# Full wwPDB EM Validation Report ⓘ

Nov 5, 2022 – 04:25 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 5VKU |
| EMDB ID | : | EMD-8703 |
| Title | : | An atomic structure of the human cytomegalovirus (HCMV) capsid with its securing layer of pp150 tegument protein |
| Authors | : | Yu, X.; Jih, J.; Jiang, J.; Zhou, H. |
| Deposited on | : | 2017-04-24 |
| Resolution | : | 3.90 Å(reported) |

This is a Full wwPDB EM Validation 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:

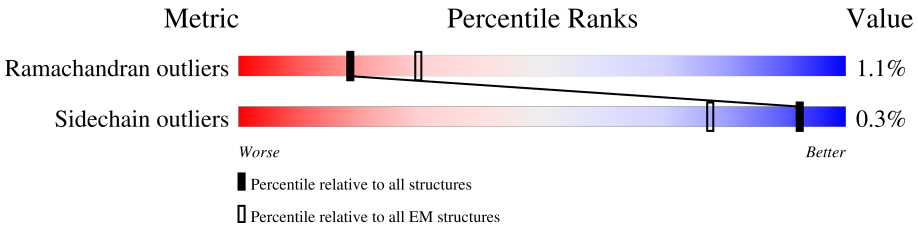
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA)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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 Å.

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




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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 0 | 285 | 58% 99% |
| 1 | 1 | 285 | 56% 99% |
| 1 | 2 | 285 | 93% 99% |
| 1 | 3 | 285 | 75% 98% |
| 1 | 4 | 285 | 53% 99% |
| 1 | 5 | 285 | 63% 99% |
| 1 | 6 | 285 | 60% 99% |
| 1 | 7 | 285 | 49% 99% |
| 1 | 8 | 285 | 59% 99% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 9 | 285 | 60% 99% |
| 1 | v | 285 | 97% 97% |
| 1 | w | 285 | 97% 99% |
| 1 | x | 285 | 85% 98% |
| 1 | y | 285 | 54% 99% |
| 1 | z | 285 | 53% 99% |
| 2 | A | 1370 | 68% 96% |
| 2 | B | 1370 | 46% 95% |
| 2 | C | 1370 | 39% 97% |
| 2 | D | 1370 | 36% 97% |
| 2 | E | 1370 | 34% 96% |
| 2 | F | 1370 | 38% 97% |
| 2 | G | 1370 | 47% 97% |
| 2 | H | 1370 | 31% 98% |
| 2 | I | 1370 | 30% 97% |
| 2 | J | 1370 | 29% 96% |
| 2 | K | 1370 | 29% 98% |
| 2 | L | 1370 | 30% 98% |
| 2 | M | 1370 | 34% 98% |
| 2 | N | 1370 | 30% 98% |
| 2 | O | 1370 | 29% 97% |
| 2 | P | 1370 | 31% 97% |
| 3 | Q | 75 | 68% 84% 16% |
| 3 | R | 75 | 67% 84% 16% |
| 3 | S | 75 | 56% 84% 16% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | T | 75 | 55% 84% 16% |
| 3 | U | 75 | 56% 84% 16% |
| 3 | V | 75 | 57% 83% 16% |
| 3 | W | 75 | 64% 84% 16% |
| 3 | X | 75 | 52% 84% 16% |
| 3 | Y | 75 | 47% 83% 16% |
| 3 | Z | 75 | 43% 84% 16% |
| 3 | a | 75 | 51% 84% 16% |
| 3 | b | 75 | 49% 83% 16% |
| 3 | c | 75 | 53% 84% 16% |
| 3 | d | 75 | 41% 84% 16% |
| 3 | e | 75 | 40% 84% 16% |
| 3 | f | 75 | 45% 84% 16% |
| 4 | g | 290 | 74% 88% 10% |
| 4 | j | 290 | 30% 98% |
| 4 | m | 290 | 39% 99% |
| 4 | p | 290 | 32% 98% |
| 4 | s | 290 | 29% 98% |
| 5 | h | 306 | 69% 92% 5% |
| 5 | i | 306 | 76% 92% 7% |
| 5 | k | 306 | 34% 93% 5% |
| 5 | l | 306 | 36% 98% |
| 5 | n | 306 | 41% 94% |
| 5 | o | 306 | 39% 94% 5% |
| 5 | q | 306 | 33% 96% |

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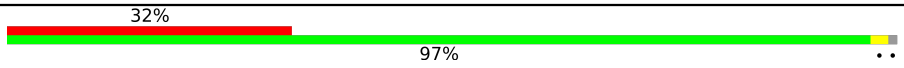
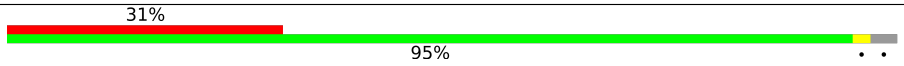
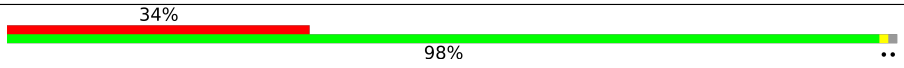
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | r | 306 |   |
| 5 | t | 306 |   |
| 5 | u | 306 |   |

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 248627 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 Tegument protein pp150.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | 1 | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | 2 | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | 3 | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | 4 | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | 5 | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | 6 | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | 7 | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | 8 | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | 9 | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | v | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | w | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | x | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | y | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |
| 1 | z | 285 | Total 2328 | C 1468 | N 426 | O 421 | S 13 | 0 | 0 |

- Molecule 2 is a protein called Major capsid protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | A | 1329 | Total | C | N | O | S | 0 | 0 |
| | | | 10527 | 6711 | 1822 | 1933 | 61 | | |
| 2 | B | 1335 | Total | C | N | O | S | 0 | 0 |
| | | | 10574 | 6733 | 1830 | 1950 | 61 | | |
| 2 | C | 1349 | Total | C | N | O | S | 0 | 0 |
| | | | 10686 | 6805 | 1852 | 1968 | 61 | | |
| 2 | D | 1346 | Total | C | N | O | S | 0 | 0 |
| | | | 10670 | 6796 | 1849 | 1964 | 61 | | |
| 2 | E | 1347 | Total | C | N | O | S | 0 | 0 |
| | | | 10676 | 6799 | 1850 | 1966 | 61 | | |
| 2 | F | 1350 | Total | C | N | O | S | 0 | 0 |
| | | | 10693 | 6809 | 1853 | 1970 | 61 | | |
| 2 | G | 1351 | Total | C | N | O | S | 0 | 0 |
| | | | 10705 | 6816 | 1854 | 1974 | 61 | | |
| 2 | H | 1352 | Total | C | N | O | S | 0 | 0 |
| | | | 10710 | 6819 | 1855 | 1975 | 61 | | |
| 2 | I | 1347 | Total | C | N | O | S | 0 | 0 |
| | | | 10676 | 6799 | 1850 | 1966 | 61 | | |
| 2 | J | 1335 | Total | C | N | O | S | 0 | 0 |
| | | | 10581 | 6739 | 1837 | 1945 | 60 | | |
| 2 | K | 1348 | Total | C | N | O | S | 0 | 0 |
| | | | 10681 | 6802 | 1851 | 1967 | 61 | | |
| 2 | L | 1353 | Total | C | N | O | S | 0 | 0 |
| | | | 10717 | 6823 | 1856 | 1977 | 61 | | |
| 2 | M | 1353 | Total | C | N | O | S | 0 | 0 |
| | | | 10717 | 6823 | 1856 | 1977 | 61 | | |
| 2 | N | 1350 | Total | C | N | O | S | 0 | 0 |
| | | | 10693 | 6809 | 1853 | 1970 | 61 | | |
| 2 | O | 1348 | Total | C | N | O | S | 0 | 0 |
| | | | 10681 | 6802 | 1851 | 1967 | 61 | | |
| 2 | P | 1348 | Total | C | N | O | S | 0 | 0 |
| | | | 10681 | 6802 | 1851 | 1967 | 61 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | Q | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | R | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | S | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | T | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | U | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | V | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | W | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | X | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | Y | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | Z | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | a | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | b | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | c | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | d | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | e | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |
| 3 | f | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 513 | 321 | 97 | 91 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | g | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2091 | 1344 | 365 | 371 | 11 | | |
| 4 | j | 290 | Total | C | N | O | S | 0 | 0 |
| | | | 2325 | 1485 | 411 | 417 | 12 | | |
| 4 | m | 290 | Total | C | N | O | S | 0 | 0 |
| | | | 2325 | 1485 | 411 | 417 | 12 | | |
| 4 | p | 290 | Total | C | N | O | S | 0 | 0 |
| | | | 2325 | 1485 | 411 | 417 | 12 | | |
| 4 | s | 290 | Total | C | N | O | S | 0 | 0 |
| | | | 2325 | 1485 | 411 | 417 | 12 | | |

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

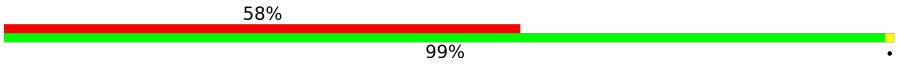
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | h | 292 | Total | C | N | O | S | 0 | 0 |
| | | | 2316 | 1490 | 399 | 409 | 18 | | |
| 5 | i | 285 | Total | C | N | O | S | 0 | 0 |
| | | | 2258 | 1454 | 386 | 401 | 17 | | |
| 5 | k | 292 | Total | C | N | O | S | 0 | 0 |
| | | | 2317 | 1491 | 399 | 408 | 19 | | |
| 5 | l | 303 | Total | C | N | O | S | 0 | 0 |
| | | | 2406 | 1541 | 419 | 428 | 18 | | |
| 5 | n | 295 | Total | C | N | O | S | 0 | 0 |
| | | | 2334 | 1501 | 402 | 412 | 19 | | |
| 5 | o | 291 | Total | C | N | O | S | 0 | 0 |
| | | | 2311 | 1484 | 398 | 411 | 18 | | |
| 5 | q | 295 | Total | C | N | O | S | 0 | 0 |
| | | | 2334 | 1501 | 402 | 412 | 19 | | |
| 5 | r | 304 | Total | C | N | O | S | 0 | 0 |
| | | | 2411 | 1544 | 420 | 429 | 18 | | |
| 5 | t | 296 | Total | C | N | O | S | 0 | 0 |
| | | | 2342 | 1505 | 403 | 415 | 19 | | |
| 5 | u | 304 | Total | C | N | O | S | 0 | 0 |
| | | | 2411 | 1544 | 420 | 429 | 18 | | |

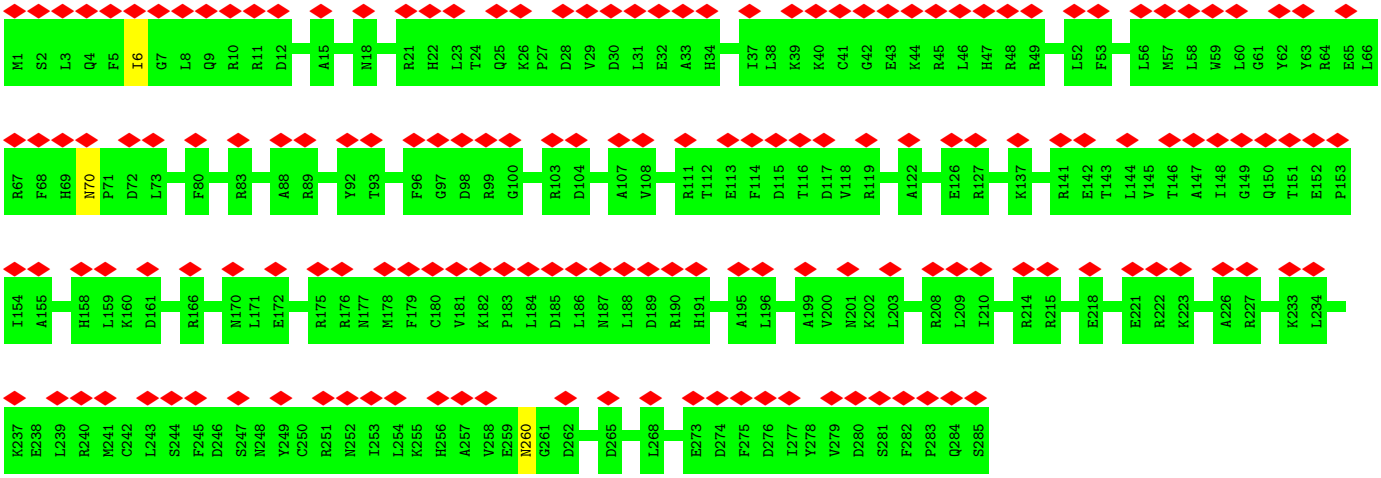
# 3 Residue-property plots (i)

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: Tegument protein pp150

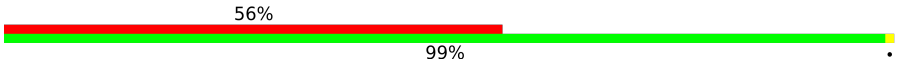
Chain 0:

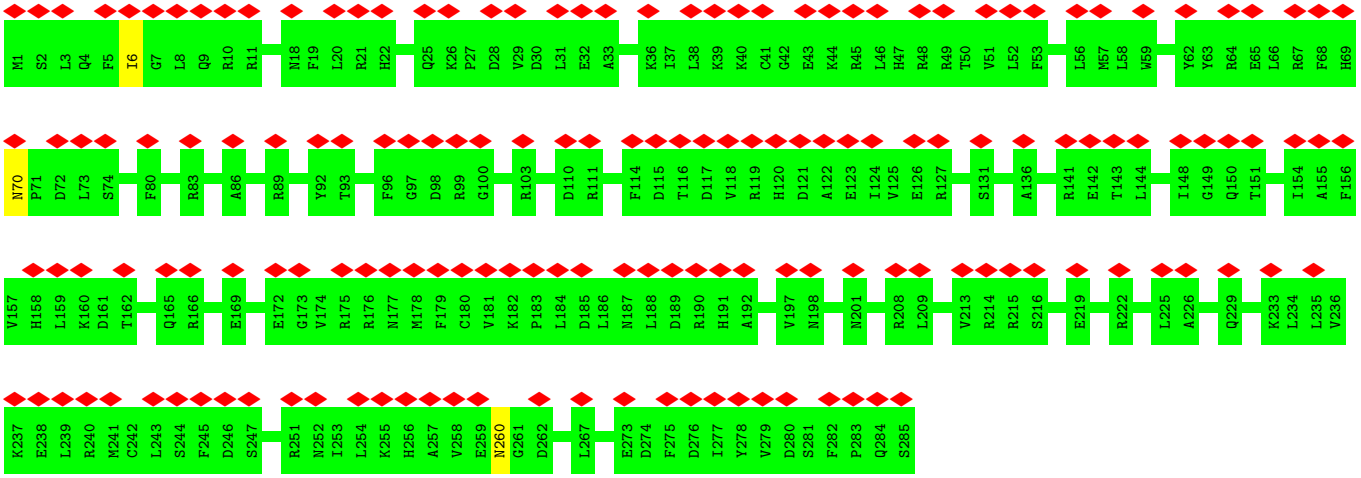



• Molecule 1: Tegument protein pp150

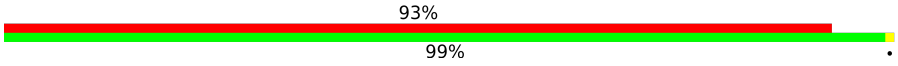
Chain 1:

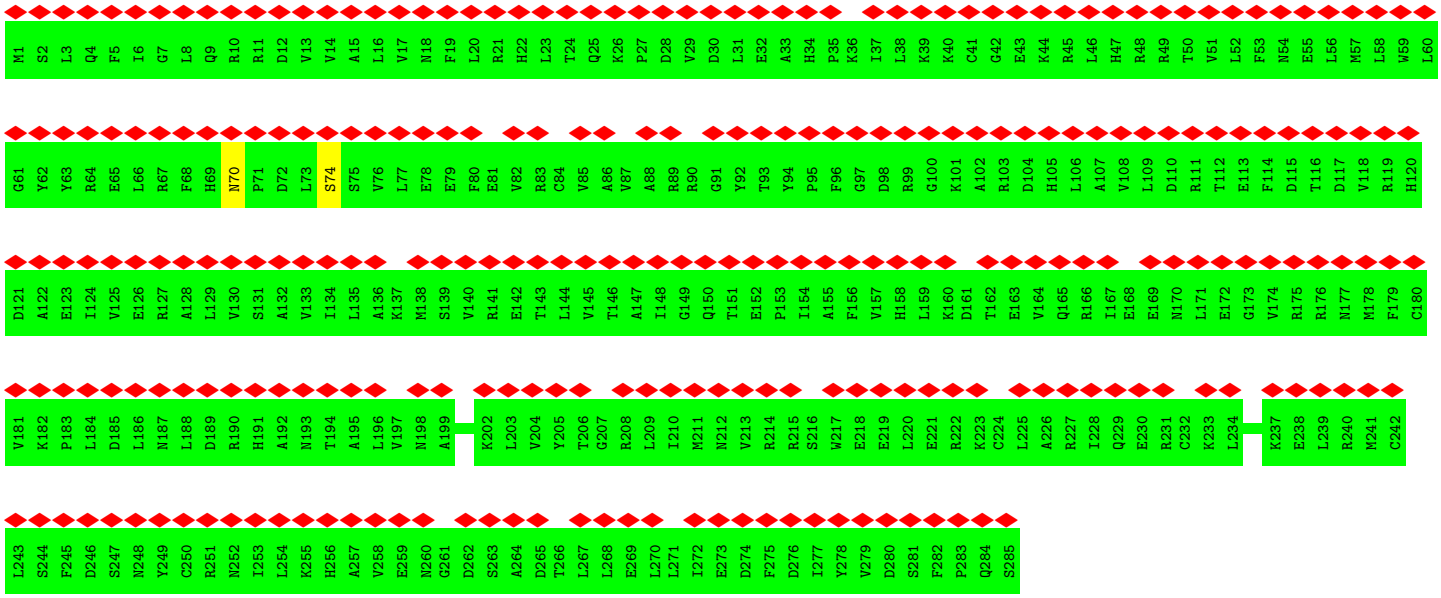



• Molecule 1: Tegument protein pp150

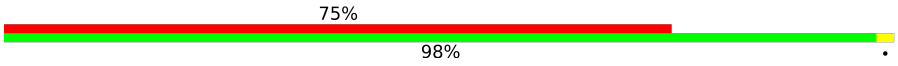
Chain 2:




• Molecule 1: Tegument protein pp150

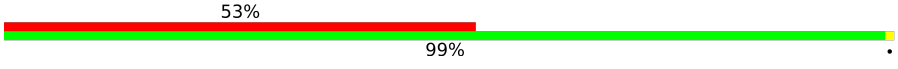
Chain 3:

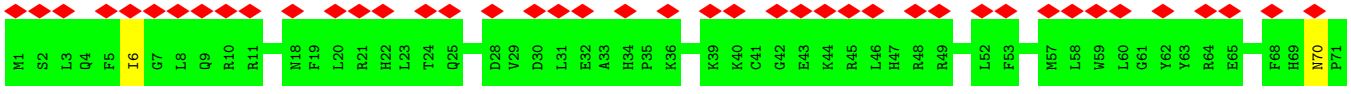


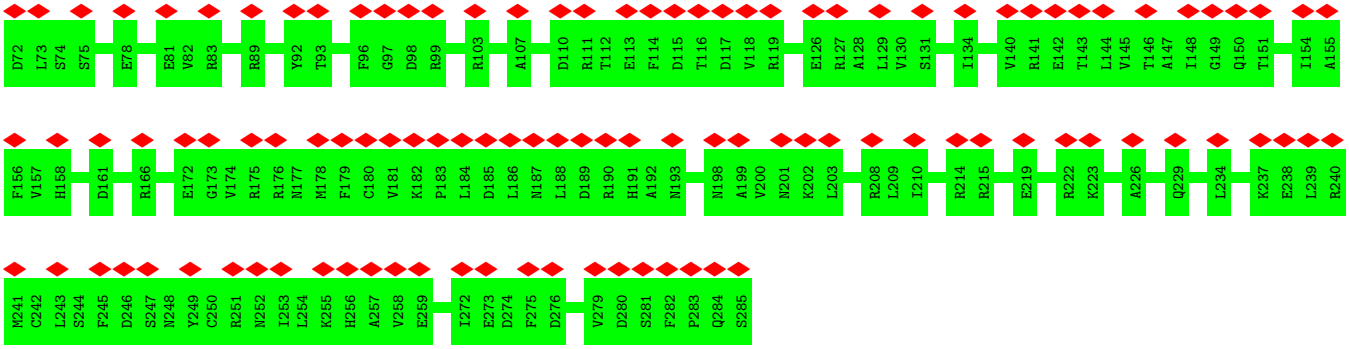


• Molecule 1: Tegument protein pp150

Chain 4:

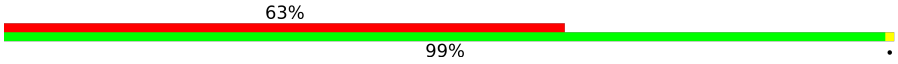


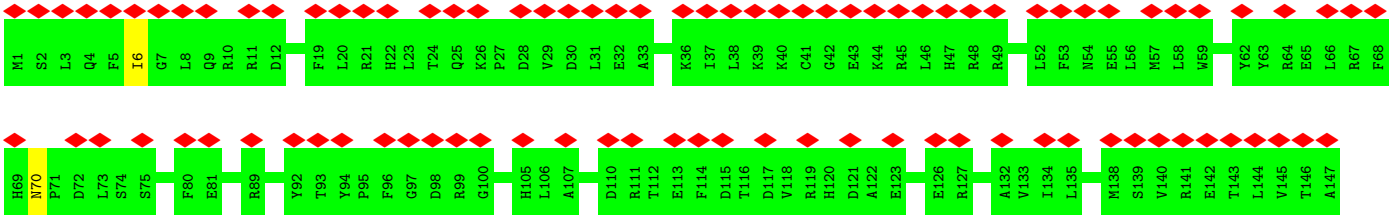






• Molecule 1: Tegument protein pp150

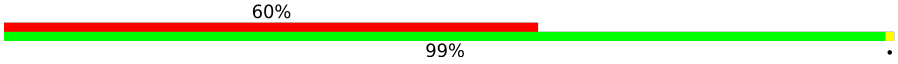
Chain 5:

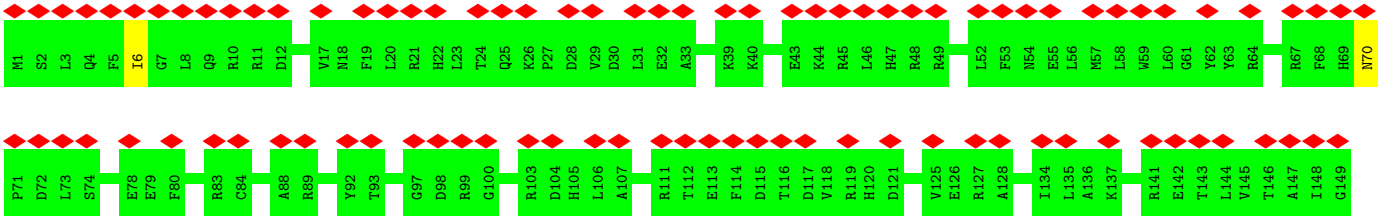


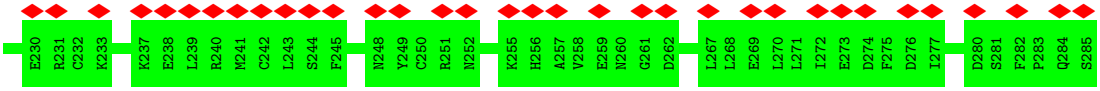




• Molecule 1: Tegument protein pp150

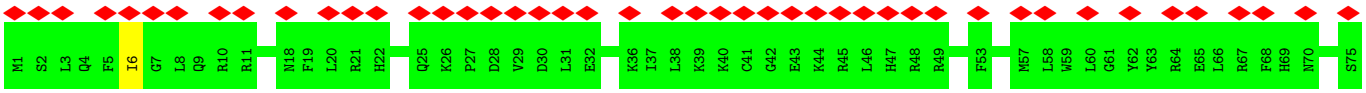
Chain 6:

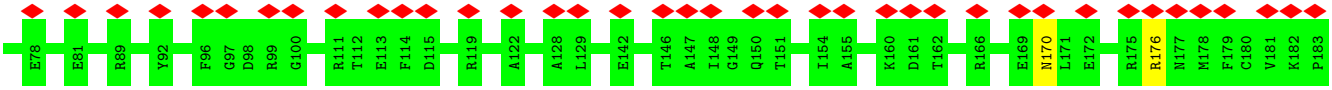


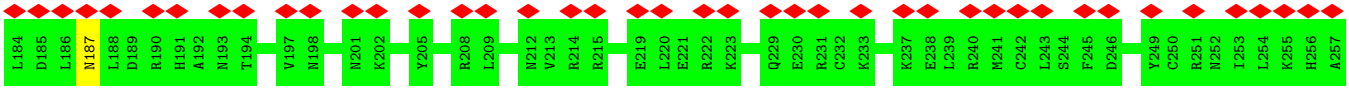



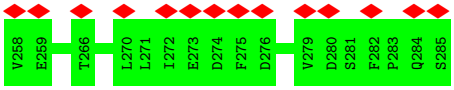



• Molecule 1: Tegument protein pp150

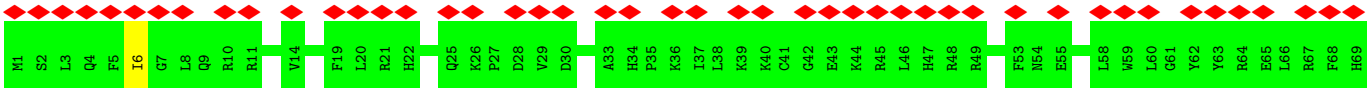



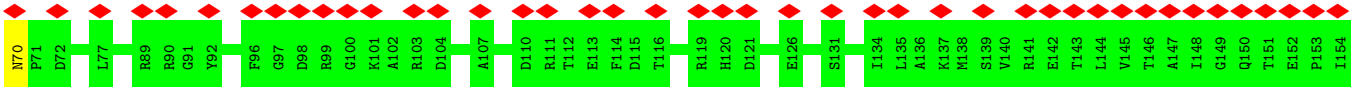



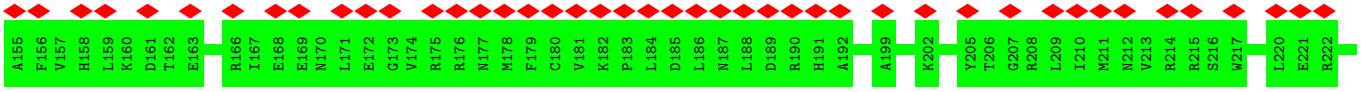



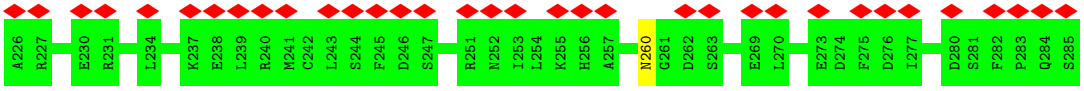




• Molecule 1: Tegument protein pp150

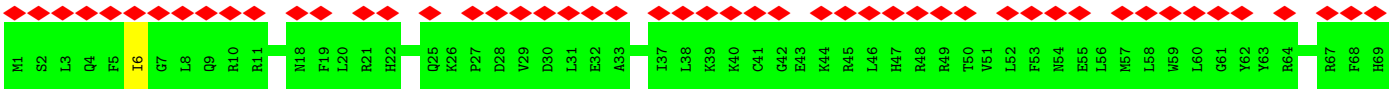



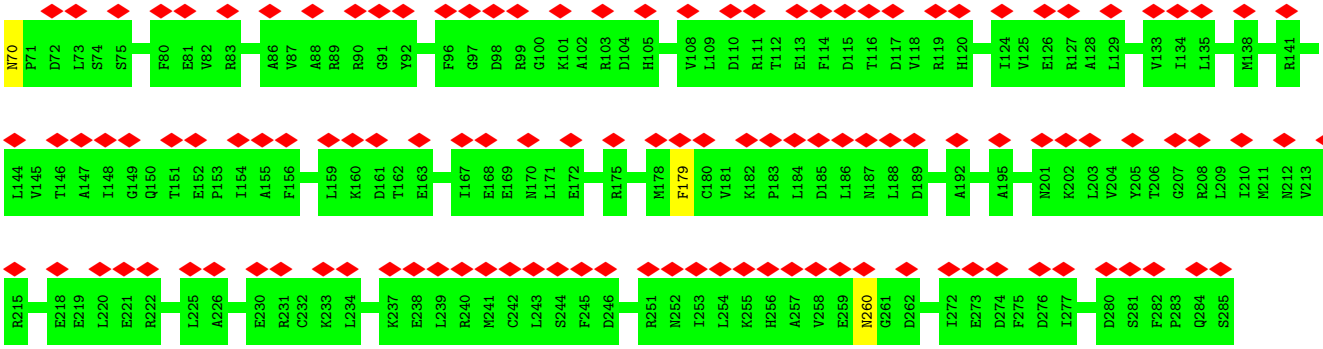



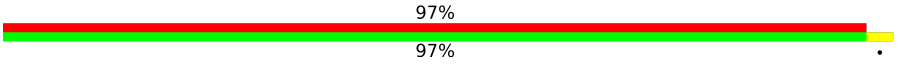

• Molecule 1: Tegument protein pp150

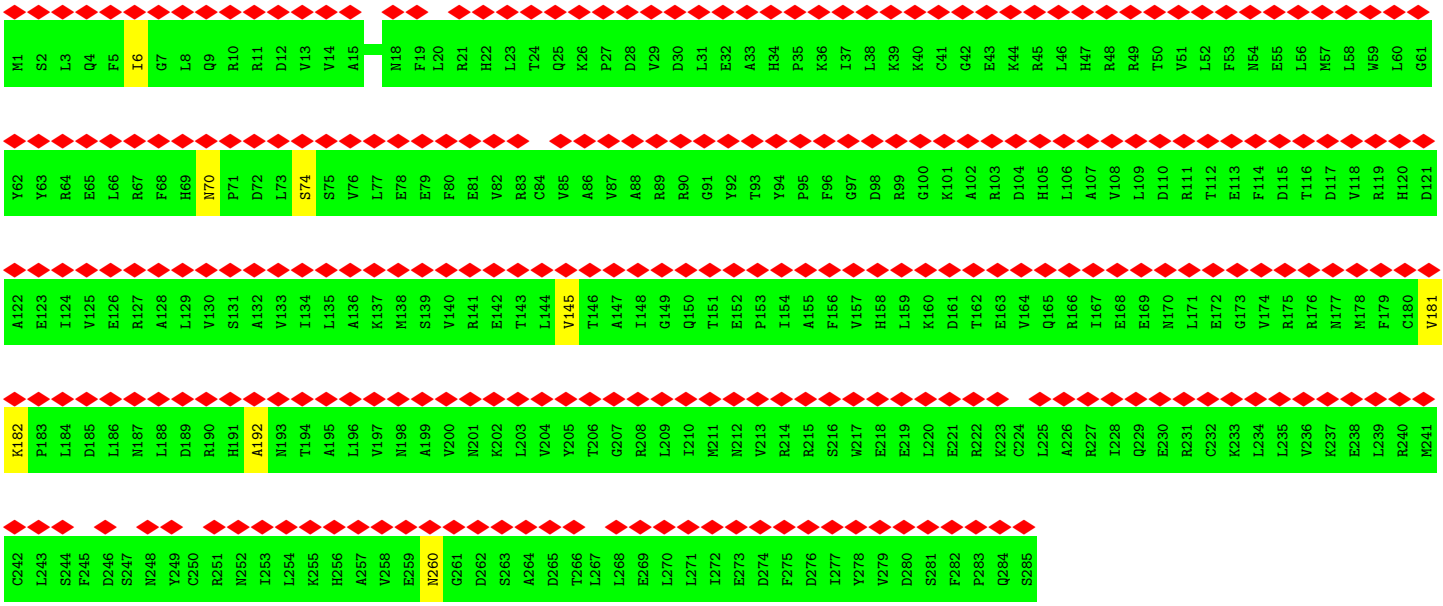






• Molecule 1: Tegument protein pp150

Chain v:




• Molecule 1: Tegument protein pp150

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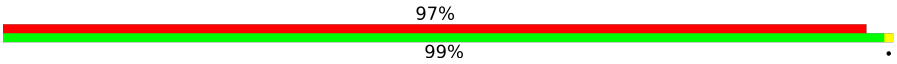
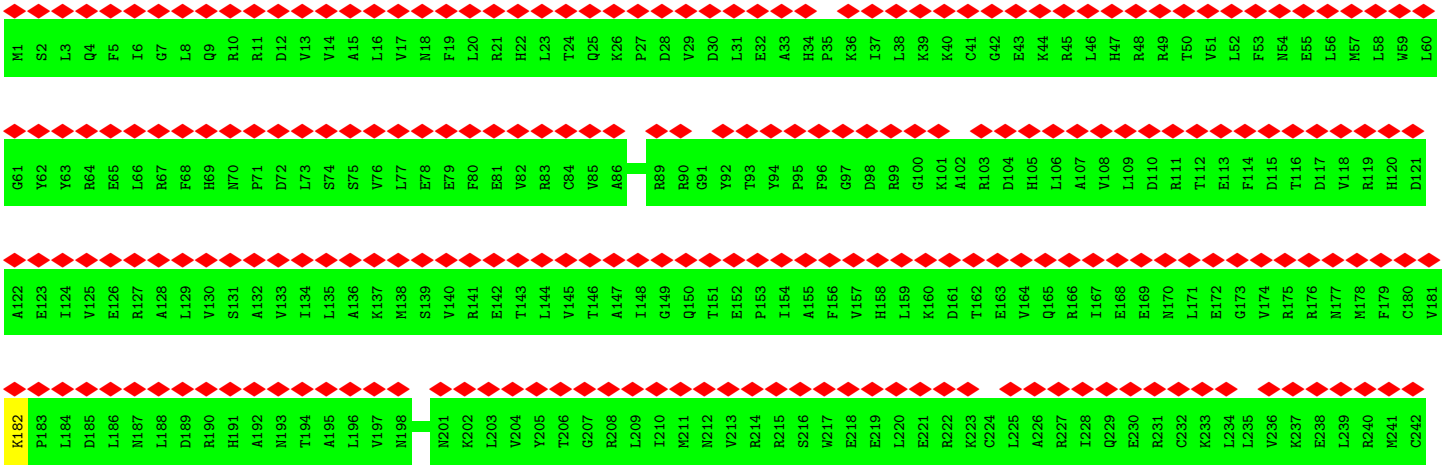
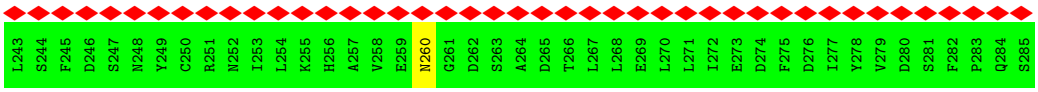
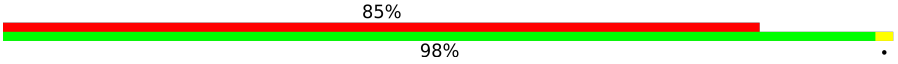


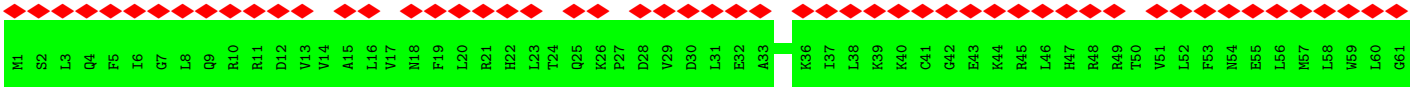



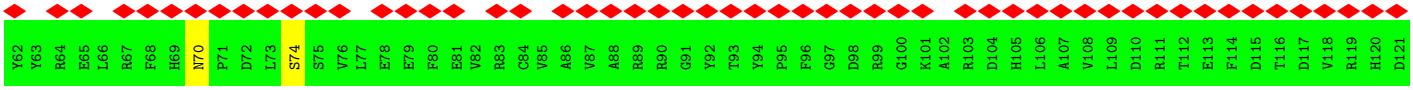


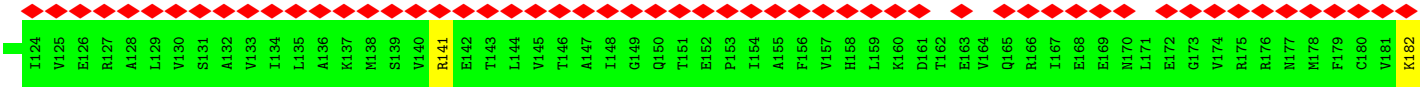

• Molecule 1: Tegument protein pp150

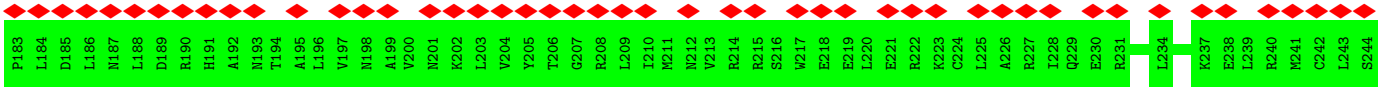
Chain x:

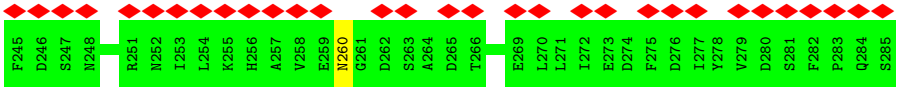


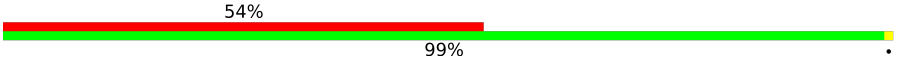



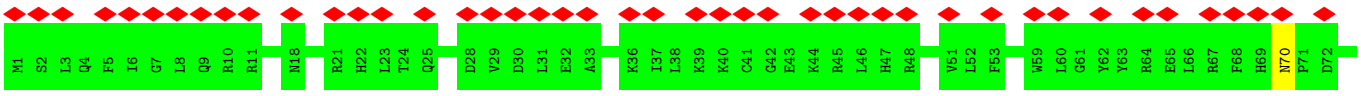



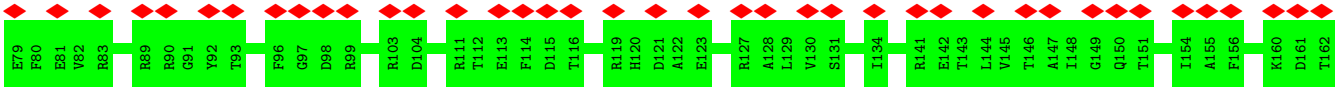



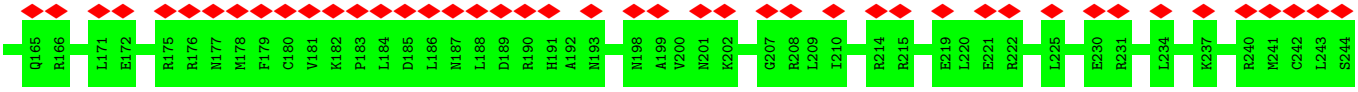

• Molecule 1: Tegument protein pp150

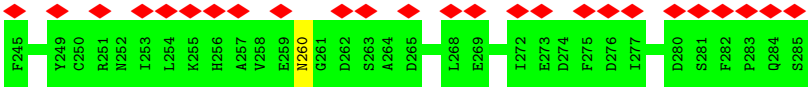
Chain y:



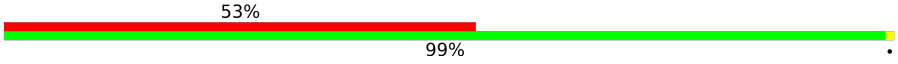



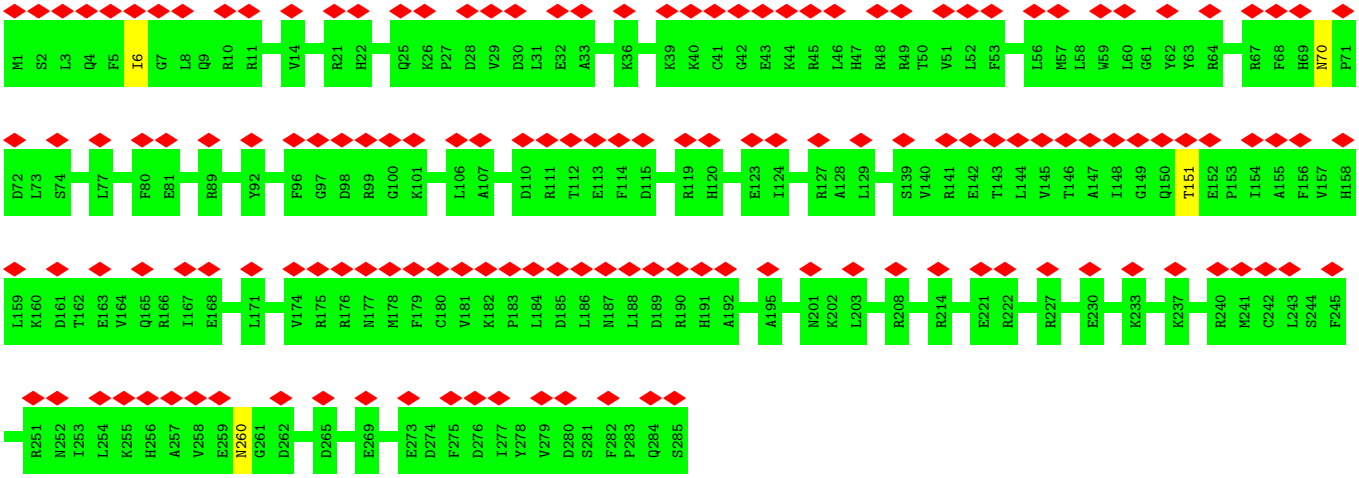




• Molecule 1: Tegument protein pp150

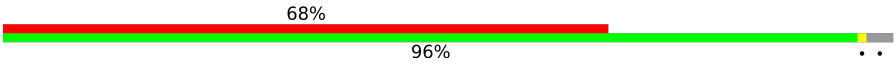
Chain z:

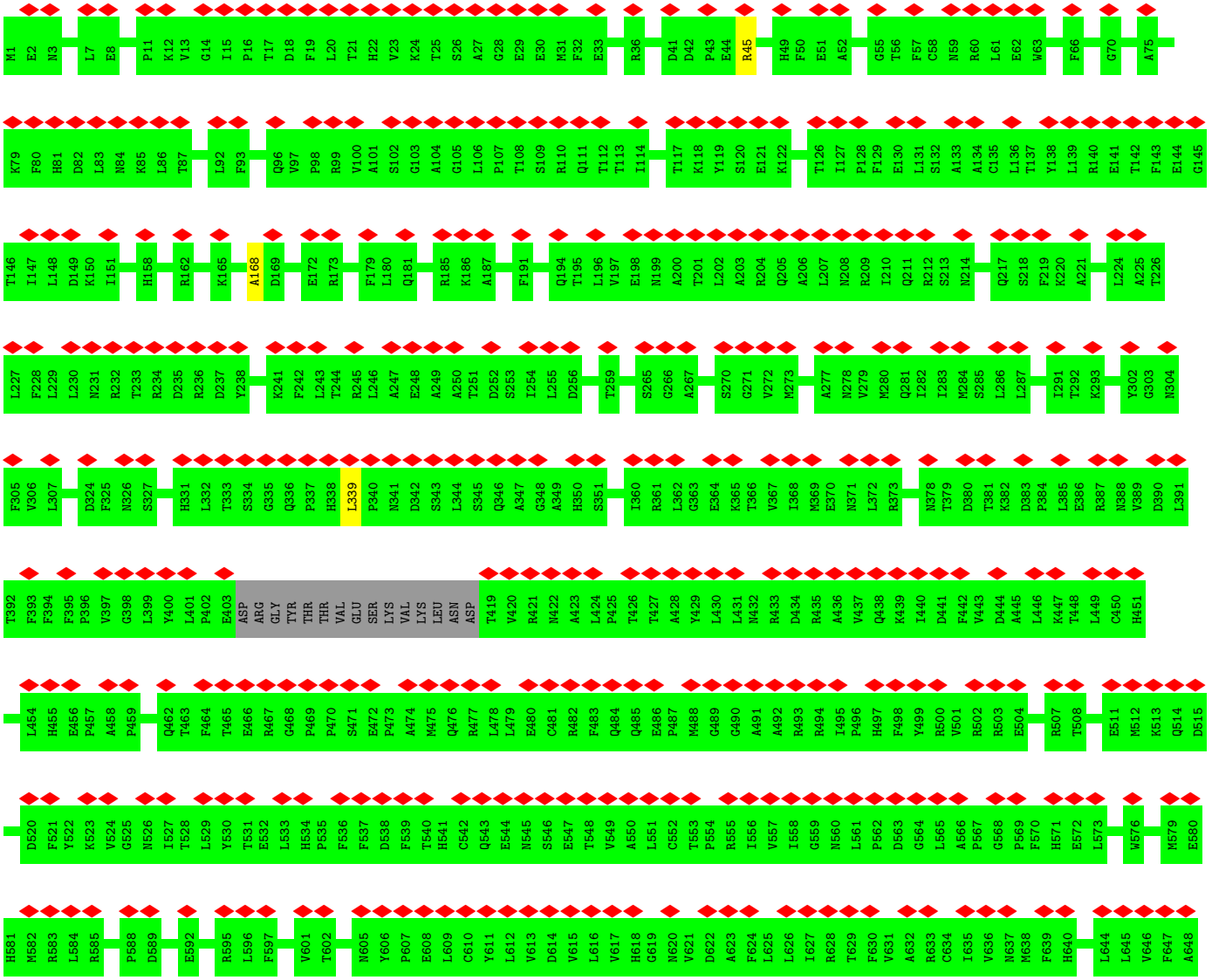


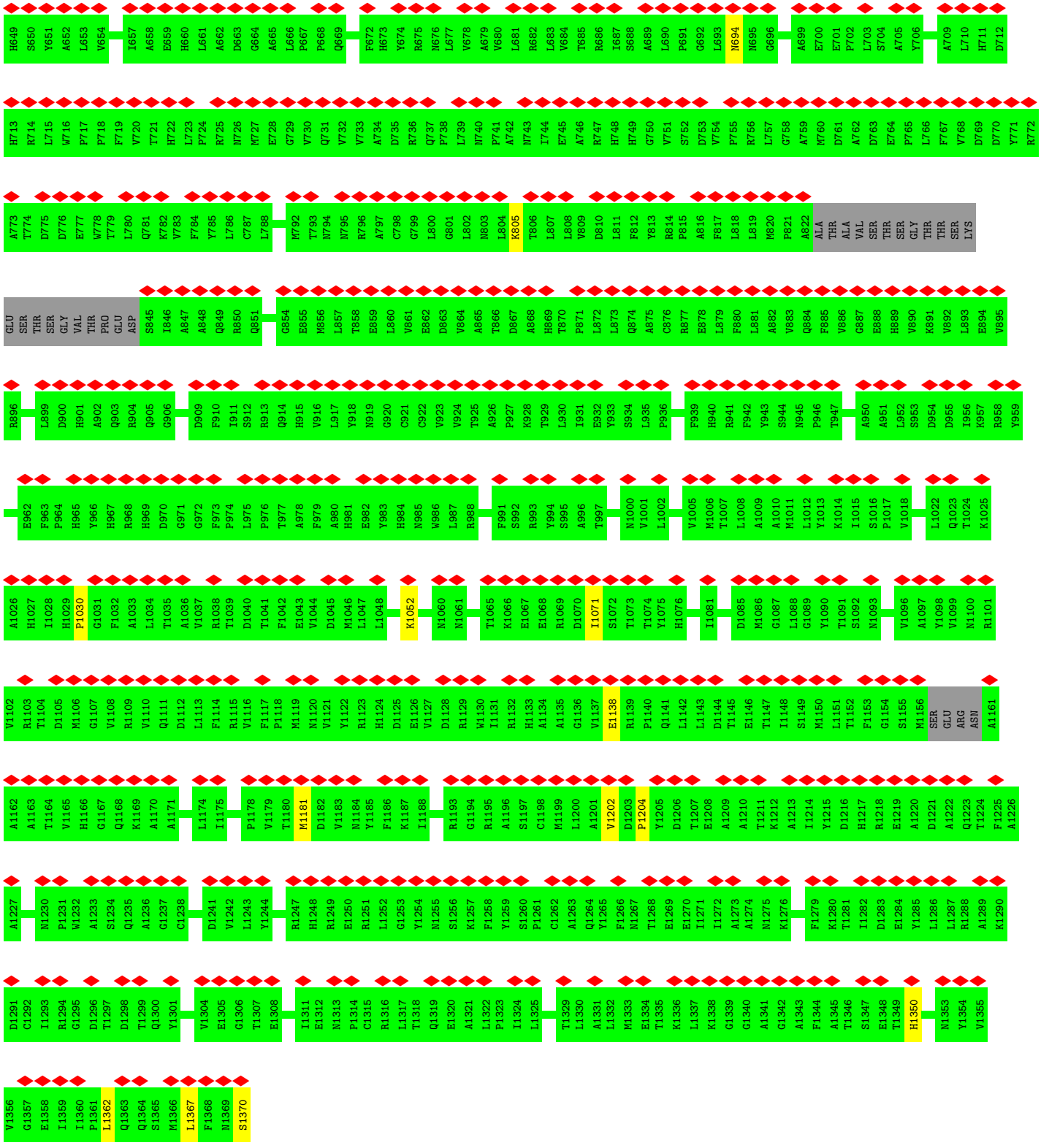



• Molecule 2: Major capsid protein

Chain A:

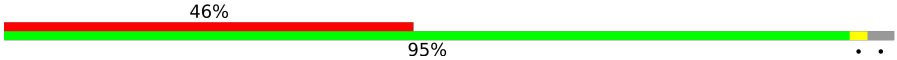


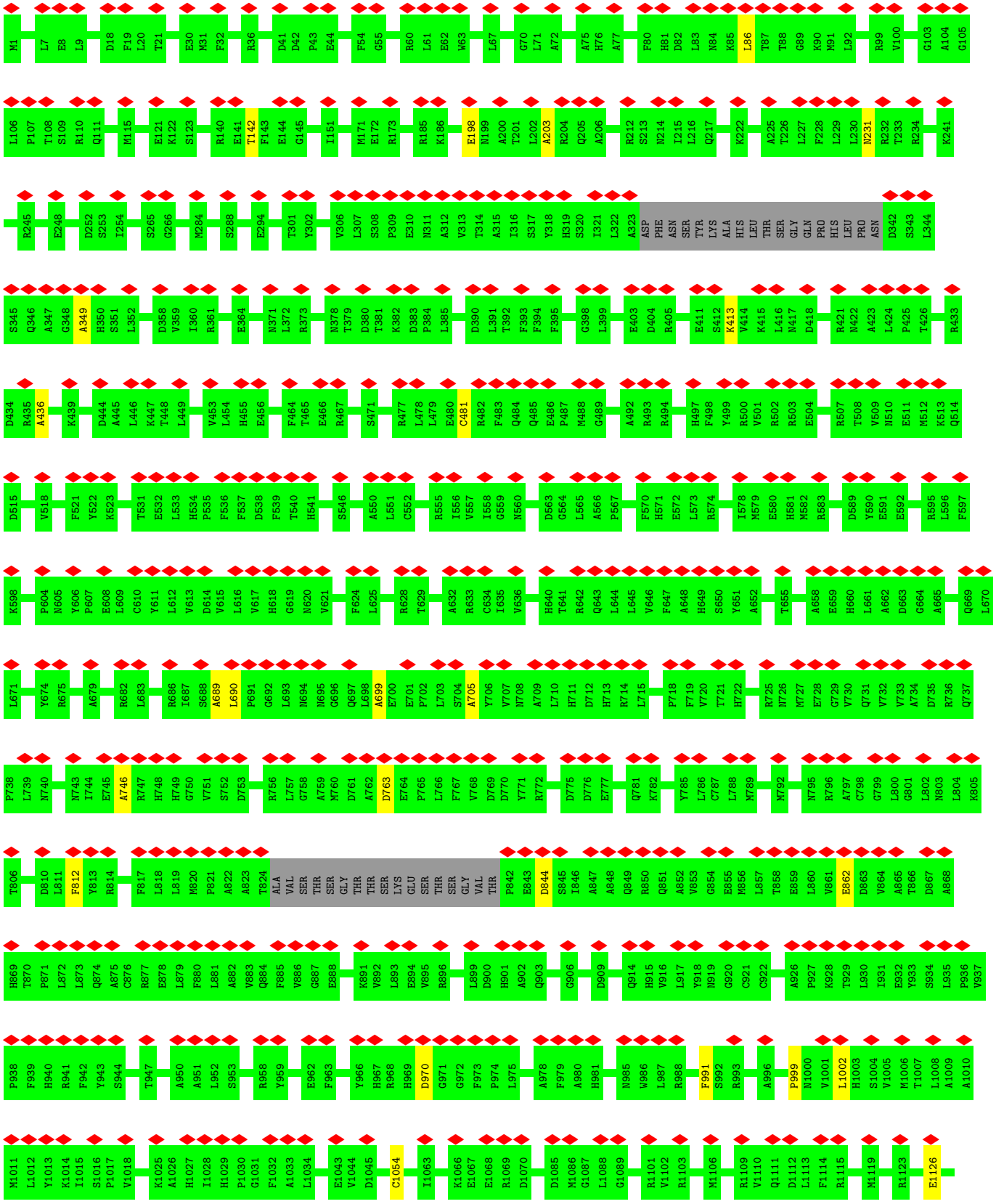






• Molecule 2: Major capsid protein

Chain B:

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L106 P107 T108 S109 R110 Q111 M115 E121 K122 S123 R140 E141 T142 F143 E144 G145 I151 M171 E172 R173 R185 K186 E198 N199 A200 T201 L202 A203 R204 Q205 A206 R212 S213 N214 I215 L216 Q217 K222 A225 T226 L227 F228 L229 L230 N231 R232 T233 R234 K241
R245 E248 D252 S253 I254 S265 G266 M284 S288 E294 T301 Y302 V306 L307 S308 P309 E310 N311 A312 V313 T314 A315 I316 S317 Y318 H319 S320 I321 L322 A323 ASP PHE ASN SER TYR LYS ALA HIS LEU THR SER GLY GLN PRO HIS LEU PRO ASN D342 S343 L344
S345 Q346 A347 G348 A349 H350 S351 L352 D358 V359 I360 R361 E364 N371 L372 R373 N378 T379 D380 T381 K382 D383 P384 L385 D390 L391 T392 F393 F394 F395 G398 L399 E403 D404 R405 E411 S412 K413 V414 K415 L416 N417 D418 R421 N422 A423 L424 P425 T426 R433
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L671 Y674 R675 A679 R682 L683 R686 I687 S688 A689 L690 P691 G692 L693 N694 N695 G696 Q697 L698 A699 E700 E701 P702 L703 S704 A705 Y706 V707 N708 A709 L710 H711 D712 H713 R714 L715 P718 F719 V720 T721 H722 R725 N726 M727 E728 G729 V730 Q731 V732 V733 A734 D735 R736 Q737
P738 L739 N740 N743 I744 E745 A746 R747 H748 H749 G750 V751 S752 D753 R756 L757 G758 A759 M760 D761 A762 D763 E764 P765 L766 F767 V768 D769 D770 Y771 R772 D775 D776 E777 Q781 K782 Y785 L786 C787 L788 M789 M792 N795 R796 A797 C798 G799 L800 G801 L802 N803 L804 K805
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P938 F939 H940 R941 F942 Y943 S944 T947 A950 A951 L952 S953 R958 Y959 E962 F963 Y966 H967 R968 H969 D970 G971 G972 F973 P974 L975 A978 F979 A980 H981 N985 W986 L987 R988 F991 S992 R993 A996 P999 N1000 V1001 L1002 H1003 S1004 V1005 M1006 T1007 L1008 A1009 A1010
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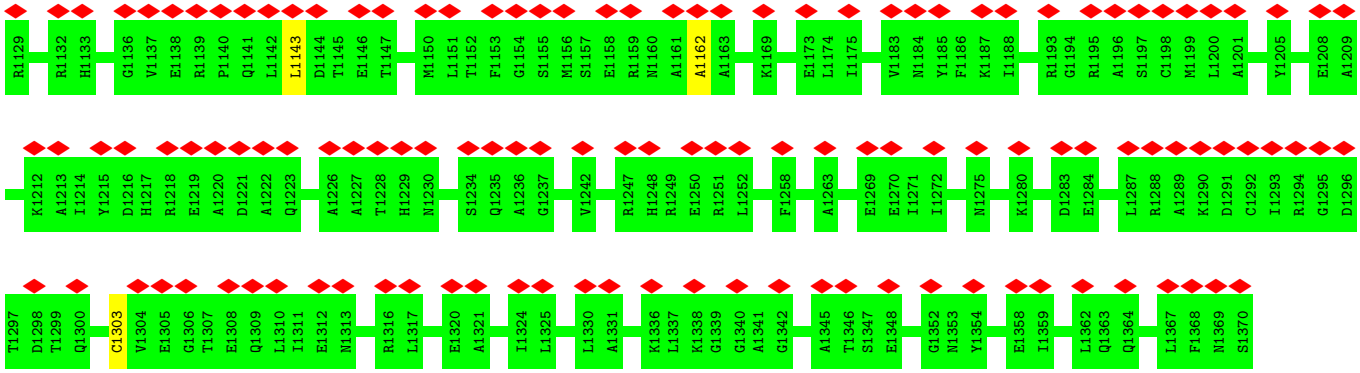
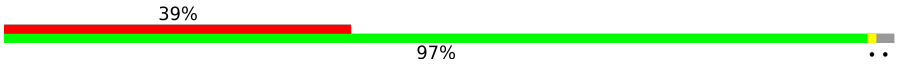
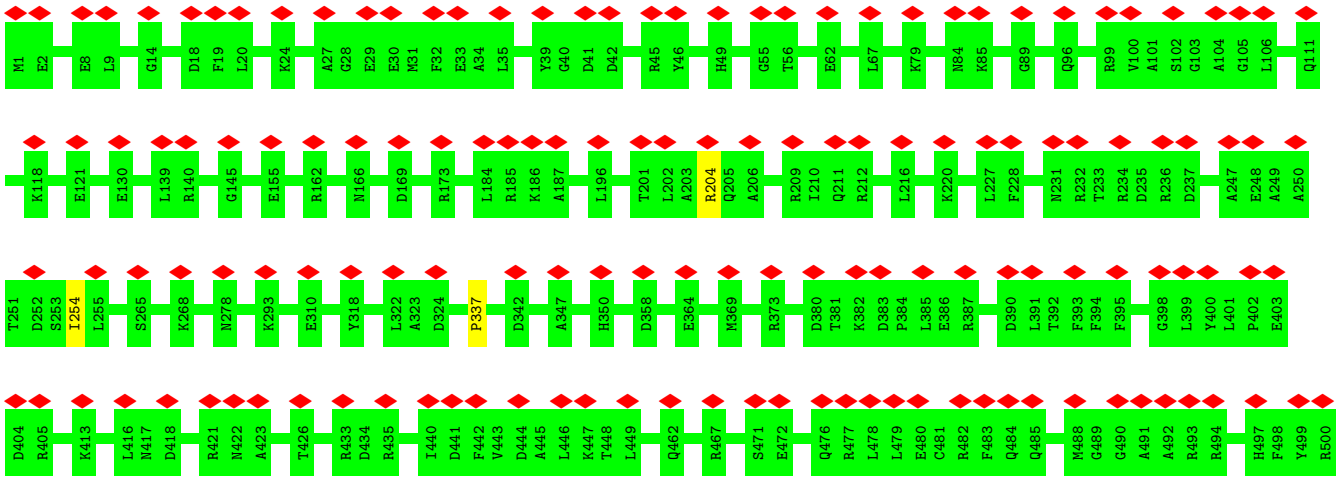



• Molecule 2: Major capsid protein

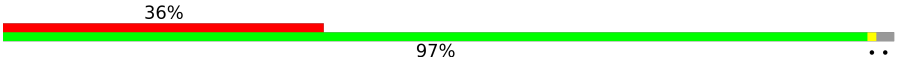
Chain C:

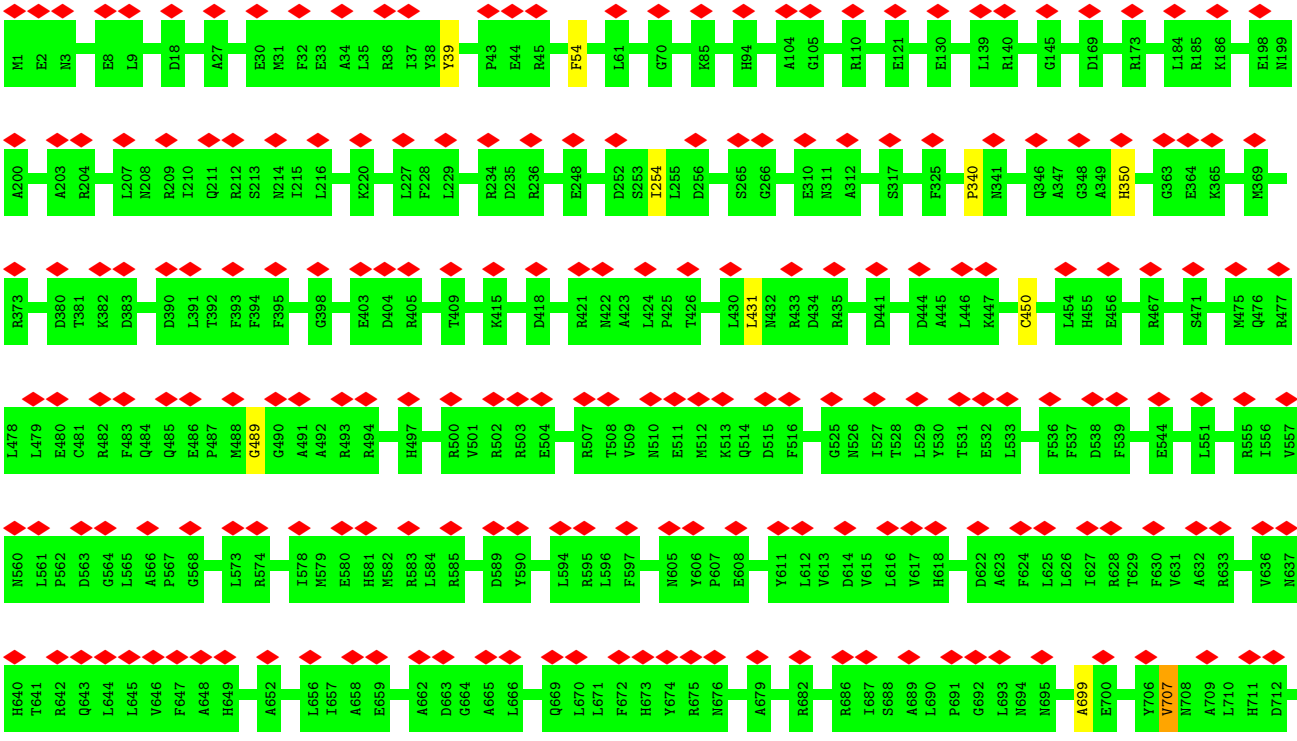


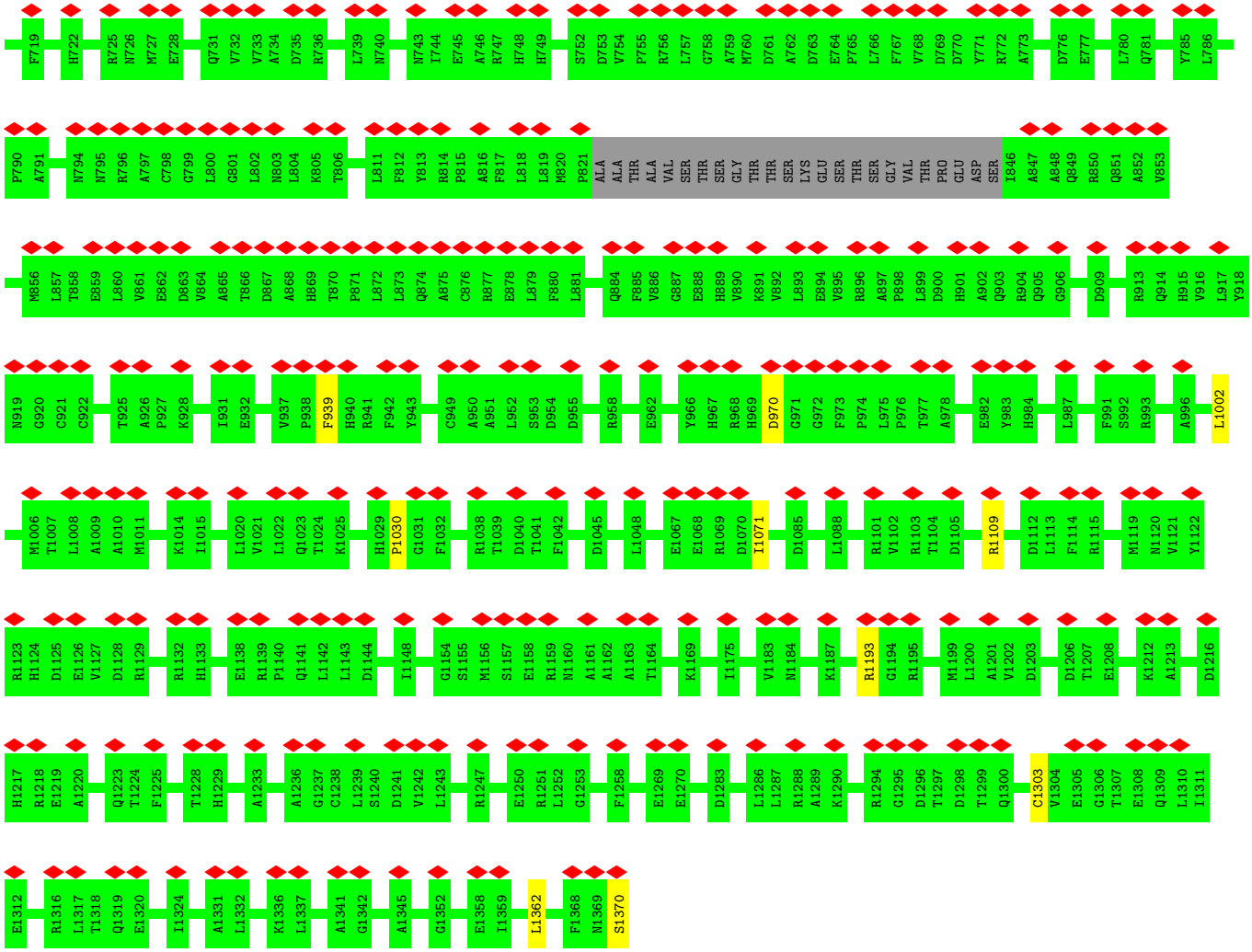




• Molecule 2: Major capsid protein

Chain D:

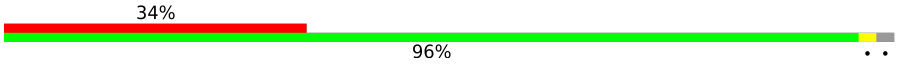


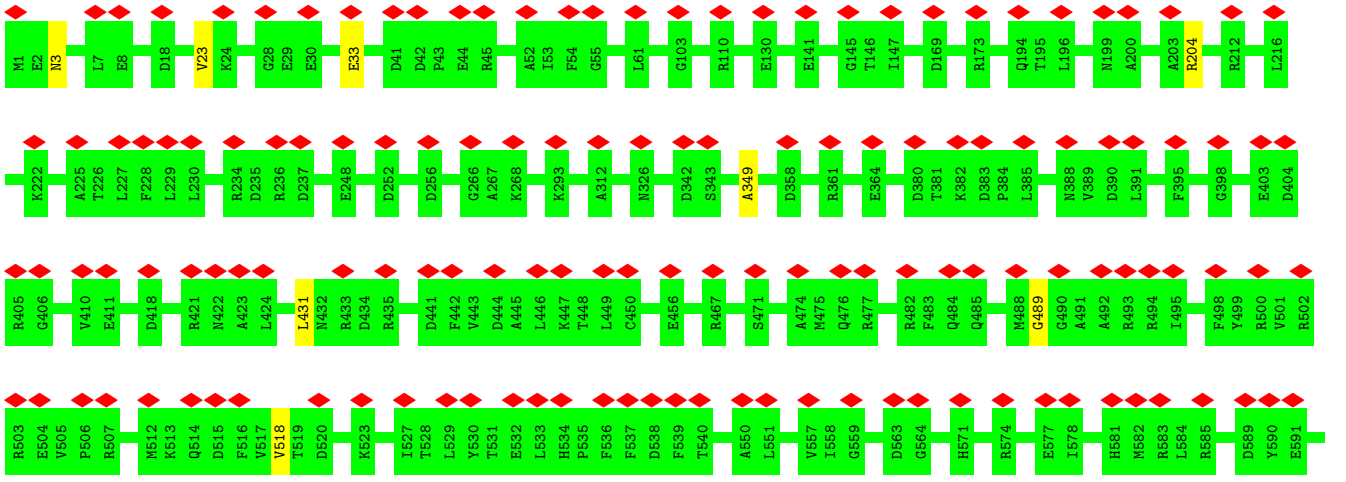






• Molecule 2: Major capsid protein

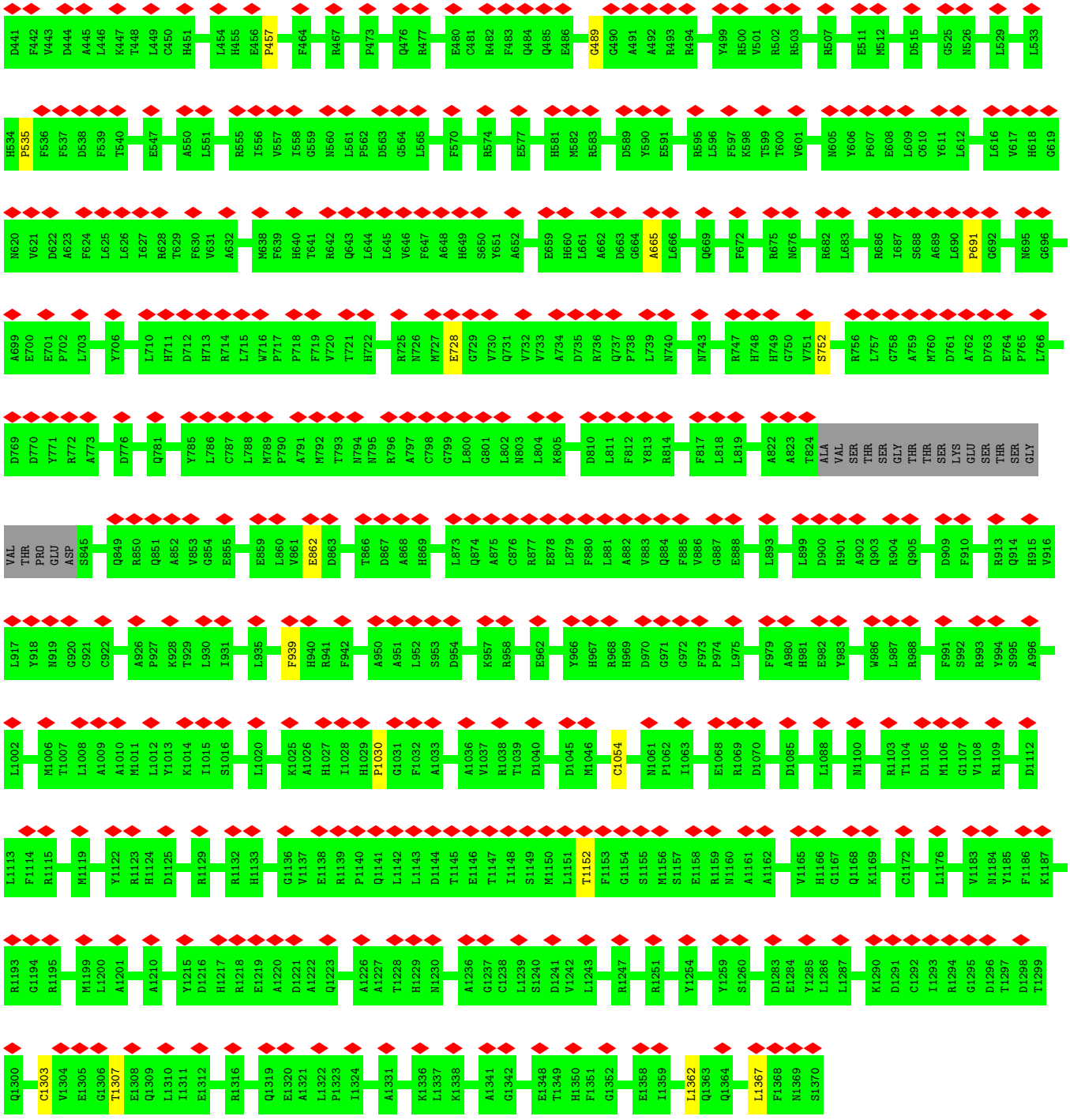
Chain E:



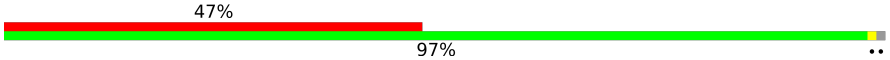
• Molecule 2: Major capsid protein

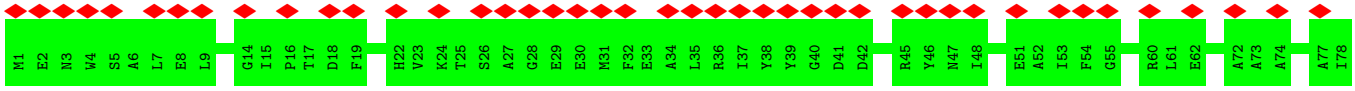
Chain F:

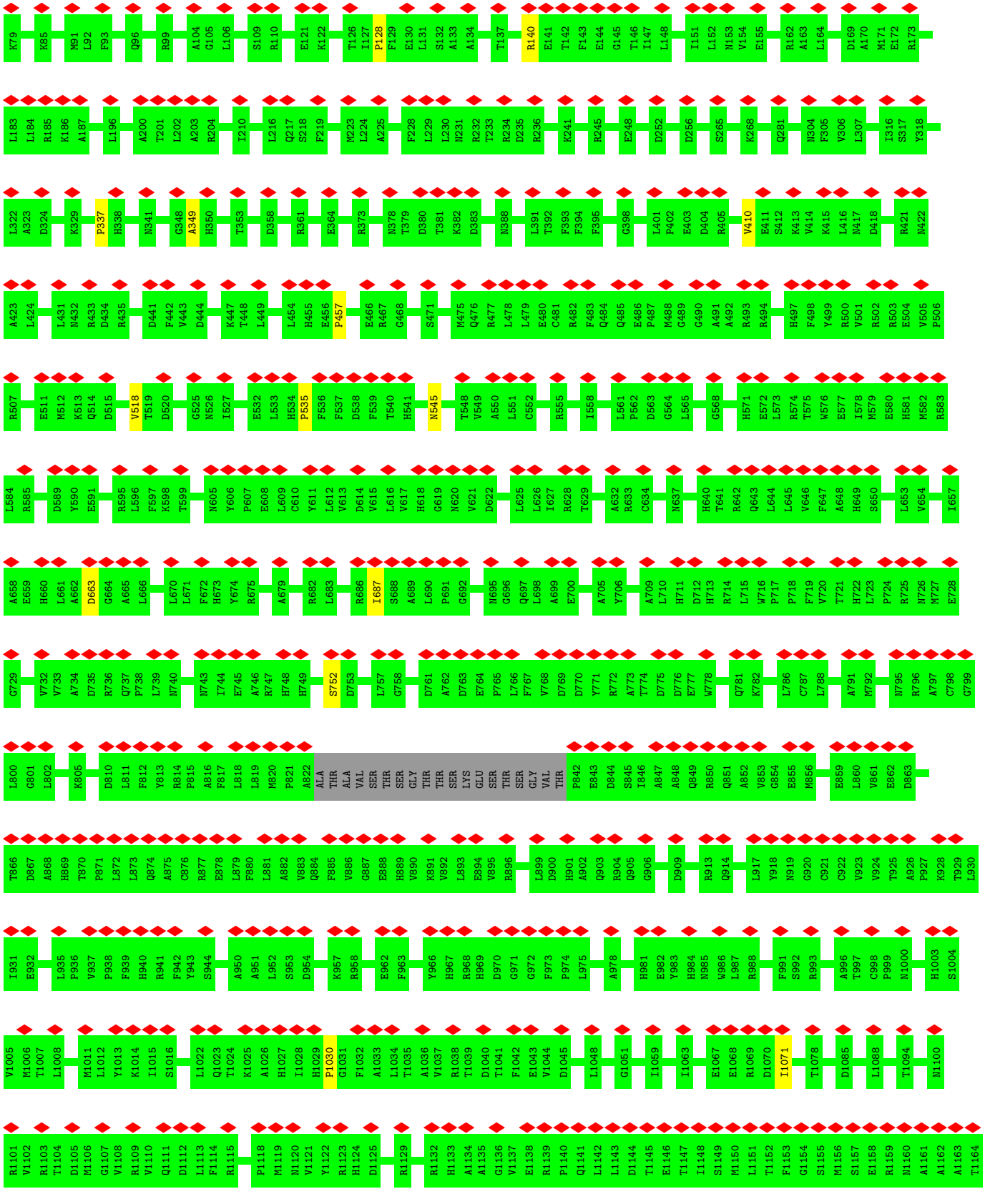



• Molecule 2: Major capsid protein

Chain G:

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L183 L184 R185 K186 A187 L196 A200 T201 L202 A203 R204 I210 L216 Q217 S218 F219 M223 L224 A225 F228 L229 L230 N231 R232 T233 R234 D235 R236 K241 R245 E248 D252 D256 S265 K268 Q281 N304 F305 V306 L307 I316 S317 Y318
L322 A323 D324 K329 P337 H338 N341 G348 A349 H350 T353 D358 R361 E364 R373 N378 T379 D380 T381 K382 D383 N388 L391 T392 F393 F394 F395 G398 L401 P402 E403 D404 R405 V410 E411 S412 K413 V414 K415 L416 N417 D418 R421 N422
A423 L424 L431 N432 R433 D434 R435 D441 F442 V443 D444 K447 T448 L449 L454 H455 E456 P457 E466 R467 G468 S471 M475 Q476 R477 L478 L479 E480 C481 R482 F483 Q484 Q485 E486 P487 M488 G489 G490 A491 A492 R493 R494 H497 F498 Y499 R500 V501 R502 R503 E504 V505 P506
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I931 E932 L935 P936 V937 P938 F939 H940 R941 F942 Y943 S944 A950 A951 L952 S953 D954 K957 R958 E962 F963 Y966 H967 R968 H969 D970 G971 G972 F973 P974 L975 A978 H981 E982 Y983 H984 N985 W986 L987 R988 F991 S992 R993 A996 T997 C998 P999 N1000 H1003 S1004
V1005 M1006 T1007 L1008 M1011 L1012 Y1013 K1014 I1015 S1016 L1022 Q1023 T1024 K1025 A1026 H1027 I1028 H1029 P1030 G1031 F1032 A1033 L1034 T1035 A1036 V1037 R1038 T1039 D1040 T1041 F1042 E1043 V1044 D1045 L1048 G1051 I1059 I1063 E1067 E1068 R1069 D1070 I1071 T1078 D1085 L1088 T1094 N1100
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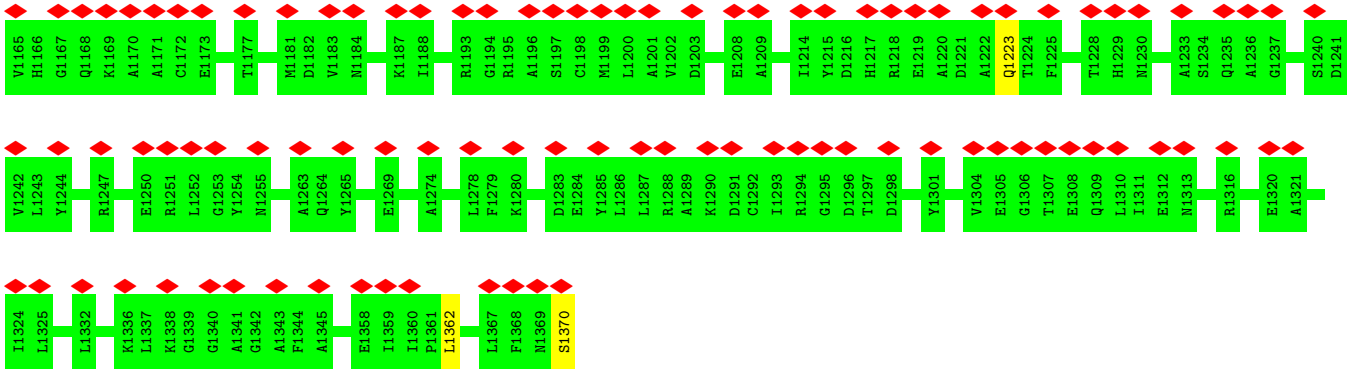
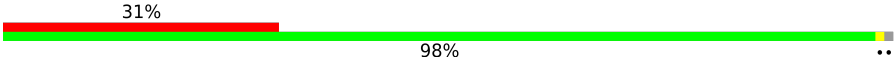
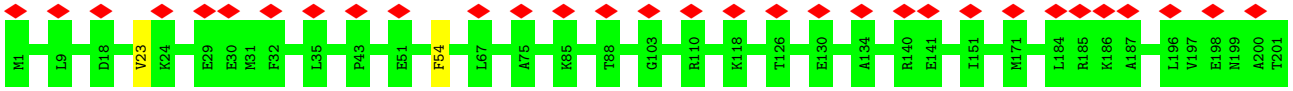
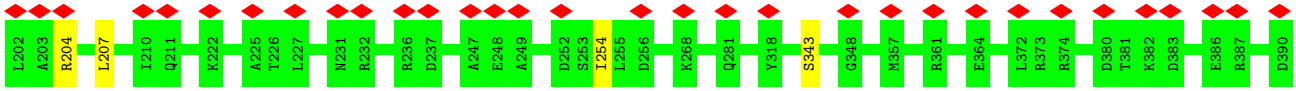


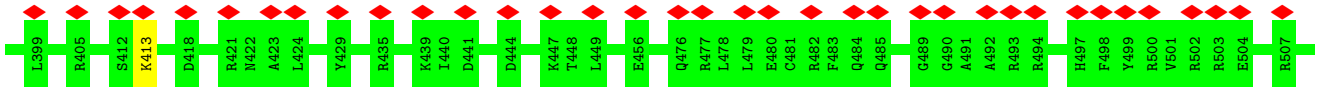

• Molecule 2: Major capsid protein

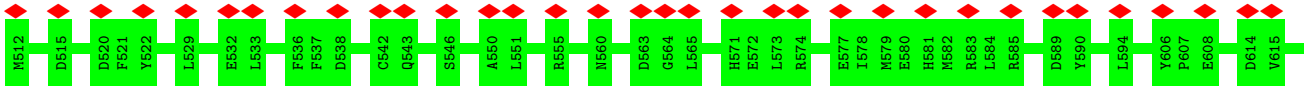
Chain H:

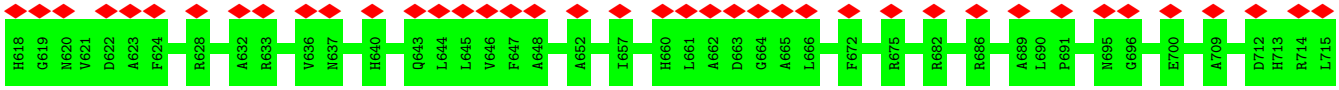


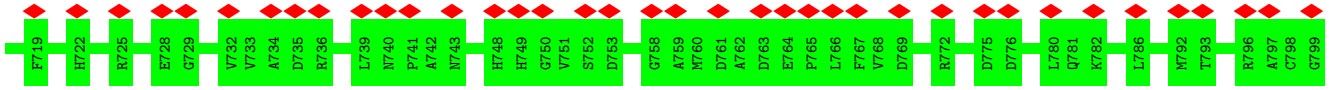



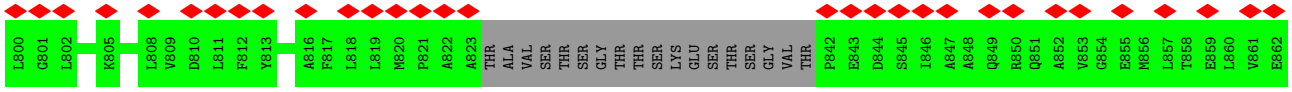



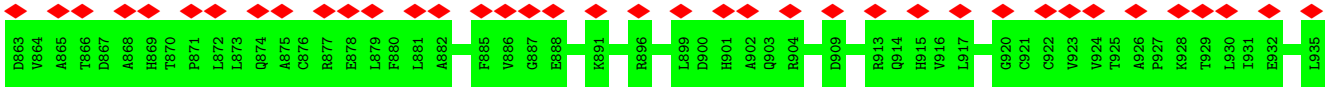



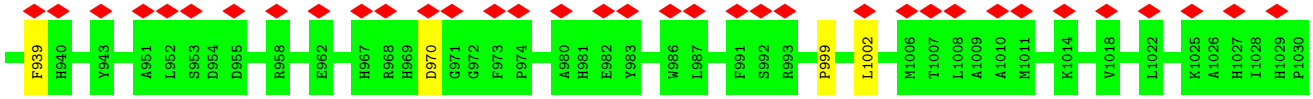



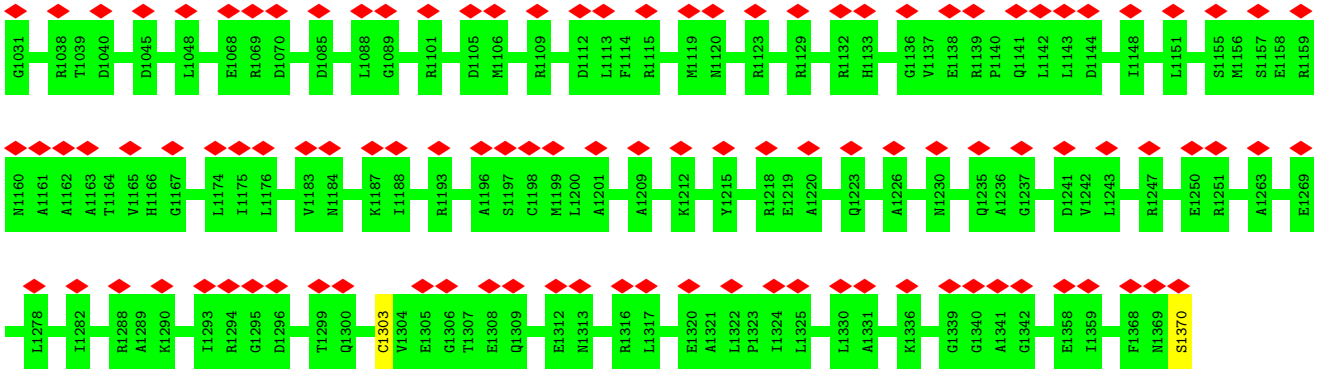



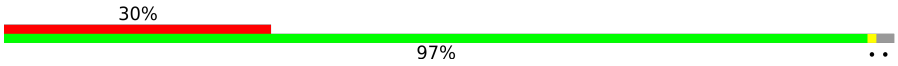



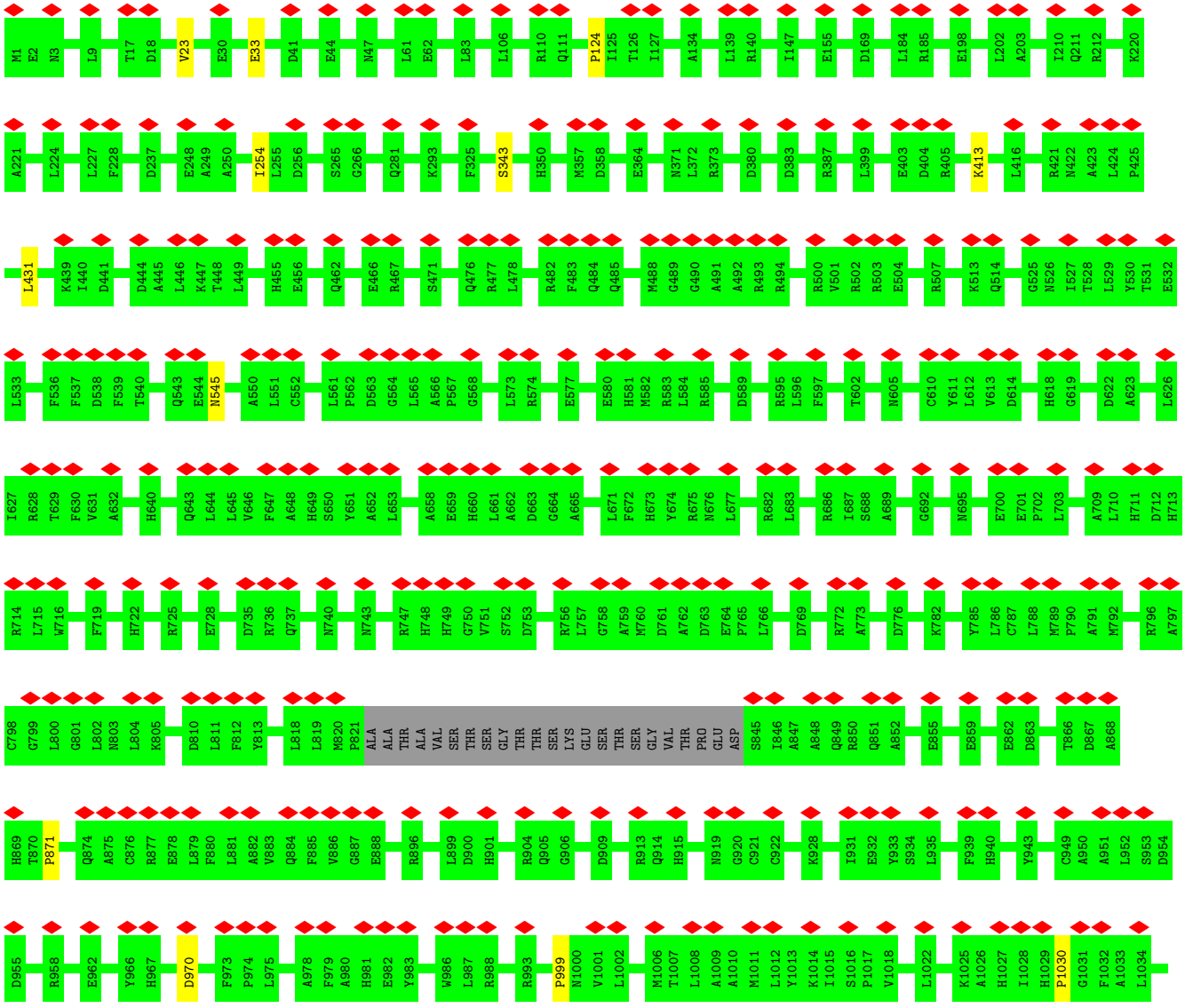



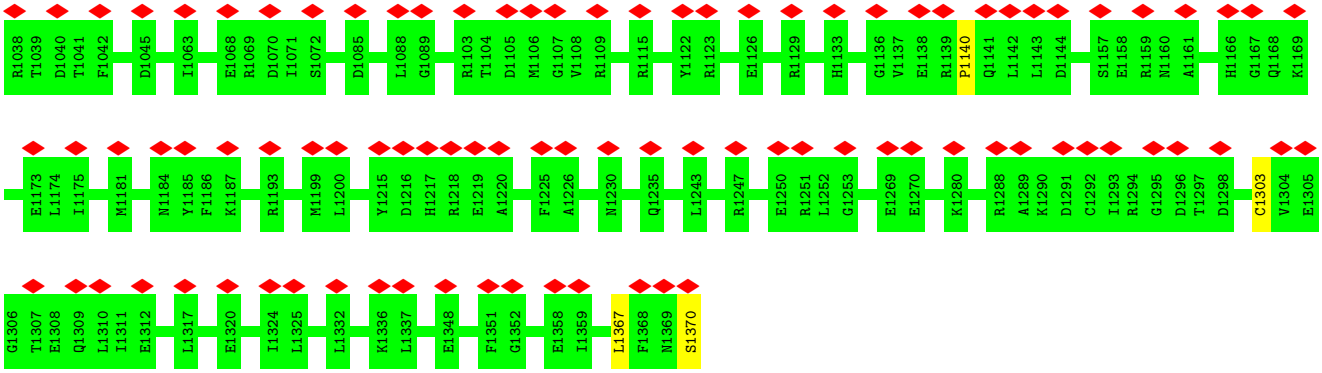



• Molecule 2: Major capsid protein

Chain I:

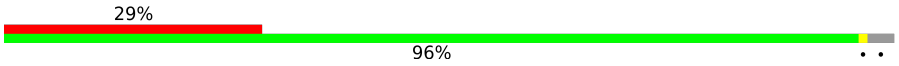


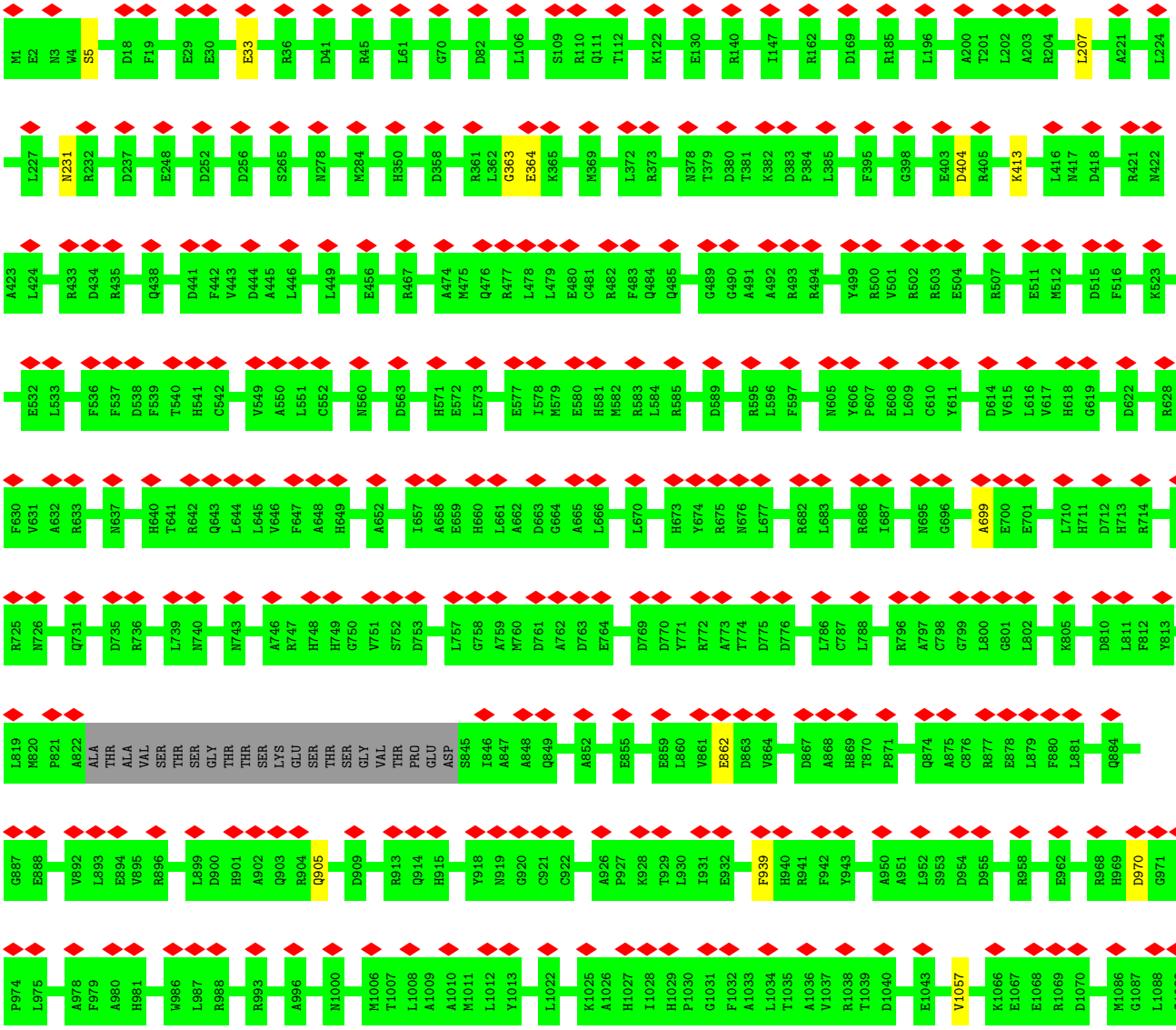



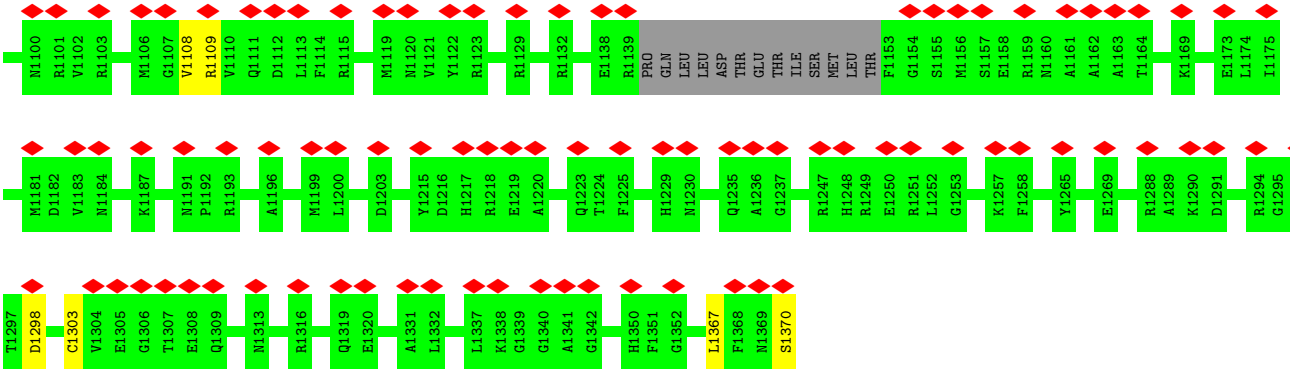



• Molecule 2: Major capsid protein

Chain J:

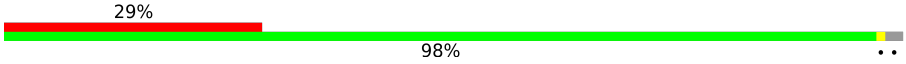


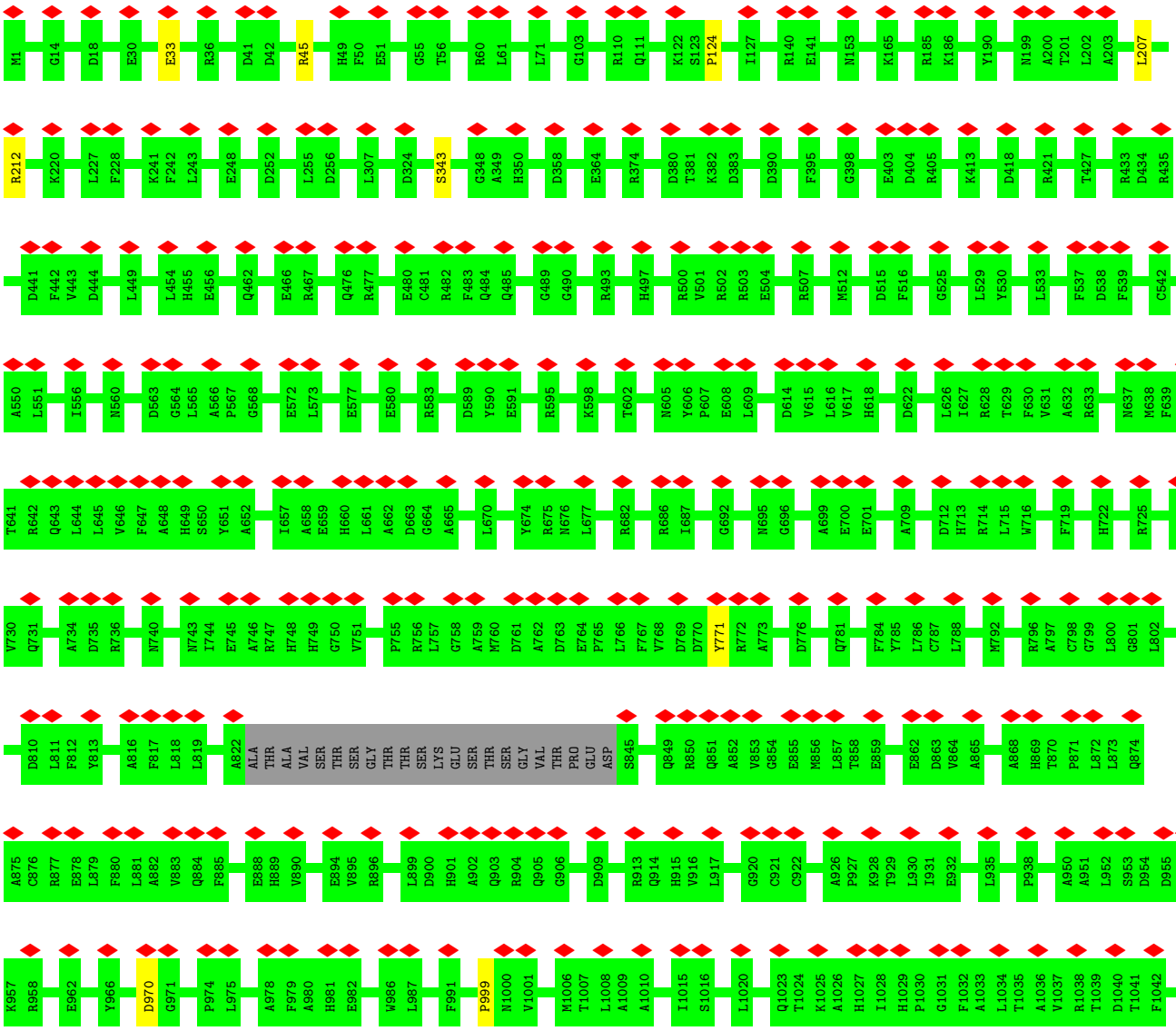



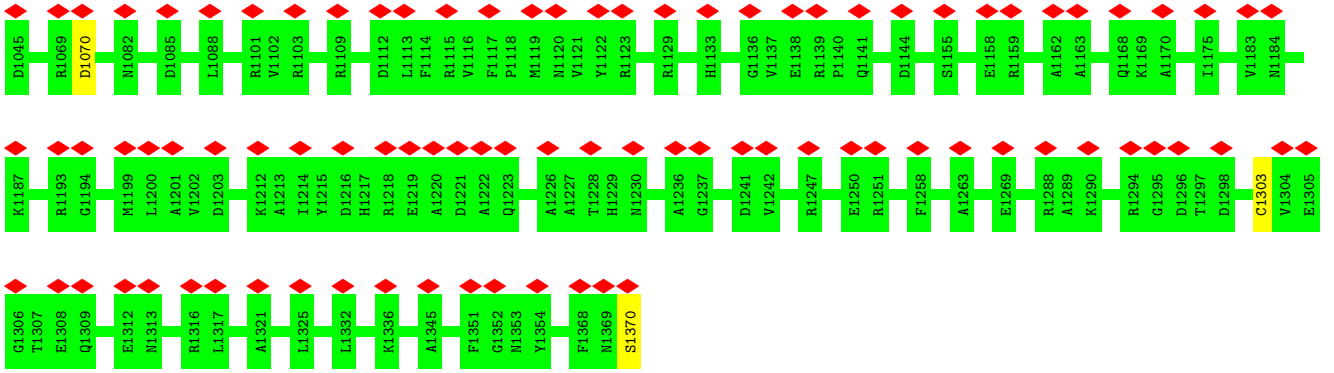



• Molecule 2: Major capsid protein

Chain K:

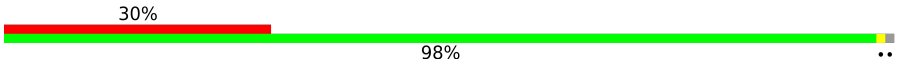


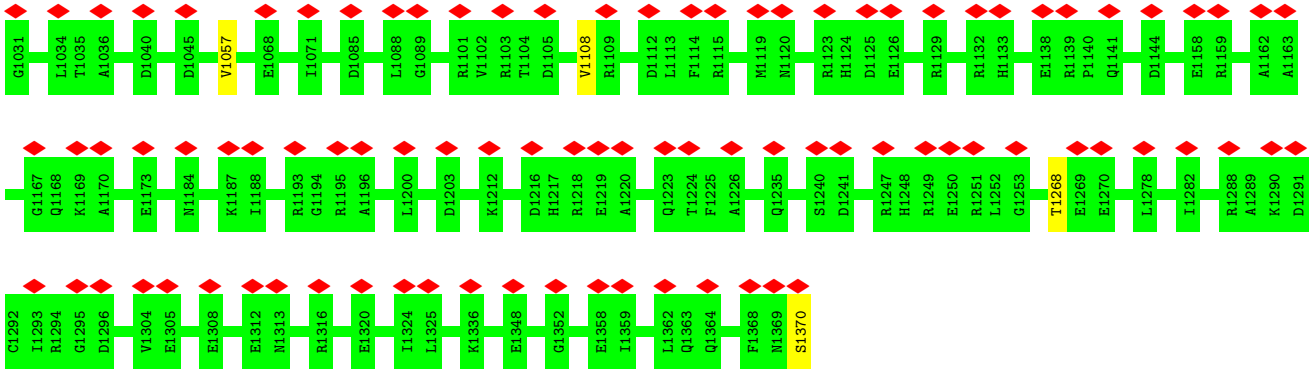






• Molecule 2: Major capsid protein

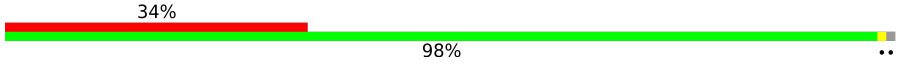
Chain L:

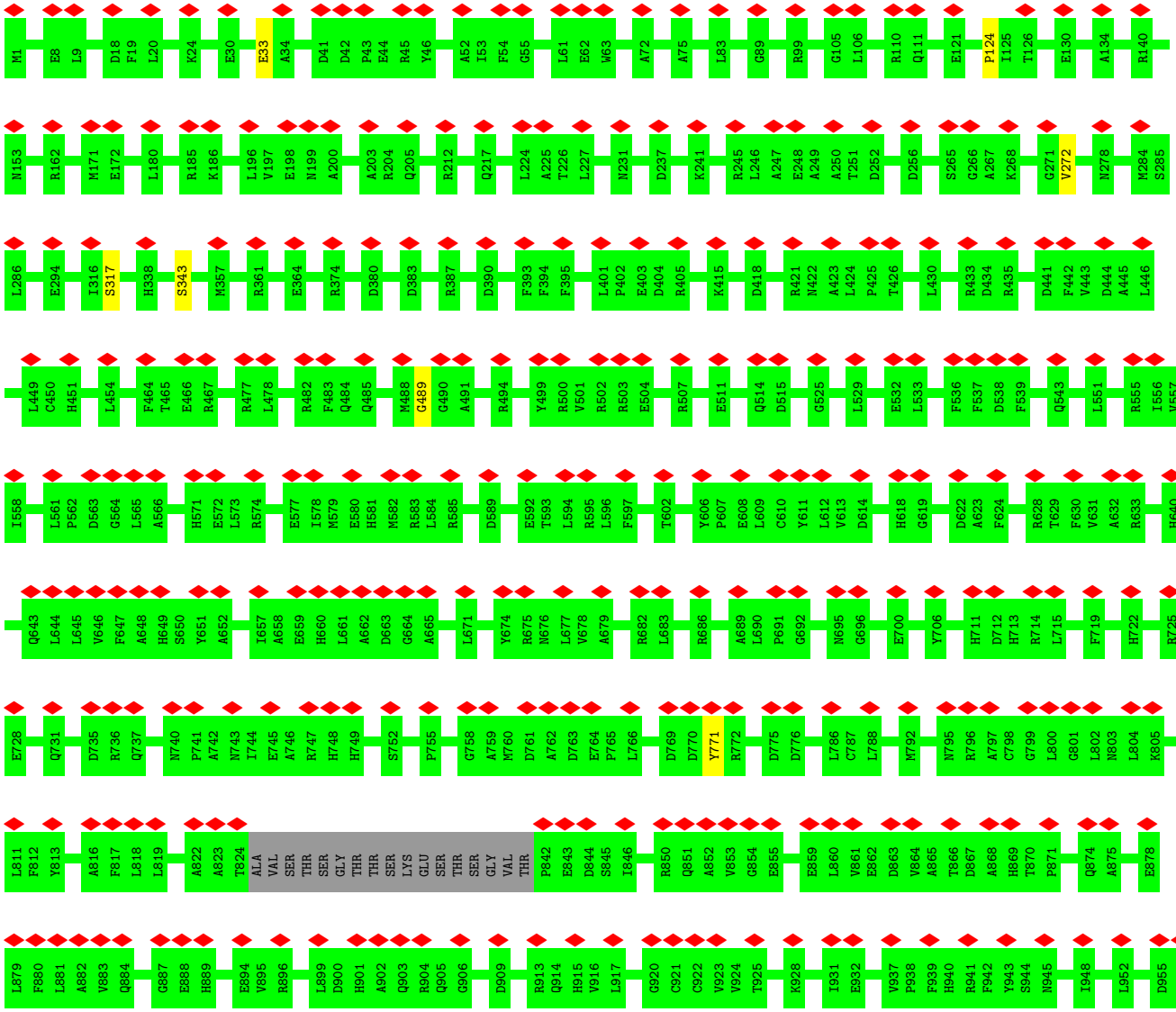


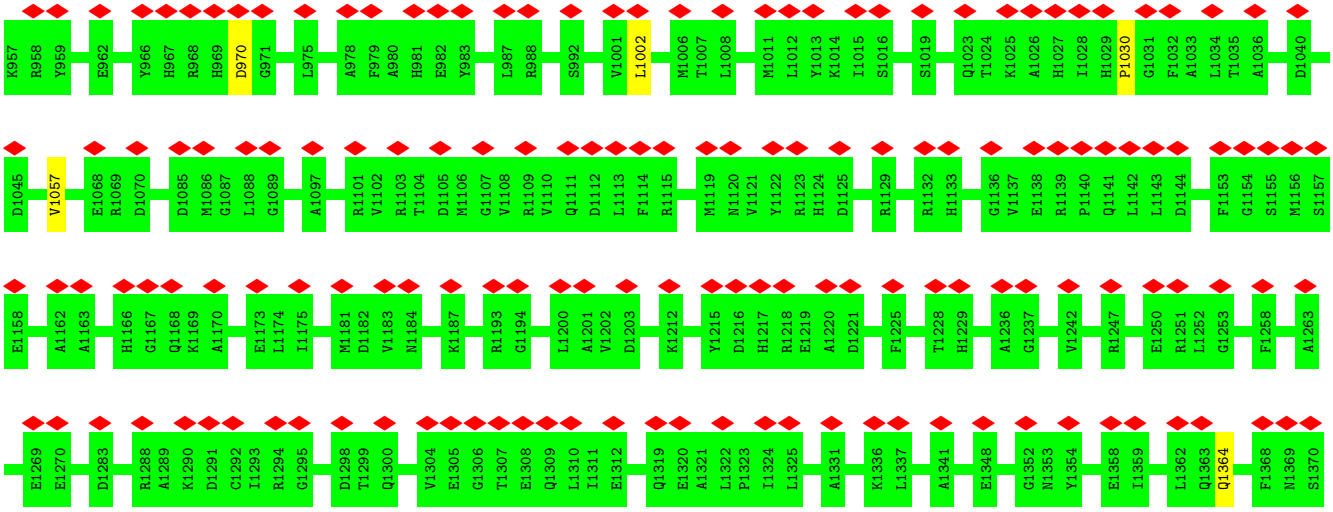




• Molecule 2: Major capsid protein

Chain M:

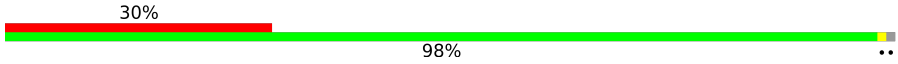


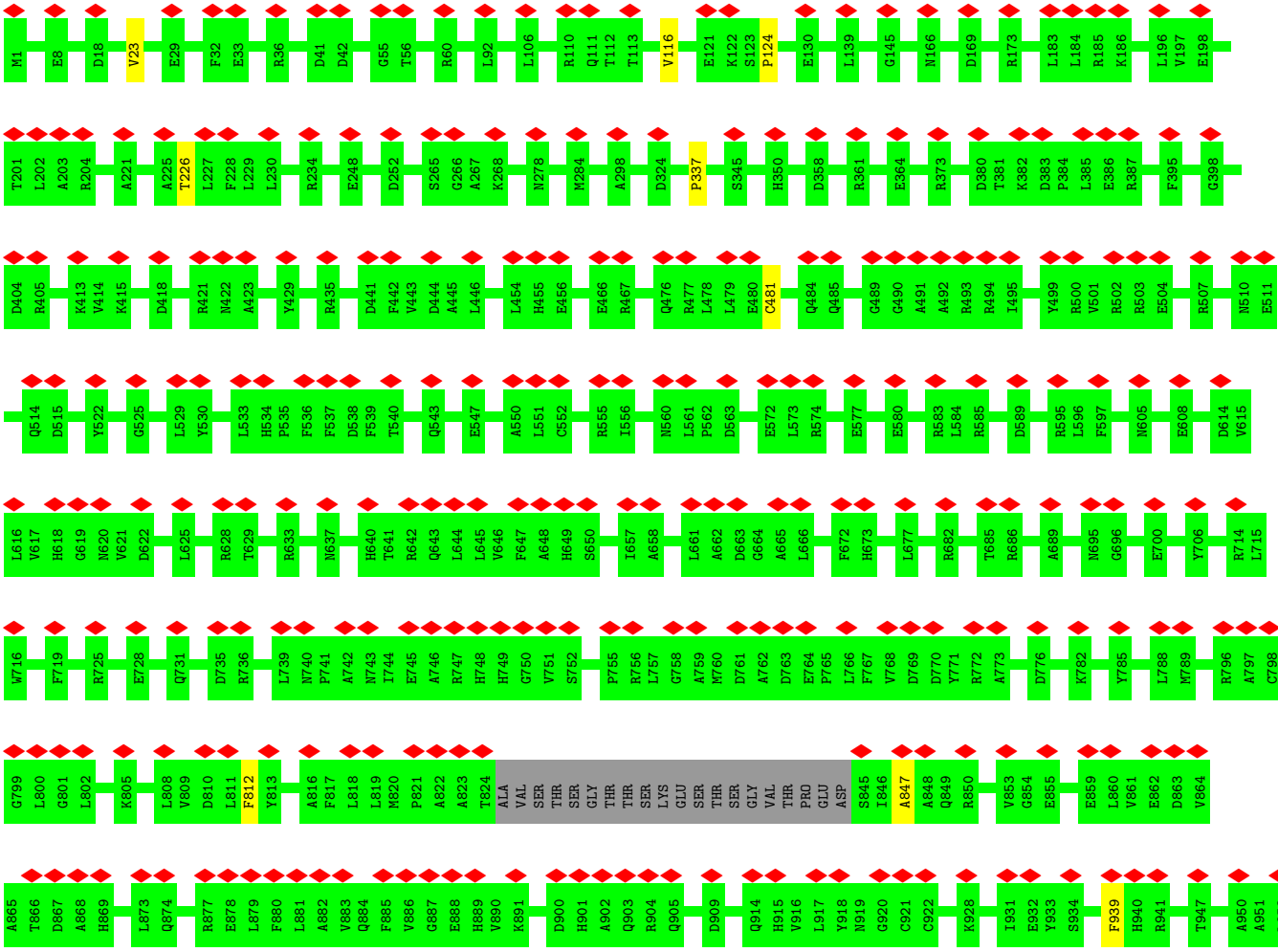



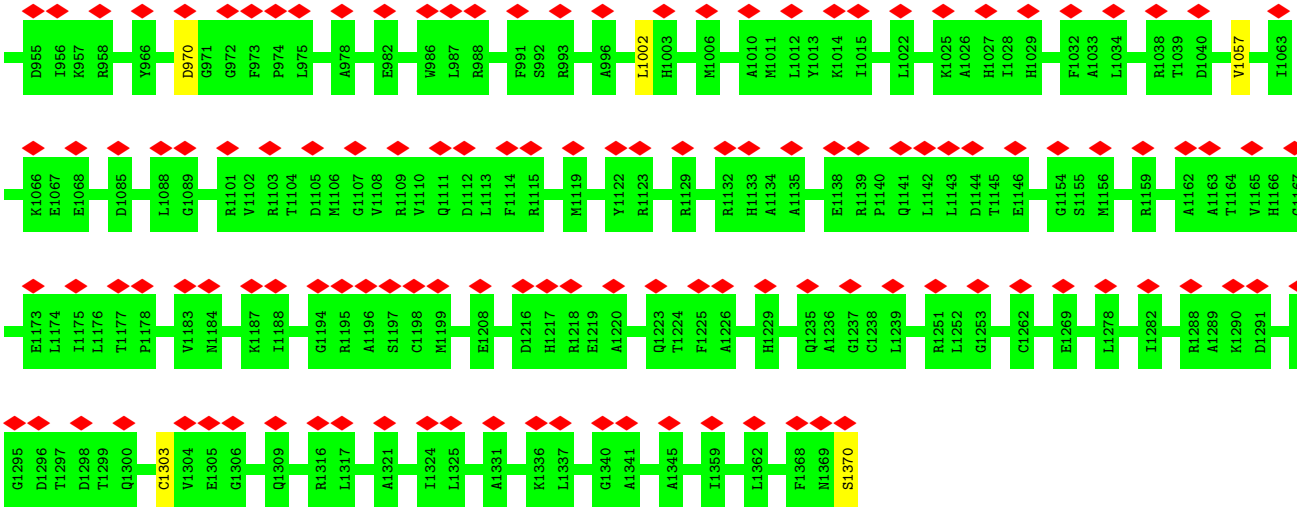



• Molecule 2: Major capsid protein

Chain N:

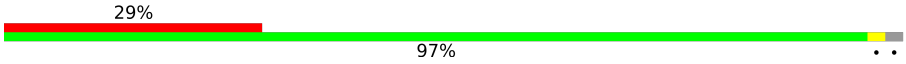


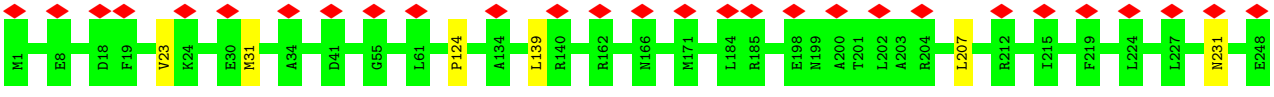



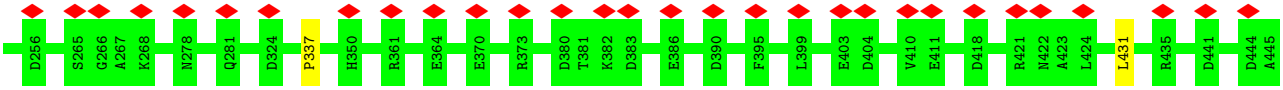


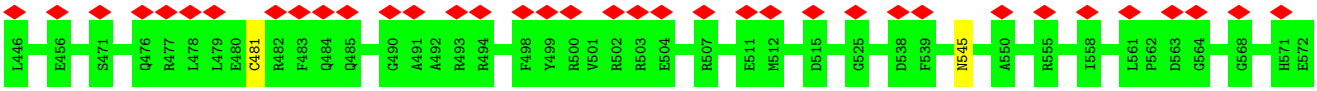

• Molecule 2: Major capsid protein

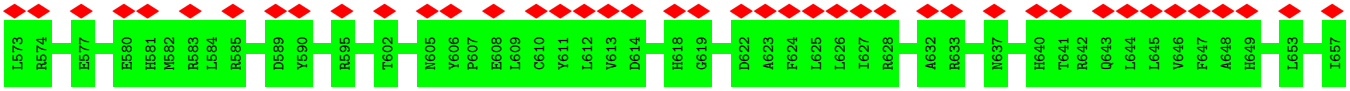
Chain O:

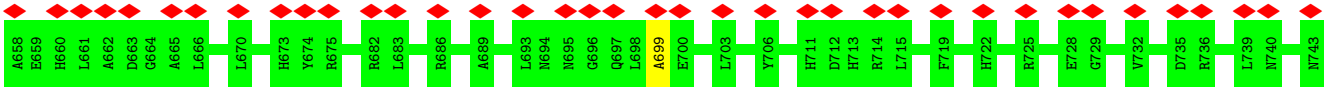


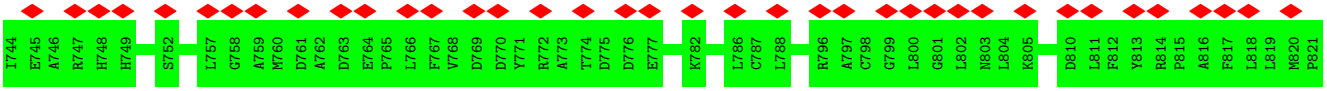



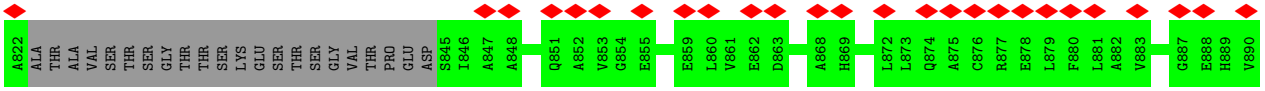



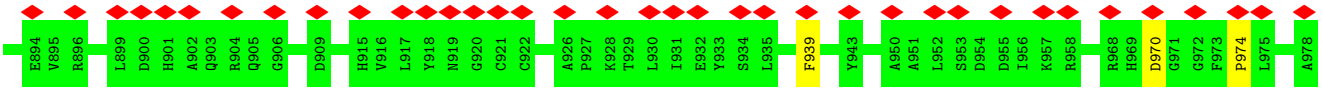



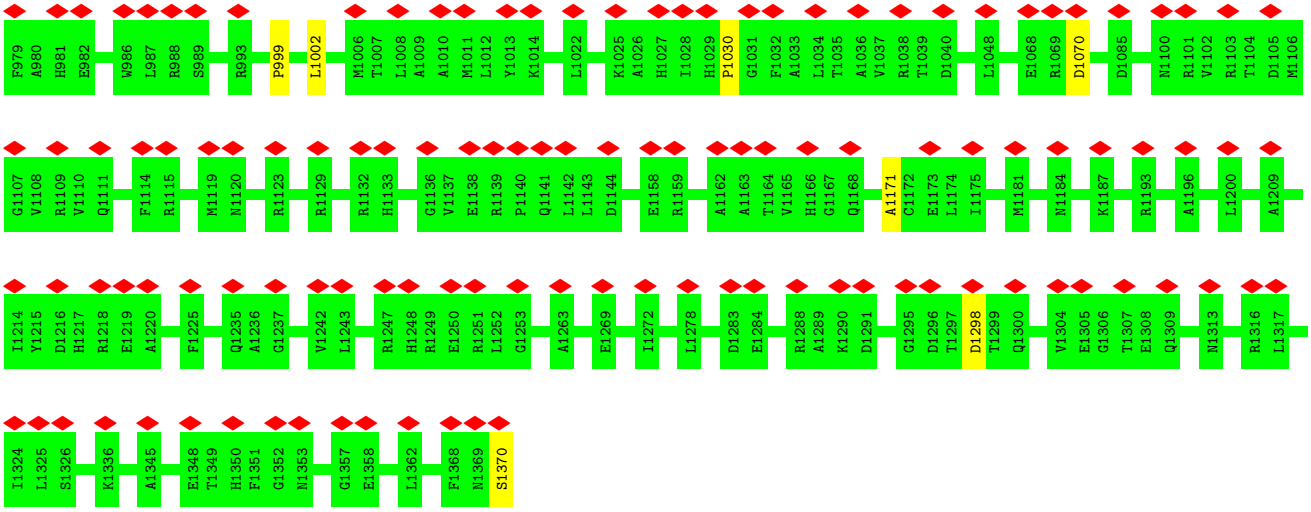



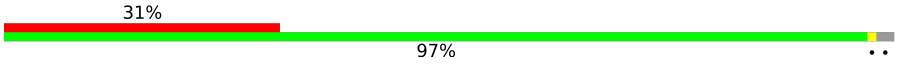



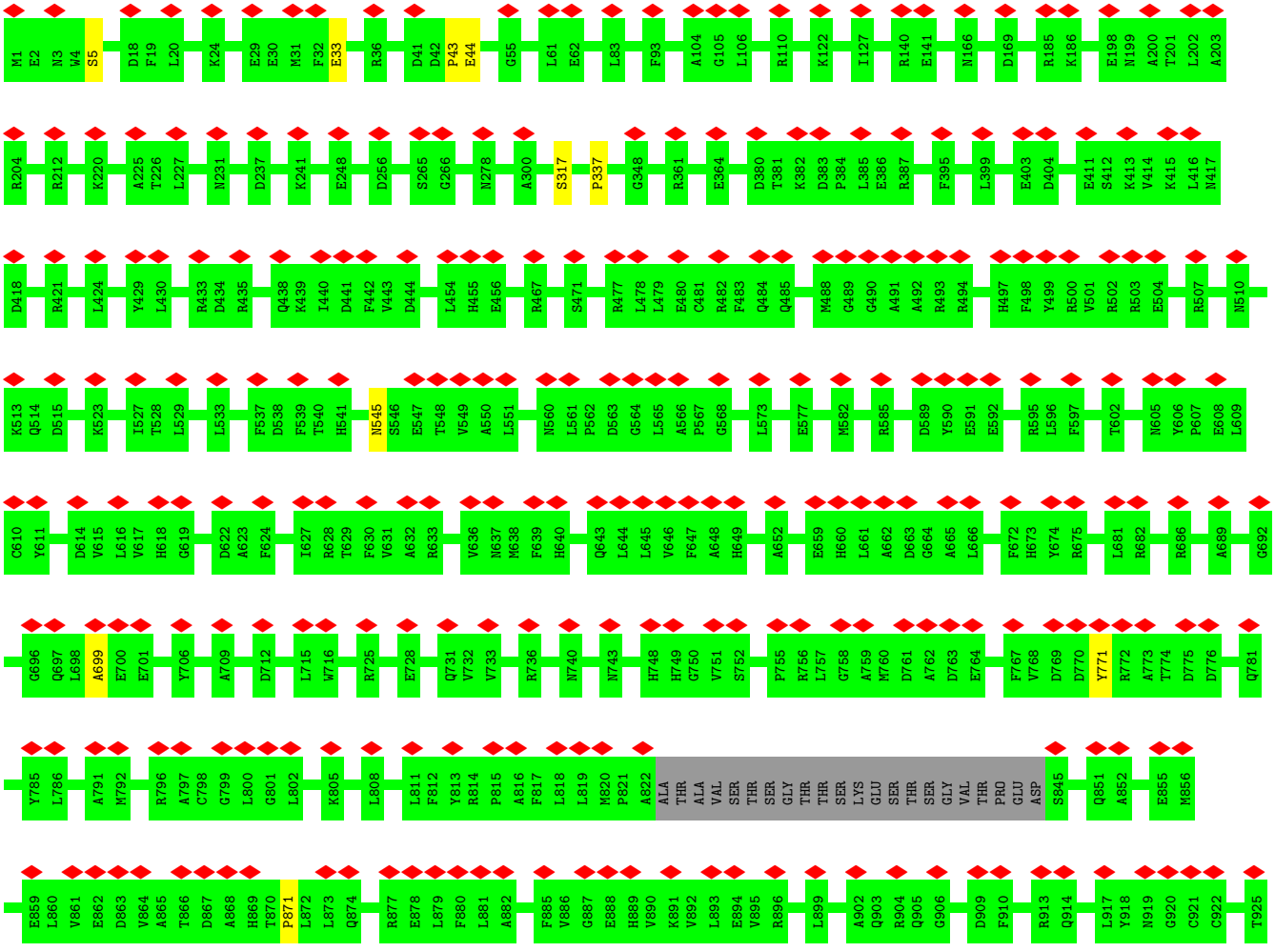



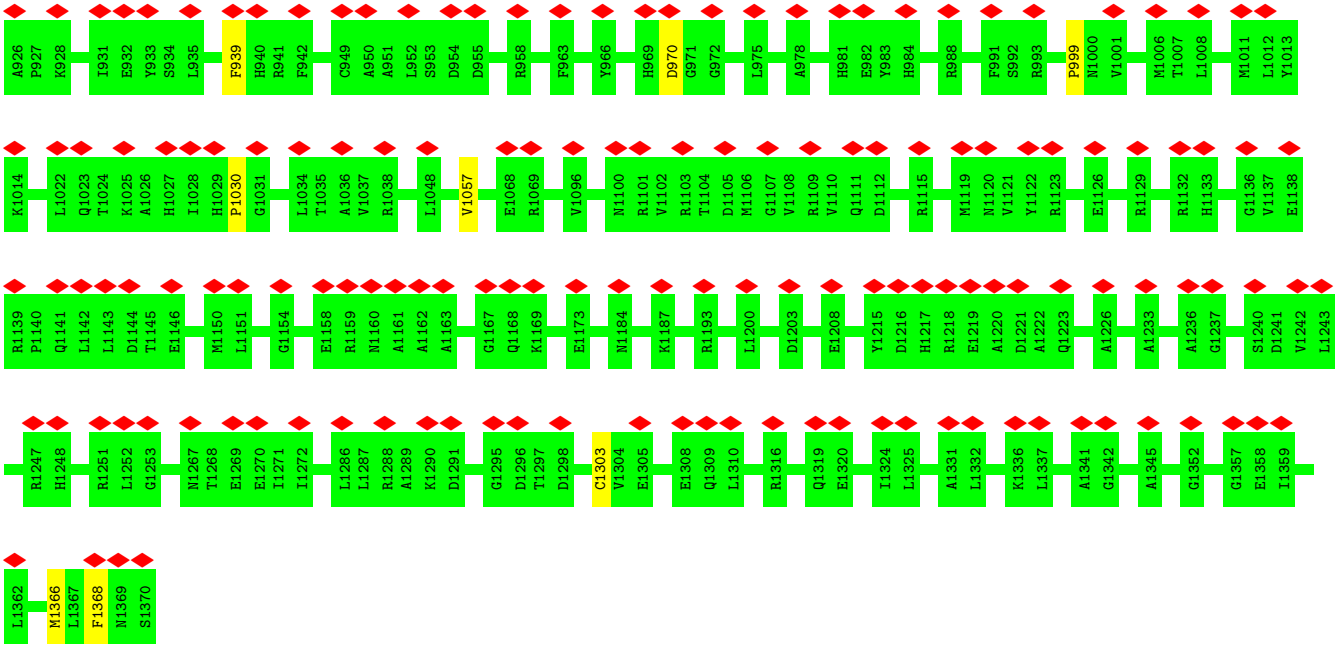



• Molecule 2: Major capsid protein

Chain P:





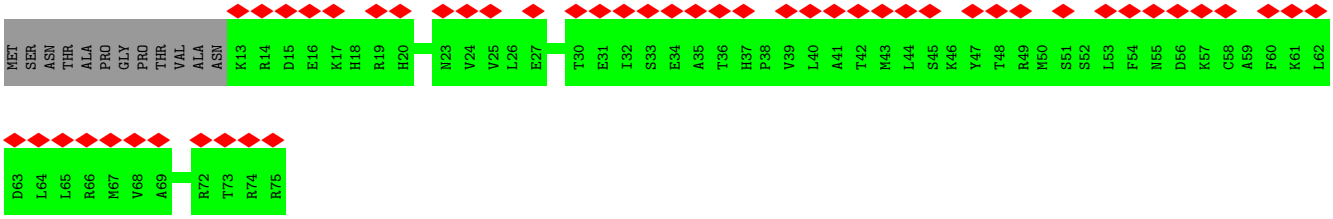

• Molecule 3: Small capsomere-interacting protein

Chain Q:



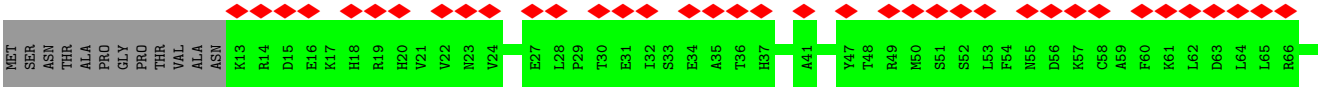
• Molecule 3: Small capsomere-interacting protein

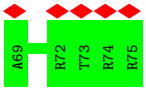
Chain R:


• Molecule 3: Small capsomere-interacting protein

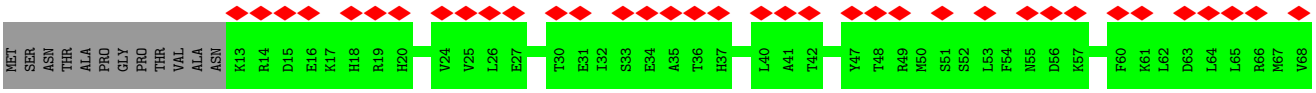
Chain S:

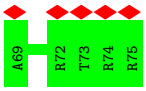






• Molecule 3: Small capsomere-interacting protein

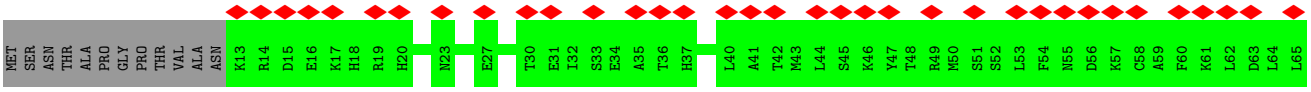
Chain T:

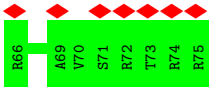




• Molecule 3: Small capsomere-interacting protein

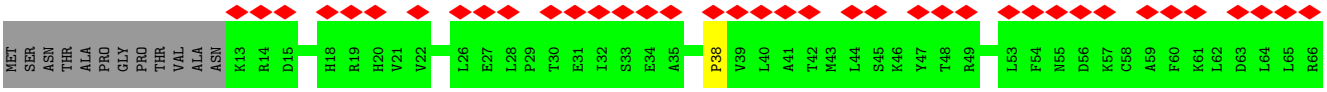
Chain U:

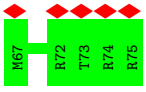




• Molecule 3: Small capsomere-interacting protein

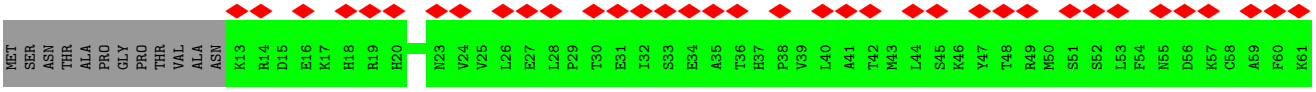
Chain V:

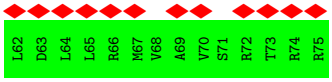




• Molecule 3: Small capsomere-interacting protein

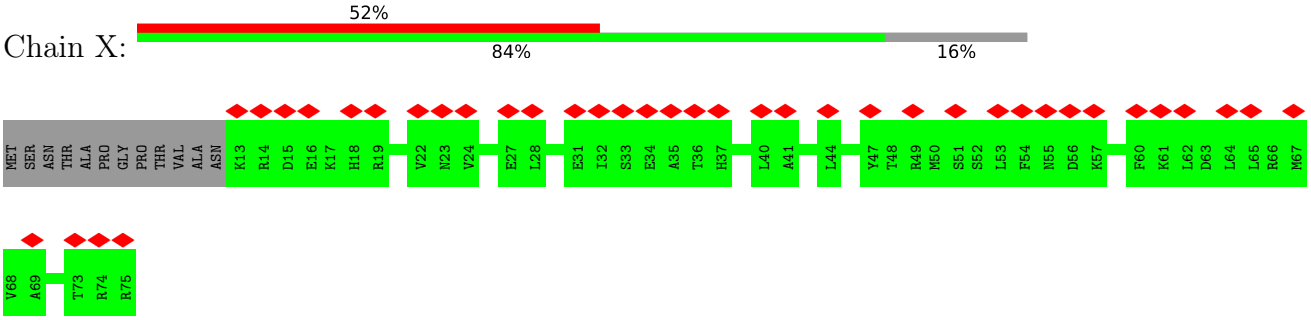
Chain W:

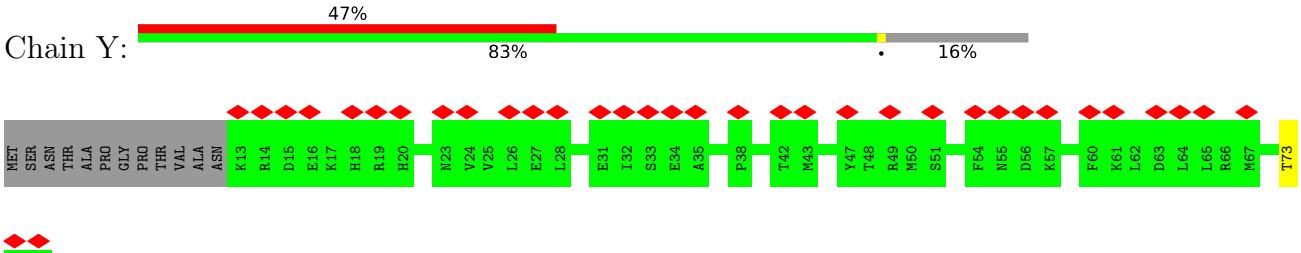

• Molecule 3: Small capsomere-interacting protein

Chain X:



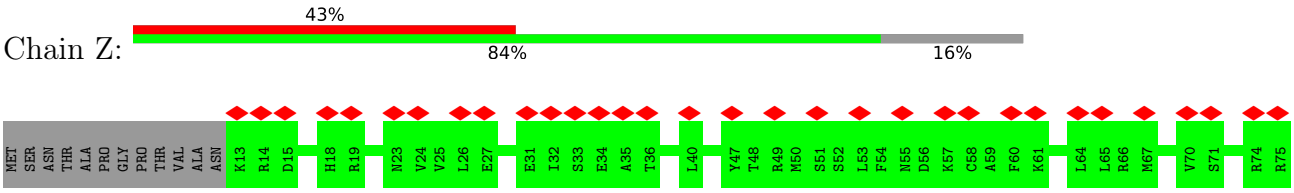

• Molecule 3: Small capsomere-interacting protein

Chain Y:



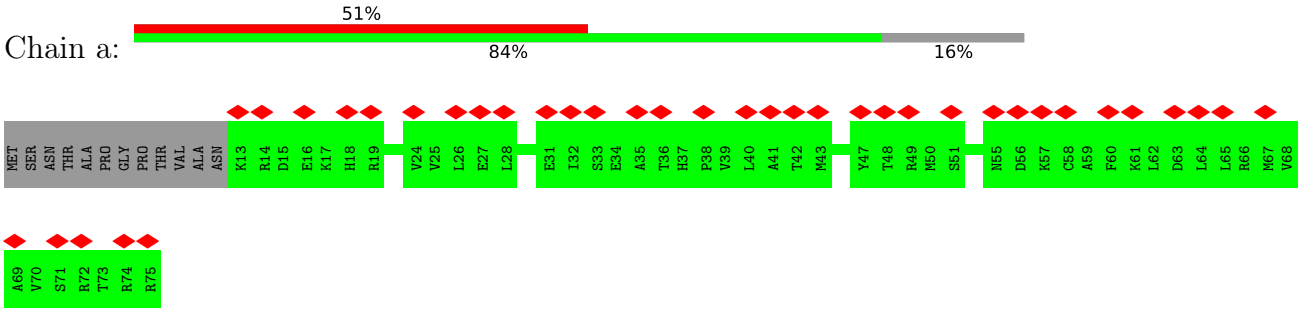

• Molecule 3: Small capsomere-interacting protein

Chain Z:



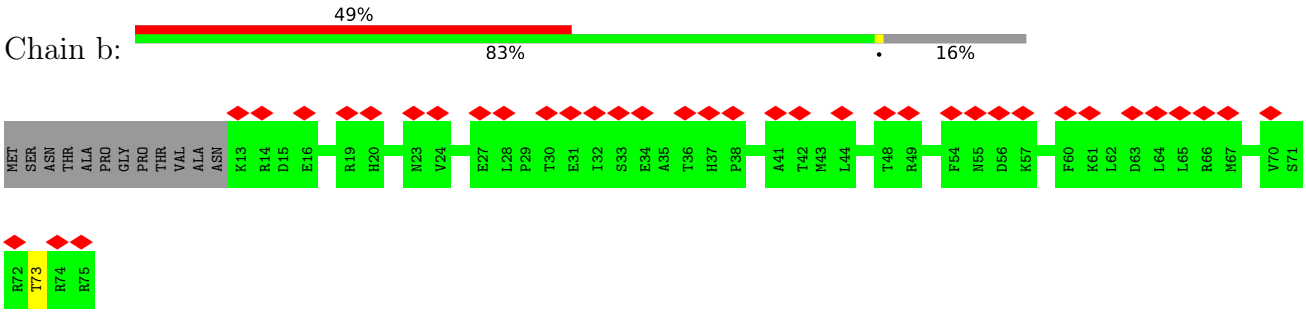

• Molecule 3: Small capsomere-interacting protein

Chain a:



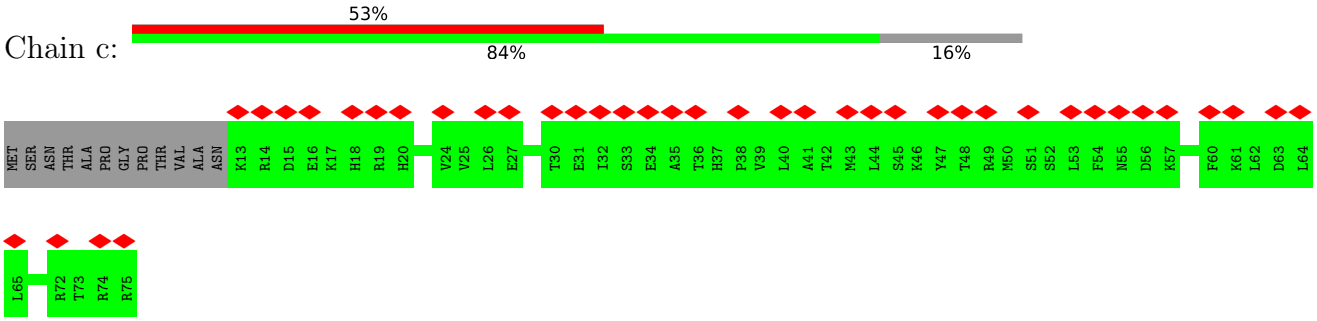

• Molecule 3: Small capsomere-interacting protein

Chain b:



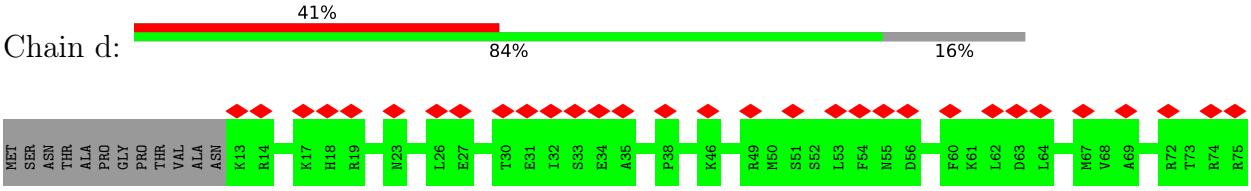
• Molecule 3: Small capsomere-interacting protein

Chain c:



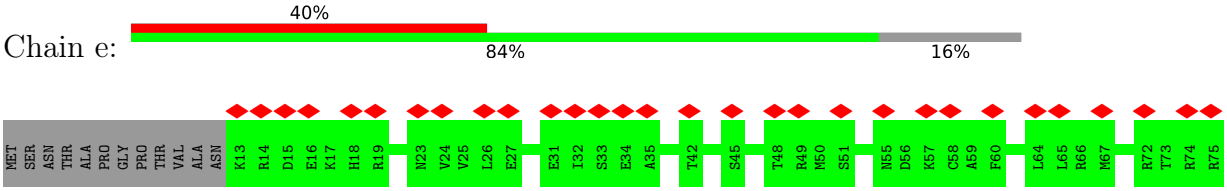

• Molecule 3: Small capsomere-interacting protein

Chain d:



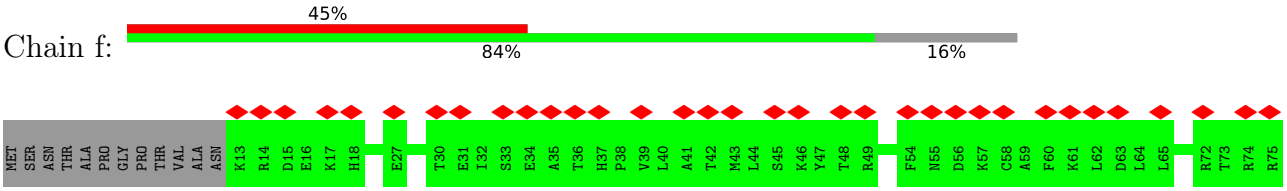

• Molecule 3: Small capsomere-interacting protein

Chain e:



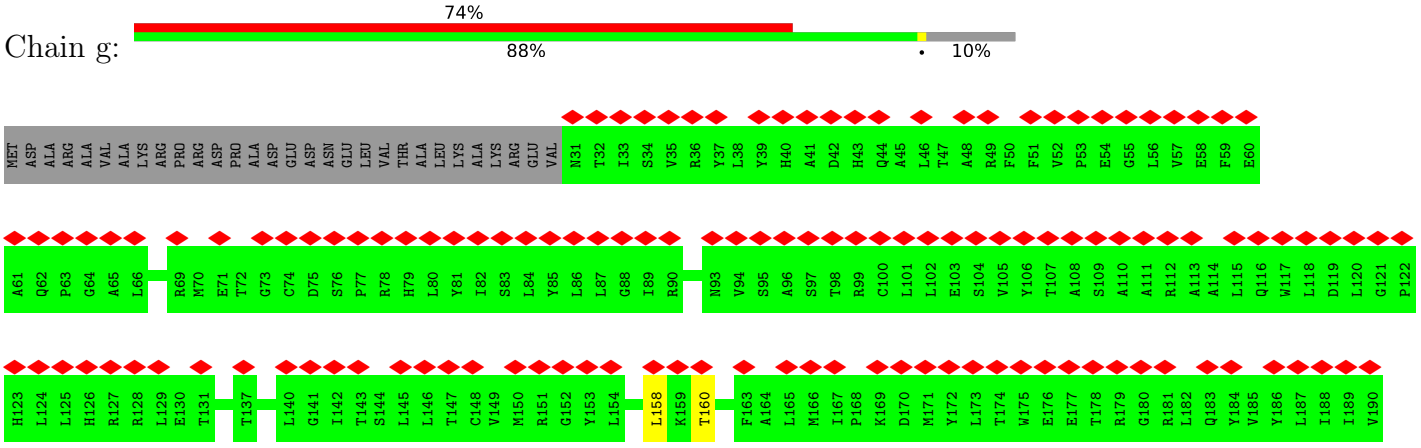

• Molecule 3: Small capsomere-interacting protein

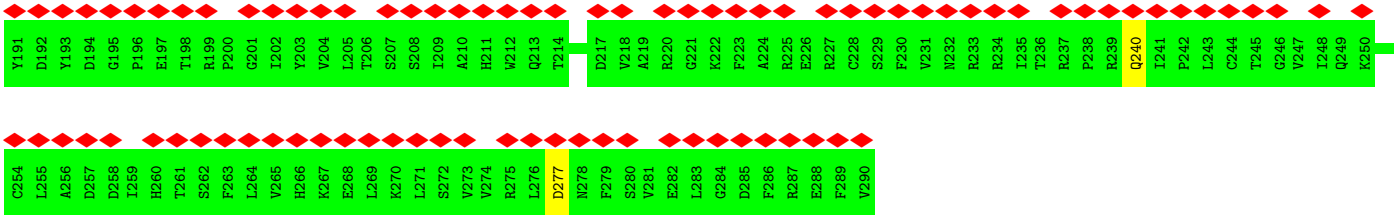
Chain f:




• Molecule 4: Triplex capsid protein 1

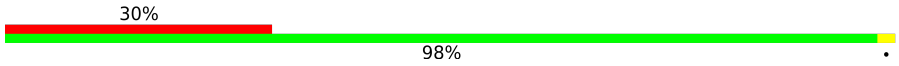
Chain g:

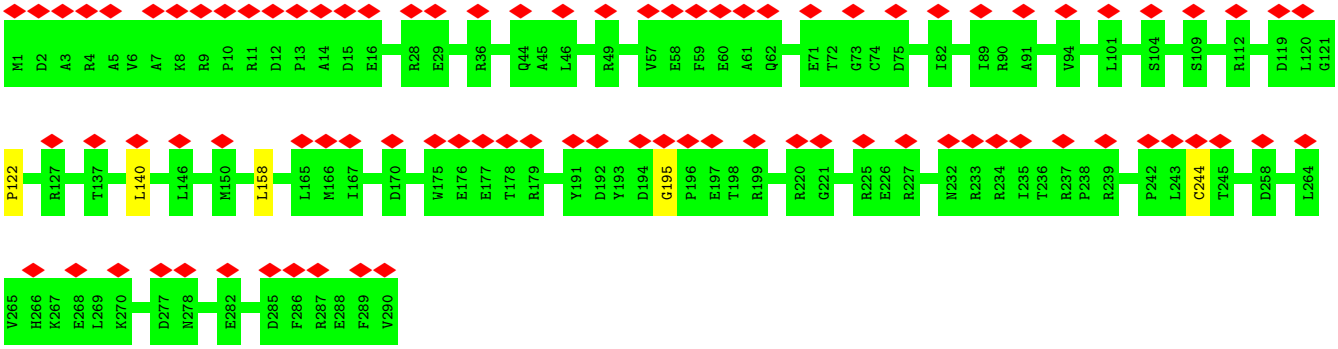





• Molecule 4: Triplex capsid protein 1

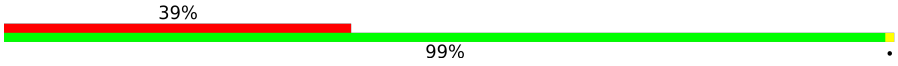
Chain j:

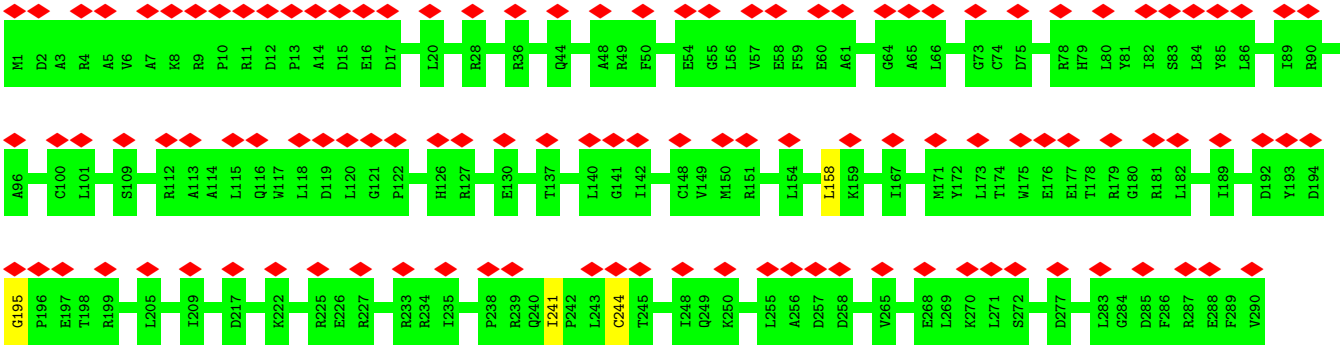



• Molecule 4: Triplex capsid protein 1

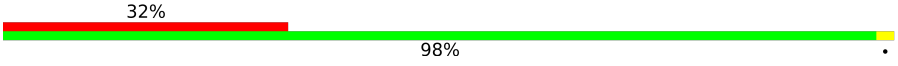
Chain m:

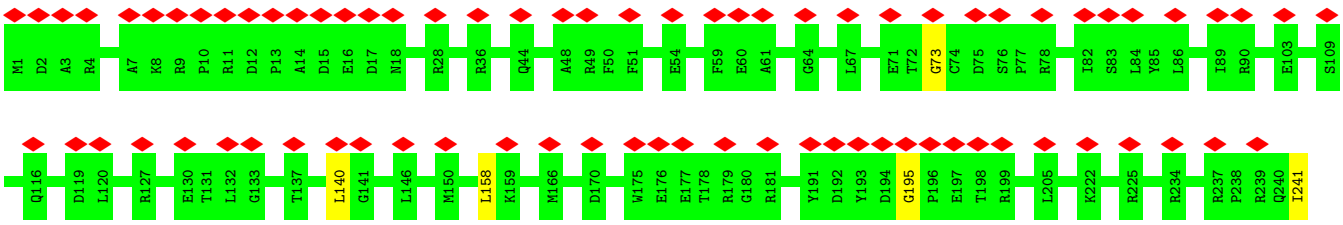


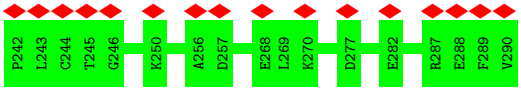




• Molecule 4: Triplex capsid protein 1

Chain p:

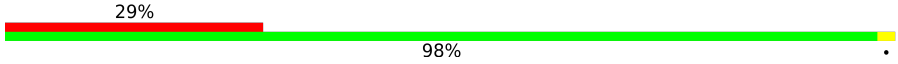


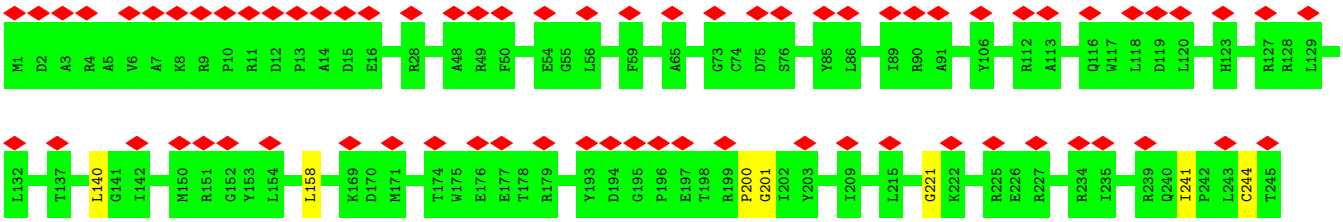






• Molecule 4: Triplex capsid protein 1

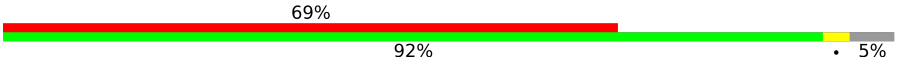
Chain s:

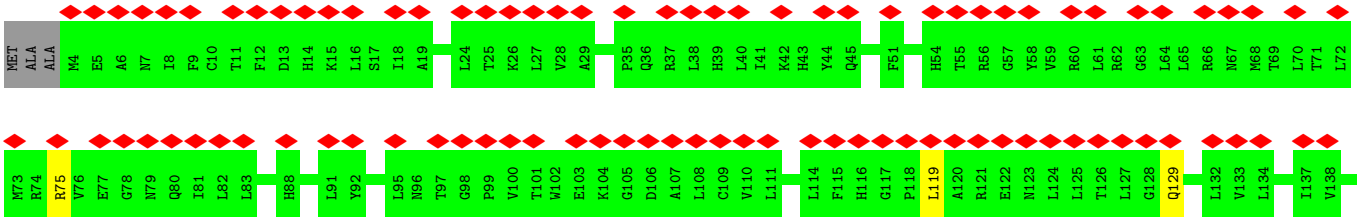


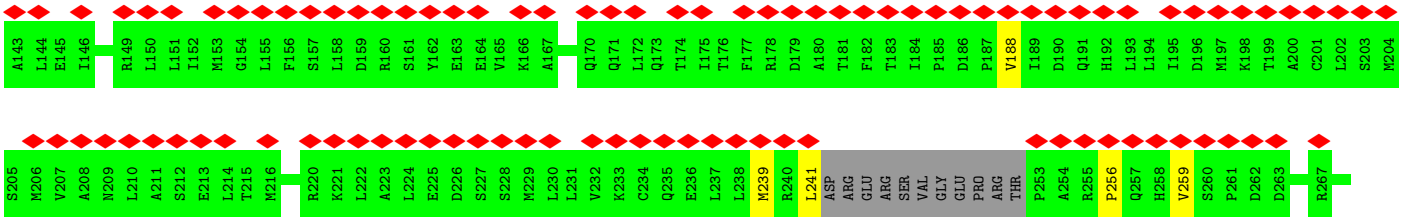



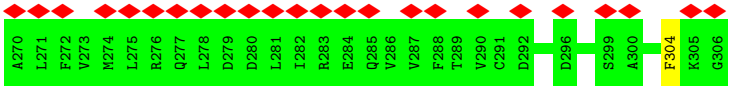

• Molecule 5: Triplex capsid protein 2

Chain h:



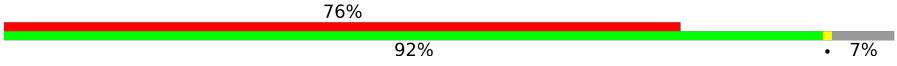



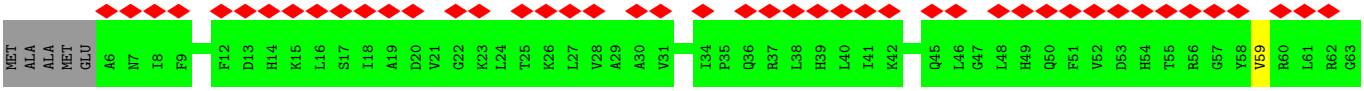



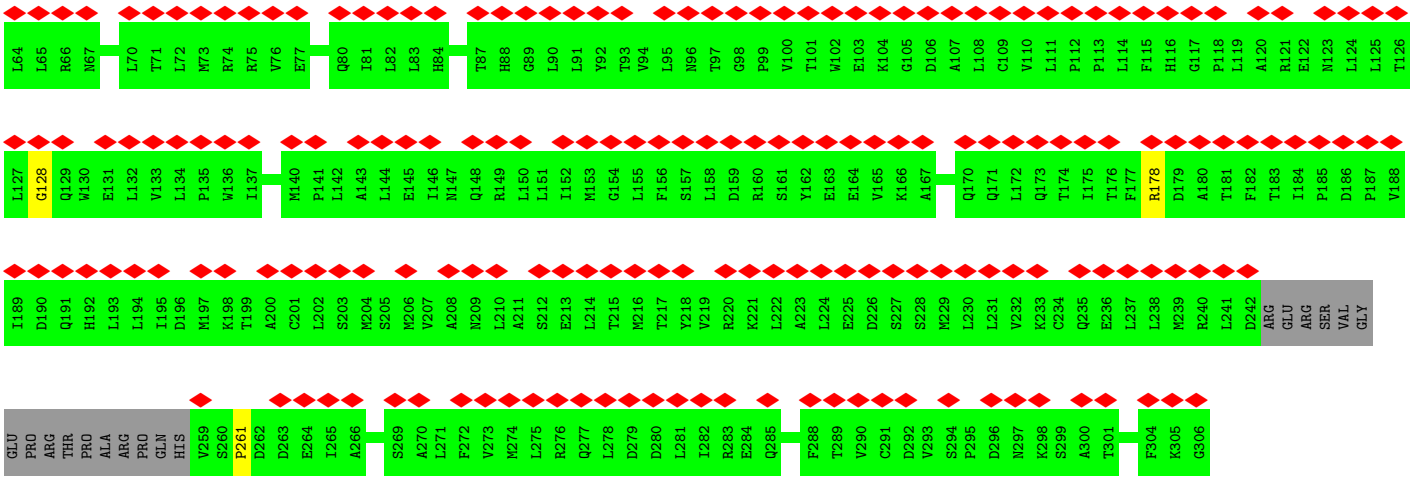




• Molecule 5: Triplex capsid protein 2

Chain i:

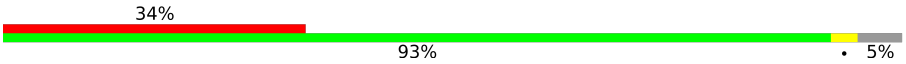


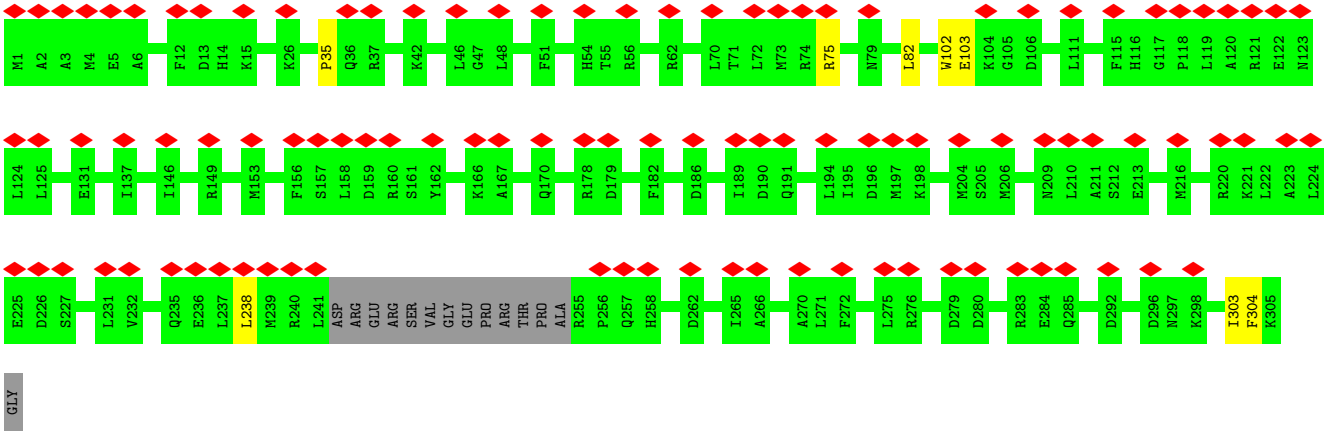






• Molecule 5: Triplex capsid protein 2

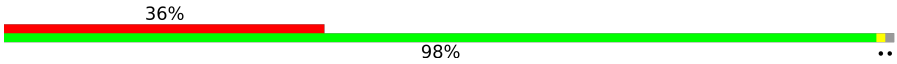
Chain k:

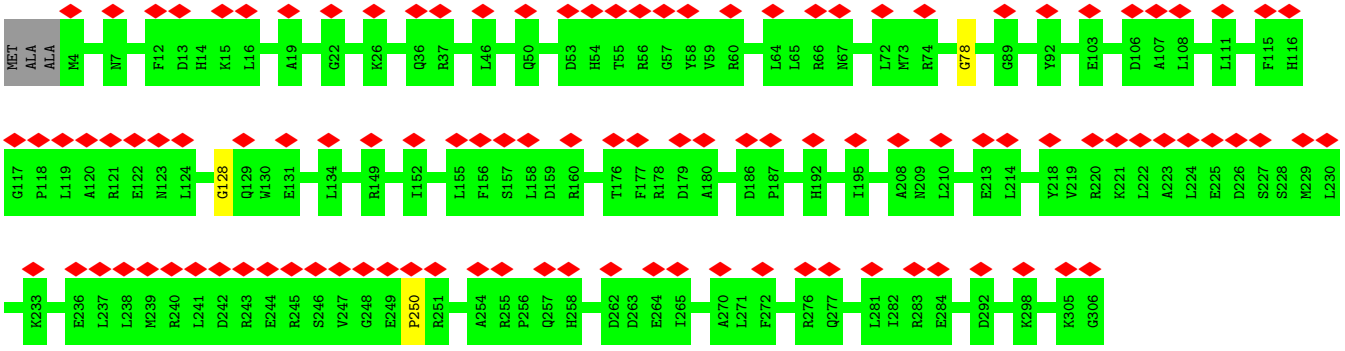



• Molecule 5: Triplex capsid protein 2

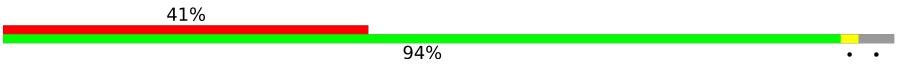
Chain l:

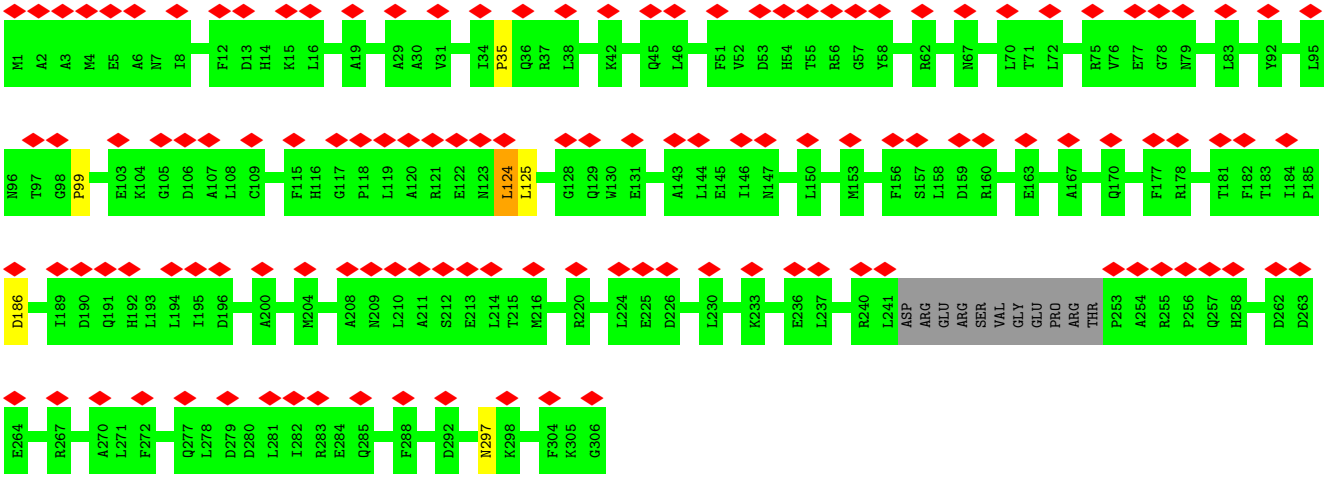



• Molecule 5: Triplex capsid protein 2

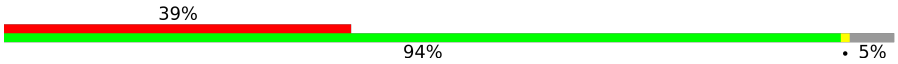
Chain n:

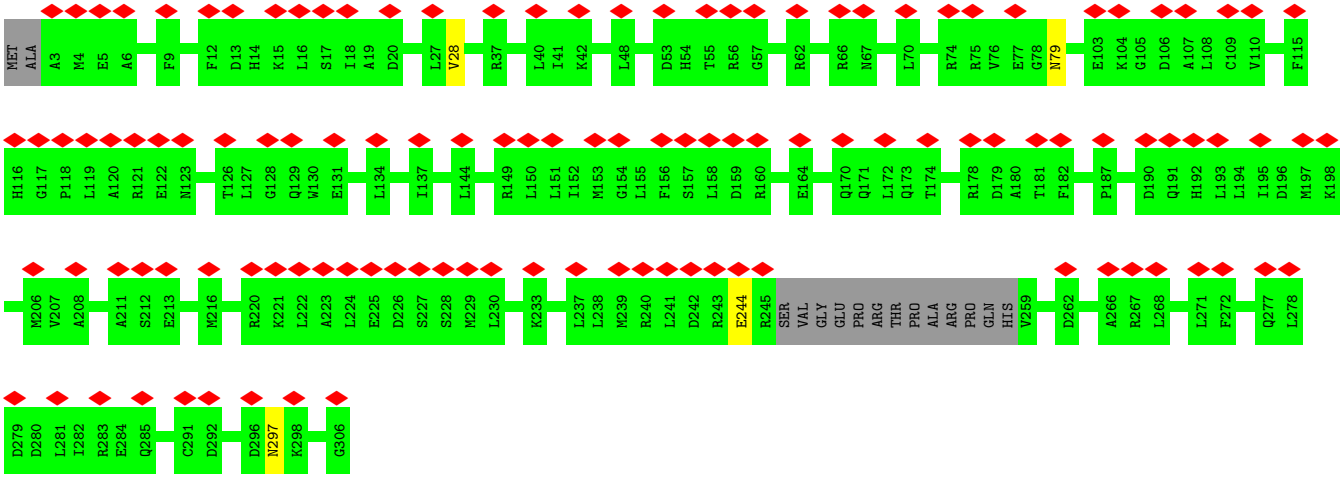





• Molecule 5: Triplex capsid protein 2

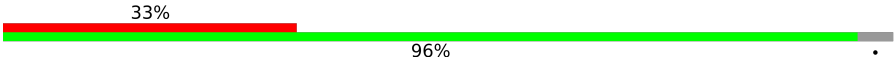
Chain o:

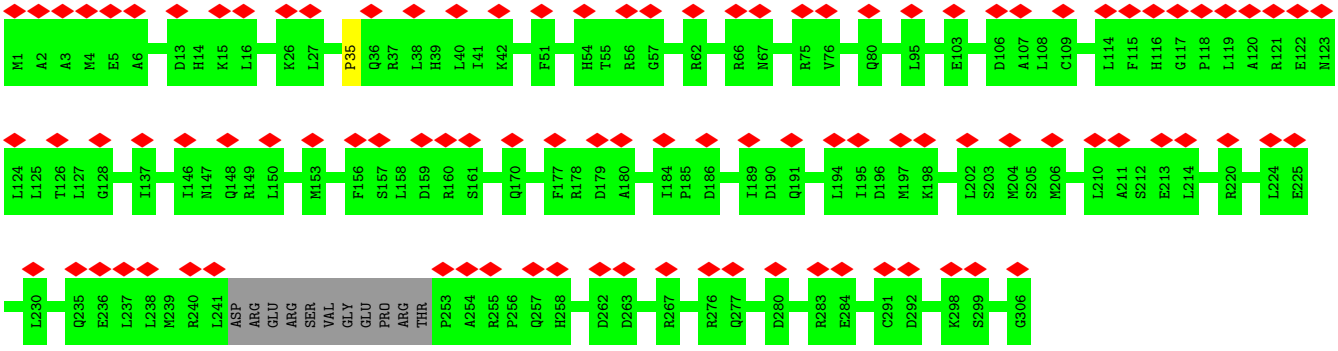



• Molecule 5: Triplex capsid protein 2

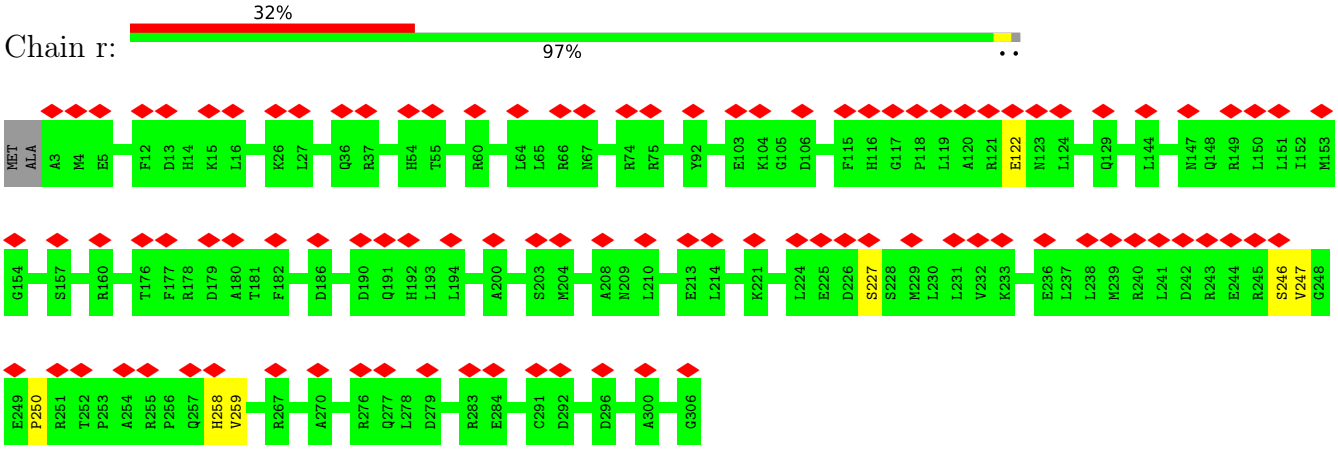
Chain q:



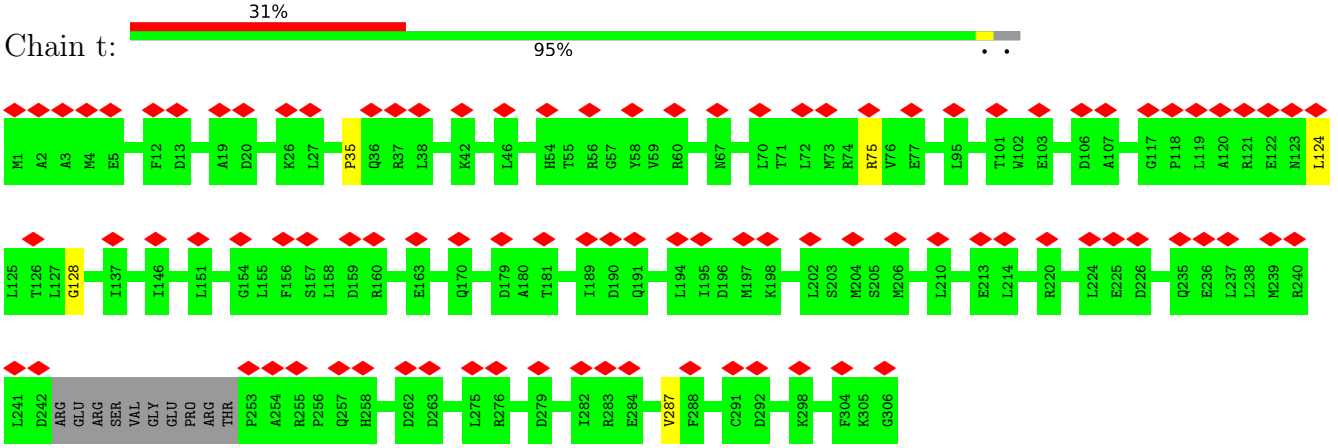

• Molecule 5: Triplex capsid protein 2

Chain r:



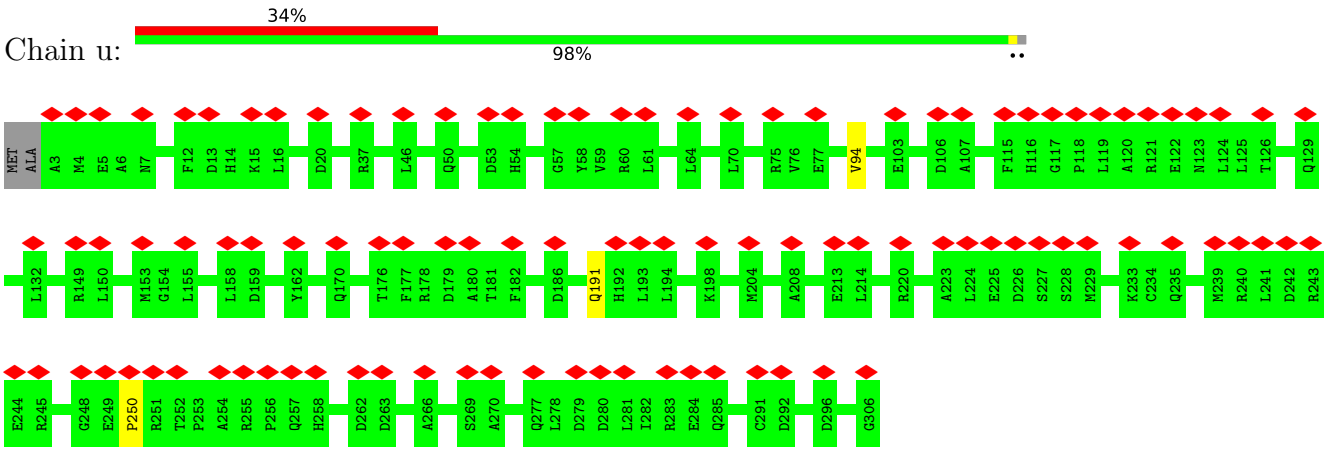

• Molecule 5: Triplex capsid protein 2

Chain t:




• Molecule 5: Triplex capsid protein 2

Chain u:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, I | Depositor |
| Number of particles used | 39600 | 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 ($e^-/Å^2$) | 2.7 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.203 | Depositor |
| Minimum map value | -0.123 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.018 | Depositor |
| Recommended contour level | 0.05 | Depositor |
| Map size (Å) | 1352.4, 1352.4, 1352.4 | wwPDB |
| Map dimensions | 840, 840, 840 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.61, 1.61, 1.61 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | 0 | 0.23 | 0/2366 | 0.37 | 0/3192 |
| 1 | 1 | 0.23 | 0/2366 | 0.38 | 0/3192 |
| 1 | 2 | 0.23 | 0/2366 | 0.38 | 0/3192 |
| 1 | 3 | 0.23 | 0/2366 | 0.37 | 0/3192 |
| 1 | 4 | 0.23 | 0/2366 | 0.38 | 0/3192 |
| 1 | 5 | 0.23 | 0/2366 | 0.37 | 0/3192 |
| 1 | 6 | 0.23 | 0/2366 | 0.37 | 0/3192 |
| 1 | 7 | 0.23 | 0/2366 | 0.38 | 0/3192 |
| 1 | 8 | 0.23 | 0/2366 | 0.37 | 0/3192 |
| 1 | 9 | 0.23 | 0/2366 | 0.38 | 0/3192 |
| 1 | v | 0.23 | 0/2366 | 0.38 | 0/3192 |
| 1 | w | 0.23 | 0/2366 | 0.38 | 0/3192 |
| 1 | x | 0.23 | 0/2366 | 0.38 | 0/3192 |
| 1 | y | 0.23 | 0/2366 | 0.37 | 0/3192 |
| 1 | z | 0.23 | 0/2366 | 0.37 | 0/3192 |
| 2 | A | 0.25 | 0/10780 | 0.44 | 0/14685 |
| 2 | B | 0.25 | 0/10824 | 0.44 | 0/14743 |
| 2 | C | 0.25 | 0/10942 | 0.44 | 1/14906 (0.0%) |
| 2 | D | 0.25 | 0/10926 | 0.44 | 0/14884 |
| 2 | E | 0.25 | 0/10932 | 0.44 | 0/14892 |
| 2 | F | 0.25 | 0/10949 | 0.43 | 0/14916 |
| 2 | G | 0.25 | 0/10962 | 0.43 | 0/14933 |
| 2 | H | 0.25 | 0/10967 | 0.43 | 0/14940 |
| 2 | I | 0.25 | 0/10932 | 0.43 | 1/14892 (0.0%) |
| 2 | J | 0.25 | 0/10835 | 0.43 | 1/14757 (0.0%) |
| 2 | K | 0.25 | 0/10937 | 0.44 | 0/14899 |
| 2 | L | 0.25 | 0/10974 | 0.43 | 0/14950 |
| 2 | M | 0.25 | 0/10974 | 0.43 | 0/14950 |
| 2 | N | 0.25 | 0/10949 | 0.43 | 0/14916 |
| 2 | O | 0.25 | 0/10937 | 0.43 | 0/14899 |
| 2 | P | 0.25 | 0/10937 | 0.43 | 0/14899 |
| 3 | Q | 0.22 | 0/520 | 0.38 | 0/697 |
| 3 | R | 0.23 | 0/520 | 0.38 | 0/697 |
| 3 | S | 0.24 | 0/520 | 0.38 | 0/697 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 3 | T | 0.24 | 0/520 | 0.38 | 0/697 |
| 3 | U | 0.23 | 0/520 | 0.38 | 0/697 |
| 3 | V | 0.23 | 0/520 | 0.37 | 0/697 |
| 3 | W | 0.23 | 0/520 | 0.37 | 0/697 |
| 3 | X | 0.23 | 0/520 | 0.38 | 0/697 |
| 3 | Y | 0.23 | 0/520 | 0.37 | 0/697 |
| 3 | Z | 0.23 | 0/520 | 0.38 | 0/697 |
| 3 | a | 0.23 | 0/520 | 0.37 | 0/697 |
| 3 | b | 0.23 | 0/520 | 0.37 | 0/697 |
| 3 | c | 0.23 | 0/520 | 0.38 | 0/697 |
| 3 | d | 0.23 | 0/520 | 0.37 | 0/697 |
| 3 | e | 0.23 | 0/520 | 0.37 | 0/697 |
| 3 | f | 0.23 | 0/520 | 0.37 | 0/697 |
| 4 | g | 0.24 | 0/2138 | 0.44 | 0/2903 |
| 4 | j | 0.25 | 0/2374 | 0.43 | 0/3221 |
| 4 | m | 0.24 | 0/2374 | 0.43 | 0/3221 |
| 4 | p | 0.25 | 0/2374 | 0.43 | 0/3221 |
| 4 | s | 0.25 | 0/2374 | 0.43 | 0/3221 |
| 5 | h | 0.25 | 0/2361 | 0.44 | 0/3206 |
| 5 | i | 0.25 | 0/2300 | 0.46 | 0/3124 |
| 5 | k | 0.25 | 0/2361 | 0.43 | 0/3207 |
| 5 | l | 0.24 | 0/2453 | 0.43 | 0/3332 |
| 5 | n | 0.24 | 0/2379 | 0.45 | 1/3230 (0.0%) |
| 5 | o | 0.24 | 0/2353 | 0.42 | 0/3193 |
| 5 | q | 0.24 | 0/2379 | 0.43 | 0/3230 |
| 5 | r | 0.24 | 0/2458 | 0.43 | 0/3339 |
| 5 | t | 0.25 | 0/2387 | 0.45 | 0/3241 |
| 5 | u | 0.24 | 0/2458 | 0.43 | 0/3339 |
| All | All | 0.25 | 0/254090 | 0.42 | 4/345321 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 1367 | LEU | CB-CG-CD2 | -6.90 | 99.26 | 111.00 |
| 2 | J | 1367 | LEU | CB-CG-CD1 | -6.42 | 100.09 | 111.00 |
| 2 | I | 1367 | LEU | CB-CG-CD2 | -5.55 | 101.56 | 111.00 |
| 5 | n | 124 | LEU | CA-CB-CG | 5.21 | 127.28 | 115.30 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 283/285 (99%) | 274 (97%) | 6 (2%) | 3 (1%) | 14 | 51 |
| 1 | 1 | 283/285 (99%) | 267 (94%) | 13 (5%) | 3 (1%) | 14 | 51 |
| 1 | 2 | 283/285 (99%) | 267 (94%) | 14 (5%) | 2 (1%) | 22 | 60 |
| 1 | 3 | 283/285 (99%) | 266 (94%) | 11 (4%) | 6 (2%) | 7 | 39 |
| 1 | 4 | 283/285 (99%) | 271 (96%) | 10 (4%) | 2 (1%) | 22 | 60 |
| 1 | 5 | 283/285 (99%) | 272 (96%) | 7 (2%) | 4 (1%) | 11 | 46 |
| 1 | 6 | 283/285 (99%) | 271 (96%) | 10 (4%) | 2 (1%) | 22 | 60 |
| 1 | 7 | 283/285 (99%) | 267 (94%) | 13 (5%) | 3 (1%) | 14 | 51 |
| 1 | 8 | 283/285 (99%) | 275 (97%) | 5 (2%) | 3 (1%) | 14 | 51 |
| 1 | 9 | 283/285 (99%) | 271 (96%) | 8 (3%) | 4 (1%) | 11 | 46 |
| 1 | v | 283/285 (99%) | 262 (93%) | 13 (5%) | 8 (3%) | 5 | 34 |
| 1 | w | 283/285 (99%) | 269 (95%) | 12 (4%) | 2 (1%) | 22 | 60 |
| 1 | x | 283/285 (99%) | 264 (93%) | 14 (5%) | 5 (2%) | 8 | 42 |
| 1 | y | 283/285 (99%) | 270 (95%) | 11 (4%) | 2 (1%) | 22 | 60 |
| 1 | z | 283/285 (99%) | 272 (96%) | 7 (2%) | 4 (1%) | 11 | 46 |
| 2 | A | 1321/1370 (96%) | 1230 (93%) | 78 (6%) | 13 (1%) | 15 | 52 |
| 2 | B | 1329/1370 (97%) | 1226 (92%) | 80 (6%) | 23 (2%) | 9 | 43 |
| 2 | C | 1345/1370 (98%) | 1259 (94%) | 71 (5%) | 15 (1%) | 14 | 51 |
| 2 | D | 1342/1370 (98%) | 1233 (92%) | 94 (7%) | 15 (1%) | 14 | 51 |
| 2 | E | 1343/1370 (98%) | 1233 (92%) | 90 (7%) | 20 (2%) | 10 | 45 |
| 2 | F | 1346/1370 (98%) | 1242 (92%) | 87 (6%) | 17 (1%) | 12 | 48 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 2 | G | 1347/1370 (98%) | 1250 (93%) | 82 (6%) | 15 (1%) | 14 51 |
| 2 | H | 1348/1370 (98%) | 1253 (93%) | 86 (6%) | 9 (1%) | 22 60 |
| 2 | I | 1343/1370 (98%) | 1243 (93%) | 88 (7%) | 12 (1%) | 17 54 |
| 2 | J | 1329/1370 (97%) | 1239 (93%) | 76 (6%) | 14 (1%) | 14 51 |
| 2 | K | 1344/1370 (98%) | 1249 (93%) | 87 (6%) | 8 (1%) | 25 63 |
| 2 | L | 1349/1370 (98%) | 1259 (93%) | 77 (6%) | 13 (1%) | 15 52 |
| 2 | M | 1349/1370 (98%) | 1250 (93%) | 89 (7%) | 10 (1%) | 22 60 |
| 2 | N | 1346/1370 (98%) | 1256 (93%) | 81 (6%) | 9 (1%) | 22 60 |
| 2 | O | 1344/1370 (98%) | 1243 (92%) | 84 (6%) | 17 (1%) | 12 48 |
| 2 | P | 1344/1370 (98%) | 1249 (93%) | 81 (6%) | 14 (1%) | 15 52 |
| 3 | Q | 61/75 (81%) | 58 (95%) | 3 (5%) | 0 | 100 100 |
| 3 | R | 61/75 (81%) | 57 (93%) | 4 (7%) | 0 | 100 100 |
| 3 | S | 61/75 (81%) | 58 (95%) | 3 (5%) | 0 | 100 100 |
| 3 | T | 61/75 (81%) | 58 (95%) | 3 (5%) | 0 | 100 100 |
| 3 | U | 61/75 (81%) | 56 (92%) | 5 (8%) | 0 | 100 100 |
| 3 | V | 61/75 (81%) | 56 (92%) | 4 (7%) | 1 (2%) | 9 44 |
| 3 | W | 61/75 (81%) | 58 (95%) | 3 (5%) | 0 | 100 100 |
| 3 | X | 61/75 (81%) | 59 (97%) | 2 (3%) | 0 | 100 100 |
| 3 | Y | 61/75 (81%) | 57 (93%) | 4 (7%) | 0 | 100 100 |
| 3 | Z | 61/75 (81%) | 58 (95%) | 3 (5%) | 0 | 100 100 |
| 3 | a | 61/75 (81%) | 59 (97%) | 2 (3%) | 0 | 100 100 |
| 3 | b | 61/75 (81%) | 58 (95%) | 3 (5%) | 0 | 100 100 |
| 3 | c | 61/75 (81%) | 60 (98%) | 1 (2%) | 0 | 100 100 |
| 3 | d | 61/75 (81%) | 58 (95%) | 3 (5%) | 0 | 100 100 |
| 3 | e | 61/75 (81%) | 57 (93%) | 4 (7%) | 0 | 100 100 |
| 3 | f | 61/75 (81%) | 58 (95%) | 3 (5%) | 0 | 100 100 |
| 4 | g | 258/290 (89%) | 234 (91%) | 21 (8%) | 3 (1%) | 13 49 |
| 4 | j | 288/290 (99%) | 267 (93%) | 17 (6%) | 4 (1%) | 11 46 |
| 4 | m | 288/290 (99%) | 272 (94%) | 14 (5%) | 2 (1%) | 22 60 |
| 4 | p | 288/290 (99%) | 269 (93%) | 16 (6%) | 3 (1%) | 15 52 |
| 4 | s | 288/290 (99%) | 266 (92%) | 17 (6%) | 5 (2%) | 9 43 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 5 | h | 288/306 (94%) | 260 (90%) | 21 (7%) | 7 (2%) | 6 37 |
| 5 | i | 281/306 (92%) | 257 (92%) | 20 (7%) | 4 (1%) | 11 46 |
| 5 | k | 288/306 (94%) | 268 (93%) | 14 (5%) | 6 (2%) | 7 39 |
| 5 | l | 301/306 (98%) | 274 (91%) | 24 (8%) | 3 (1%) | 15 52 |
| 5 | n | 291/306 (95%) | 271 (93%) | 15 (5%) | 5 (2%) | 9 43 |
| 5 | o | 287/306 (94%) | 266 (93%) | 18 (6%) | 3 (1%) | 15 52 |
| 5 | q | 291/306 (95%) | 279 (96%) | 11 (4%) | 1 (0%) | 41 75 |
| 5 | r | 302/306 (99%) | 275 (91%) | 21 (7%) | 6 (2%) | 7 40 |
| 5 | t | 292/306 (95%) | 269 (92%) | 19 (6%) | 4 (1%) | 11 46 |
| 5 | u | 302/306 (99%) | 275 (91%) | 24 (8%) | 3 (1%) | 15 52 |
| All | All | 31023/31905 (97%) | 28879 (93%) | 1807 (6%) | 337 (1%) | 18 51 |

All (337) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 3 | 183 | PRO |
| 2 | A | 694 | ASN |
| 2 | A | 805 | LYS |
| 2 | B | 203 | ALA |
| 2 | B | 844 | ASP |
| 2 | B | 1054 | CYS |
| 2 | B | 1162 | ALA |
| 2 | C | 254 | ILE |
| 2 | C | 1002 | LEU |
| 2 | D | 39 | TYR |
| 2 | D | 970 | ASP |
| 2 | E | 691 | PRO |
| 2 | E | 1162 | ALA |
| 2 | E | 1183 | VAL |
| 2 | F | 337 | PRO |
| 2 | F | 340 | PRO |
| 2 | H | 970 | ASP |
| 2 | J | 862 | GLU |
| 2 | J | 970 | ASP |
| 2 | K | 771 | TYR |
| 2 | K | 970 | ASP |
| 2 | N | 970 | ASP |
| 2 | N | 1002 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | O | 1002 | LEU |
| 2 | P | 337 | PRO |
| 5 | l | 250 | PRO |
| 1 | 1 | 6 | ILE |
| 1 | 2 | 74 | SER |
| 1 | 3 | 190 | ARG |
| 1 | 9 | 179 | PHE |
| 2 | A | 45 | ARG |
| 2 | A | 1052 | LYS |
| 2 | A | 1138 | GLU |
| 2 | A | 1204 | PRO |
| 2 | B | 198 | GLU |
| 2 | B | 689 | ALA |
| 2 | B | 699 | ALA |
| 2 | B | 763 | ASP |
| 2 | B | 862 | GLU |
| 2 | B | 1002 | LEU |
| 2 | C | 699 | ALA |
| 2 | C | 769 | ASP |
| 2 | C | 898 | PRO |
| 2 | D | 254 | ILE |
| 2 | D | 340 | PRO |
| 2 | D | 350 | HIS |
| 2 | D | 489 | GLY |
| 2 | D | 699 | ALA |
| 2 | D | 1071 | ILE |
| 2 | D | 1109 | ARG |
| 2 | D | 1193 | ARG |
| 2 | E | 23 | VAL |
| 2 | E | 33 | GLU |
| 2 | E | 693 | LEU |
| 2 | E | 699 | ALA |
| 2 | E | 970 | ASP |
| 2 | E | 1054 | CYS |
| 2 | F | 144 | GLU |
| 2 | F | 691 | PRO |
| 2 | F | 728 | GLU |
| 2 | F | 1054 | CYS |
| 2 | G | 545 | ASN |
| 2 | G | 663 | ASP |
| 2 | H | 23 | VAL |
| 2 | H | 254 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 23 | VAL |
| 2 | I | 33 | GLU |
| 2 | I | 413 | LYS |
| 2 | I | 545 | ASN |
| 2 | I | 871 | PRO |
| 2 | J | 33 | GLU |
| 2 | J | 364 | GLU |
| 2 | J | 699 | ALA |
| 2 | K | 33 | GLU |
| 2 | L | 254 | ILE |
| 2 | L | 699 | ALA |
| 2 | L | 970 | ASP |
| 2 | L | 1002 | LEU |
| 2 | M | 33 | GLU |
| 2 | M | 272 | VAL |
| 2 | M | 771 | TYR |
| 2 | M | 970 | ASP |
| 2 | M | 1002 | LEU |
| 2 | N | 23 | VAL |
| 2 | O | 139 | LEU |
| 2 | O | 481 | CYS |
| 2 | O | 699 | ALA |
| 2 | O | 970 | ASP |
| 2 | O | 1070 | ASP |
| 2 | P | 43 | PRO |
| 2 | P | 317 | SER |
| 2 | P | 871 | PRO |
| 2 | P | 970 | ASP |
| 4 | g | 277 | ASP |
| 5 | h | 129 | GLN |
| 5 | h | 259 | VAL |
| 5 | i | 178 | ARG |
| 5 | k | 35 | PRO |
| 5 | k | 304 | PHE |
| 5 | n | 35 | PRO |
| 5 | o | 28 | VAL |
| 5 | o | 244 | GLU |
| 4 | p | 73 | GLY |
| 5 | q | 35 | PRO |
| 5 | r | 259 | VAL |
| 4 | s | 200 | PRO |
| 5 | t | 75 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | v | 74 | SER |
| 1 | 0 | 260 | ASN |
| 1 | 3 | 191 | HIS |
| 1 | 5 | 70 | ASN |
| 1 | 5 | 241 | MET |
| 1 | 8 | 6 | ILE |
| 2 | A | 168 | ALA |
| 2 | A | 1181 | MET |
| 2 | B | 746 | ALA |
| 2 | B | 991 | PHE |
| 2 | C | 337 | PRO |
| 2 | C | 862 | GLU |
| 2 | C | 1227 | ALA |
| 2 | D | 1002 | LEU |
| 2 | E | 3 | ASN |
| 2 | E | 349 | ALA |
| 2 | E | 518 | VAL |
| 2 | E | 688 | SER |
| 2 | E | 898 | PRO |
| 2 | E | 929 | THR |
| 2 | F | 862 | GLU |
| 2 | G | 518 | VAL |
| 2 | G | 752 | SER |
| 2 | I | 254 | ILE |
| 2 | I | 343 | SER |
| 2 | I | 970 | ASP |
| 2 | J | 404 | ASP |
| 2 | J | 413 | LYS |
| 2 | J | 1298 | ASP |
| 2 | K | 45 | ARG |
| 2 | K | 124 | PRO |
| 2 | K | 343 | SER |
| 2 | K | 1070 | ASP |
| 2 | L | 22 | HIS |
| 2 | L | 33 | GLU |
| 2 | M | 317 | SER |
| 2 | M | 343 | SER |
| 2 | M | 489 | GLY |
| 2 | N | 812 | PHE |
| 2 | N | 847 | ALA |
| 2 | O | 545 | ASN |
| 2 | O | 939 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | O | 1298 | ASP |
| 2 | P | 44 | GLU |
| 2 | P | 545 | ASN |
| 2 | P | 699 | ALA |
| 5 | h | 75 | ARG |
| 4 | j | 122 | PRO |
| 4 | j | 140 | LEU |
| 4 | j | 195 | GLY |
| 5 | k | 102 | TRP |
| 5 | k | 303 | ILE |
| 5 | n | 124 | LEU |
| 4 | p | 140 | LEU |
| 5 | r | 122 | GLU |
| 5 | r | 247 | VAL |
| 4 | s | 140 | LEU |
| 4 | s | 201 | GLY |
| 5 | t | 35 | PRO |
| 5 | u | 250 | PRO |
| 1 | v | 192 | ALA |
| 1 | v | 260 | ASN |
| 1 | w | 260 | ASN |
| 1 | x | 260 | ASN |
| 1 | y | 260 | ASN |
| 1 | z | 151 | THR |
| 1 | z | 260 | ASN |
| 1 | 0 | 70 | ASN |
| 1 | 1 | 70 | ASN |
| 1 | 1 | 260 | ASN |
| 1 | 3 | 70 | ASN |
| 1 | 5 | 260 | ASN |
| 1 | 7 | 176 | ARG |
| 1 | 8 | 260 | ASN |
| 1 | 9 | 6 | ILE |
| 1 | 9 | 70 | ASN |
| 2 | B | 413 | LYS |
| 2 | B | 436 | ALA |
| 2 | B | 812 | PHE |
| 2 | B | 1126 | GLU |
| 2 | C | 847 | ALA |
| 2 | C | 1142 | LEU |
| 2 | D | 54 | PHE |
| 2 | E | 999 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | F | 128 | PRO |
| 2 | F | 489 | GLY |
| 2 | F | 665 | ALA |
| 2 | F | 752 | SER |
| 2 | F | 939 | PHE |
| 2 | F | 1307 | THR |
| 2 | G | 140 | ARG |
| 2 | G | 337 | PRO |
| 2 | G | 1223 | GLN |
| 2 | H | 413 | LYS |
| 2 | H | 939 | PHE |
| 2 | H | 1002 | LEU |
| 2 | J | 939 | PHE |
| 2 | J | 1109 | ARG |
| 2 | L | 481 | CYS |
| 2 | L | 735 | ASP |
| 2 | L | 939 | PHE |
| 2 | L | 999 | PRO |
| 2 | L | 1268 | THR |
| 2 | N | 481 | CYS |
| 2 | N | 939 | PHE |
| 2 | O | 124 | PRO |
| 2 | O | 974 | PRO |
| 2 | O | 999 | PRO |
| 2 | P | 771 | TYR |
| 4 | g | 240 | GLN |
| 4 | j | 244 | CYS |
| 5 | k | 75 | ARG |
| 5 | l | 128 | GLY |
| 4 | m | 244 | CYS |
| 5 | n | 125 | LEU |
| 5 | r | 227 | SER |
| 5 | r | 258 | HIS |
| 4 | s | 244 | CYS |
| 1 | x | 74 | SER |
| 1 | z | 70 | ASN |
| 1 | 3 | 6 | ILE |
| 1 | 4 | 6 | ILE |
| 1 | 4 | 70 | ASN |
| 1 | 5 | 6 | ILE |
| 1 | 7 | 187 | ASN |
| 1 | 8 | 70 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 9 | 260 | ASN |
| 2 | A | 1030 | PRO |
| 2 | A | 1202 | VAL |
| 2 | A | 1350 | HIS |
| 2 | B | 349 | ALA |
| 2 | B | 690 | LEU |
| 2 | B | 705 | ALA |
| 2 | B | 970 | ASP |
| 2 | B | 999 | PRO |
| 2 | B | 1143 | LEU |
| 2 | C | 695 | ASN |
| 2 | C | 1054 | CYS |
| 2 | C | 1109 | ARG |
| 2 | D | 939 | PHE |
| 2 | E | 939 | PHE |
| 2 | E | 1171 | ALA |
| 2 | E | 1323 | PRO |
| 2 | F | 1152 | THR |
| 2 | G | 349 | ALA |
| 2 | H | 54 | PHE |
| 2 | H | 999 | PRO |
| 2 | I | 124 | PRO |
| 2 | I | 1140 | PRO |
| 2 | J | 5 | SER |
| 2 | J | 905 | GLN |
| 2 | K | 999 | PRO |
| 2 | L | 124 | PRO |
| 2 | L | 1108 | VAL |
| 2 | N | 124 | PRO |
| 2 | O | 31 | MET |
| 2 | O | 337 | PRO |
| 2 | O | 1030 | PRO |
| 2 | O | 1171 | ALA |
| 2 | P | 5 | SER |
| 2 | P | 939 | PHE |
| 2 | P | 999 | PRO |
| 3 | V | 38 | PRO |
| 4 | g | 160 | THR |
| 5 | h | 256 | PRO |
| 5 | h | 304 | PHE |
| 5 | i | 261 | PRO |
| 5 | k | 103 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | o | 79 | ASN |
| 5 | u | 191 | GLN |
| 1 | v | 145 | VAL |
| 1 | v | 182 | LYS |
| 1 | w | 182 | LYS |
| 1 | x | 182 | LYS |
| 1 | y | 70 | ASN |
| 1 | 0 | 6 | ILE |
| 1 | 3 | 260 | ASN |
| 1 | 6 | 6 | ILE |
| 1 | 6 | 70 | ASN |
| 2 | B | 481 | CYS |
| 2 | D | 707 | VAL |
| 2 | D | 1030 | PRO |
| 2 | G | 128 | PRO |
| 2 | G | 410 | VAL |
| 2 | G | 535 | PRO |
| 2 | G | 687 | ILE |
| 2 | H | 343 | SER |
| 2 | P | 33 | GLU |
| 5 | h | 119 | LEU |
| 5 | i | 59 | VAL |
| 4 | s | 221 | GLY |
| 1 | x | 141 | ARG |
| 1 | 7 | 6 | ILE |
| 2 | F | 535 | PRO |
| 2 | F | 1030 | PRO |
| 2 | G | 457 | PRO |
| 2 | J | 1108 | VAL |
| 2 | N | 337 | PRO |
| 4 | m | 195 | GLY |
| 1 | v | 6 | ILE |
| 1 | v | 181 | VAL |
| 2 | A | 1071 | ILE |
| 5 | h | 188 | VAL |
| 5 | l | 78 | GLY |
| 5 | n | 186 | ASP |
| 1 | 2 | 70 | ASN |
| 2 | A | 339 | LEU |
| 2 | E | 489 | GLY |
| 2 | G | 1030 | PRO |
| 2 | G | 1071 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 999 | PRO |
| 2 | J | 363 | GLY |
| 2 | O | 23 | VAL |
| 5 | i | 128 | GLY |
| 5 | t | 287 | VAL |
| 1 | x | 70 | ASN |
| 2 | C | 535 | PRO |
| 2 | C | 861 | VAL |
| 2 | F | 457 | PRO |
| 2 | M | 124 | PRO |
| 2 | M | 1030 | PRO |
| 2 | P | 1030 | PRO |
| 5 | n | 99 | PRO |
| 4 | p | 195 | GLY |
| 5 | u | 94 | VAL |
| 1 | z | 6 | ILE |
| 2 | I | 1030 | PRO |
| 5 | t | 128 | GLY |
| 1 | v | 70 | ASN |
| 5 | r | 250 | PRO |

### 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 | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 1 | 1 | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 1 | 2 | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 1 | 3 | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 1 | 4 | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 1 | 5 | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 1 | 6 | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 1 | 7 | 256/257 (100%) | 255 (100%) | 1 (0%) | 91 | 94 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | 8 | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 1 | 9 | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 1 | v | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 1 | w | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 1 | x | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 1 | y | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 1 | z | 256/257 (100%) | 256 (100%) | 0 | 100 | 100 |
| 2 | A | 1156/1192 (97%) | 1153 (100%) | 3 (0%) | 92 | 95 |
| 2 | B | 1162/1192 (98%) | 1158 (100%) | 4 (0%) | 92 | 95 |
| 2 | C | 1174/1192 (98%) | 1171 (100%) | 3 (0%) | 92 | 95 |
| 2 | D | 1173/1192 (98%) | 1167 (100%) | 6 (0%) | 88 | 93 |
| 2 | E | 1174/1192 (98%) | 1166 (99%) | 8 (1%) | 84 | 90 |
| 2 | F | 1175/1192 (99%) | 1170 (100%) | 5 (0%) | 91 | 94 |
| 2 | G | 1177/1192 (99%) | 1175 (100%) | 2 (0%) | 93 | 96 |
| 2 | H | 1177/1192 (99%) | 1173 (100%) | 4 (0%) | 92 | 95 |
| 2 | I | 1174/1192 (98%) | 1171 (100%) | 3 (0%) | 92 | 95 |
| 2 | J | 1161/1192 (97%) | 1156 (100%) | 5 (0%) | 91 | 94 |
| 2 | K | 1174/1192 (98%) | 1170 (100%) | 4 (0%) | 92 | 95 |
| 2 | L | 1178/1192 (99%) | 1176 (100%) | 2 (0%) | 93 | 96 |
| 2 | M | 1178/1192 (99%) | 1176 (100%) | 2 (0%) | 93 | 96 |
| 2 | N | 1175/1192 (99%) | 1170 (100%) | 5 (0%) | 91 | 94 |
| 2 | O | 1174/1192 (98%) | 1170 (100%) | 4 (0%) | 92 | 95 |
| 2 | P | 1174/1192 (98%) | 1170 (100%) | 4 (0%) | 92 | 95 |
| 3 | Q | 59/68 (87%) | 59 (100%) | 0 | 100 | 100 |
| 3 | R | 59/68 (87%) | 59 (100%) | 0 | 100 | 100 |
| 3 | S | 59/68 (87%) | 59 (100%) | 0 | 100 | 100 |
| 3 | T | 59/68 (87%) | 59 (100%) | 0 | 100 | 100 |
| 3 | U | 59/68 (87%) | 59 (100%) | 0 | 100 | 100 |
| 3 | V | 59/68 (87%) | 59 (100%) | 0 | 100 | 100 |
| 3 | W | 59/68 (87%) | 59 (100%) | 0 | 100 | 100 |
| 3 | X | 59/68 (87%) | 59 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 3 | Y | 59/68 (87%) | 58 (98%) | 1 (2%) | 60 78 |
| 3 | Z | 59/68 (87%) | 59 (100%) | 0 | 100 100 |
| 3 | a | 59/68 (87%) | 59 (100%) | 0 | 100 100 |
| 3 | b | 59/68 (87%) | 58 (98%) | 1 (2%) | 60 78 |
| 3 | c | 59/68 (87%) | 59 (100%) | 0 | 100 100 |
| 3 | d | 59/68 (87%) | 59 (100%) | 0 | 100 100 |
| 3 | e | 59/68 (87%) | 59 (100%) | 0 | 100 100 |
| 3 | f | 59/68 (87%) | 59 (100%) | 0 | 100 100 |
| 4 | g | 228/252 (90%) | 227 (100%) | 1 (0%) | 91 94 |
| 4 | j | 252/252 (100%) | 251 (100%) | 1 (0%) | 91 94 |
| 4 | m | 252/252 (100%) | 250 (99%) | 2 (1%) | 81 89 |
| 4 | p | 252/252 (100%) | 250 (99%) | 2 (1%) | 81 89 |
| 4 | s | 252/252 (100%) | 250 (99%) | 2 (1%) | 81 89 |
| 5 | h | 262/273 (96%) | 260 (99%) | 2 (1%) | 81 89 |
| 5 | i | 256/273 (94%) | 256 (100%) | 0 | 100 100 |
| 5 | k | 262/273 (96%) | 260 (99%) | 2 (1%) | 81 89 |
| 5 | l | 272/273 (100%) | 272 (100%) | 0 | 100 100 |
| 5 | n | 263/273 (96%) | 262 (100%) | 1 (0%) | 91 94 |
| 5 | o | 261/273 (96%) | 260 (100%) | 1 (0%) | 91 94 |
| 5 | q | 263/273 (96%) | 263 (100%) | 0 | 100 100 |
| 5 | r | 272/273 (100%) | 271 (100%) | 1 (0%) | 91 94 |
| 5 | t | 264/273 (97%) | 263 (100%) | 1 (0%) | 91 94 |
| 5 | u | 272/273 (100%) | 272 (100%) | 0 | 100 100 |
| All | All | 27423/28005 (98%) | 27340 (100%) | 83 (0%) | 92 95 |

All (83) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 7 | 170 | ASN |
| 2 | A | 1362 | LEU |
| 2 | A | 1367 | LEU |
| 2 | A | 1370 | SER |
| 2 | B | 86 | LEU |
| 2 | B | 142 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 231 | ASN |
| 2 | B | 1303 | CYS |
| 2 | C | 204 | ARG |
| 2 | C | 637 | ASN |
| 2 | C | 1370 | SER |
| 2 | D | 431 | LEU |
| 2 | D | 450 | CYS |
| 2 | D | 707 | VAL |
| 2 | D | 1303 | CYS |
| 2 | D | 1362 | LEU |
| 2 | D | 1370 | SER |
| 2 | E | 204 | ARG |
| 2 | E | 431 | LEU |
| 2 | E | 708 | ASN |
| 2 | E | 739 | LEU |
| 2 | E | 1183 | VAL |
| 2 | E | 1303 | CYS |
| 2 | E | 1362 | LEU |
| 2 | E | 1370 | SER |
| 2 | F | 207 | LEU |
| 2 | F | 226 | THR |
| 2 | F | 1303 | CYS |
| 2 | F | 1362 | LEU |
| 2 | F | 1367 | LEU |
| 2 | G | 1362 | LEU |
| 2 | G | 1370 | SER |
| 2 | H | 204 | ARG |
| 2 | H | 207 | LEU |
| 2 | H | 1303 | CYS |
| 2 | H | 1370 | SER |
| 2 | I | 431 | LEU |
| 2 | I | 1303 | CYS |
| 2 | I | 1370 | SER |
| 2 | J | 207 | LEU |
| 2 | J | 231 | ASN |
| 2 | J | 1057 | VAL |
| 2 | J | 1303 | CYS |
| 2 | J | 1370 | SER |
| 2 | K | 207 | LEU |
| 2 | K | 212 | ARG |
| 2 | K | 1303 | CYS |
| 2 | K | 1370 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | L | 1057 | VAL |
| 2 | L | 1370 | SER |
| 2 | M | 1057 | VAL |
| 2 | M | 1364 | GLN |
| 2 | N | 116 | VAL |
| 2 | N | 226 | THR |
| 2 | N | 1057 | VAL |
| 2 | N | 1303 | CYS |
| 2 | N | 1370 | SER |
| 2 | O | 207 | LEU |
| 2 | O | 231 | ASN |
| 2 | O | 431 | LEU |
| 2 | O | 1370 | SER |
| 2 | P | 1057 | VAL |
| 2 | P | 1303 | CYS |
| 2 | P | 1366 | MET |
| 2 | P | 1368 | PHE |
| 3 | Y | 73 | THR |
| 3 | b | 73 | THR |
| 4 | g | 158 | LEU |
| 5 | h | 239 | MET |
| 5 | h | 241 | LEU |
| 4 | j | 158 | LEU |
| 5 | k | 82 | LEU |
| 5 | k | 238 | LEU |
| 4 | m | 158 | LEU |
| 4 | m | 241 | ILE |
| 5 | n | 297 | ASN |
| 5 | o | 297 | ASN |
| 4 | p | 158 | LEU |
| 4 | p | 241 | ILE |
| 5 | r | 246 | SER |
| 4 | s | 158 | LEU |
| 4 | s | 241 | ILE |
| 5 | t | 124 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 534 | HIS |
| 2 | A | 560 | ASN |
| 2 | A | 984 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 1191 | ASN |
| 2 | B | 422 | ASN |
| 2 | B | 748 | HIS |
| 2 | B | 795 | ASN |
| 2 | B | 914 | GLN |
| 2 | B | 940 | HIS |
| 2 | B | 1080 | ASN |
| 2 | B | 1319 | GLN |
| 2 | B | 1364 | GLN |
| 2 | C | 22 | HIS |
| 2 | C | 903 | GLN |
| 2 | C | 914 | GLN |
| 2 | C | 940 | HIS |
| 2 | C | 1191 | ASN |
| 2 | D | 422 | ASN |
| 2 | D | 514 | GLN |
| 2 | D | 694 | ASN |
| 2 | D | 1080 | ASN |
| 2 | E | 534 | HIS |
| 2 | E | 605 | ASN |
| 2 | E | 903 | GLN |
| 2 | E | 914 | GLN |
| 2 | E | 940 | HIS |
| 2 | E | 1093 | ASN |
| 2 | E | 1264 | GLN |
| 2 | E | 1313 | ASN |
| 2 | G | 96 | GLN |
| 2 | G | 231 | ASN |
| 2 | G | 455 | HIS |
| 2 | G | 803 | ASN |
| 2 | G | 1079 | GLN |
| 2 | G | 1120 | ASN |
| 2 | G | 1264 | GLN |
| 2 | G | 1313 | ASN |
| 2 | G | 1353 | ASN |
| 2 | H | 59 | ASN |
| 2 | H | 214 | ASN |
| 2 | H | 618 | HIS |
| 2 | H | 711 | HIS |
| 2 | H | 919 | ASN |
| 2 | H | 1133 | HIS |
| 2 | I | 605 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 889 | HIS |
| 2 | I | 901 | HIS |
| 2 | I | 985 | ASN |
| 2 | J | 199 | ASN |
| 2 | J | 560 | ASN |
| 2 | J | 889 | HIS |
| 2 | J | 901 | HIS |
| 2 | J | 945 | ASN |
| 2 | J | 969 | HIS |
| 2 | J | 1313 | ASN |
| 2 | J | 1364 | GLN |
| 2 | K | 438 | GLN |
| 2 | K | 749 | HIS |
| 2 | K | 889 | HIS |
| 2 | K | 901 | HIS |
| 2 | K | 919 | ASN |
| 2 | K | 945 | ASN |
| 2 | K | 969 | HIS |
| 2 | K | 1124 | HIS |
| 2 | L | 462 | GLN |
| 2 | L | 618 | HIS |
| 2 | L | 889 | HIS |
| 2 | L | 903 | GLN |
| 2 | L | 919 | ASN |
| 2 | L | 945 | ASN |
| 2 | L | 1027 | HIS |
| 2 | L | 1235 | GLN |
| 2 | M | 889 | HIS |
| 2 | M | 945 | ASN |
| 2 | N | 618 | HIS |
| 2 | N | 889 | HIS |
| 2 | N | 1023 | GLN |
| 2 | O | 889 | HIS |
| 2 | O | 914 | GLN |
| 2 | O | 1235 | GLN |
| 2 | P | 94 | HIS |
| 2 | P | 231 | ASN |
| 2 | P | 618 | HIS |
| 2 | P | 889 | HIS |
| 2 | P | 1223 | GLN |
| 2 | P | 1235 | GLN |
| 2 | P | 1255 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | V | 37 | HIS |
| 4 | g | 211 | HIS |
| 5 | h | 80 | GLN |
| 5 | h | 88 | HIS |
| 5 | l | 80 | GLN |
| 5 | o | 43 | HIS |
| 5 | o | 80 | GLN |
| 4 | p | 211 | HIS |
| 5 | q | 297 | ASN |
| 4 | s | 211 | HIS |
| 5 | t | 39 | HIS |
| 5 | t | 173 | GLN |
| 5 | t | 192 | HIS |
| 1 | v | 170 | ASN |
| 1 | w | 256 | HIS |

#### 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 monosaccharides 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.

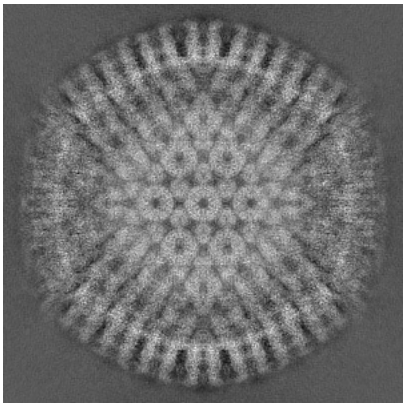
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8703. These allow visual inspection of the internal detail of the map and identification of artifacts.

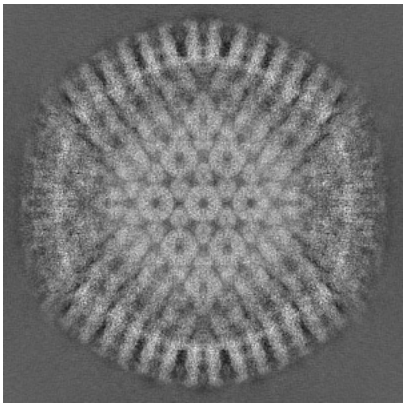
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

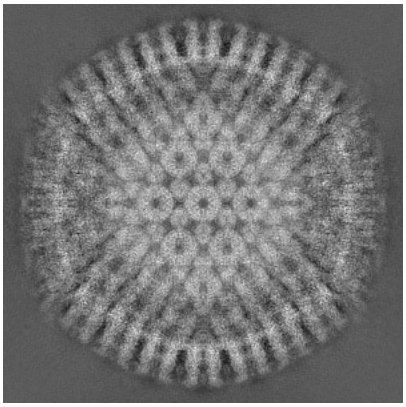
### 6.1.1 Primary map



X



Y

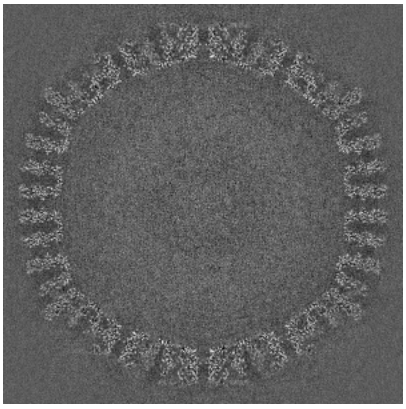


Z

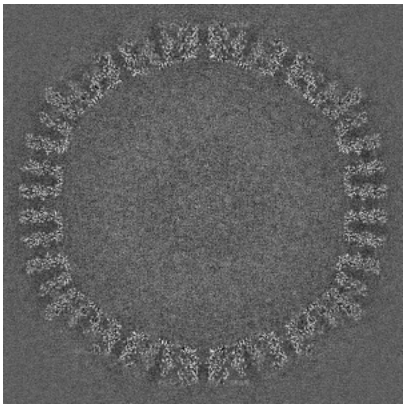
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

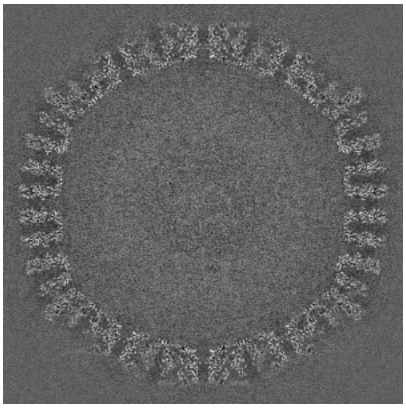
### 6.2.1 Primary map



X Index: 420



Y Index: 420

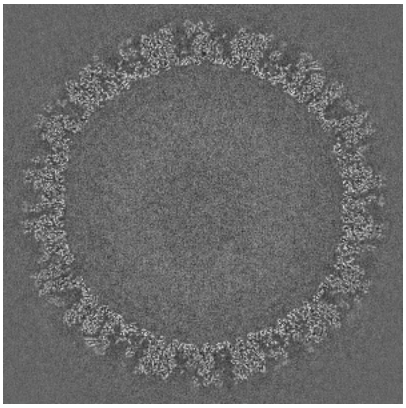


Z Index: 420

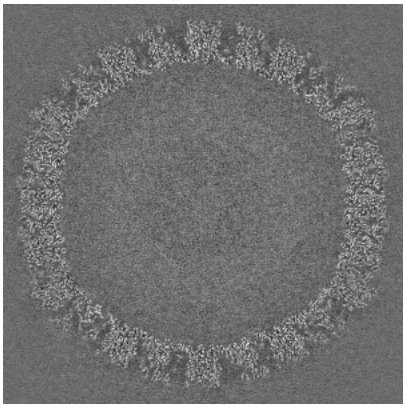
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

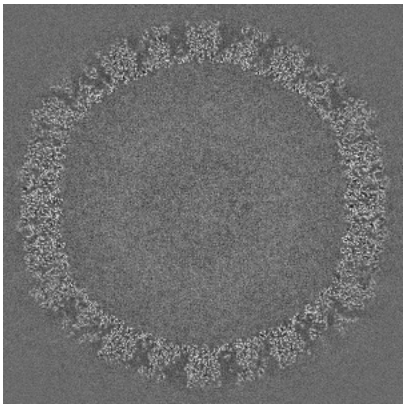
### 6.3.1 Primary map



X Index: 352



Y Index: 401



Z Index: 439

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

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

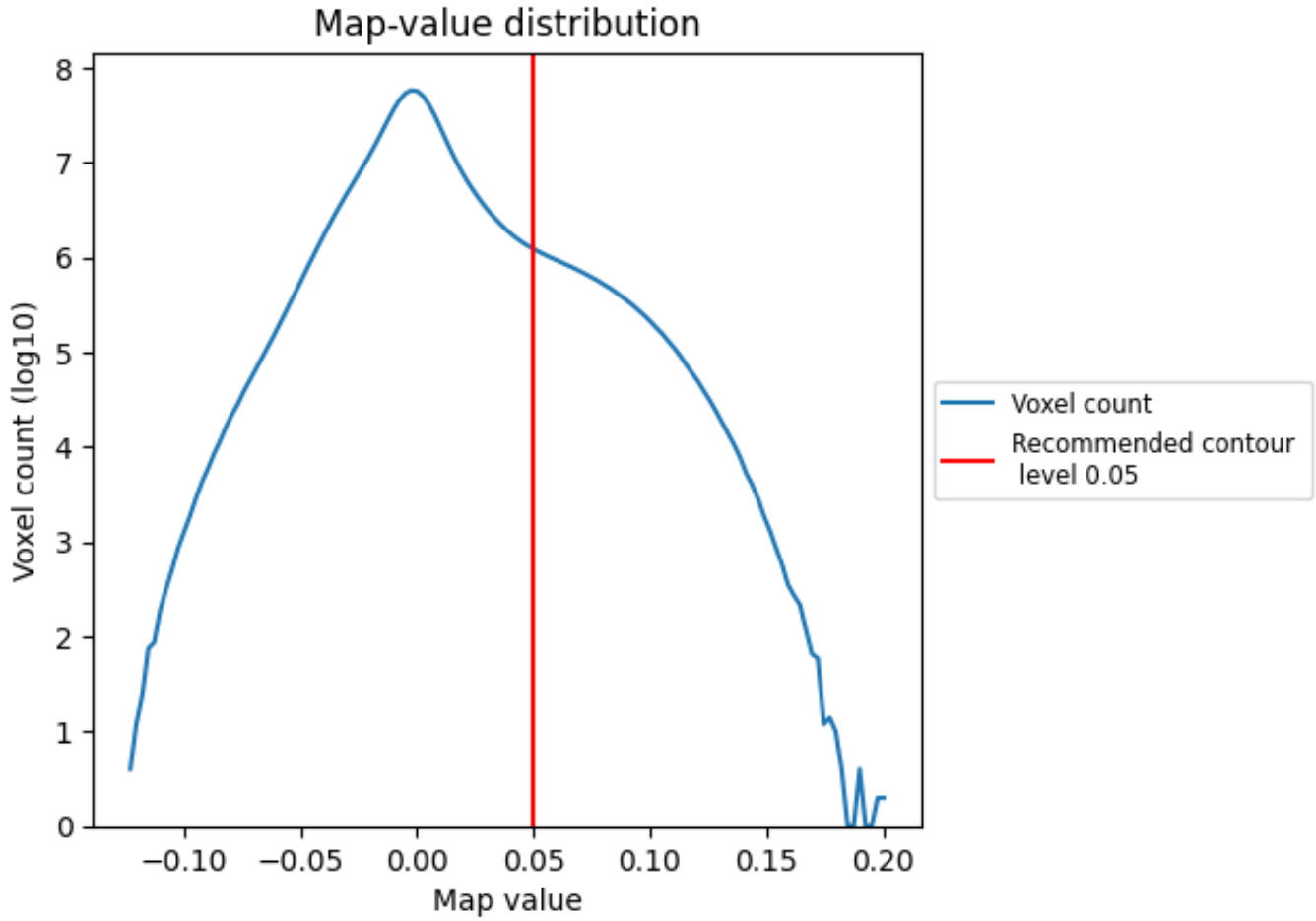
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

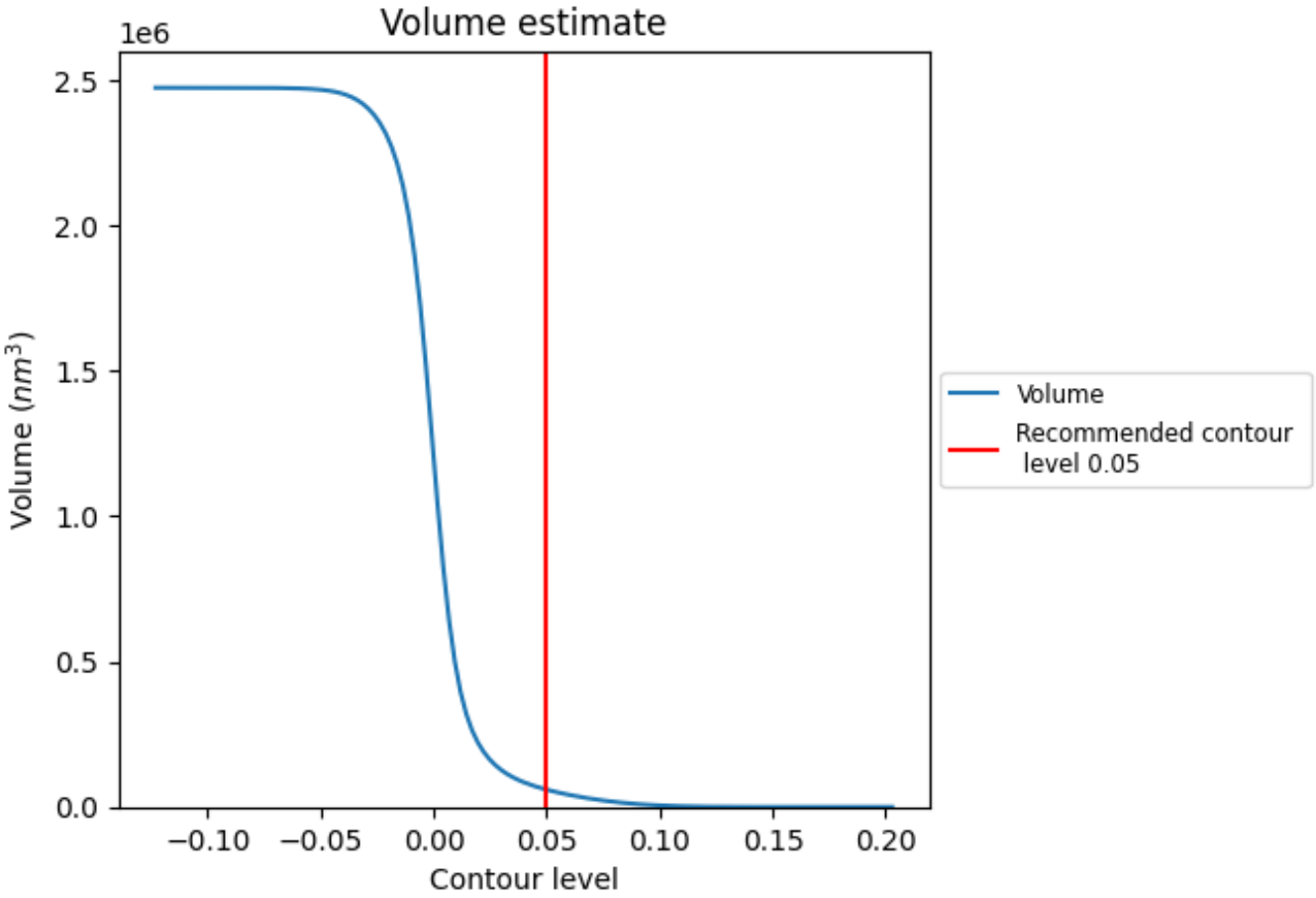
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

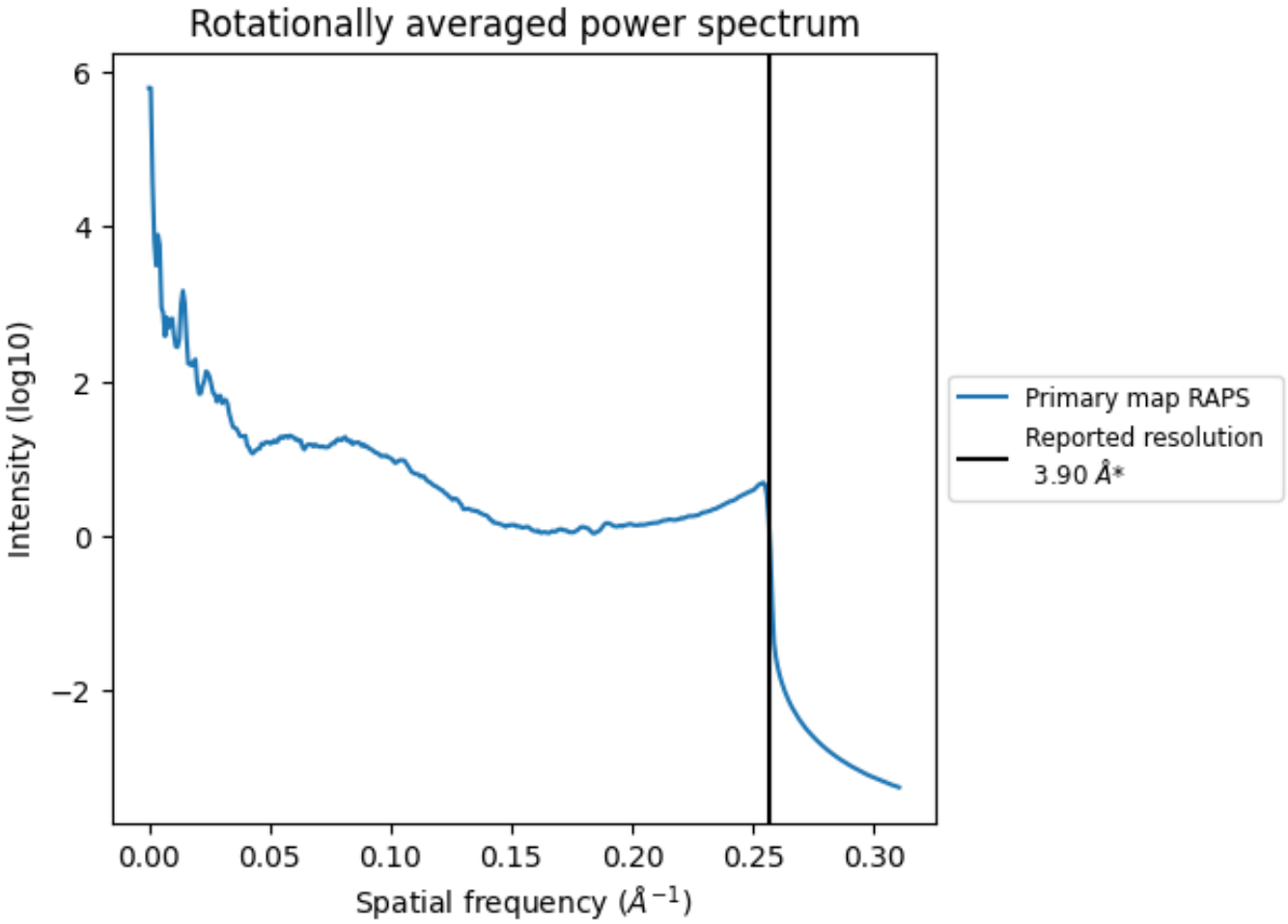
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 59607 $nm^3$; this corresponds to an approximate mass of 53844 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 0.256 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

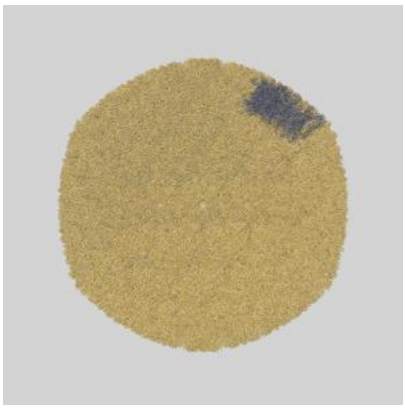
This section was not generated. No FSC curve or half-maps provided.

# 9 Map-model fit

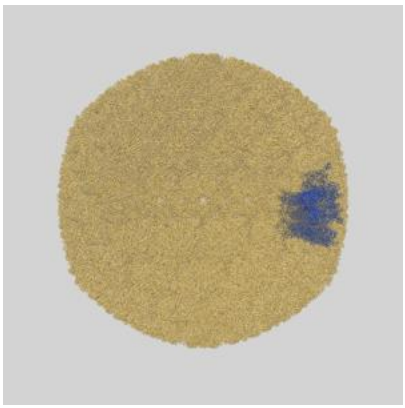
This section contains information regarding the fit between EMDB map EMD-8703 and PDB model 5VKU. Per-residue inclusion information can be found in section 3 on page 10.

## 9.1 Map-model overlays

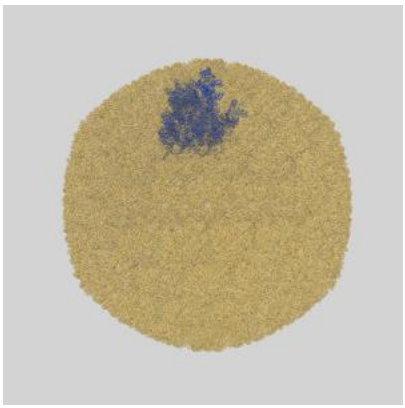
### 9.1.1 Map-model overlay



X

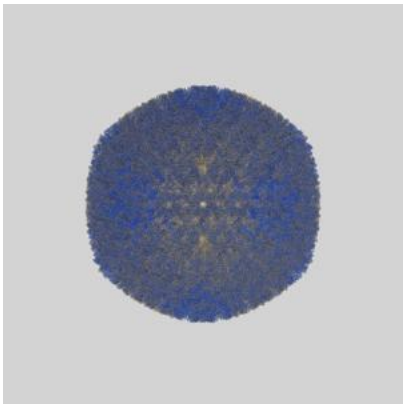


Y

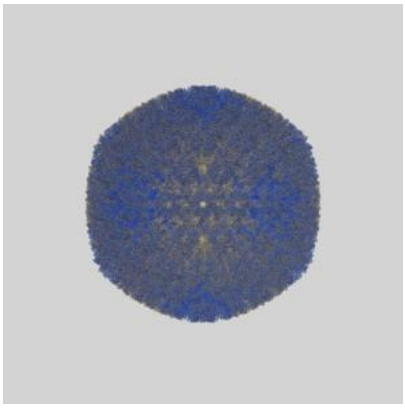


Z

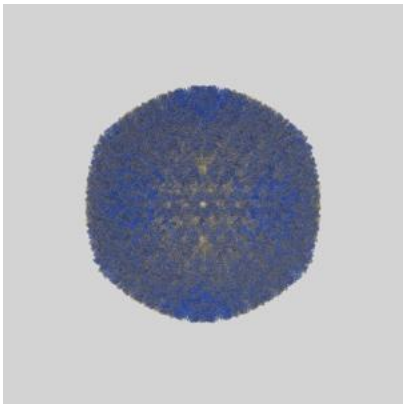
### 9.1.2 Map-model assembly overlay



X



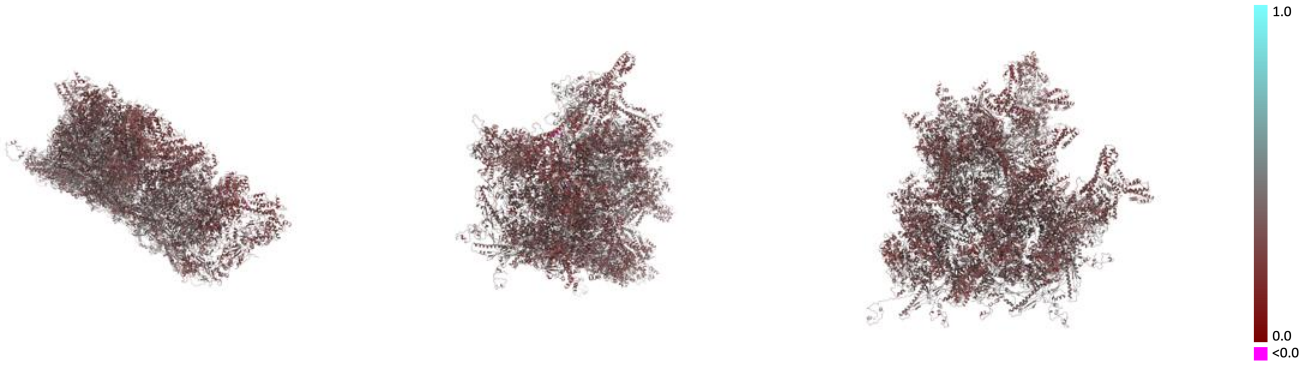
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

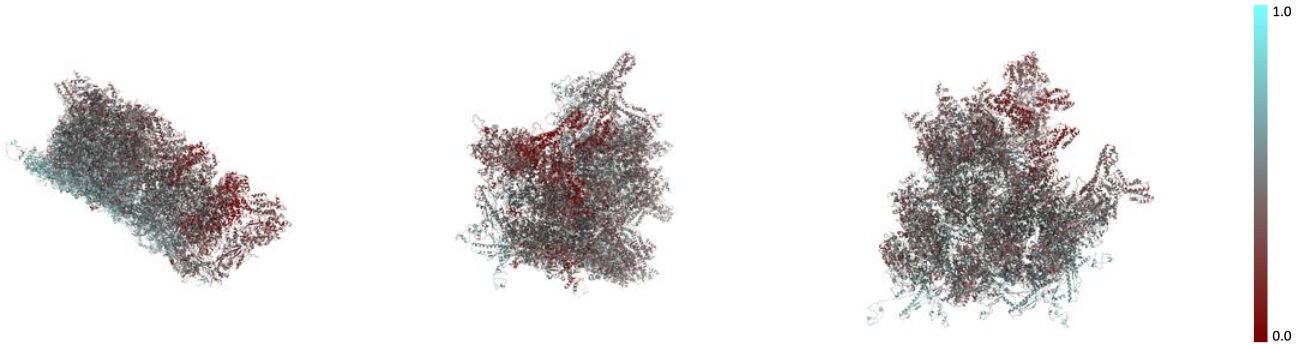
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

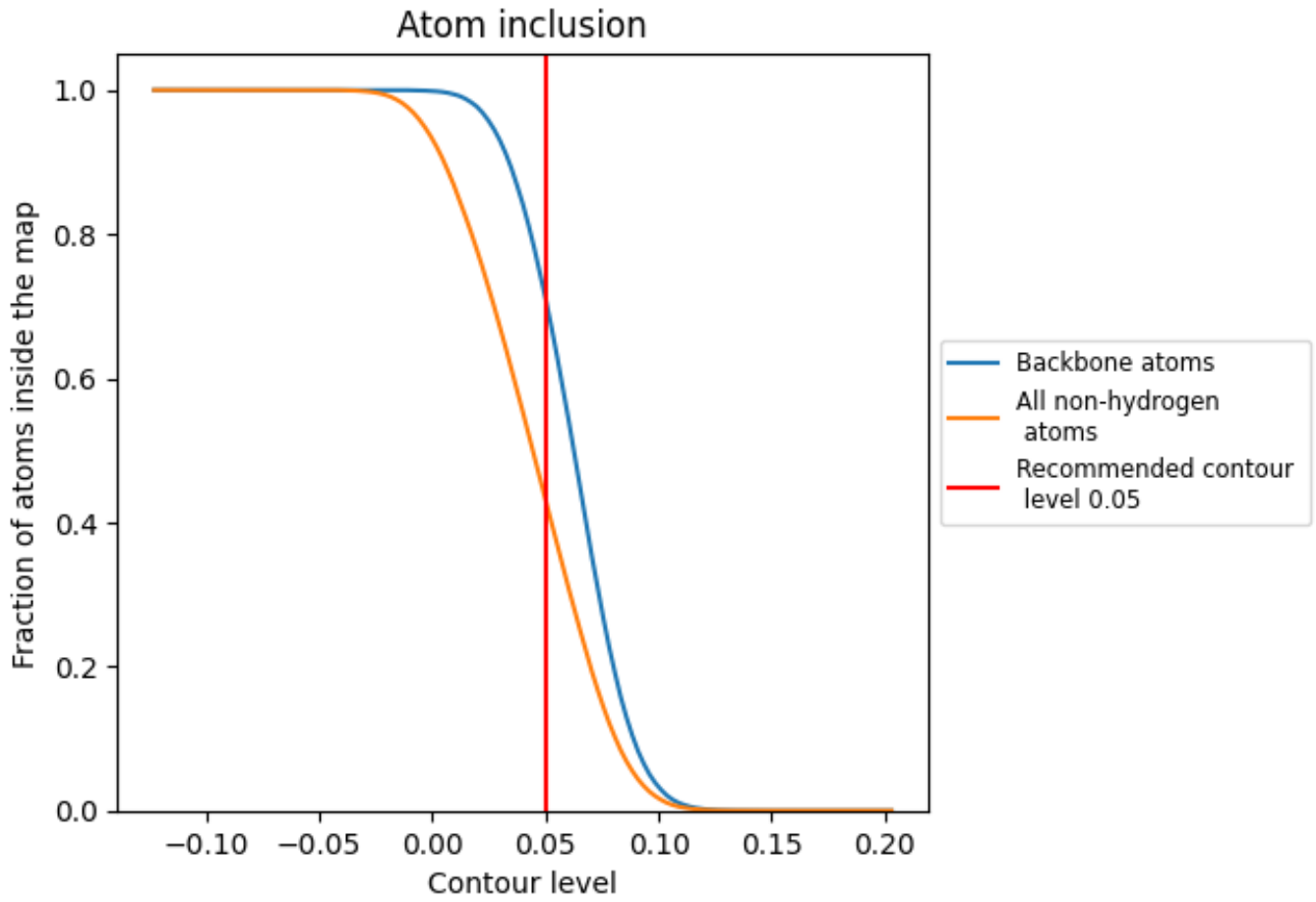
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

## 9.4 Atom inclusion (i)




At the recommended contour level, 71% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.4313 | 0.3470 |
| 0 | 0.3764 | 0.3020 |
| 1 | 0.3733 | 0.3070 |
| 2 | 0.1322 | 0.2890 |
| 3 | 0.2689 | 0.2770 |
| 4 | 0.4038 | 0.3190 |
| 5 | 0.3454 | 0.2850 |
| 6 | 0.3684 | 0.3050 |
| 7 | 0.4096 | 0.3090 |
| 8 | 0.3799 | 0.3030 |
| 9 | 0.3768 | 0.3140 |
| A | 0.3054 | 0.3280 |
| B | 0.4121 | 0.3430 |
| C | 0.4474 | 0.3540 |
| D | 0.4704 | 0.3600 |
| E | 0.4719 | 0.3630 |
| F | 0.4492 | 0.3580 |
| G | 0.4132 | 0.3450 |
| H | 0.4857 | 0.3590 |
| I | 0.4924 | 0.3670 |
| J | 0.4902 | 0.3660 |
| K | 0.4936 | 0.3690 |
| L | 0.4950 | 0.3710 |
| M | 0.4799 | 0.3610 |
| N | 0.4914 | 0.3670 |
| O | 0.4953 | 0.3670 |
| P | 0.4942 | 0.3650 |
| Q | 0.1727 | 0.2680 |
| R | 0.2631 | 0.2730 |
| S | 0.3052 | 0.2740 |
| T | 0.3333 | 0.2920 |
| U | 0.3333 | 0.2860 |
| V | 0.3253 | 0.2910 |
| W | 0.2851 | 0.2920 |
| X | 0.3715 | 0.2930 |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| Chain | Atom inclusion | Q-score |
|---|---|---|
| Y | 0.3755 | 0.3030 |
| Z | 0.3916 | 0.3170 |
| a | 0.3735 | 0.3000 |
| b | 0.3755 | 0.2850 |
| c | 0.3594 | 0.2890 |
| d | 0.3876 | 0.3160 |
| e | 0.3795 | 0.3000 |
| f | 0.3675 | 0.2860 |
| g | 0.2419 | 0.3340 |
| h | 0.2850 | 0.3180 |
| i | 0.2498 | 0.3320 |
| j | 0.4907 | 0.3740 |
| k | 0.4690 | 0.3600 |
| l | 0.4504 | 0.3620 |
| m | 0.4583 | 0.3500 |
| n | 0.4446 | 0.3520 |
| o | 0.4504 | 0.3530 |
| p | 0.4774 | 0.3570 |
| q | 0.4686 | 0.3630 |
| r | 0.4655 | 0.3550 |
| s | 0.4894 | 0.3710 |
| t | 0.4796 | 0.3690 |
| u | 0.4592 | 0.3580 |
| v | 0.0796 | 0.2740 |
| w | 0.0933 | 0.2480 |
| x | 0.2158 | 0.2720 |
| y | 0.3914 | 0.3270 |
| z | 0.3852 | 0.3050 |