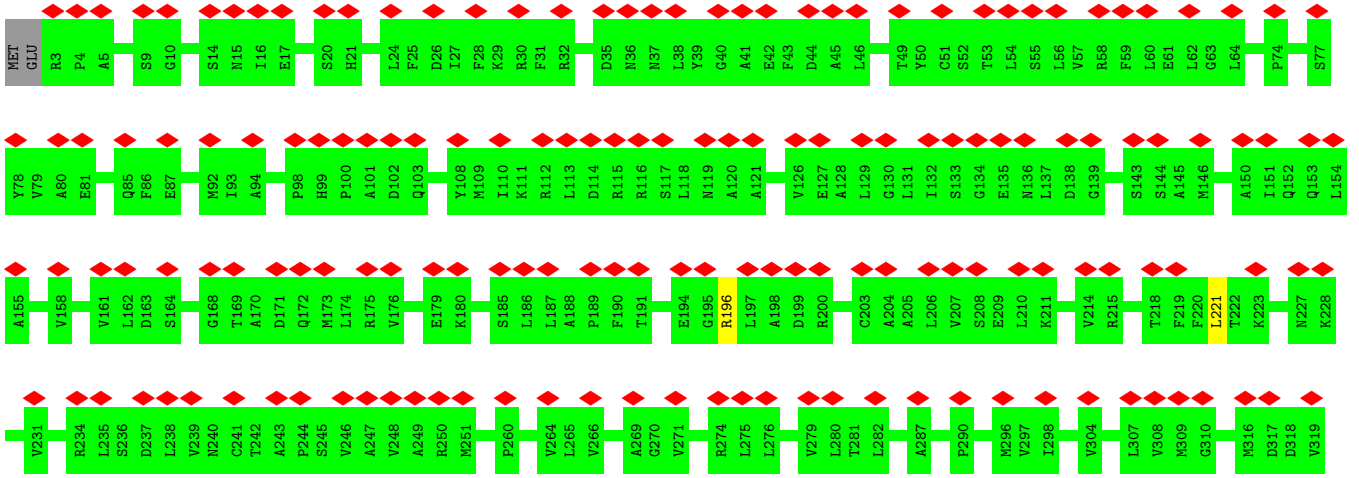
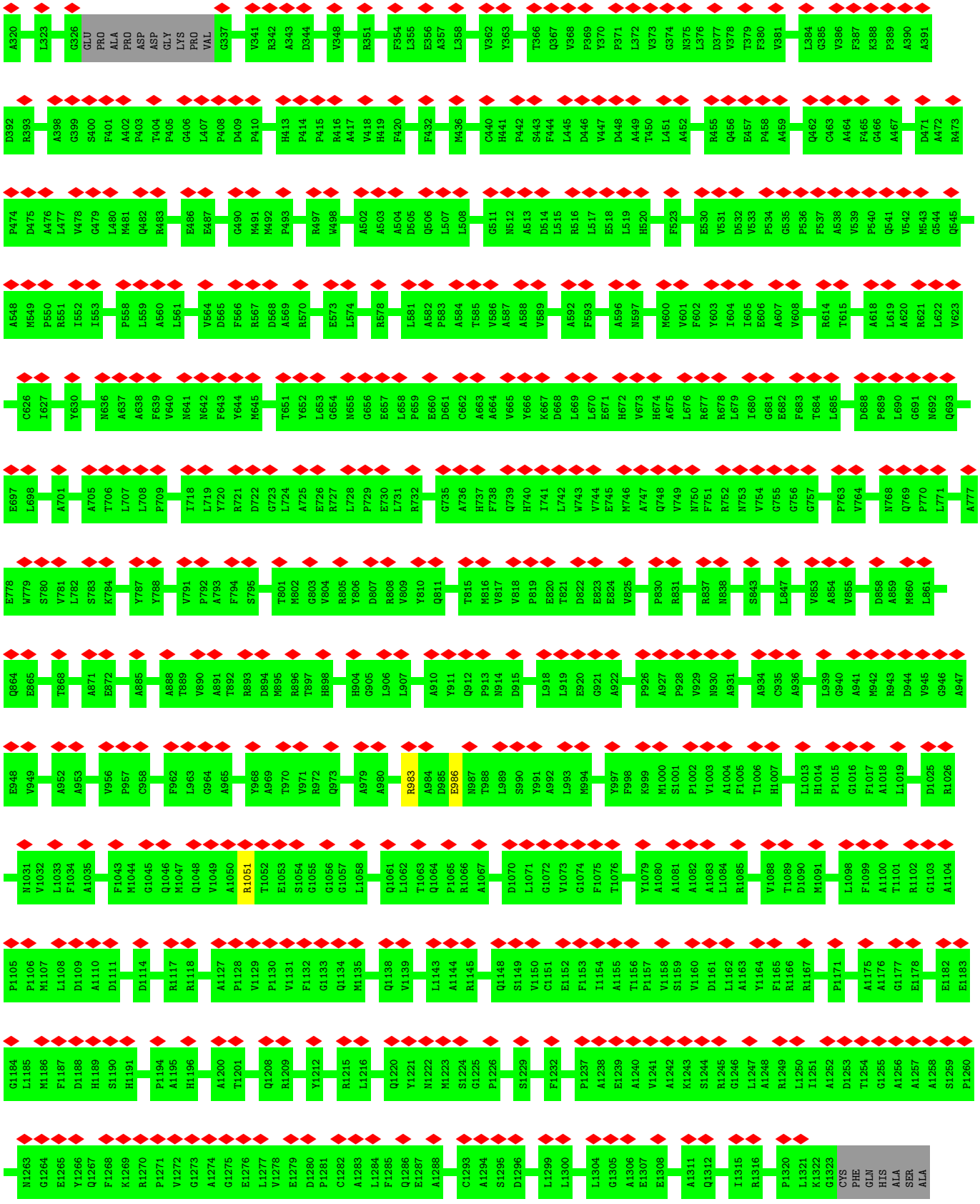
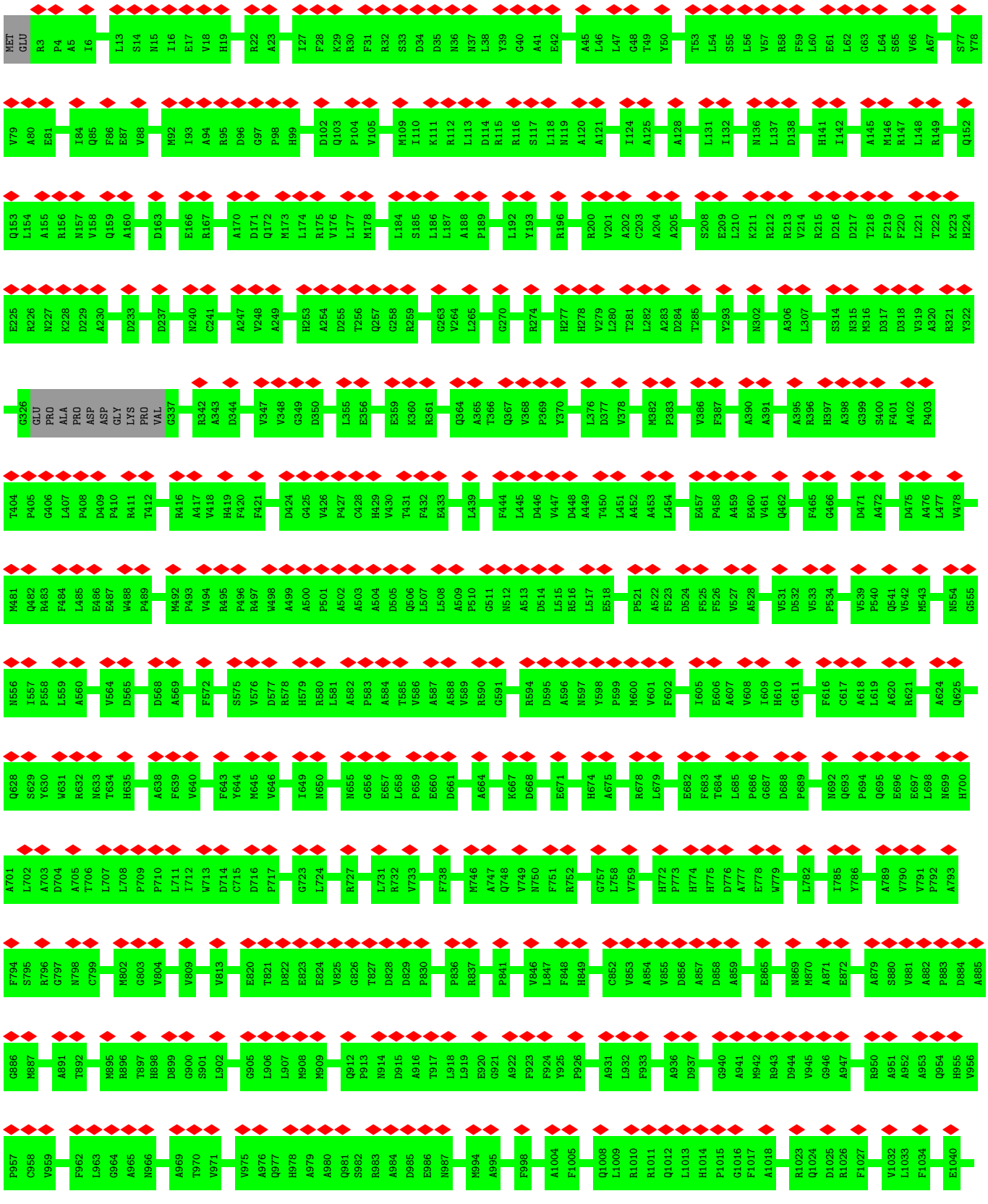




- Molecule 1: Major capsid protein

Chain q:

52%
99%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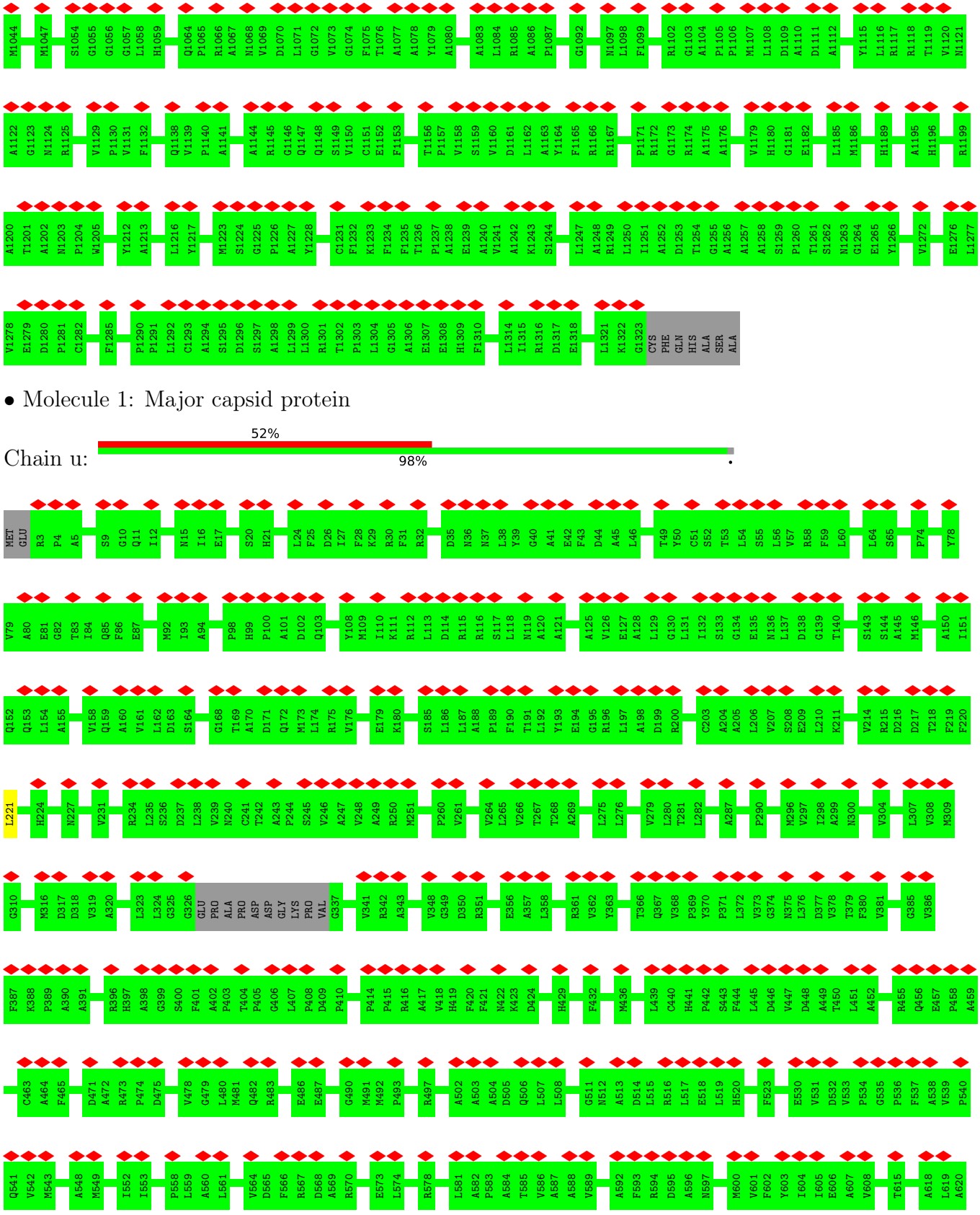

• Molecule 1: Major capsid protein

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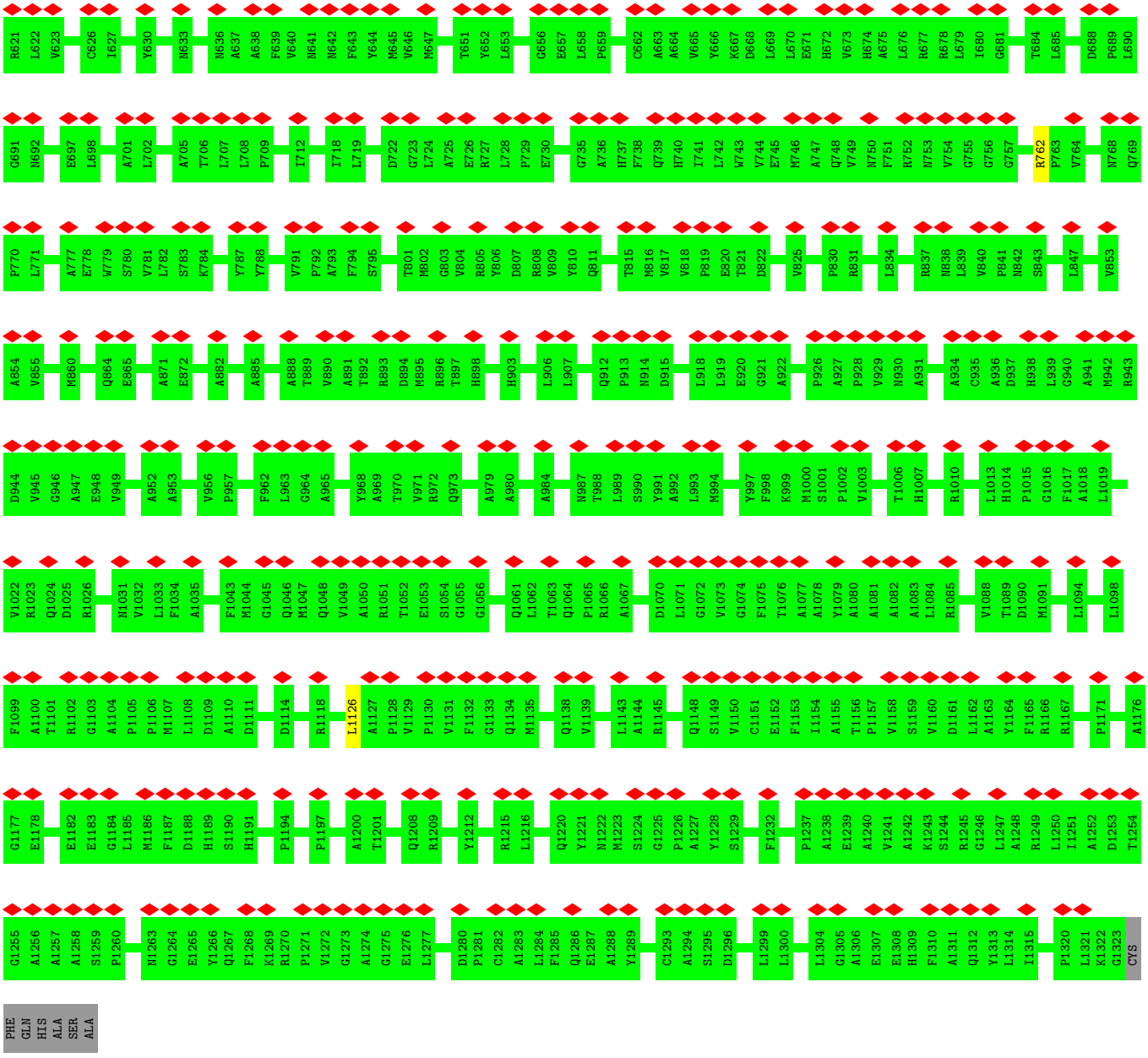

• Molecule 1: Major capsid protein

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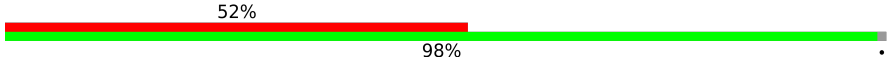

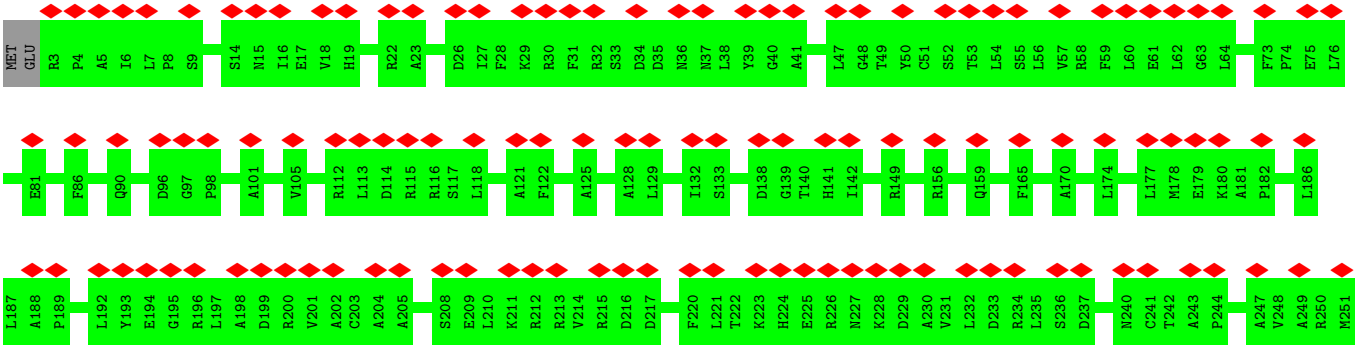

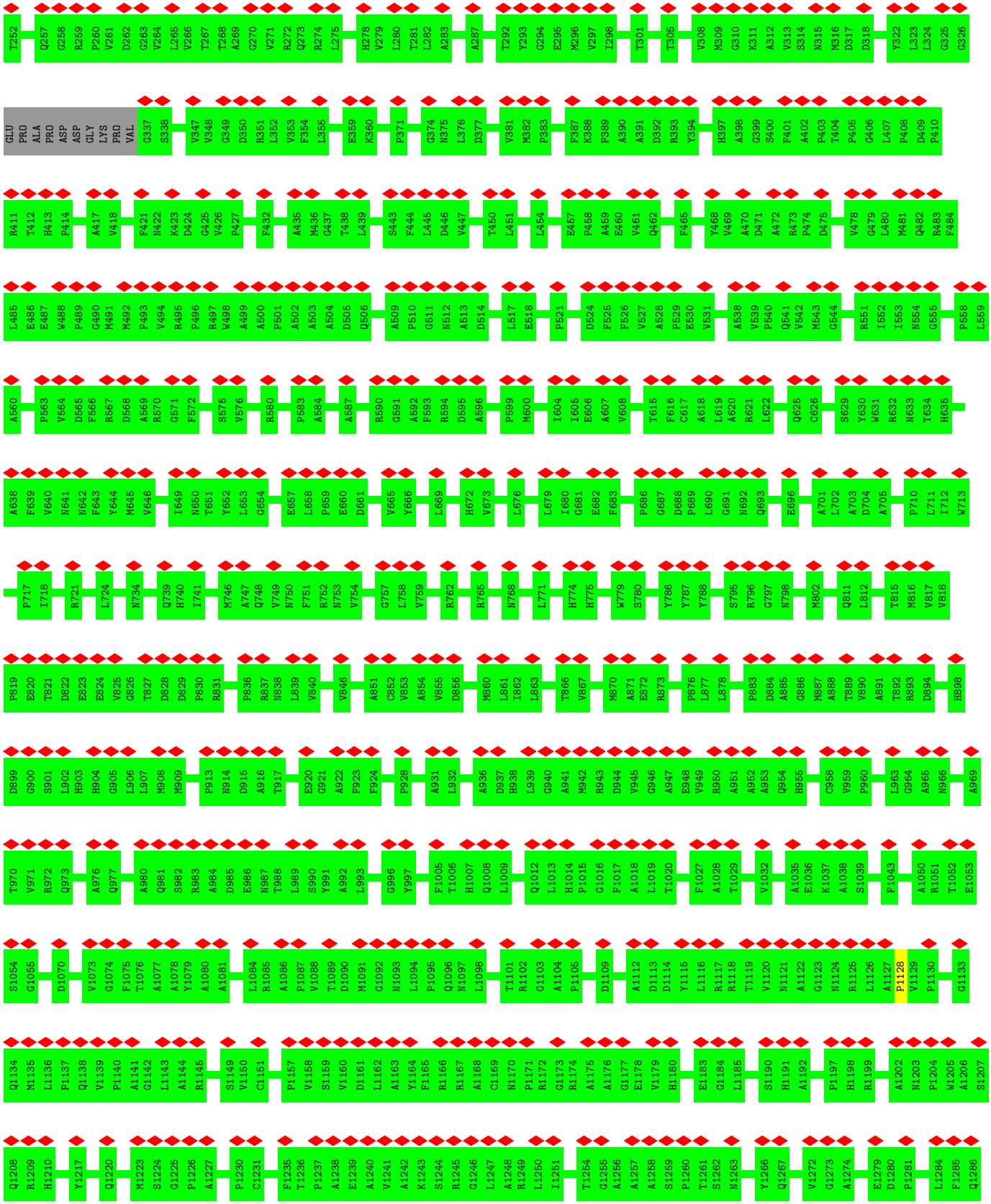
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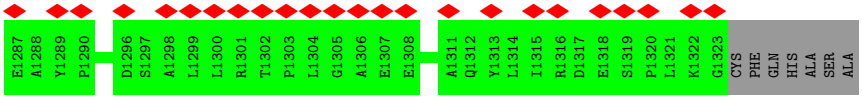
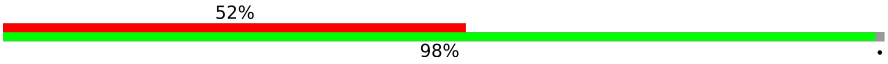
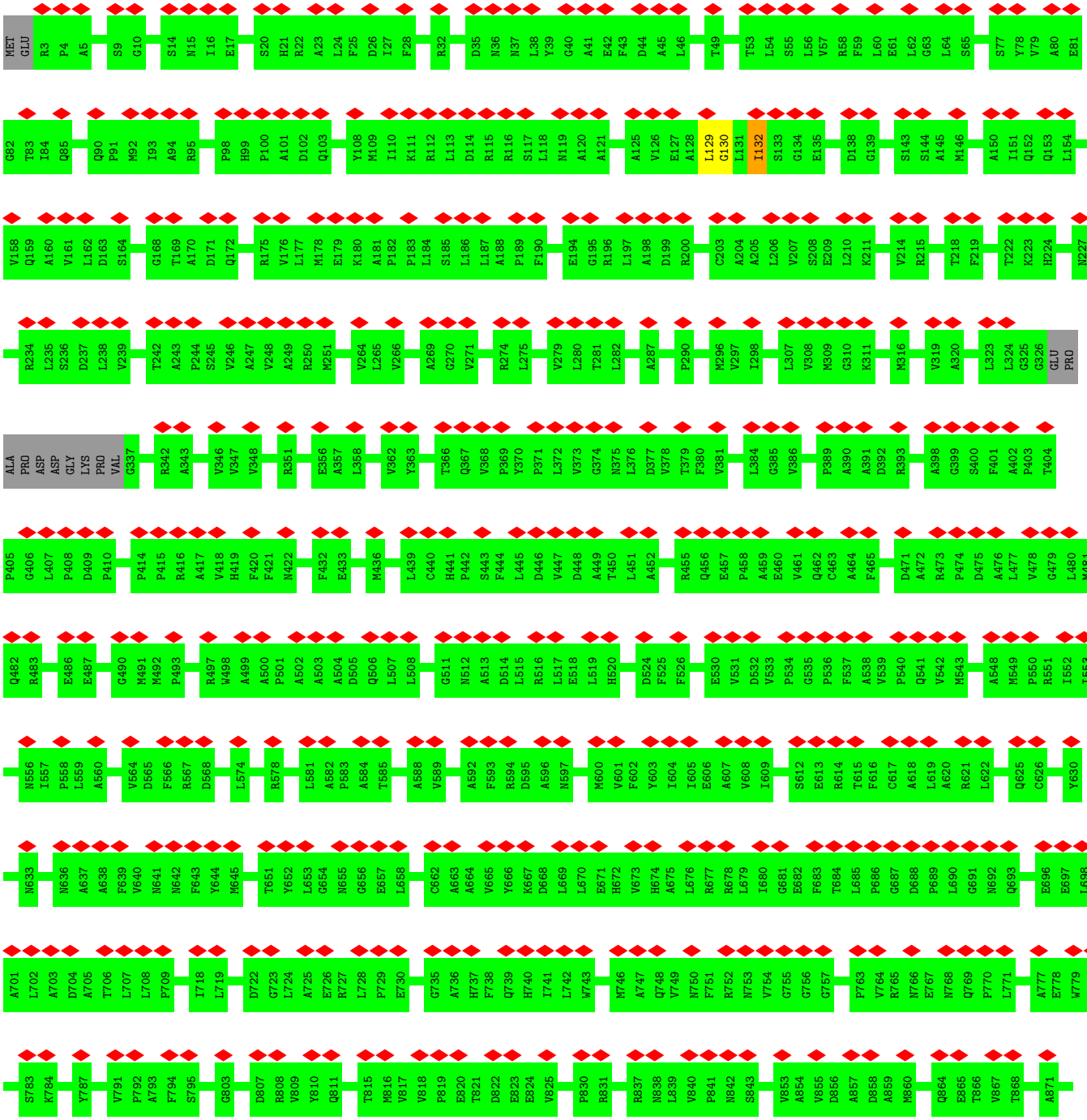
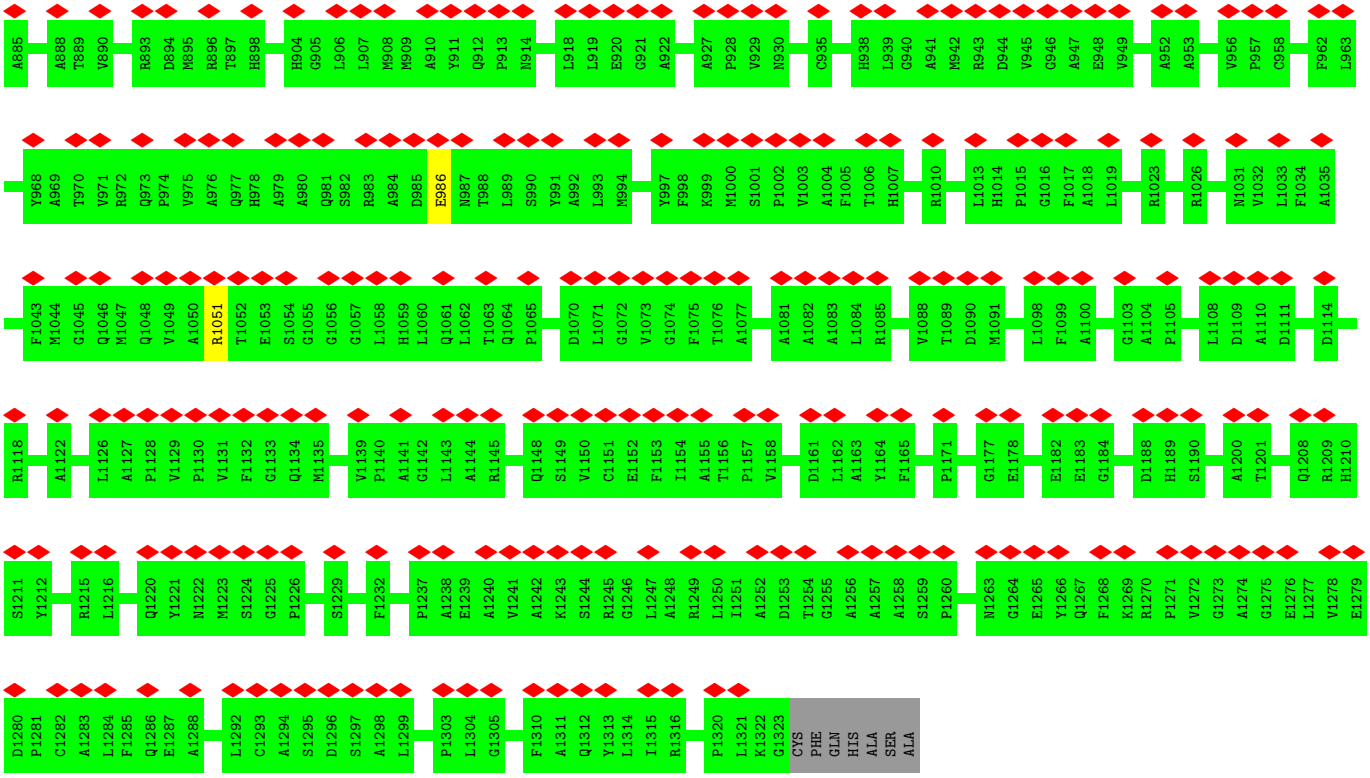


• Molecule 1: Major capsid protein

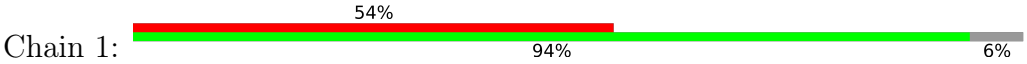
Chain y:

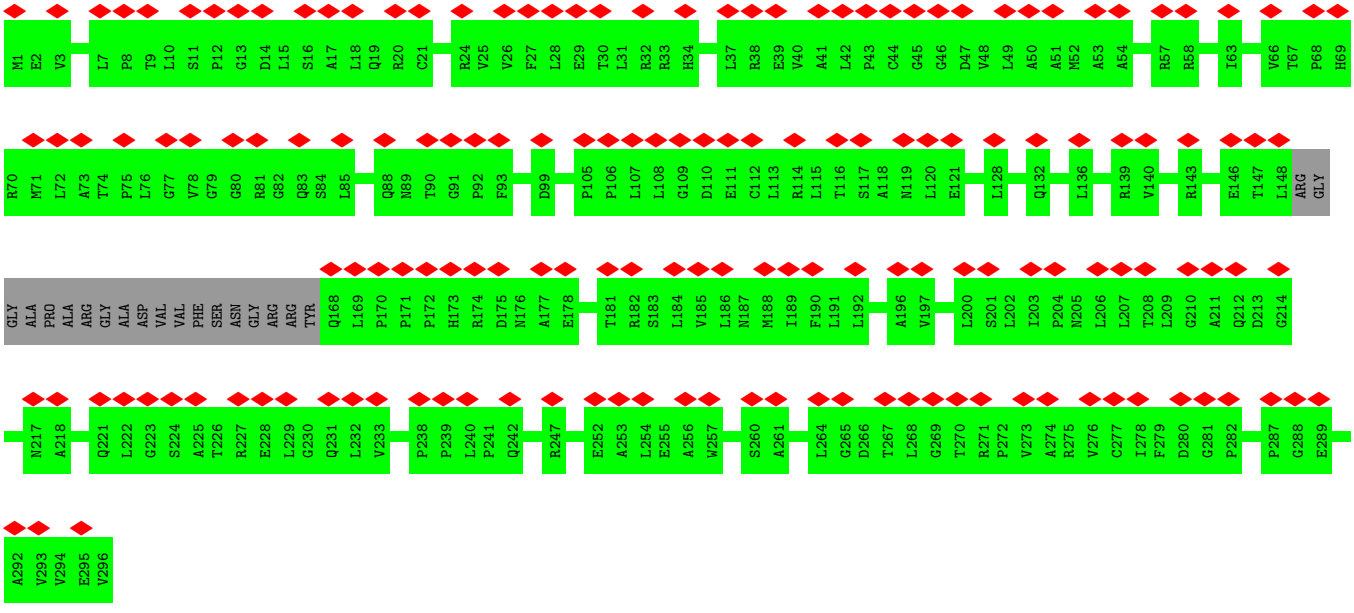




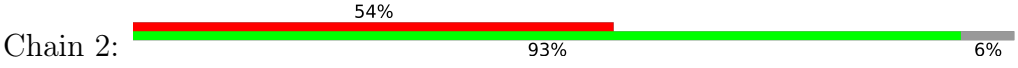


• Molecule 2: Triplex capsid protein 2





• Molecule 2: Triplex capsid protein 2



• Molecule 2: Triplex capsid protein 2

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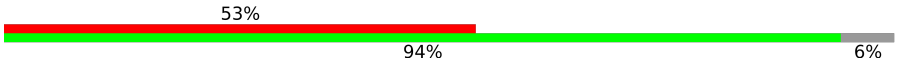

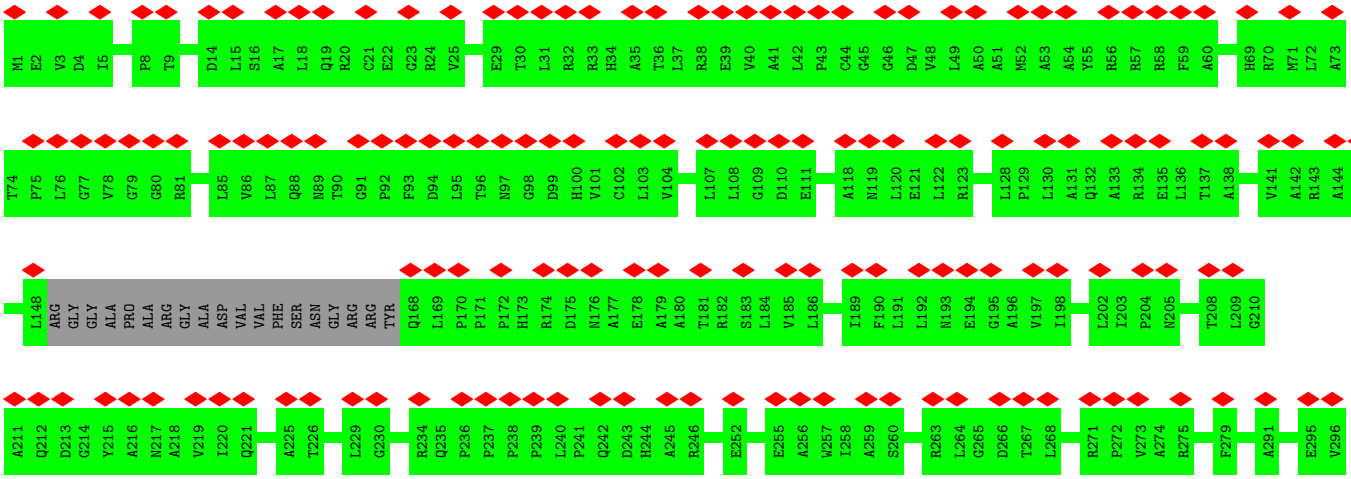

• Molecule 2: Triplex capsid protein 2

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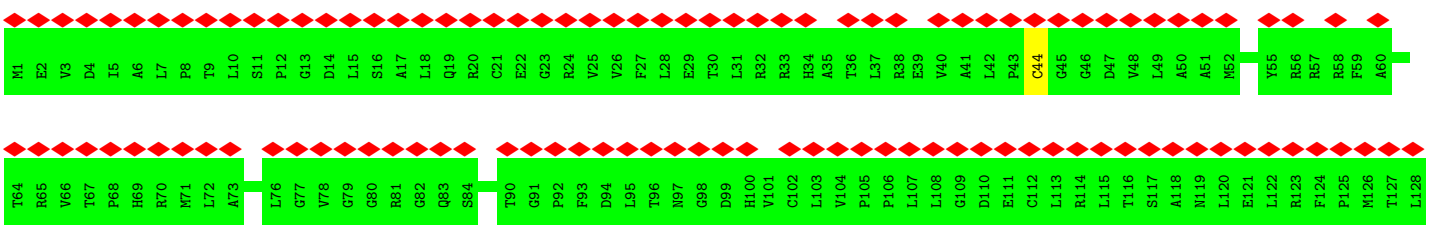
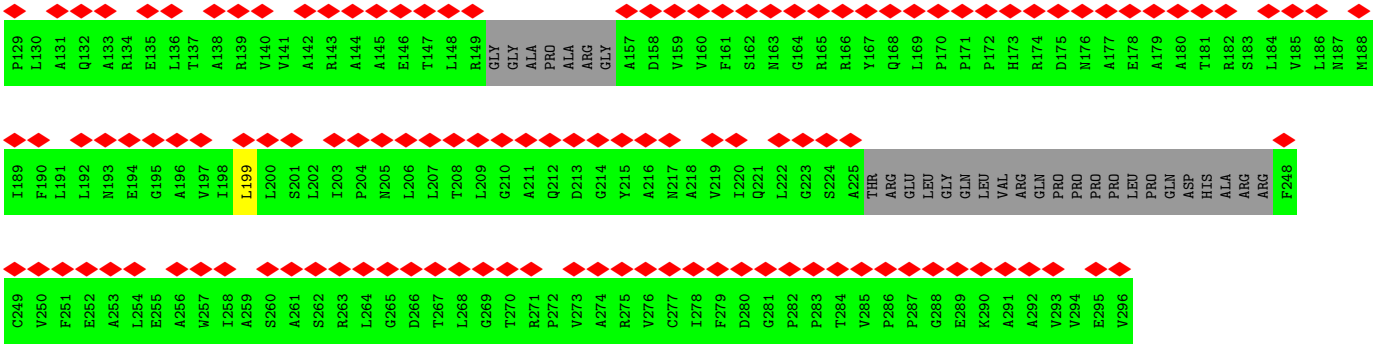
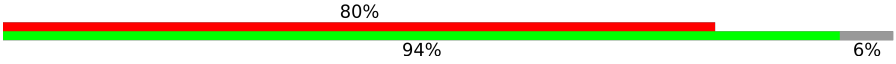
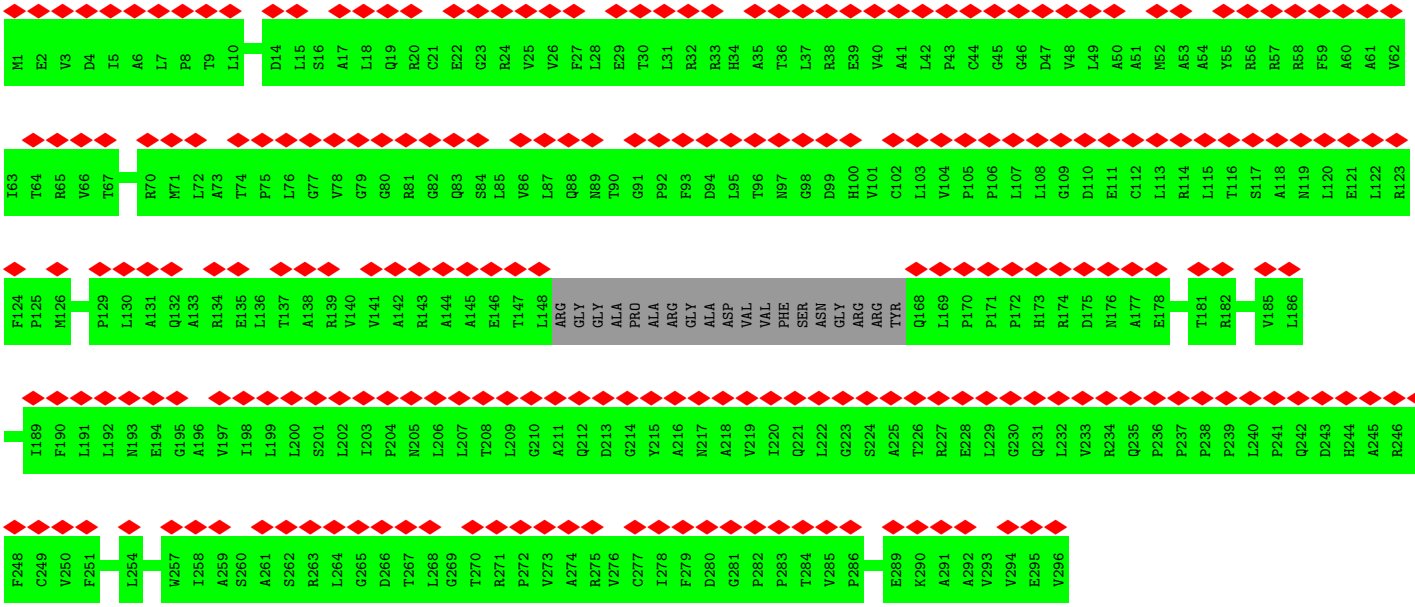




• Molecule 2: Triplex capsid protein 2

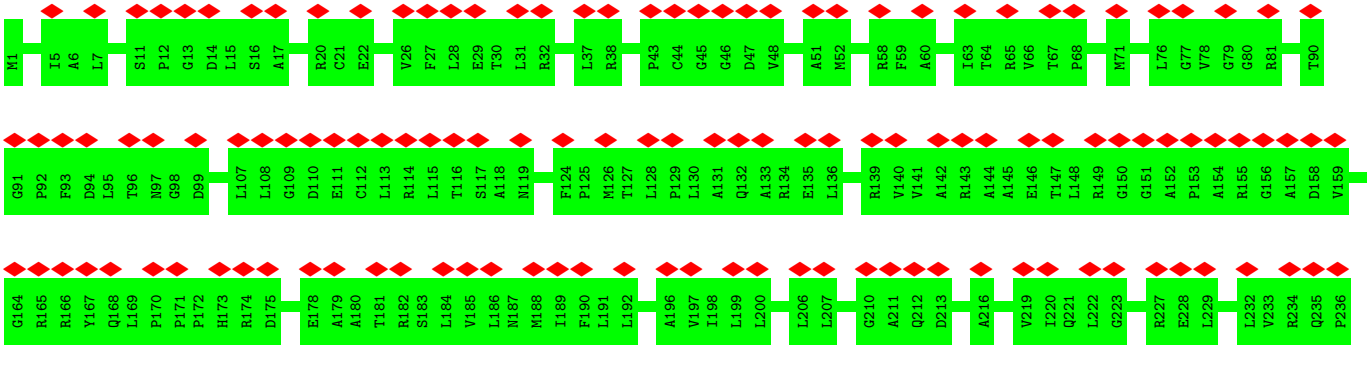
Chain k:

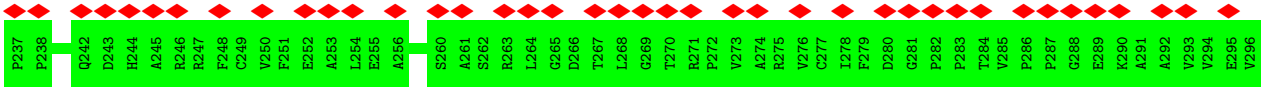




• Molecule 2: Triplex capsid protein 2

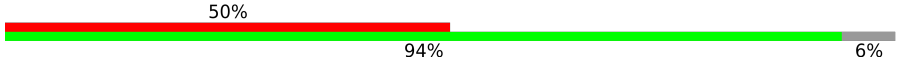
Chain o:

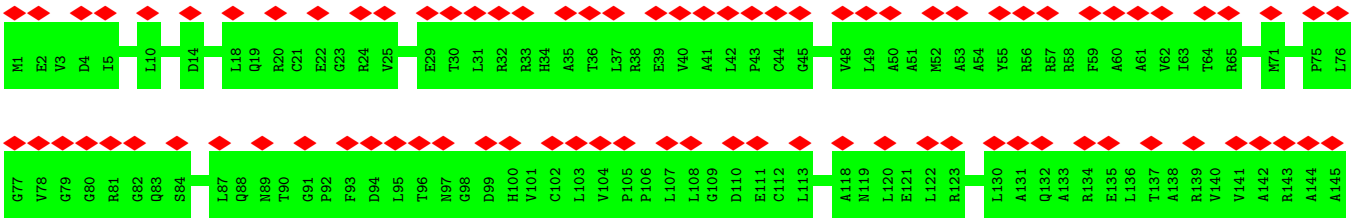




• Molecule 2: Triplex capsid protein 2

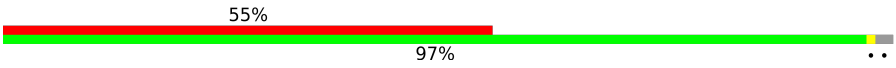
Chain s:

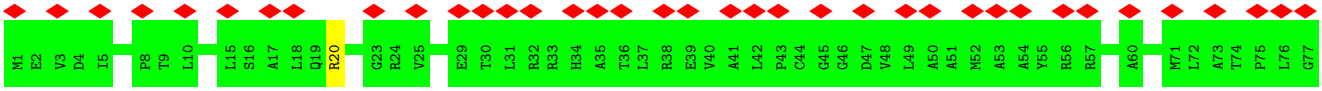




• Molecule 2: Triplex capsid protein 2

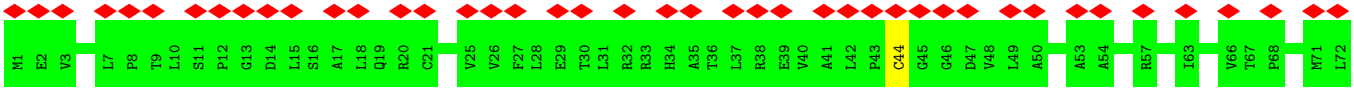
Chain v:

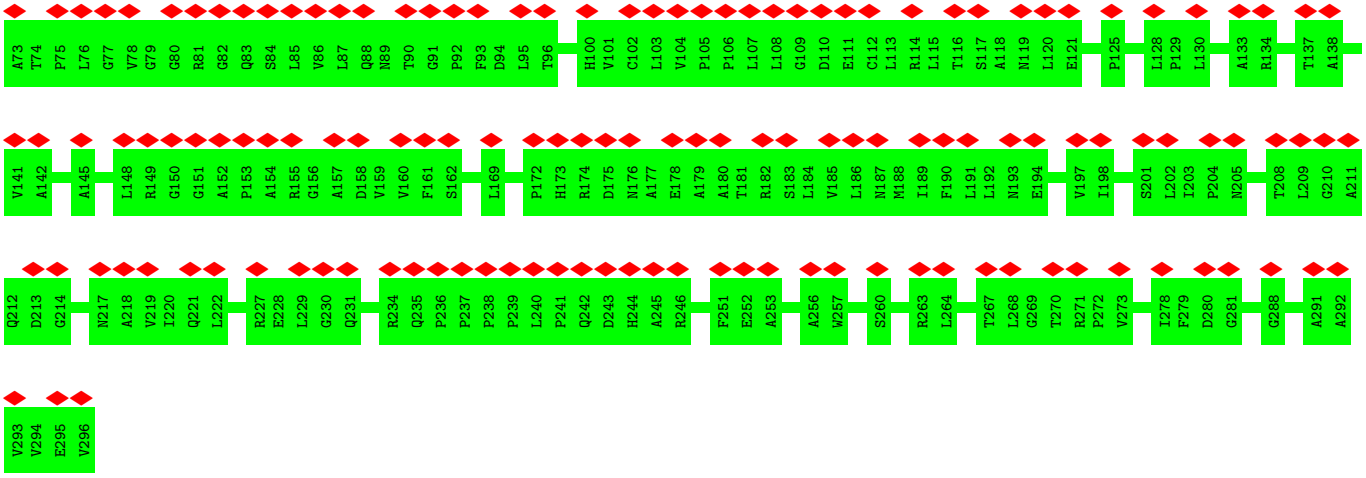




• Molecule 2: Triplex capsid protein 2

Chain x:



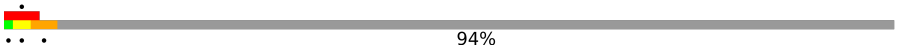


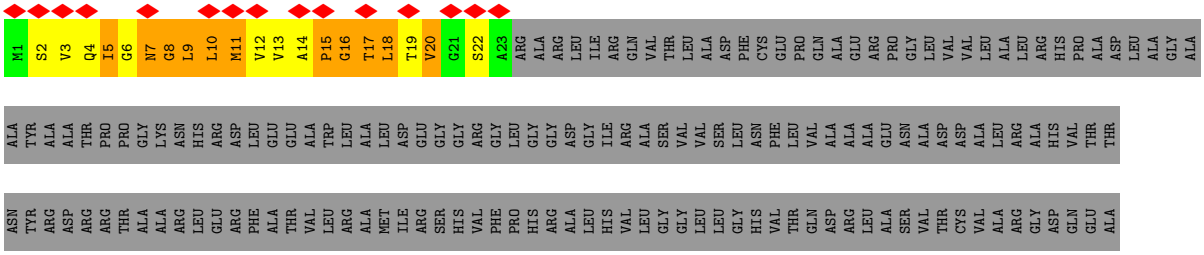
• Molecule 2: Triplex capsid protein 2

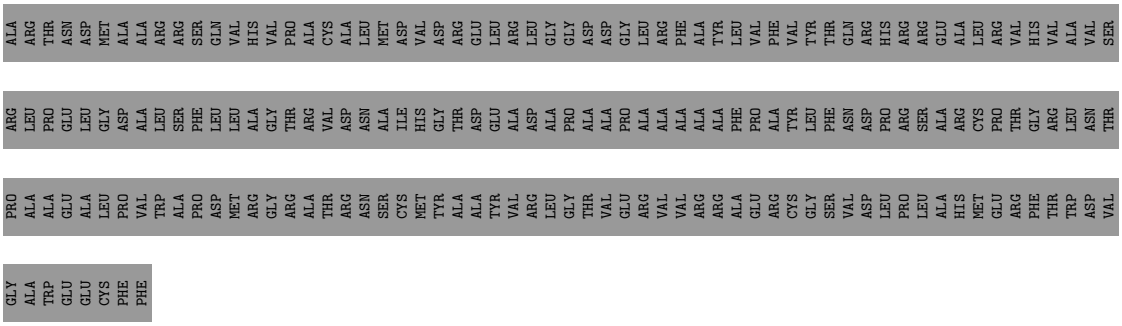
Chain z:

• Molecule 3: Triplex capsid protein 1

Chain B:

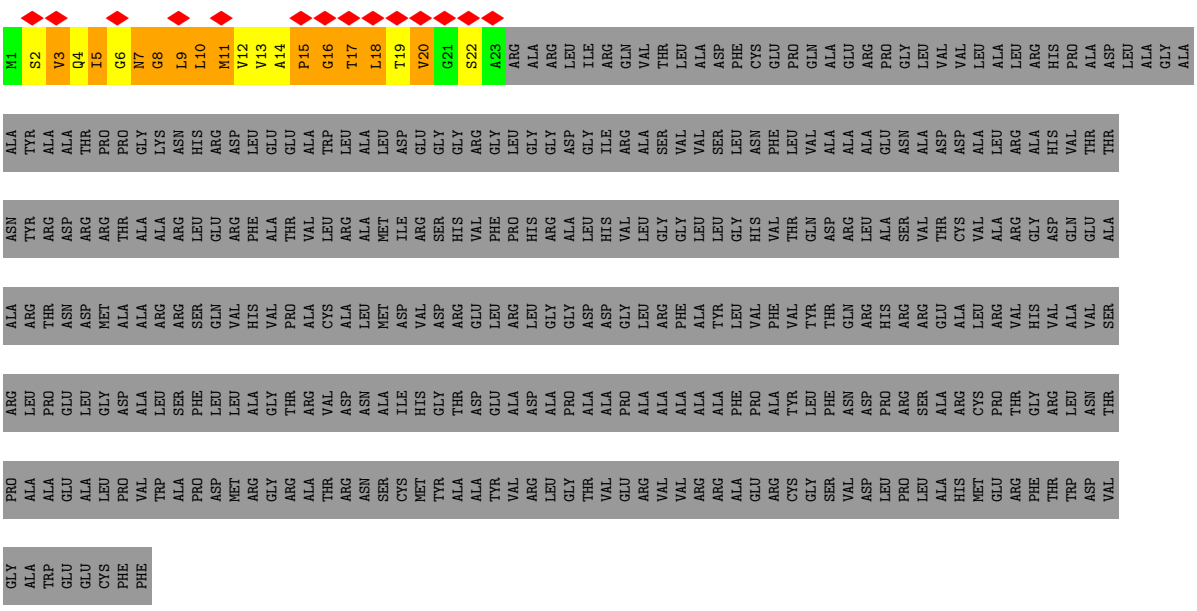






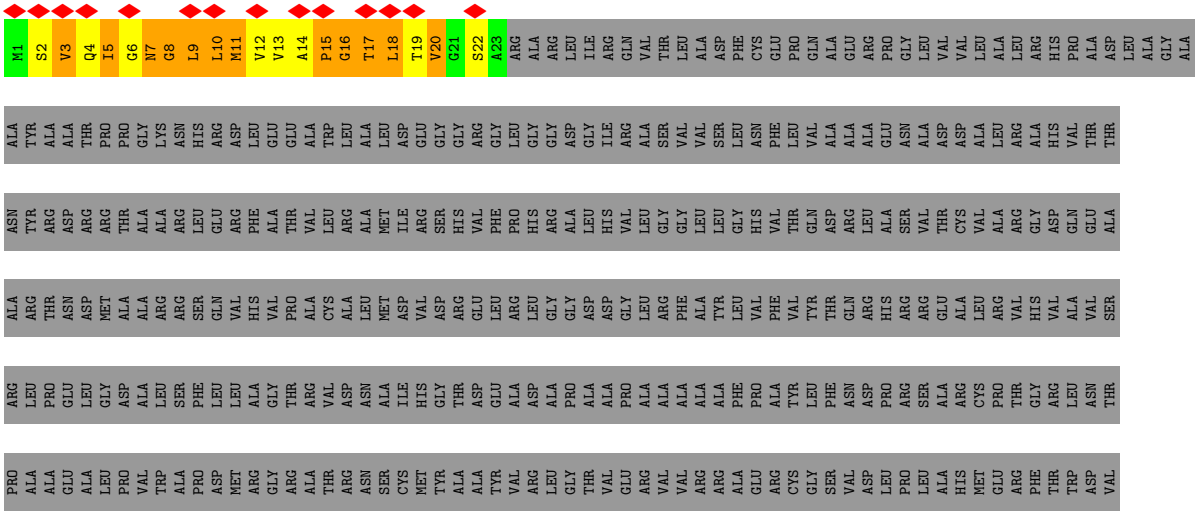
• Molecule 3: Triplex capsid protein 1

Chain C: 94%



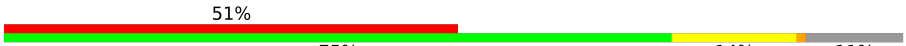
• Molecule 3: Triplex capsid protein 1

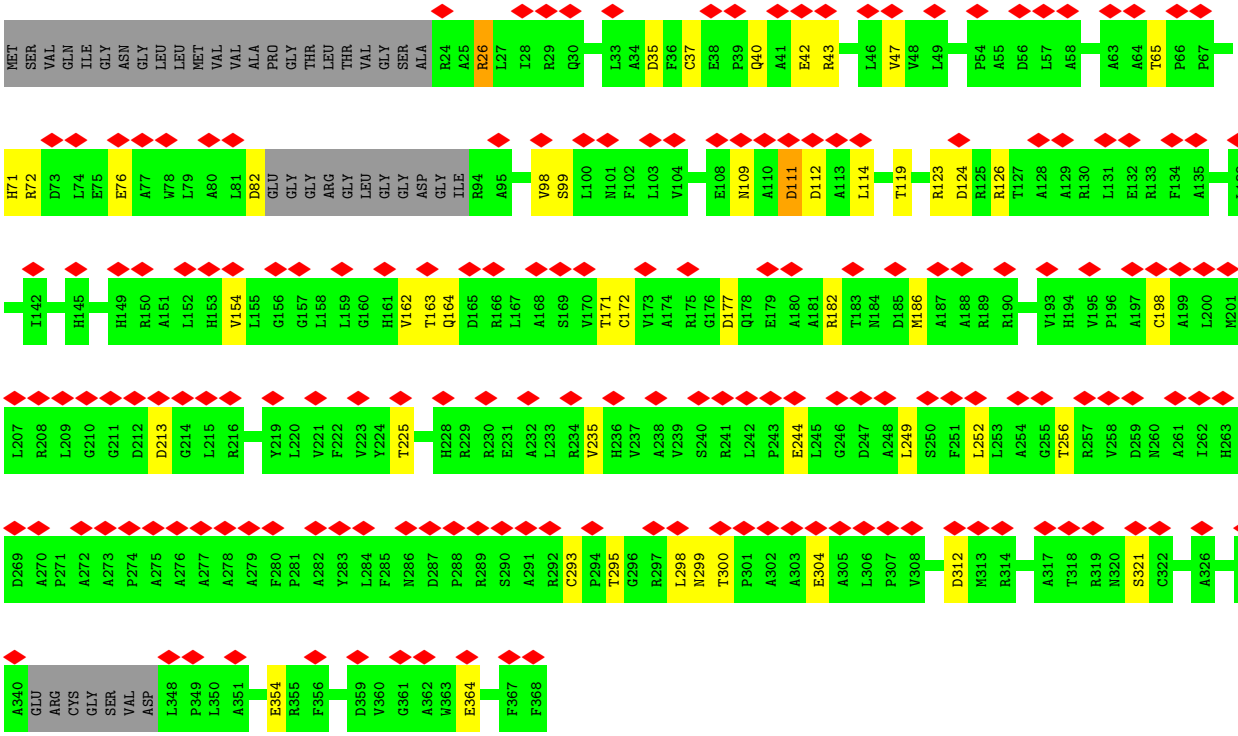
Chain D: 94%



• Molecule 3: Triplex capsid protein 1

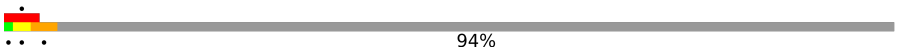
Chain T:

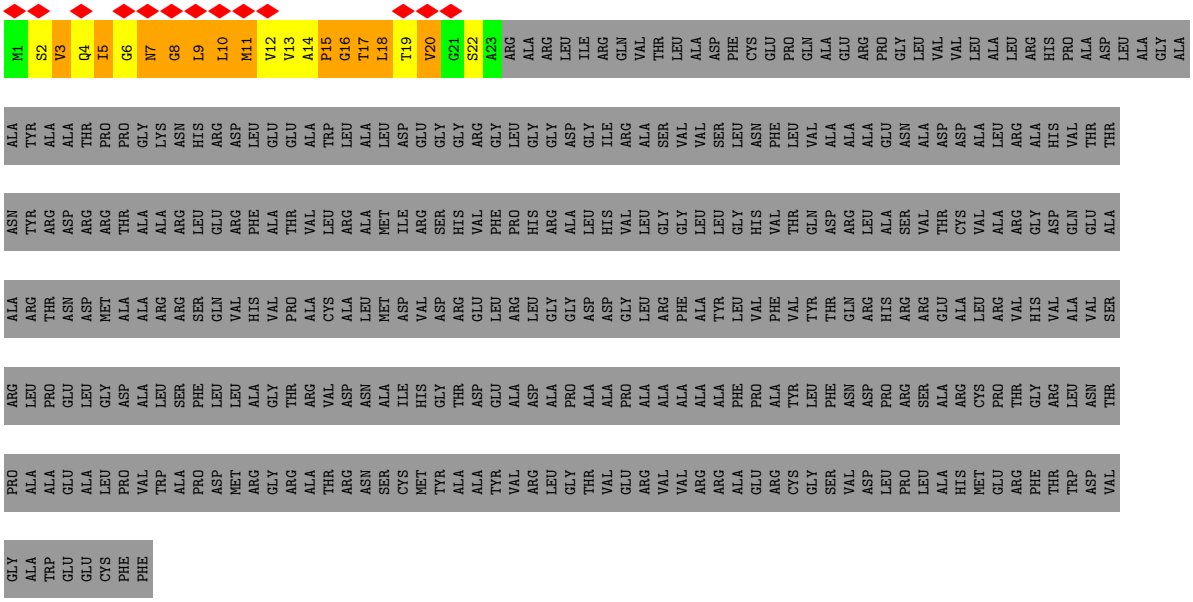




• Molecule 3: Triplex capsid protein 1

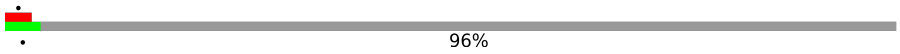
Chain W:

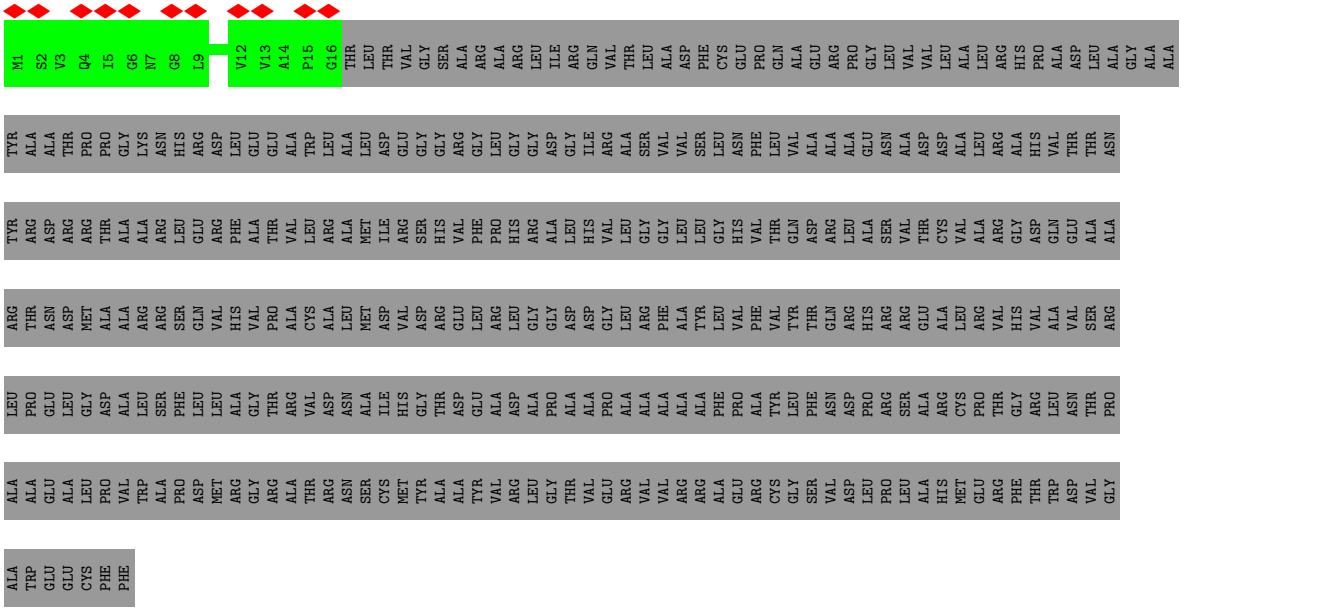




• Molecule 3: Triplex capsid protein 1

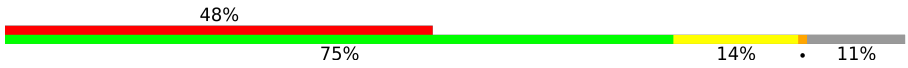
Chain d:

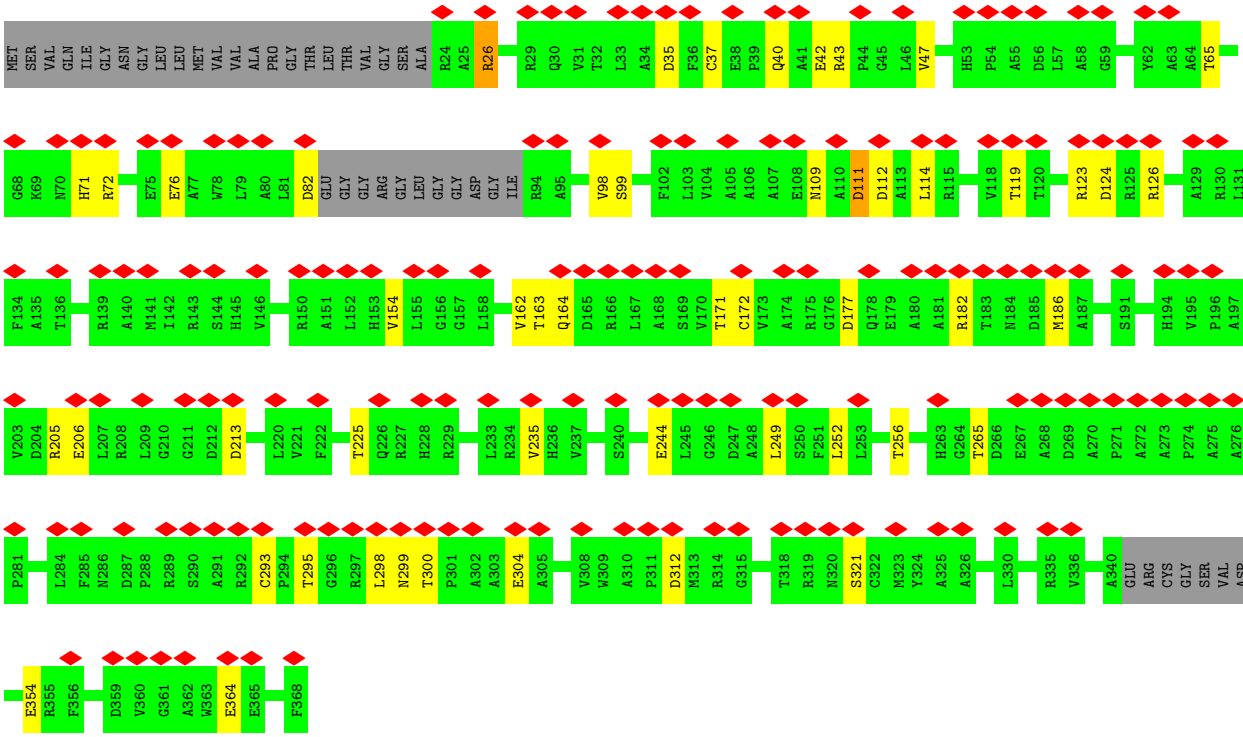




• Molecule 3: Triplex capsid protein 1

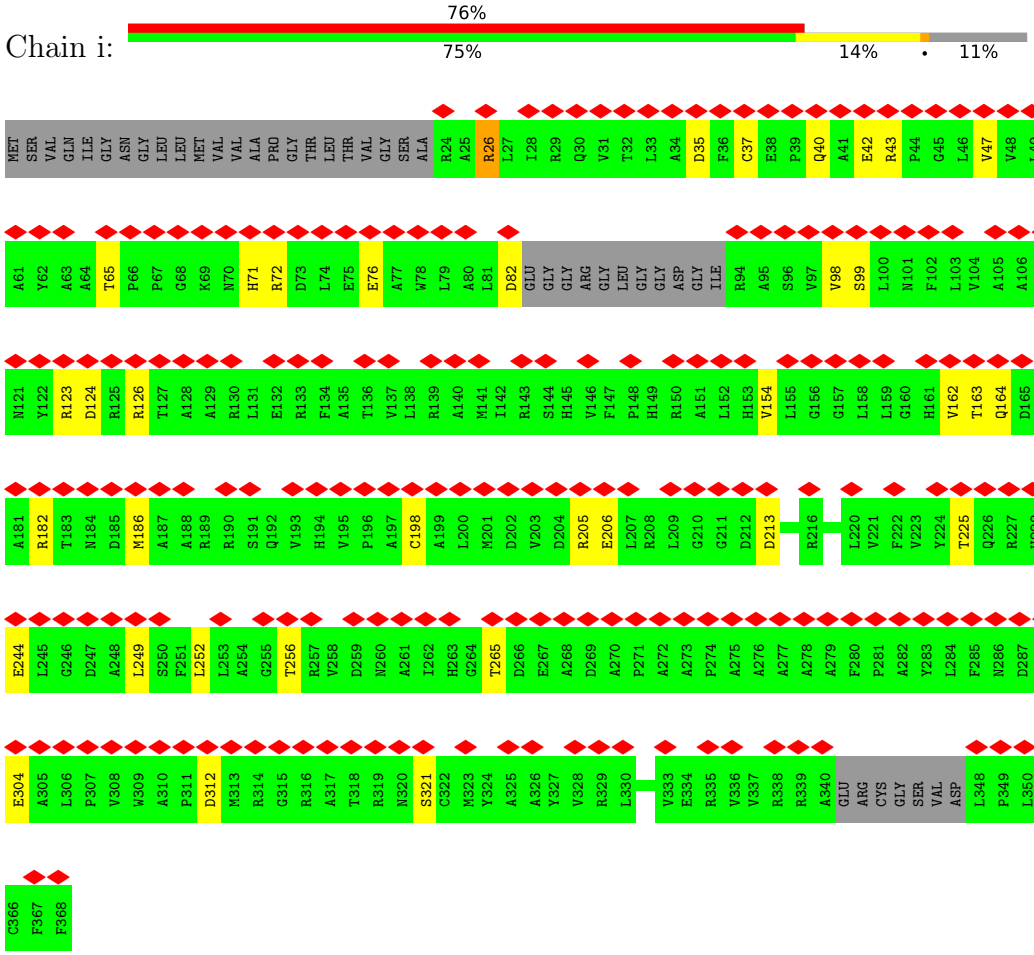
Chain h:





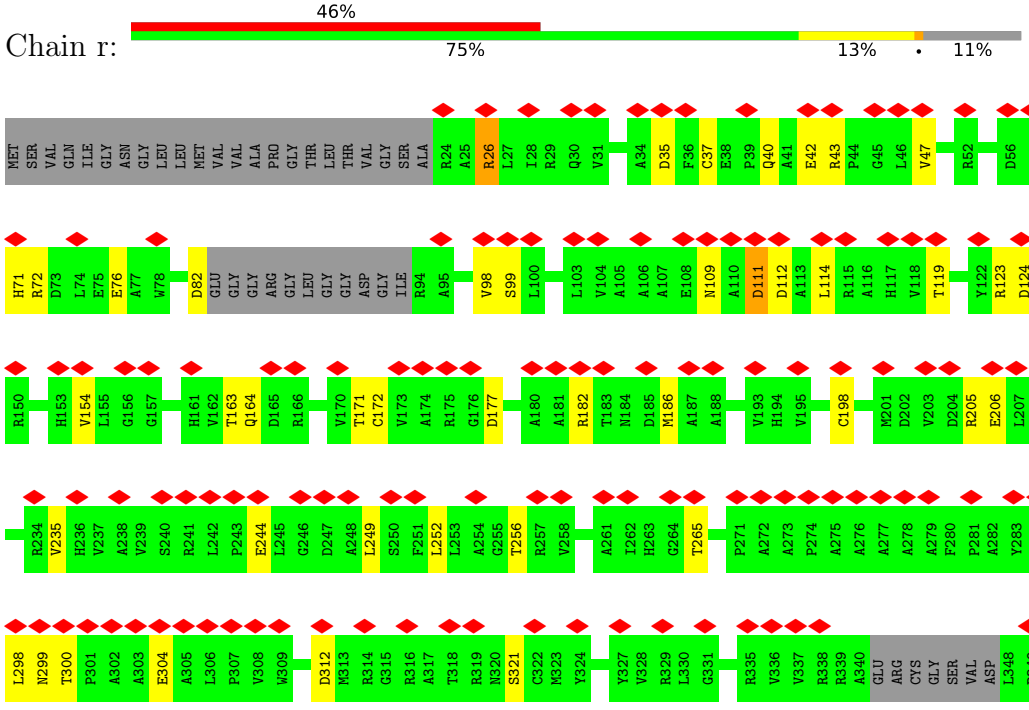
• Molecule 3: Triplex capsid protein 1

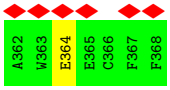
Chain i:



• Molecule 3: Triplex capsid protein 1

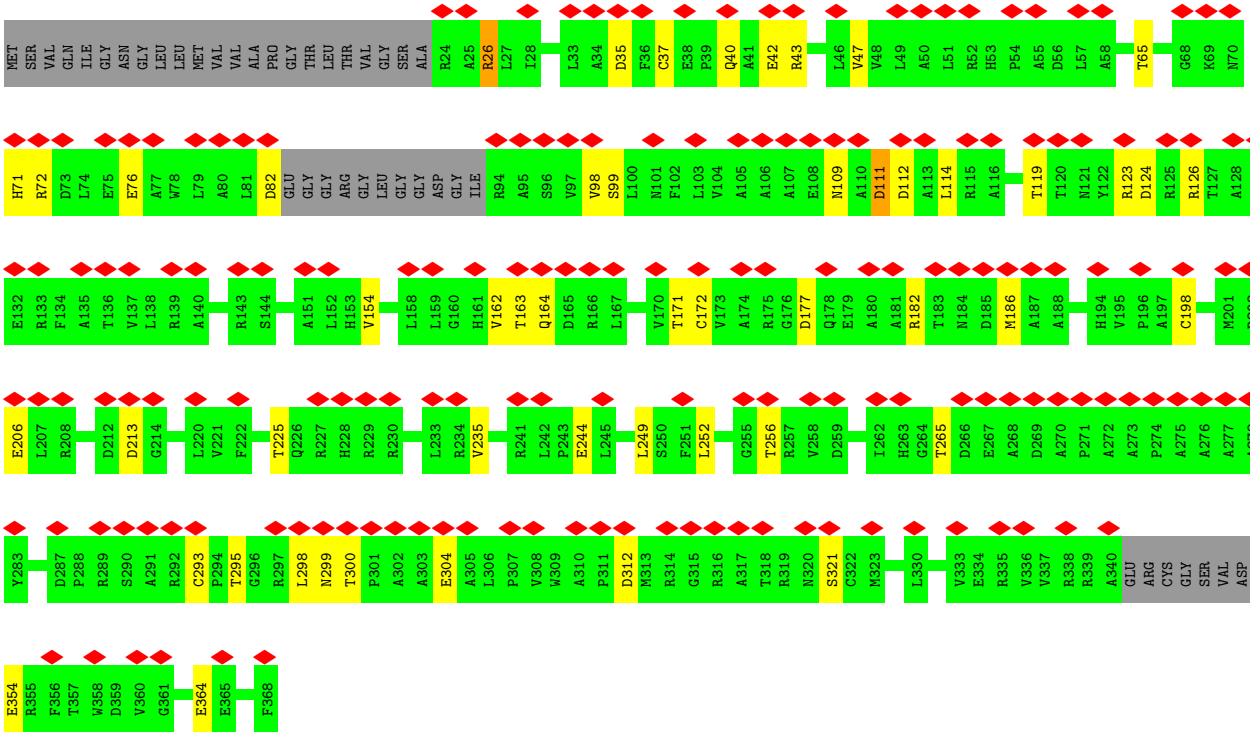
Chain r:





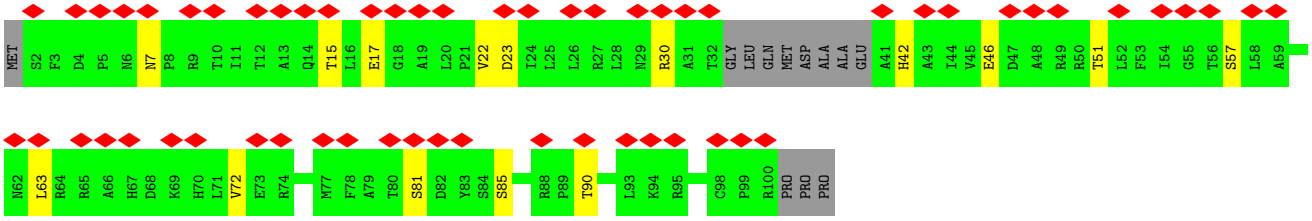
• Molecule 3: Triplex capsid protein 1

Chain t:



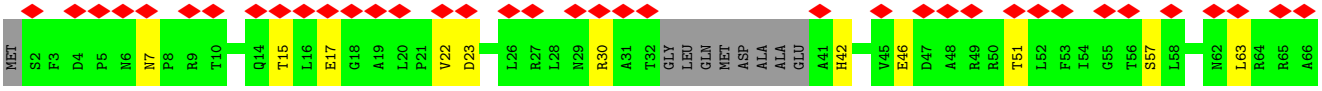
• Molecule 4: Small capsomere-interacting protein

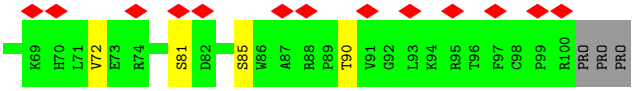
Chain E:



• Molecule 4: Small capsomere-interacting protein

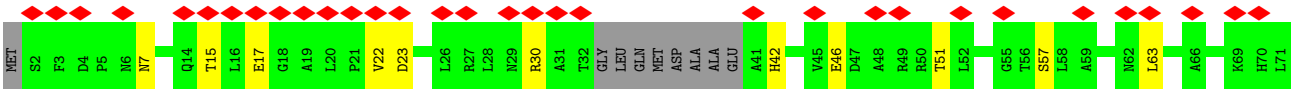
Chain F:

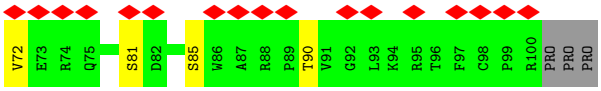




• Molecule 4: Small capsomere-interacting protein

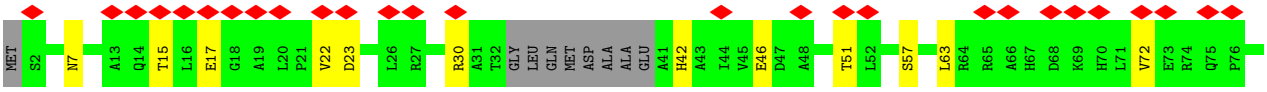
Chain G:

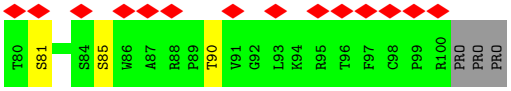




• Molecule 4: Small capsomere-interacting protein

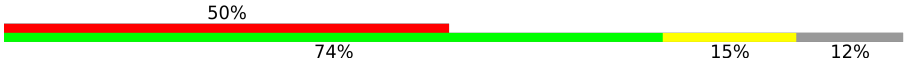
Chain H:

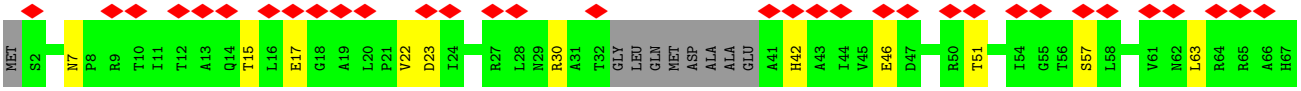


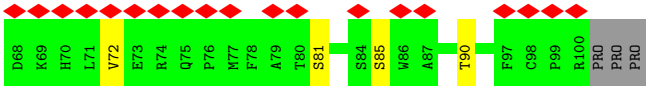


• Molecule 4: Small capsomere-interacting protein

Chain I:

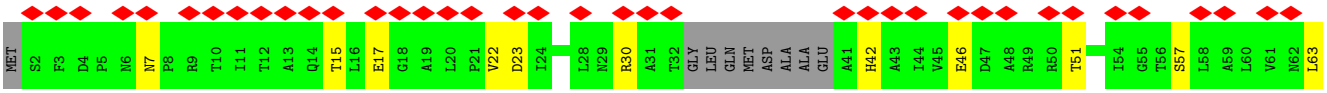


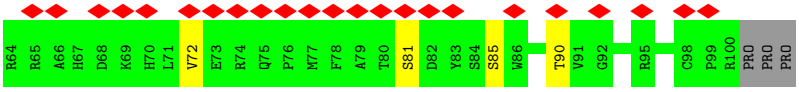




• Molecule 4: Small capsomere-interacting protein

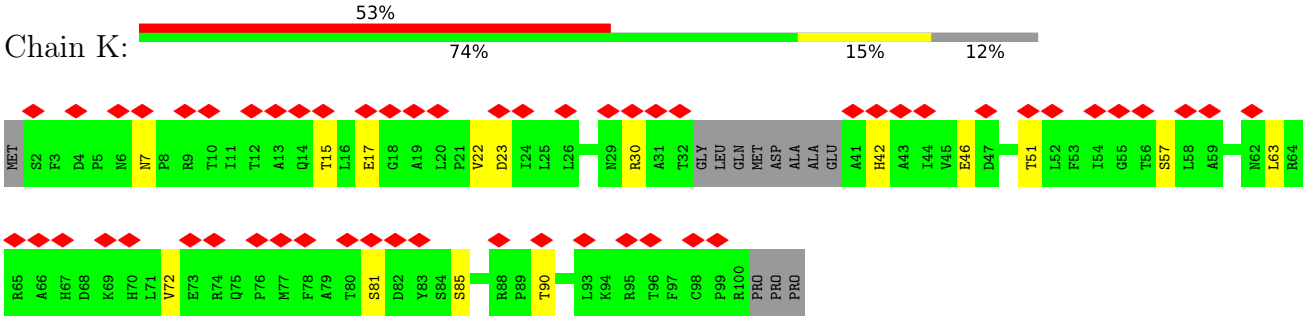
Chain J:





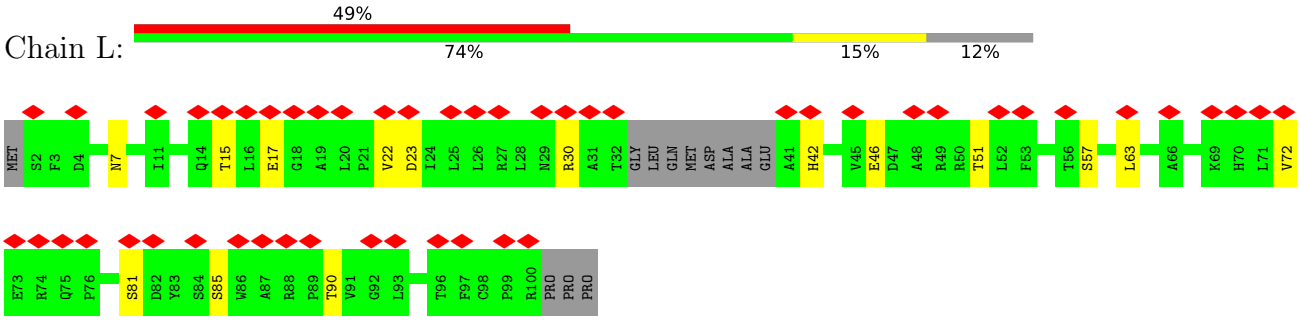
• Molecule 4: Small capsomere-interacting protein

Chain K:



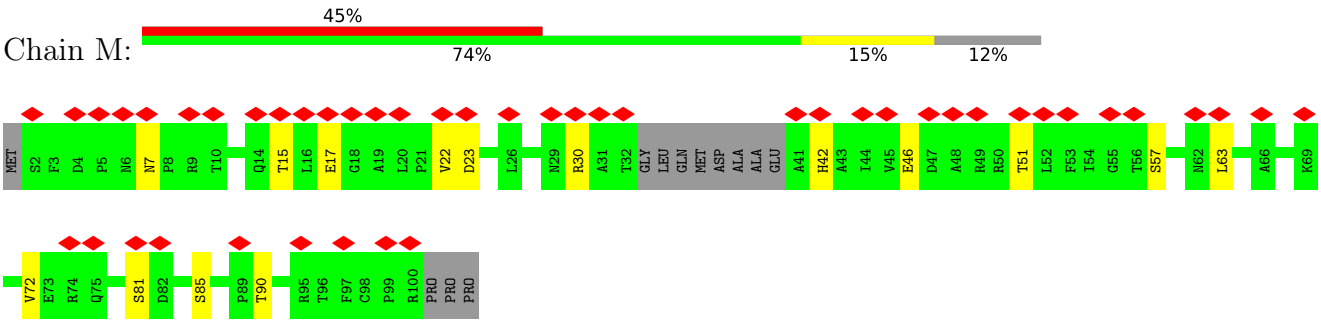
• Molecule 4: Small capsomere-interacting protein

Chain L:



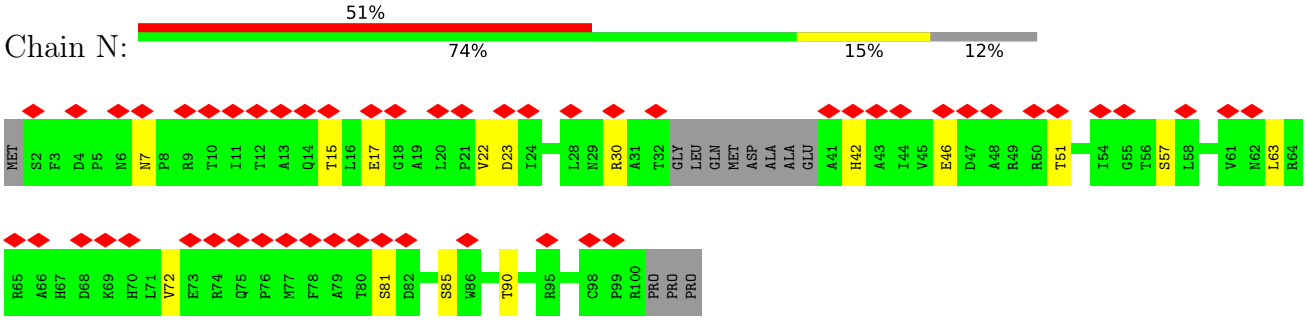
• Molecule 4: Small capsomere-interacting protein

Chain M:



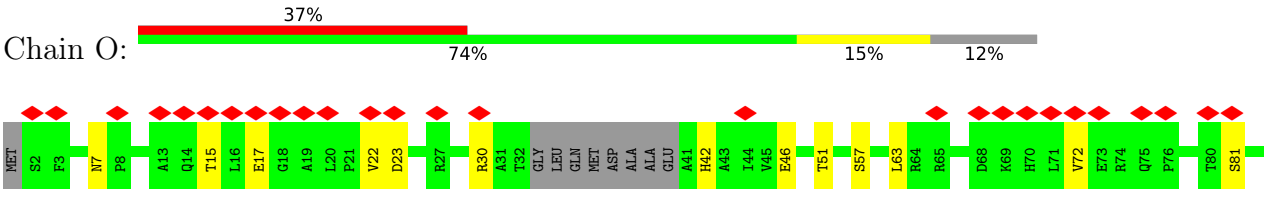
• Molecule 4: Small capsomere-interacting protein

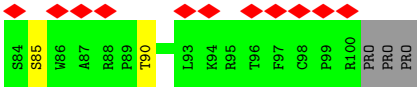
Chain N:



• Molecule 4: Small capsomere-interacting protein

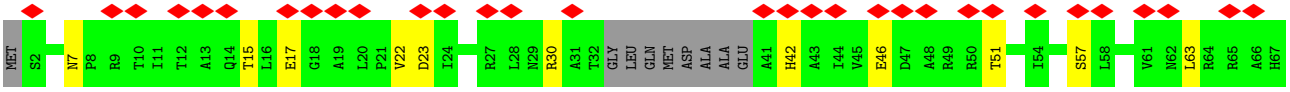
Chain O:

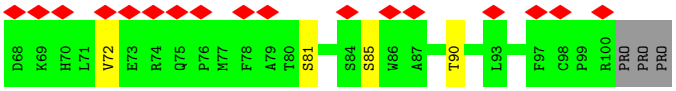




• Molecule 4: Small capsomere-interacting protein

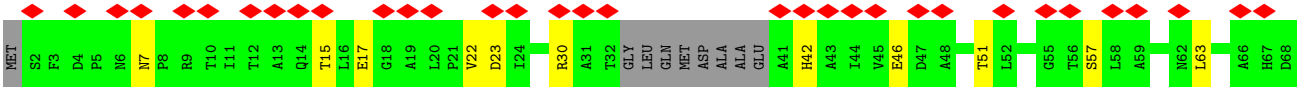
Chain P:

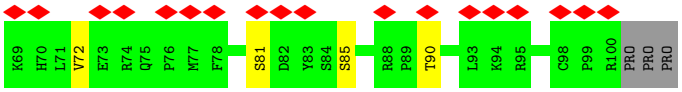




• Molecule 4: Small capsomere-interacting protein

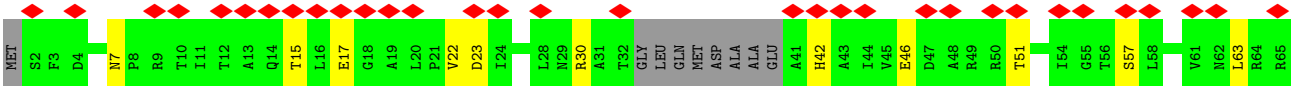
Chain Q:

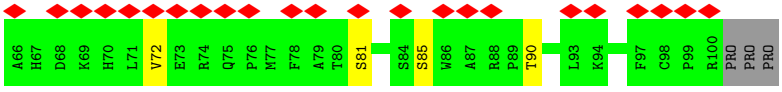




• Molecule 4: Small capsomere-interacting protein

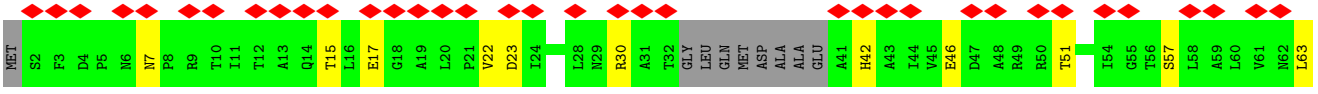
Chain R:

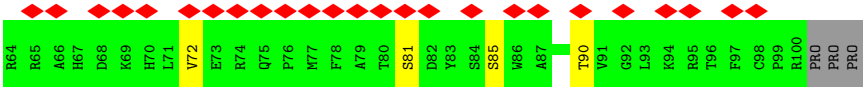




• Molecule 4: Small capsomere-interacting protein

Chain V:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8899	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	9.650	Depositor
Minimum map value	-5.599	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.860	Depositor
Recommended contour level	2	Depositor
Map size (Å)	1429.76, 1429.76, 1429.76	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.117, 1.117, 1.117	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	0	0.34	0/10384	0.47	0/14158
1	A	0.37	1/10366 (0.0%)	0.57	13/14132 (0.1%)
1	S	0.32	0/10229	0.47	0/13950
1	U	0.37	0/10384	0.48	2/14158 (0.0%)
1	a	0.33	0/10225	0.48	1/13938 (0.0%)
1	e	0.28	0/8938	0.50	0/12175
1	f	0.37	0/10384	0.48	1/14158 (0.0%)
1	g	0.36	0/10379	0.49	2/14150 (0.0%)
1	l	0.35	0/10384	0.48	0/14158
1	m	0.36	0/10384	0.48	0/14158
1	n	0.35	0/10384	0.48	1/14158 (0.0%)
1	p	0.34	0/10384	0.48	1/14158 (0.0%)
1	q	0.34	0/10384	0.47	0/14158
1	u	0.36	0/10384	0.48	1/14158 (0.0%)
1	w	0.36	0/10384	0.48	0/14158
1	y	0.35	0/10384	0.49	4/14158 (0.0%)
2	1	0.30	0/2127	0.50	0/2903
2	2	0.29	0/2127	0.51	0/2903
2	3	0.30	0/2127	0.50	0/2903
2	j	0.31	0/2043	0.54	1/2783 (0.0%)
2	k	0.28	0/2127	0.49	0/2903
2	o	0.32	0/2272	0.50	0/3099
2	s	0.33	0/2127	0.49	0/2903
2	v	0.31	0/2230	0.48	0/3041
2	x	0.30	0/2272	0.53	0/3099
2	z	0.29	0/2272	0.50	0/3099
3	B	1.95	6/152 (3.9%)	2.52	15/206 (7.3%)
3	C	1.95	6/152 (3.9%)	2.53	15/206 (7.3%)
3	D	1.95	6/152 (3.9%)	2.53	15/206 (7.3%)
3	T	0.33	0/2591	0.62	2/3521 (0.1%)
3	W	1.95	7/152 (4.6%)	2.52	15/206 (7.3%)
3	d	0.27	0/108	0.51	0/145
3	h	0.33	0/2591	0.62	2/3521 (0.1%)
3	i	0.33	0/2591	0.61	2/3521 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
3	r	0.33	0/2591	0.62	2/3521 (0.1%)
3	t	0.33	0/2591	0.61	2/3521 (0.1%)
4	E	0.28	0/736	0.50	0/999
4	F	0.28	0/736	0.50	0/999
4	G	0.28	0/736	0.50	0/999
4	H	0.28	0/736	0.50	0/999
4	I	0.28	0/736	0.50	0/999
4	J	0.28	0/736	0.50	0/999
4	K	0.28	0/736	0.50	0/999
4	L	0.28	0/736	0.50	0/999
4	M	0.28	0/736	0.50	0/999
4	N	0.28	0/736	0.50	0/999
4	O	0.28	0/736	0.50	0/999
4	P	0.28	0/736	0.50	0/999
4	Q	0.28	0/736	0.50	0/999
4	R	0.28	0/736	0.50	0/999
4	V	0.28	0/736	0.50	0/999
All	All	0.36	26/210796 (0.0%)	0.51	97/287278 (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
1	0	0	2
1	A	0	1
1	U	0	1
1	n	0	3
1	u	0	1
1	y	0	1
2	v	0	1
3	B	0	6
3	C	0	6
3	D	0	6
3	W	0	6
All	All	0	34

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	8	GLY	N-CA	8.82	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	8	GLY	N-CA	8.80	1.59	1.46
3	W	8	GLY	N-CA	8.78	1.59	1.46
3	B	8	GLY	N-CA	8.73	1.59	1.46
3	B	16	GLY	N-CA	7.64	1.57	1.46

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162	LEU	CB-CG-CD2	-21.90	73.78	111.00
3	W	17	THR	CA-CB-CG2	12.04	129.25	112.40
3	D	17	THR	CA-CB-CG2	12.03	129.24	112.40
3	B	17	THR	CA-CB-CG2	12.00	129.21	112.40
3	C	17	THR	CA-CB-CG2	12.00	129.20	112.40

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	762	ARG	Peptide
1	0	984	ALA	Peptide
1	A	163	ASP	Peptide
3	B	5	ILE	Peptide
3	B	6	GLY	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	0	1307/1330 (98%)	1171 (90%)	135 (10%)	1 (0%)	48	83
1	A	1302/1330 (98%)	1159 (89%)	138 (11%)	5 (0%)	30	68
1	S	1285/1330 (97%)	1146 (89%)	136 (11%)	3 (0%)	44	78
1	U	1307/1330 (98%)	1168 (89%)	137 (10%)	2 (0%)	44	78
1	a	1281/1330 (96%)	1137 (89%)	144 (11%)	0	100	100
1	e	1102/1330 (83%)	987 (90%)	114 (10%)	1 (0%)	48	83
1	f	1307/1330 (98%)	1162 (89%)	142 (11%)	3 (0%)	44	78
1	g	1304/1330 (98%)	1158 (89%)	146 (11%)	0	100	100
1	l	1307/1330 (98%)	1168 (89%)	138 (11%)	1 (0%)	48	83
1	m	1307/1330 (98%)	1163 (89%)	144 (11%)	0	100	100
1	n	1307/1330 (98%)	1163 (89%)	140 (11%)	4 (0%)	37	72
1	p	1307/1330 (98%)	1167 (89%)	139 (11%)	1 (0%)	48	83
1	q	1307/1330 (98%)	1183 (90%)	124 (10%)	0	100	100
1	u	1307/1330 (98%)	1156 (88%)	150 (12%)	1 (0%)	48	83
1	w	1307/1330 (98%)	1174 (90%)	132 (10%)	1 (0%)	48	83
1	y	1307/1330 (98%)	1168 (89%)	138 (11%)	1 (0%)	48	83
2	1	273/296 (92%)	252 (92%)	21 (8%)	0	100	100
2	2	273/296 (92%)	252 (92%)	21 (8%)	0	100	100
2	3	273/296 (92%)	250 (92%)	23 (8%)	0	100	100
2	j	261/296 (88%)	236 (90%)	25 (10%)	0	100	100
2	k	273/296 (92%)	252 (92%)	21 (8%)	0	100	100
2	o	294/296 (99%)	263 (90%)	31 (10%)	0	100	100
2	s	273/296 (92%)	248 (91%)	25 (9%)	0	100	100
2	v	285/296 (96%)	257 (90%)	28 (10%)	0	100	100
2	x	294/296 (99%)	258 (88%)	36 (12%)	0	100	100
2	z	294/296 (99%)	262 (89%)	32 (11%)	0	100	100
3	B	21/368 (6%)	11 (52%)	6 (29%)	4 (19%)	0	2
3	C	21/368 (6%)	11 (52%)	6 (29%)	4 (19%)	0	2
3	D	21/368 (6%)	11 (52%)	6 (29%)	4 (19%)	0	2
3	T	321/368 (87%)	293 (91%)	28 (9%)	0	100	100
3	W	21/368 (6%)	11 (52%)	6 (29%)	4 (19%)	0	2
3	d	14/368 (4%)	12 (86%)	2 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	h	321/368 (87%)	292 (91%)	29 (9%)	0	100	100
3	i	321/368 (87%)	292 (91%)	29 (9%)	0	100	100
3	r	321/368 (87%)	293 (91%)	28 (9%)	0	100	100
3	t	321/368 (87%)	293 (91%)	28 (9%)	0	100	100
4	E	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	F	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	G	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	H	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	I	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	J	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	K	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	L	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	M	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	N	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	O	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	P	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	Q	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	R	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
4	V	87/103 (84%)	81 (93%)	6 (7%)	0	100	100
All	All	26452/29465 (90%)	23694 (90%)	2718 (10%)	40 (0%)	45	78

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	SER
3	B	13	VAL
3	B	16	GLY
3	B	20	VAL
3	C	13	VAL

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	0	1057/1072 (99%)	1056 (100%)	1 (0%)	92 94
1	A	1056/1072 (98%)	1050 (99%)	6 (1%)	84 88
1	S	1042/1072 (97%)	1042 (100%)	0	100 100
1	U	1057/1072 (99%)	1057 (100%)	0	100 100
1	a	1040/1072 (97%)	1040 (100%)	0	100 100
1	e	909/1072 (85%)	908 (100%)	1 (0%)	92 94
1	f	1057/1072 (99%)	1056 (100%)	1 (0%)	92 94
1	g	1057/1072 (99%)	1056 (100%)	1 (0%)	92 94
1	l	1057/1072 (99%)	1056 (100%)	1 (0%)	92 94
1	m	1057/1072 (99%)	1057 (100%)	0	100 100
1	n	1057/1072 (99%)	1057 (100%)	0	100 100
1	p	1057/1072 (99%)	1054 (100%)	3 (0%)	91 91
1	q	1057/1072 (99%)	1057 (100%)	0	100 100
1	u	1057/1072 (99%)	1057 (100%)	0	100 100
1	w	1057/1072 (99%)	1057 (100%)	0	100 100
1	y	1057/1072 (99%)	1056 (100%)	1 (0%)	92 94
2	1	223/235 (95%)	223 (100%)	0	100 100
2	2	223/235 (95%)	222 (100%)	1 (0%)	89 90
2	3	223/235 (95%)	223 (100%)	0	100 100
2	j	213/235 (91%)	212 (100%)	1 (0%)	86 89
2	k	223/235 (95%)	223 (100%)	0	100 100
2	o	235/235 (100%)	235 (100%)	0	100 100
2	s	223/235 (95%)	223 (100%)	0	100 100
2	v	233/235 (99%)	232 (100%)	1 (0%)	89 90
2	x	235/235 (100%)	234 (100%)	1 (0%)	89 90
2	z	235/235 (100%)	235 (100%)	0	100 100
3	B	17/279 (6%)	8 (47%)	9 (53%)	0 0
3	C	17/279 (6%)	7 (41%)	10 (59%)	0 0
3	D	17/279 (6%)	7 (41%)	10 (59%)	0 0
3	T	251/279 (90%)	199 (79%)	52 (21%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	W	17/279 (6%)	7 (41%)	10 (59%)	0 0
3	d	12/279 (4%)	12 (100%)	0	100 100
3	h	251/279 (90%)	199 (79%)	52 (21%)	1 6
3	i	251/279 (90%)	199 (79%)	52 (21%)	1 6
3	r	251/279 (90%)	200 (80%)	51 (20%)	1 6
3	t	251/279 (90%)	199 (79%)	52 (21%)	1 6
4	E	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	F	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	G	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	H	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	I	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	J	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	K	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	L	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	M	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	N	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	O	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	P	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	Q	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	R	78/87 (90%)	63 (81%)	15 (19%)	1 7
4	V	78/87 (90%)	63 (81%)	15 (19%)	1 7
All	All	21502/23597 (91%)	20960 (98%)	542 (2%)	43 62

5 of 542 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	r	177	ASP
3	r	265	THR
3	r	172	CYS
3	t	206	GLU
4	O	46	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 432 such sidechains are listed below:

Mol	Chain	Res	Type
1	l	938	HIS
2	o	163	ASN
1	y	172	GLN
1	l	1121	ASN
1	m	966	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

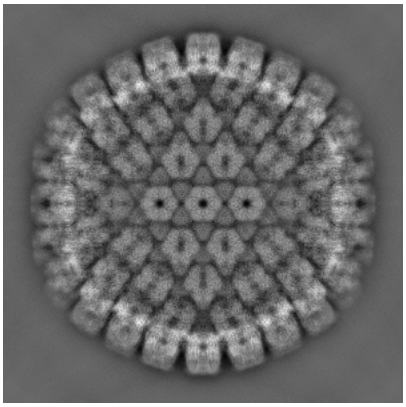
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31612. These allow visual inspection of the internal detail of the map and identification of artifacts.

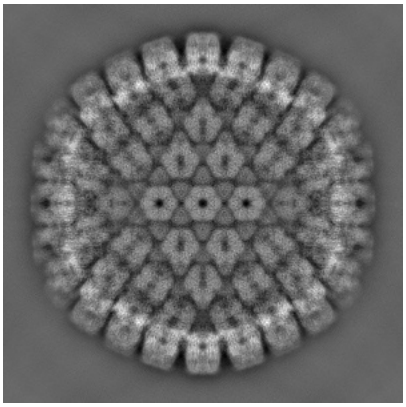
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

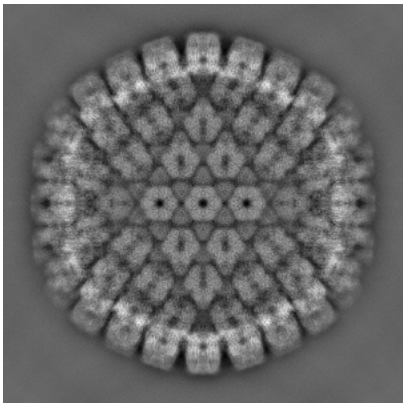
6.1.1 Primary map



X



Y

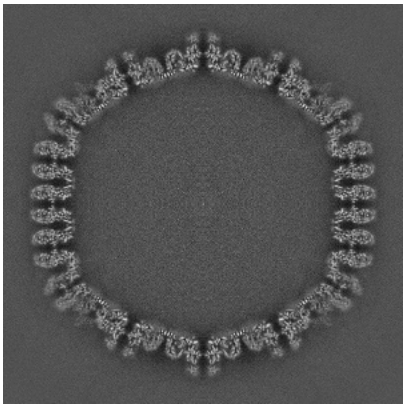


Z

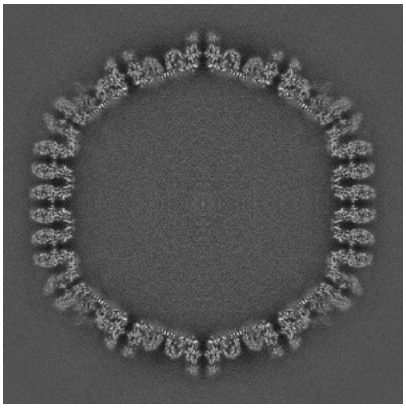
The images above show the map projected in three orthogonal directions.

6.2 Central slices

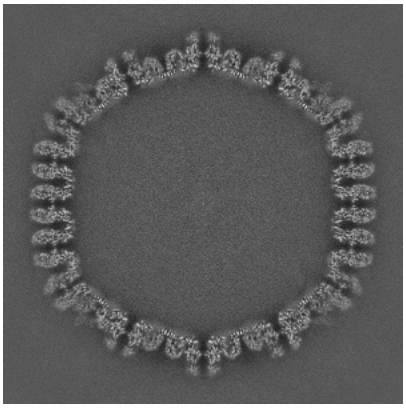
6.2.1 Primary map



X Index: 640



Y Index: 640

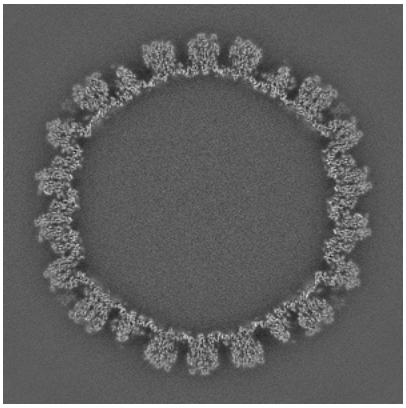


Z Index: 640

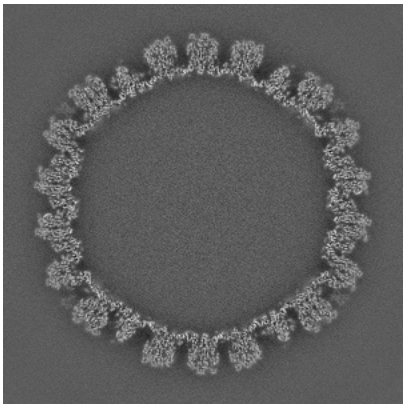
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

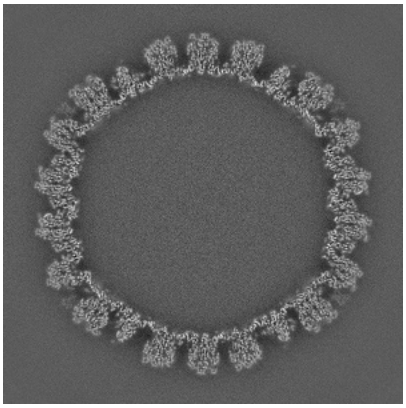
6.3.1 Primary map



X Index: 746



Y Index: 534

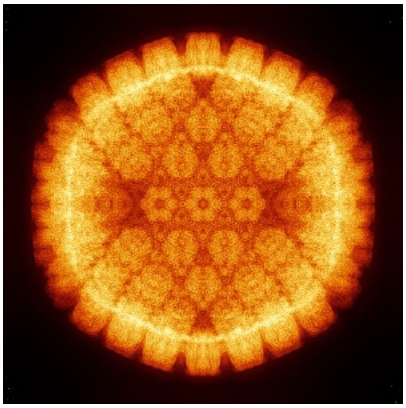


Z Index: 533

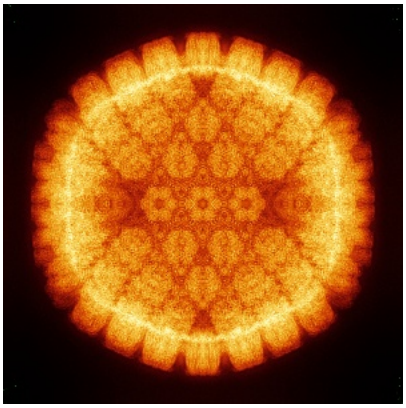
The images above show the largest variance slices of the map in three orthogonal directions.

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

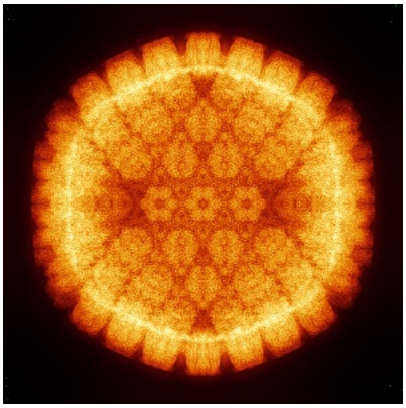
6.4.1 Primary map



X



Y

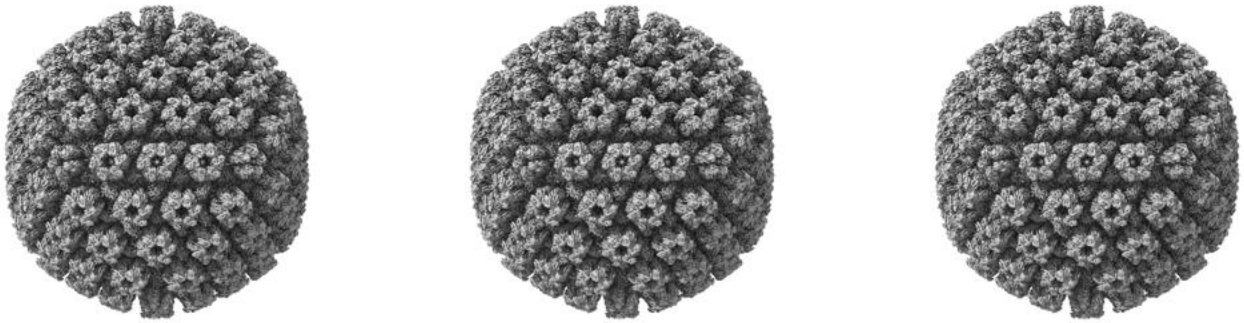


Z

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

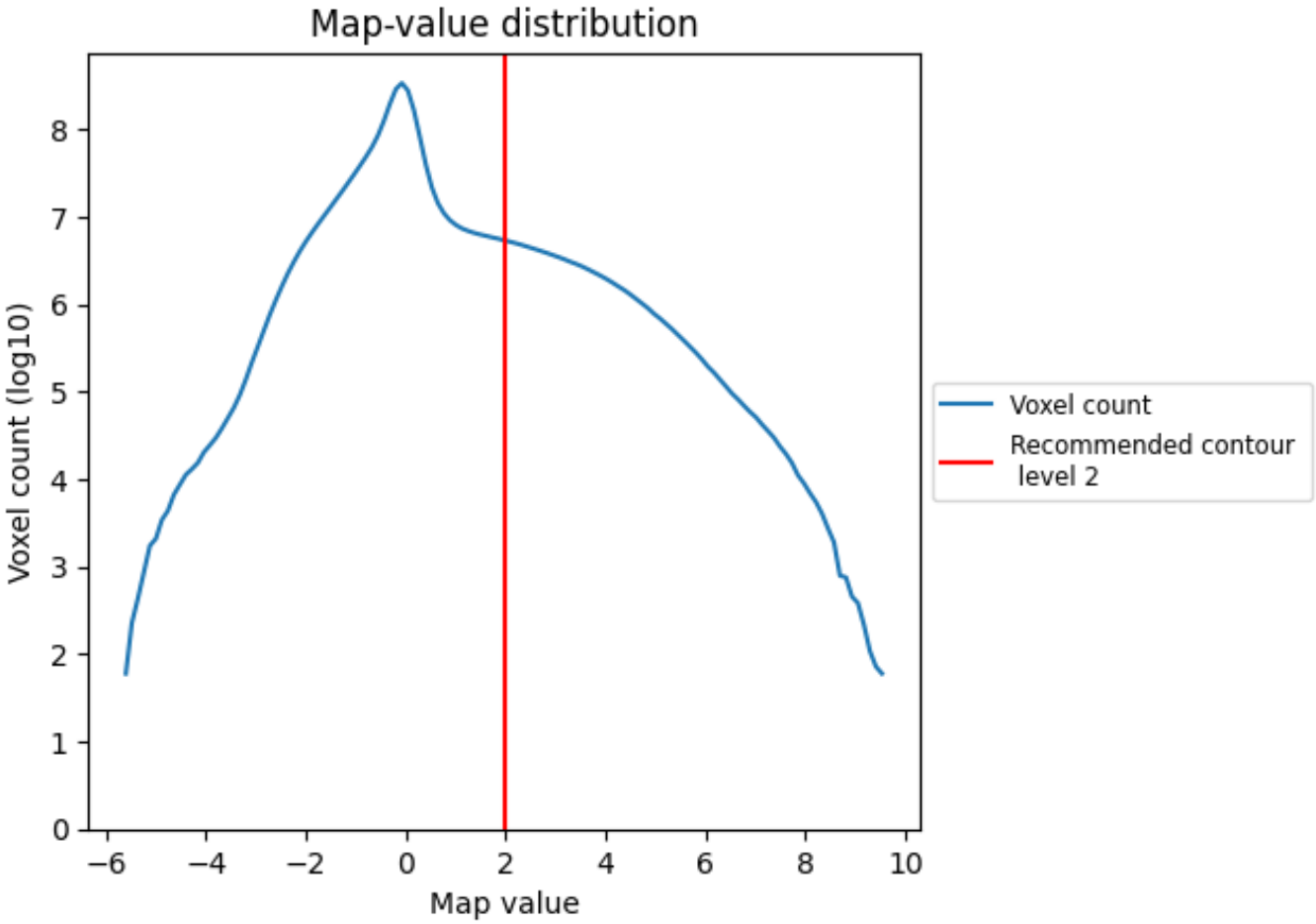
6.6 Mask visualisation (i)

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

7 Map analysis

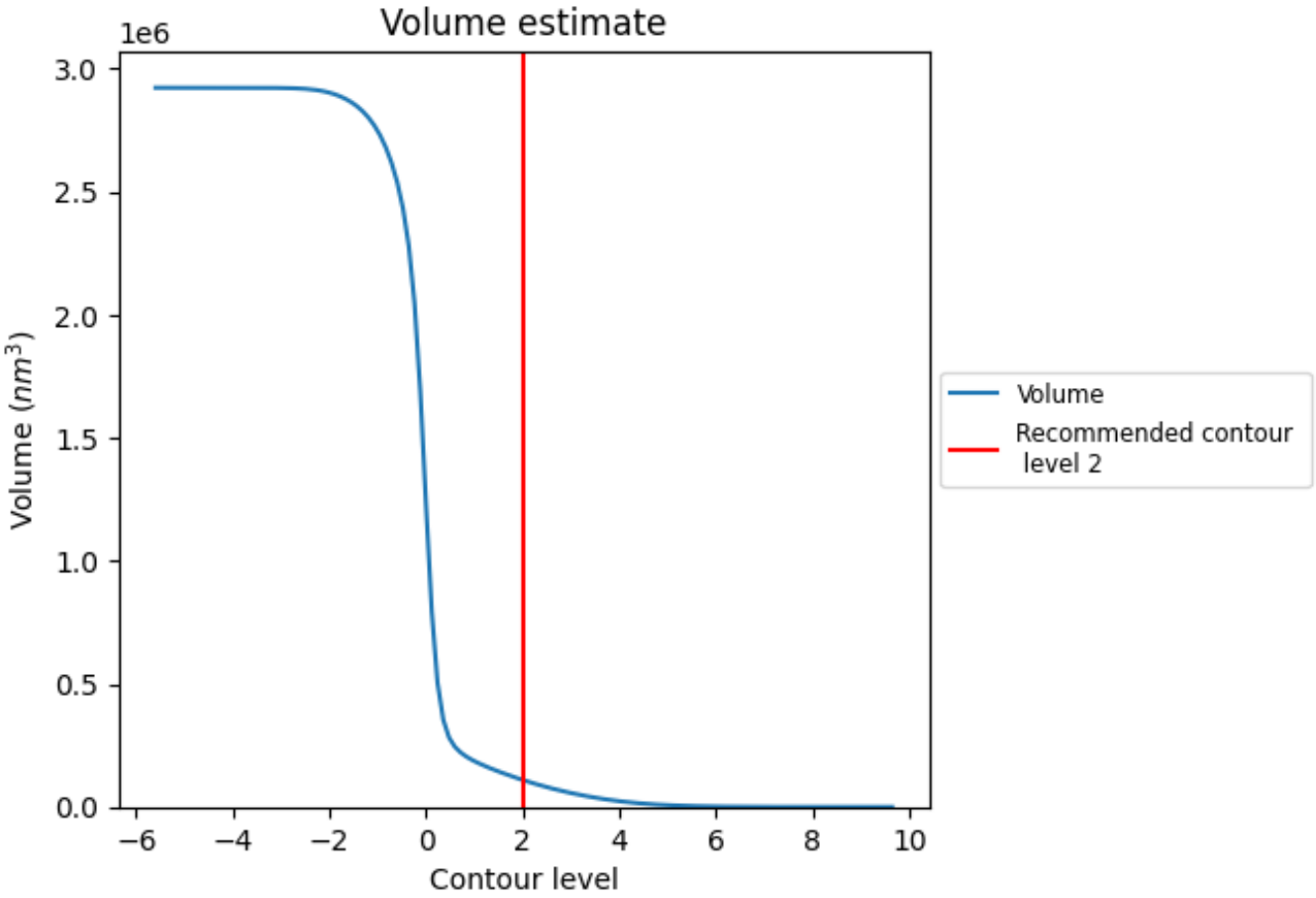
This section contains the results of statistical analysis of the map.

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.

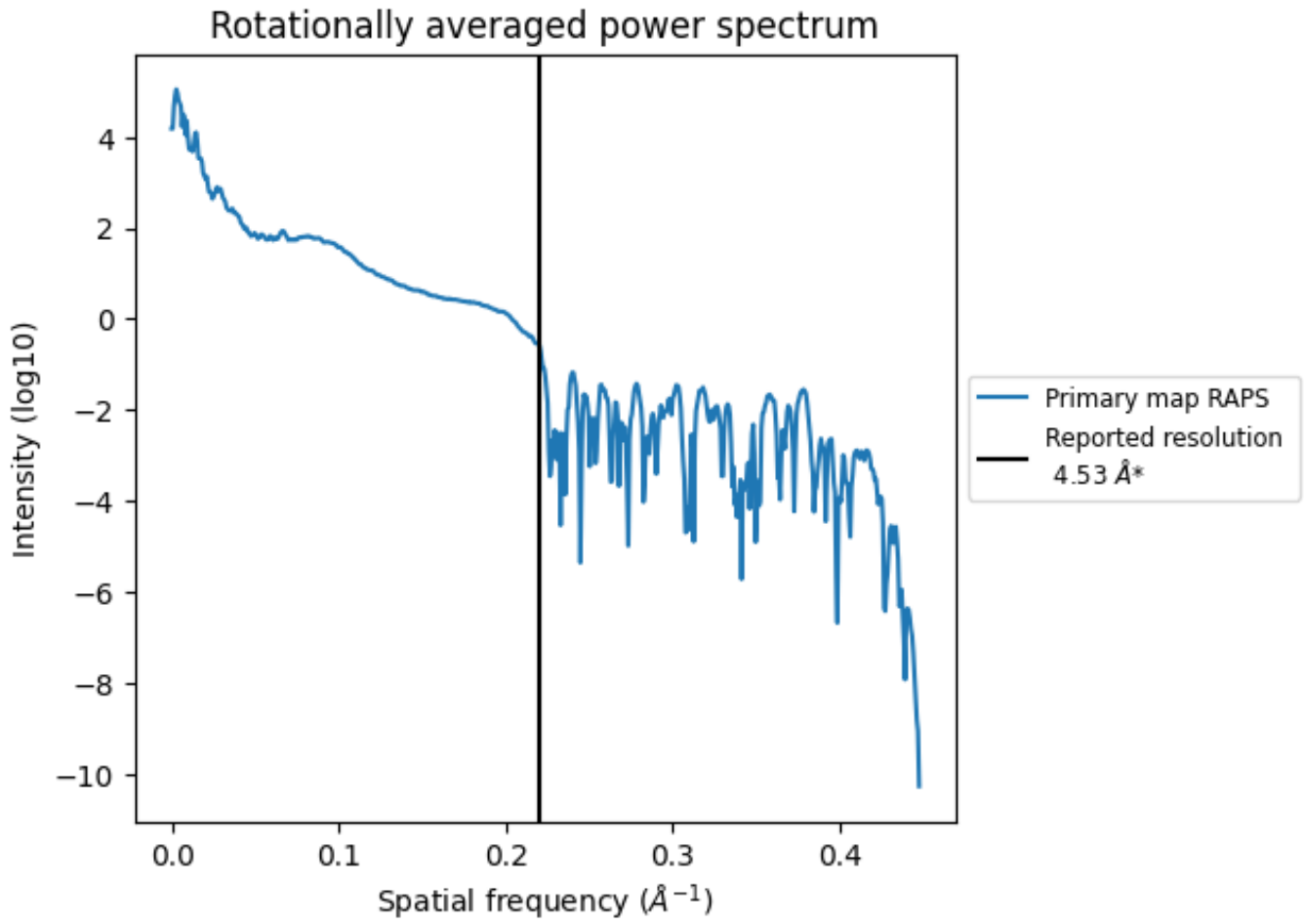
7.2 Volume estimate (i)



The volume at the recommended contour level is 109801 nm^3; this corresponds to an approximate mass of 99186 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 0.221 Å^{-1}

8 Fourier-Shell correlation (i)

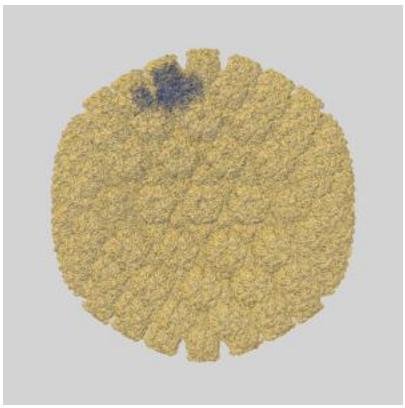
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

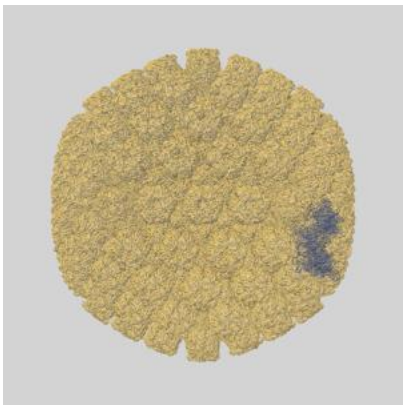
This section contains information regarding the fit between EMDB map EMD-31612 and PDB model 7FJ3. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

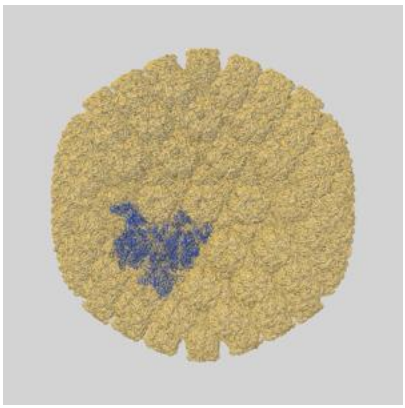
9.1.1 Map-model overlay



X

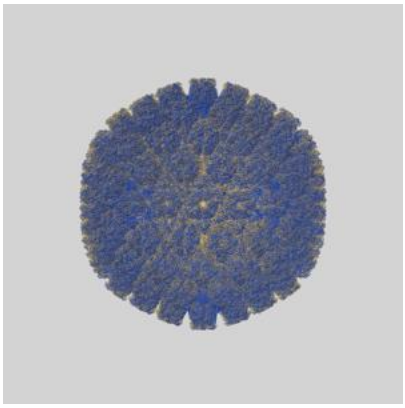


Y

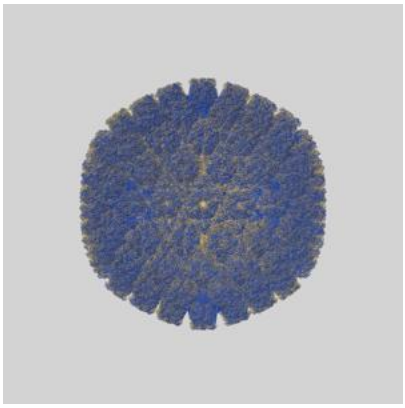


Z

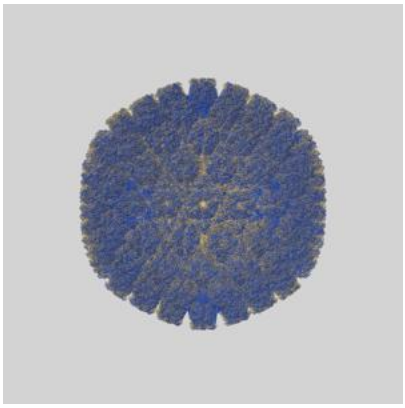
9.1.2 Map-model assembly overlay



X



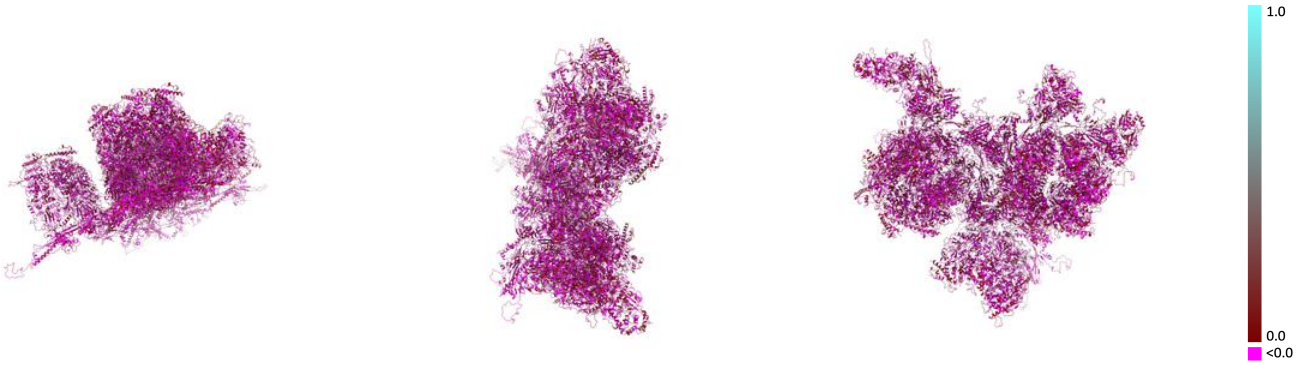
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 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.

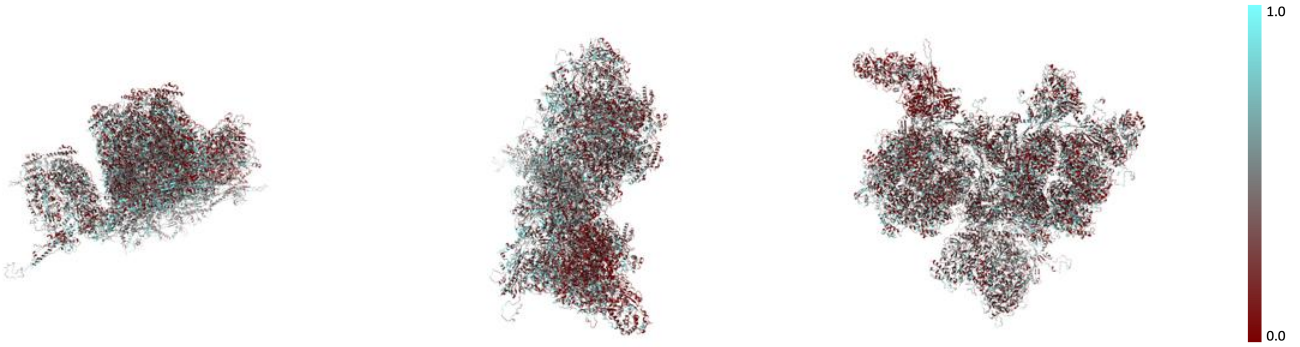
9.2 Q-score mapped to coordinate model



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.

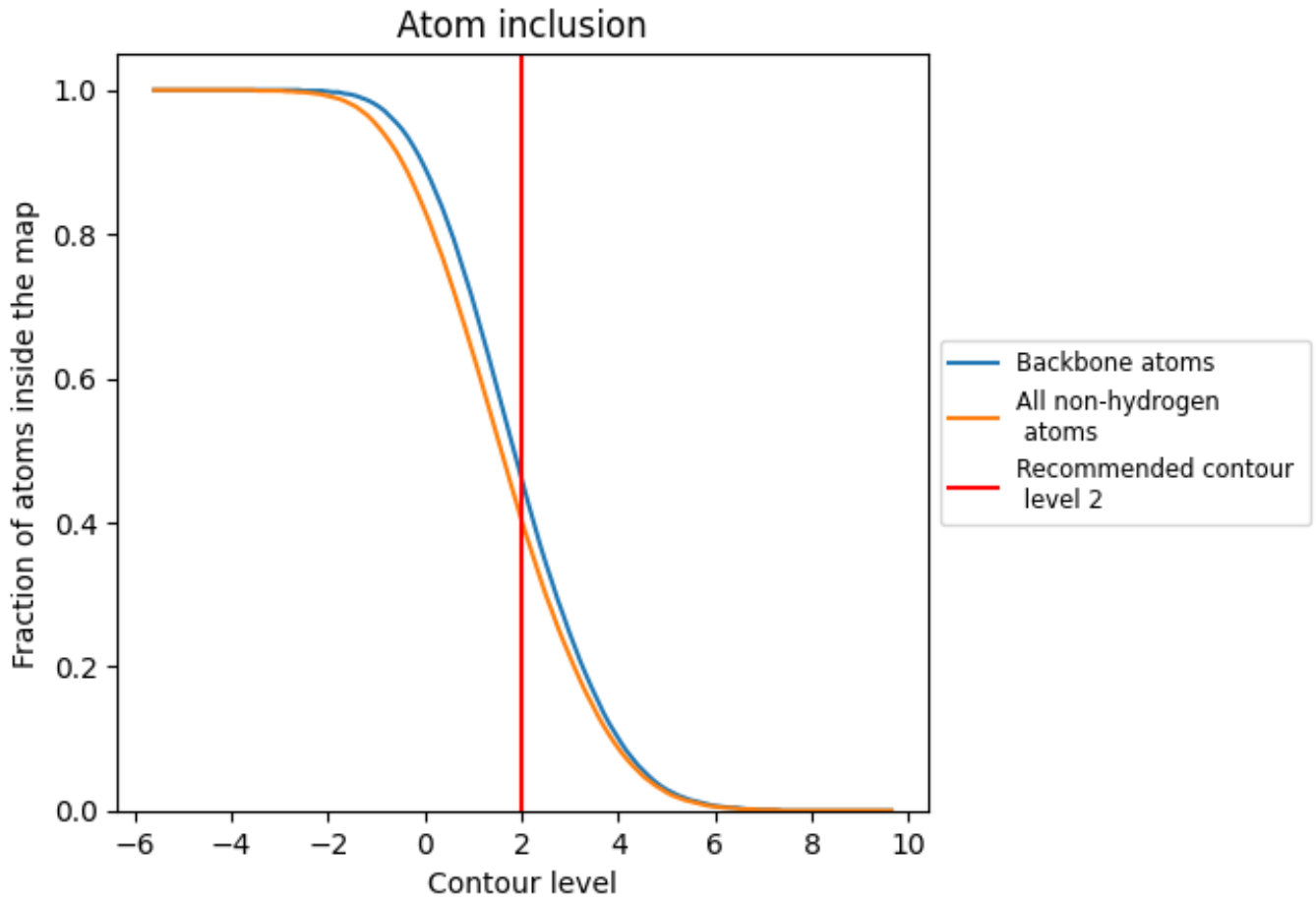
9.3 Atom inclusion mapped to coordinate model



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 (2).

9.4 Atom inclusion (i)



At the recommended contour level, 46% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4030	0.0230
0	0.4090	0.0140
1	0.3840	0.0330
2	0.3890	0.0420
3	0.3970	0.0420
A	0.4310	0.0220
B	0.2960	0.0130
C	0.3160	-0.0010
D	0.3750	0.0420
E	0.3420	0.0280
F	0.4080	0.0500
G	0.4070	0.0350
H	0.4470	0.0910
I	0.3640	0.0840
J	0.3270	0.0600
K	0.3770	0.0520
L	0.4130	0.0710
M	0.4560	0.0680
N	0.3930	0.0720
O	0.4460	0.0890
P	0.4380	0.0900
Q	0.4410	0.0580
R	0.3700	0.0540
S	0.4080	0.0250
T	0.3850	0.0280
U	0.4240	0.0160
V	0.3300	0.0490
W	0.3620	0.0350
a	0.4180	0.0160
d	0.3240	-0.0070
e	0.3040	0.0320
f	0.4240	0.0070
g	0.4180	0.0140
h	0.4190	0.0120
i	0.1370	0.0220

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Chain	Atom inclusion	Q-score
j	0.1260	0.0550
k	0.1260	0.0370
l	0.4350	0.0180
m	0.4400	0.0200
n	0.4270	0.0180
o	0.3910	0.0380
p	0.4220	0.0190
q	0.4200	0.0180
r	0.4220	0.0480
s	0.3940	0.0200
t	0.4010	0.0480
u	0.4320	0.0120
v	0.3900	0.0260
w	0.4230	0.0170
x	0.3730	0.0540
y	0.4200	0.0150
z	0.3620	0.0320