



# wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 11:30 AM UTC

PDB ID : 6LGN / pdb\_00006lgn  
EMDB ID : EMD-0881  
Title : The atomic structure of varicella zoster virus C-capsid  
Authors : Li, S.; Zheng, Q.  
Deposited on : 2019-12-05  
Resolution : 5.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

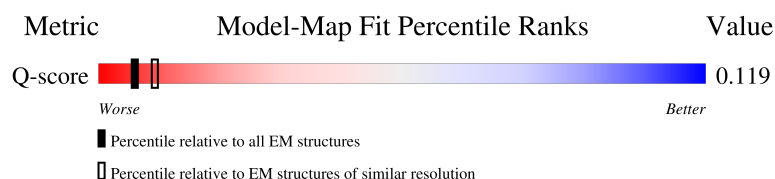
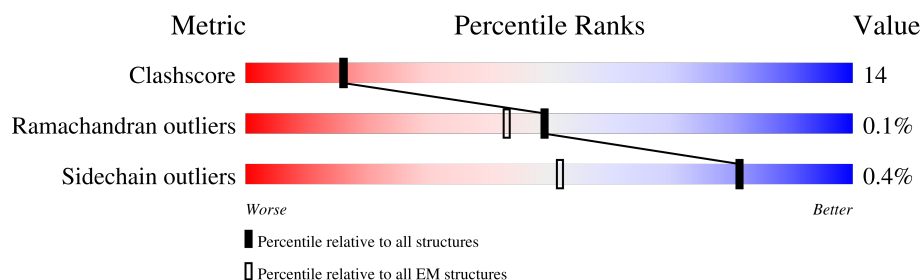
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

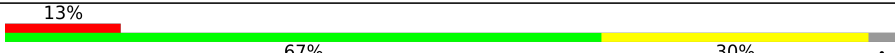
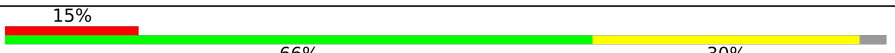
The reported resolution of this entry is 5.30 Å.

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<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 625 ( 4.80 - 5.80 )                                      |

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 1396   |  |
| 1   | B     | 1396   |  |
| 1   | C     | 1396   |  |
| 1   | E     | 1396   |  |

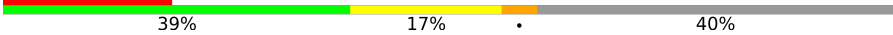
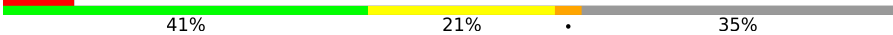
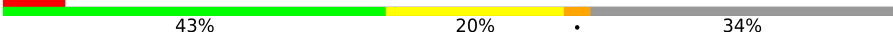
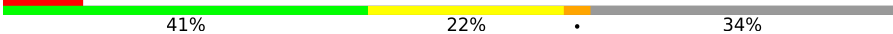
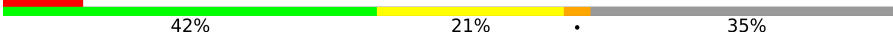
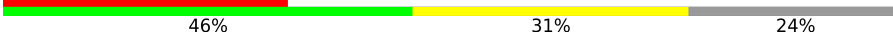
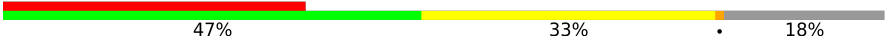
Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 1396   |                  |
| 1   | G     | 1396   |                  |
| 1   | M     | 1396   |                  |
| 1   | N     | 1396   |                  |
| 1   | O     | 1396   |                  |
| 1   | P     | 1396   |                  |
| 1   | Q     | 1396   |                  |
| 1   | R     | 1396   |                  |
| 1   | S     | 1396   |                  |
| 1   | T     | 1396   |                  |
| 1   | U     | 1396   |                  |
| 1   | z     | 1396   |                  |
| 2   | D     | 235    |                  |
| 2   | H     | 235    |                  |
| 2   | I     | 235    |                  |
| 2   | J     | 235    |                  |
| 2   | K     | 235    |                  |
| 2   | L     | 235    |                  |
| 2   | V     | 235    |                  |
| 2   | W     | 235    |                  |
| 2   | X     | 235    |                  |
| 2   | Y     | 235    |                  |
| 2   | Z     | 235    |                  |
| 2   | a     | 235    |                  |
| 2   | b     | 235    |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | c     | 235    |    |
| 2   | d     | 235    |    |
| 3   | e     | 483    |    |
| 3   | f     | 483    |    |
| 3   | g     | 483    |    |
| 3   | h     | 483    |    |
| 3   | i     | 483    |    |
| 4   | j     | 316    |    |
| 4   | k     | 316    |    |
| 4   | l     | 316    |    |
| 4   | m     | 316    |    |
| 4   | n     | 316    |   |
| 4   | o     | 316    |  |
| 4   | p     | 316    |  |
| 4   | q     | 316    |  |
| 4   | r     | 316    |  |
| 4   | s     | 316    |  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 207987 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Major capsid protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1354     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10592 | 6695 | 1880 | 1949 | 68 |         |       |
| 1   | M     | 1353     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10582 | 6690 | 1876 | 1948 | 68 |         |       |
| 1   | N     | 1353     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10582 | 6690 | 1876 | 1948 | 68 |         |       |
| 1   | O     | 1355     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10600 | 6701 | 1881 | 1950 | 68 |         |       |
| 1   | P     | 1355     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10600 | 6701 | 1881 | 1950 | 68 |         |       |
| 1   | Q     | 1354     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10592 | 6695 | 1880 | 1949 | 68 |         |       |
| 1   | R     | 1353     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10582 | 6690 | 1876 | 1948 | 68 |         |       |
| 1   | S     | 1355     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10600 | 6701 | 1881 | 1950 | 68 |         |       |
| 1   | T     | 1354     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10592 | 6695 | 1880 | 1949 | 68 |         |       |
| 1   | U     | 1331     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10422 | 6590 | 1847 | 1919 | 66 |         |       |
| 1   | B     | 1355     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10600 | 6701 | 1881 | 1950 | 68 |         |       |
| 1   | C     | 1354     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10592 | 6695 | 1880 | 1949 | 68 |         |       |
| 1   | E     | 1353     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10582 | 6689 | 1877 | 1948 | 68 |         |       |
| 1   | F     | 1354     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10592 | 6695 | 1880 | 1949 | 68 |         |       |
| 1   | G     | 1295     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10133 | 6401 | 1804 | 1863 | 65 |         |       |
| 1   | z     | 607      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 4709  | 2970 | 830  | 878  | 31 |         |       |

- Molecule 2 is a protein called Small capsomere-interacting protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | D     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 481 | 146 | 136 | 2 |         |       |
| 2   | V     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 481 | 146 | 136 | 2 |         |       |
| 2   | W     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 481 | 146 | 136 | 2 |         |       |
| 2   | X     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 481 | 146 | 136 | 2 |         |       |
| 2   | Y     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 481 | 146 | 136 | 2 |         |       |
| 2   | Z     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 481 | 146 | 136 | 2 |         |       |
| 2   | a     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 481 | 146 | 136 | 2 |         |       |
| 2   | b     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 754   | 475 | 142 | 135 | 2 |         |       |
| 2   | c     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 481 | 146 | 136 | 2 |         |       |
| 2   | d     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 481 | 146 | 136 | 2 |         |       |
| 2   | H     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 754   | 475 | 142 | 135 | 2 |         |       |
| 2   | I     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 481 | 146 | 136 | 2 |         |       |
| 2   | J     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 481 | 146 | 136 | 2 |         |       |
| 2   | K     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 481 | 146 | 136 | 2 |         |       |
| 2   | L     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 481 | 146 | 136 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | e     | 289      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2294  | 1451 | 411 | 417 | 15 |         |       |
| 3   | f     | 316      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2492  | 1574 | 448 | 455 | 15 |         |       |
| 3   | g     | 317      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2497  | 1576 | 448 | 458 | 15 |         |       |
| 3   | h     | 317      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2496  | 1575 | 448 | 458 | 15 |         |       |
| 3   | i     | 316      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2490  | 1572 | 447 | 456 | 15 |         |       |

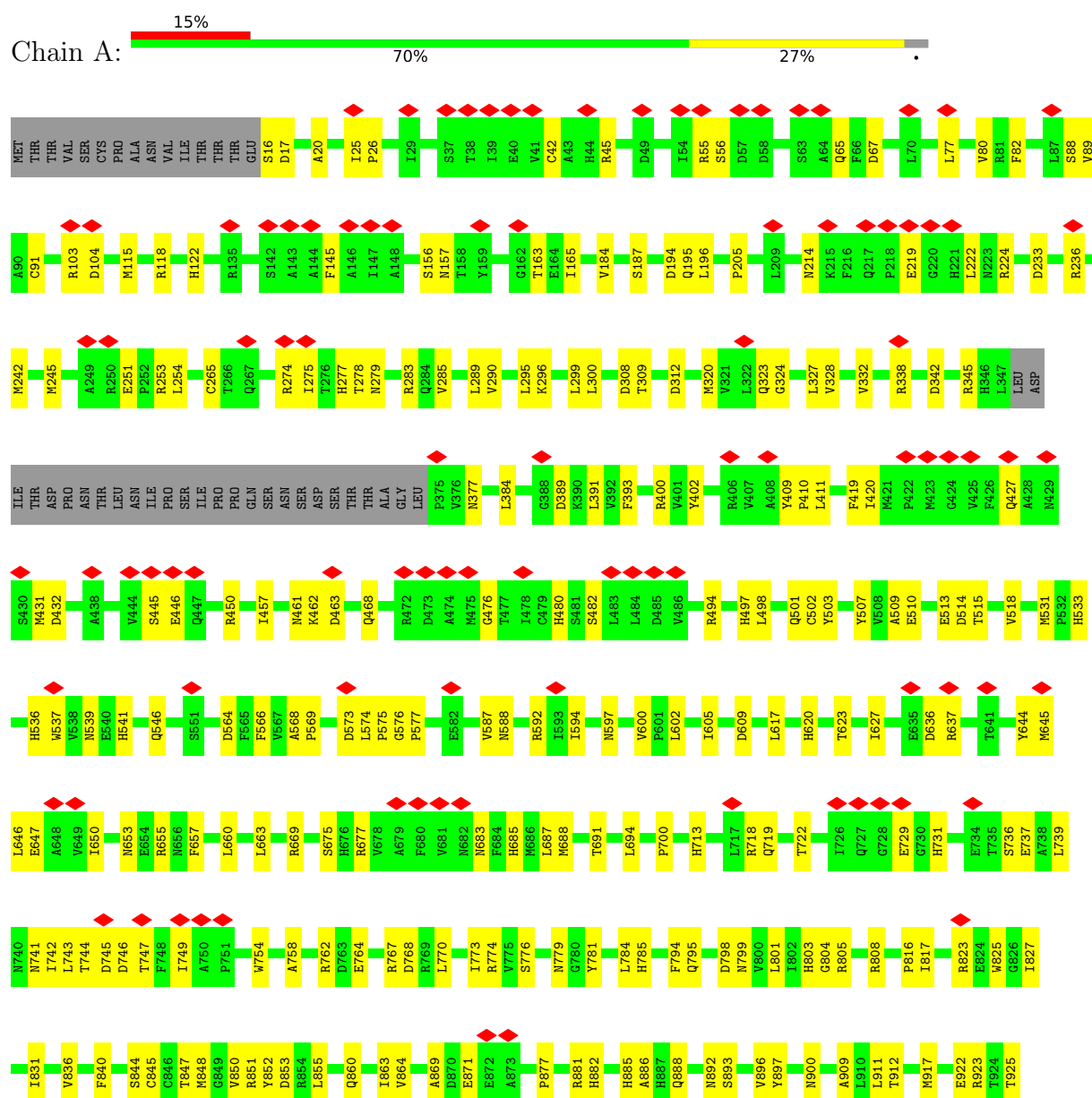
- Molecule 4 is a protein called Triplex capsid protein 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | j     | 241      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1837  | 1180 | 310 | 337 | 10 |         |       |
| 4   | o     | 258      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1969  | 1259 | 334 | 366 | 10 |         |       |
| 4   | k     | 275      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2090  | 1336 | 355 | 389 | 10 |         |       |
| 4   | p     | 304      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2325  | 1480 | 403 | 429 | 13 |         |       |
| 4   | l     | 263      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2010  | 1286 | 342 | 372 | 10 |         |       |
| 4   | q     | 301      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2307  | 1469 | 400 | 426 | 12 |         |       |
| 4   | m     | 267      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2028  | 1296 | 346 | 376 | 10 |         |       |
| 4   | r     | 315      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2407  | 1532 | 420 | 443 | 12 |         |       |
| 4   | n     | 265      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2019  | 1291 | 344 | 374 | 10 |         |       |
| 4   | s     | 304      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2321  | 1477 | 403 | 429 | 12 |         |       |

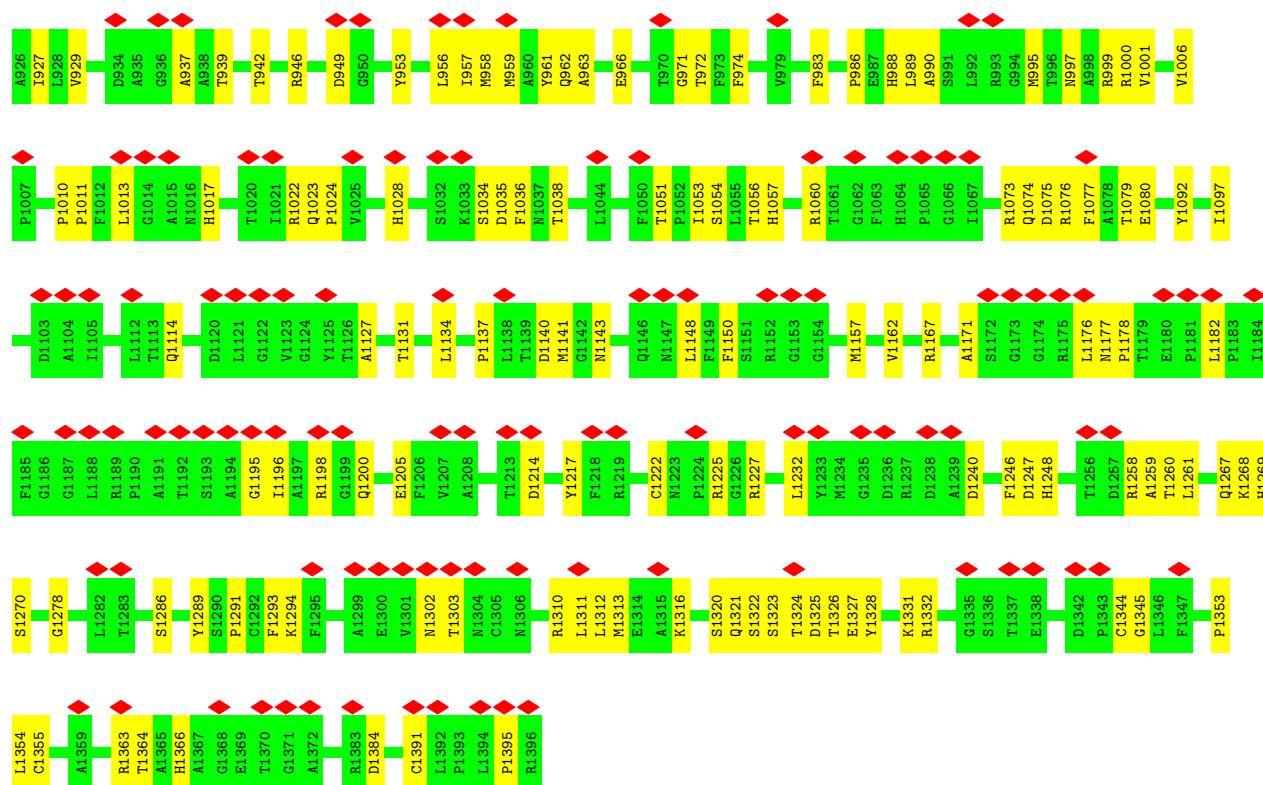
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

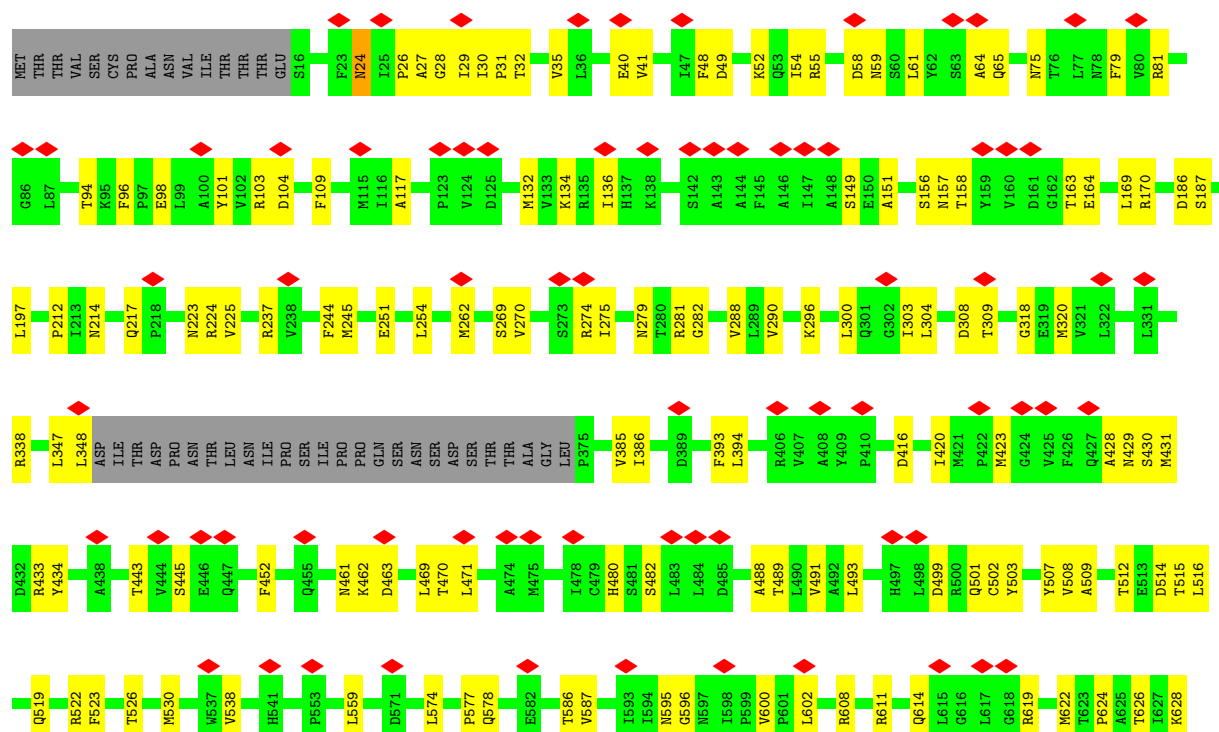
#### • Molecule 1: Major capsid protein

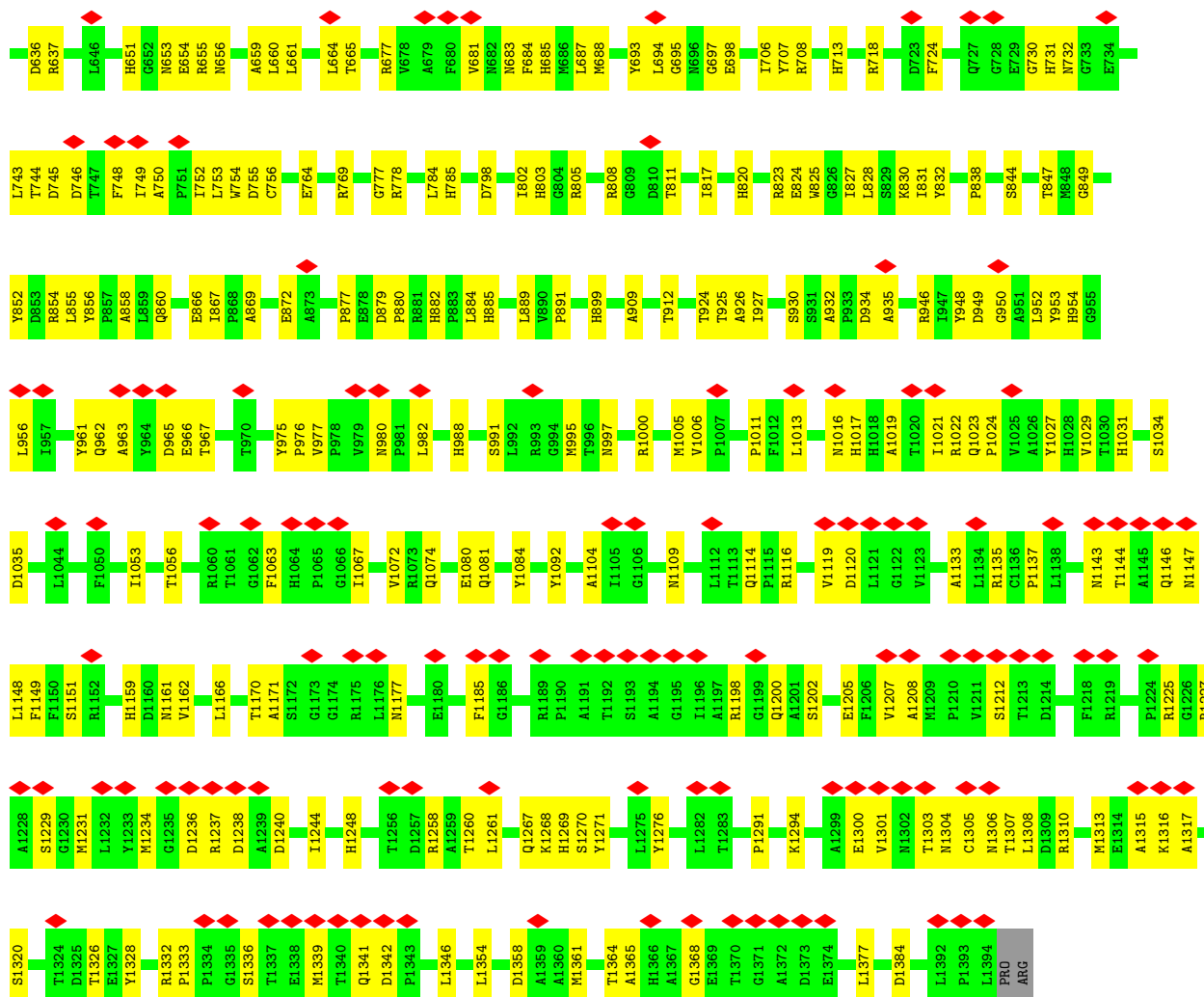




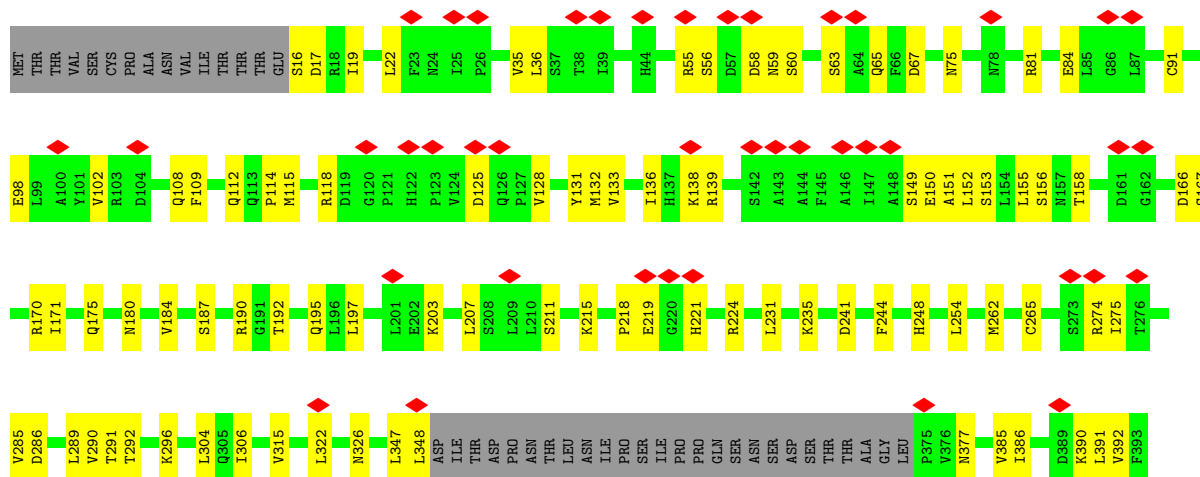


• Molecule 1: Major capsid protein

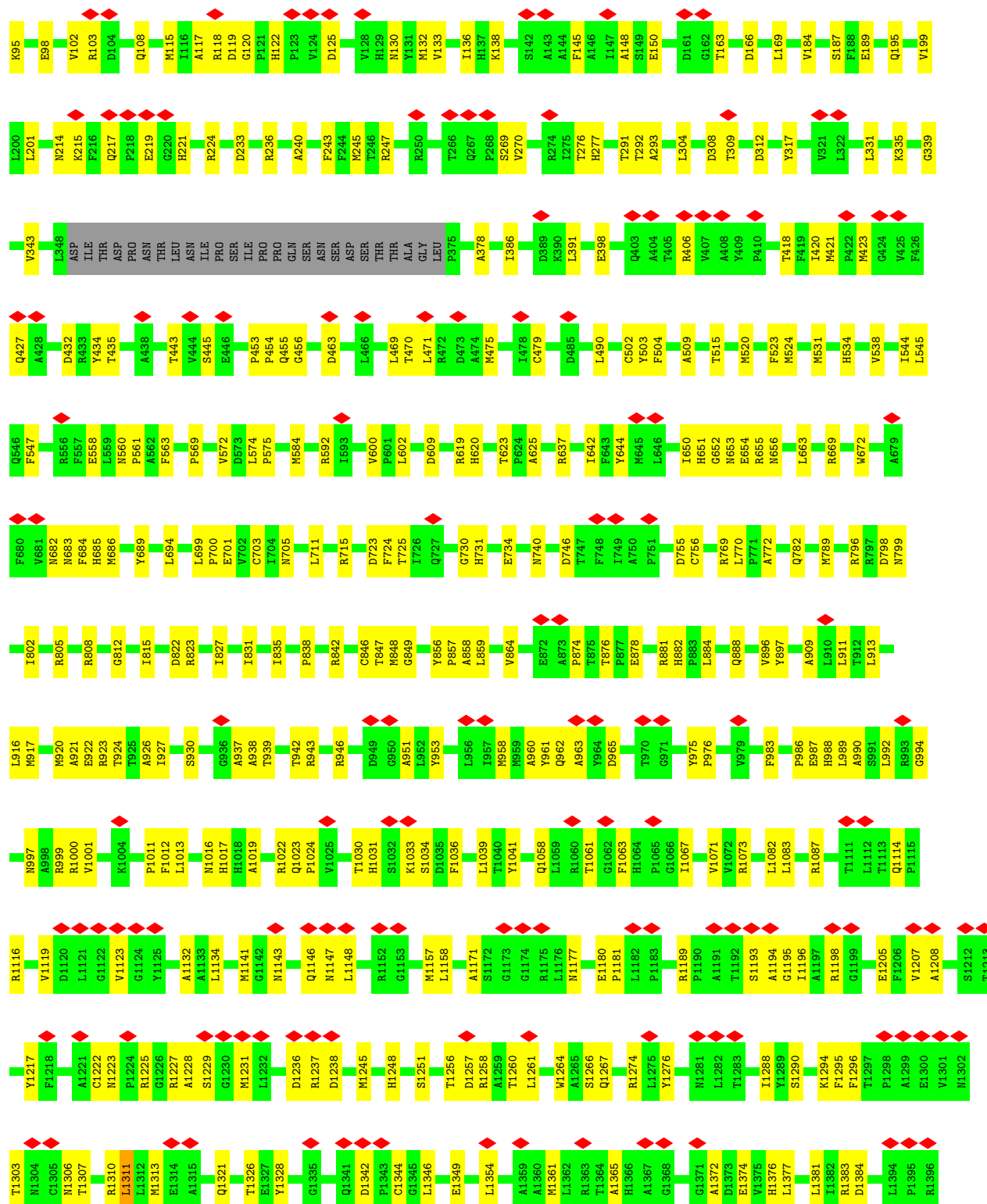




• Molecule 1: Major capsid protein







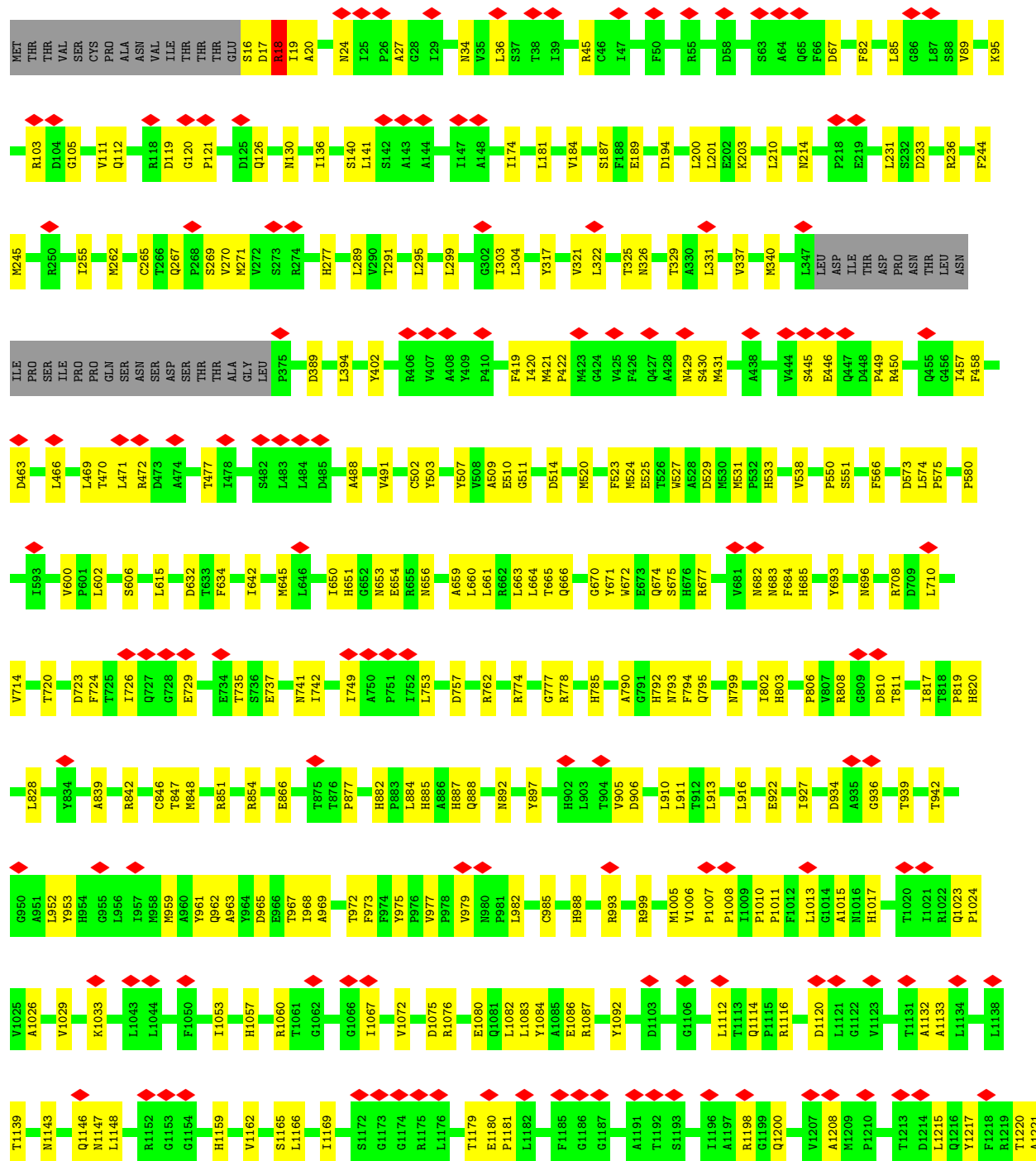
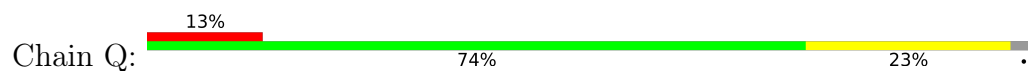
• Molecule 1: Major capsid protein

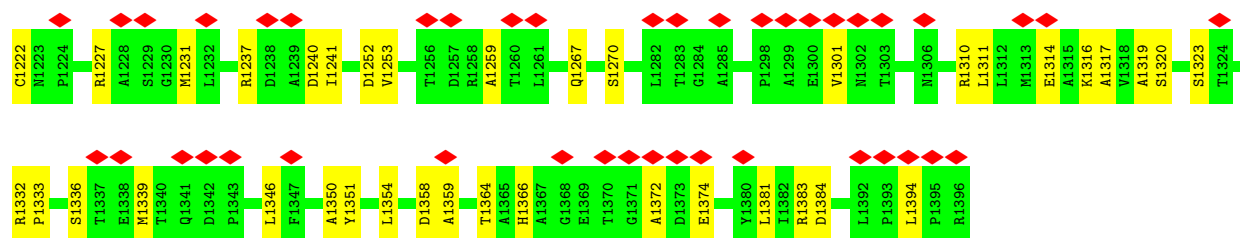




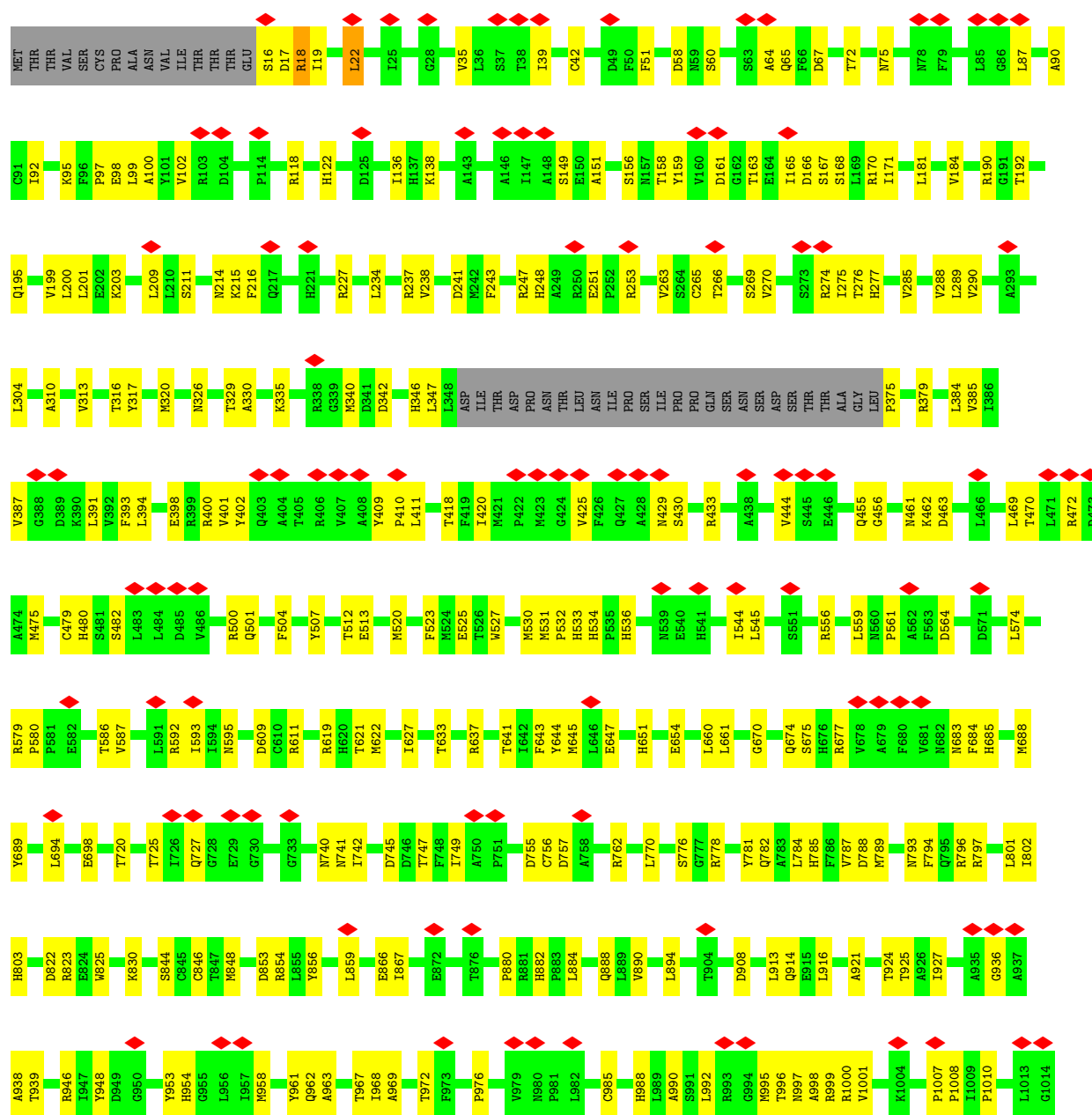


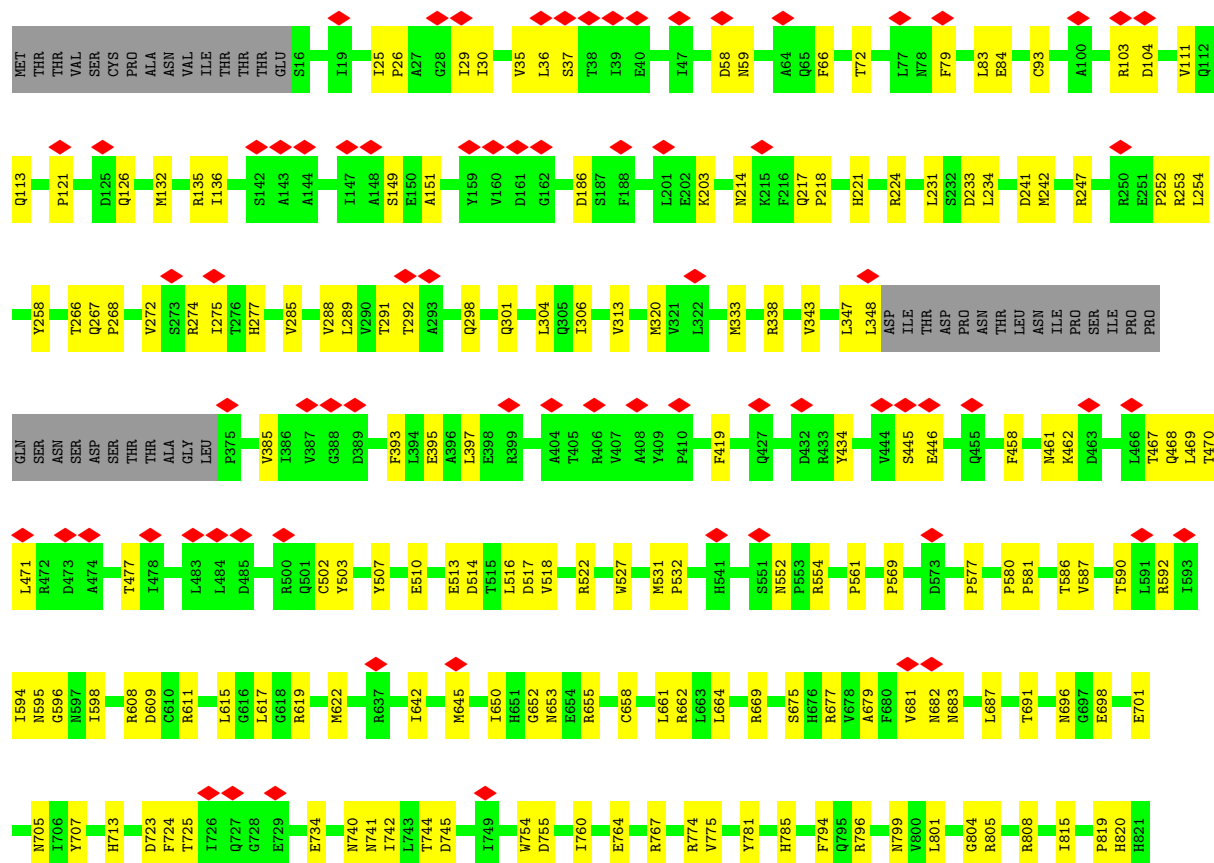
• Molecule 1: Major capsid protein



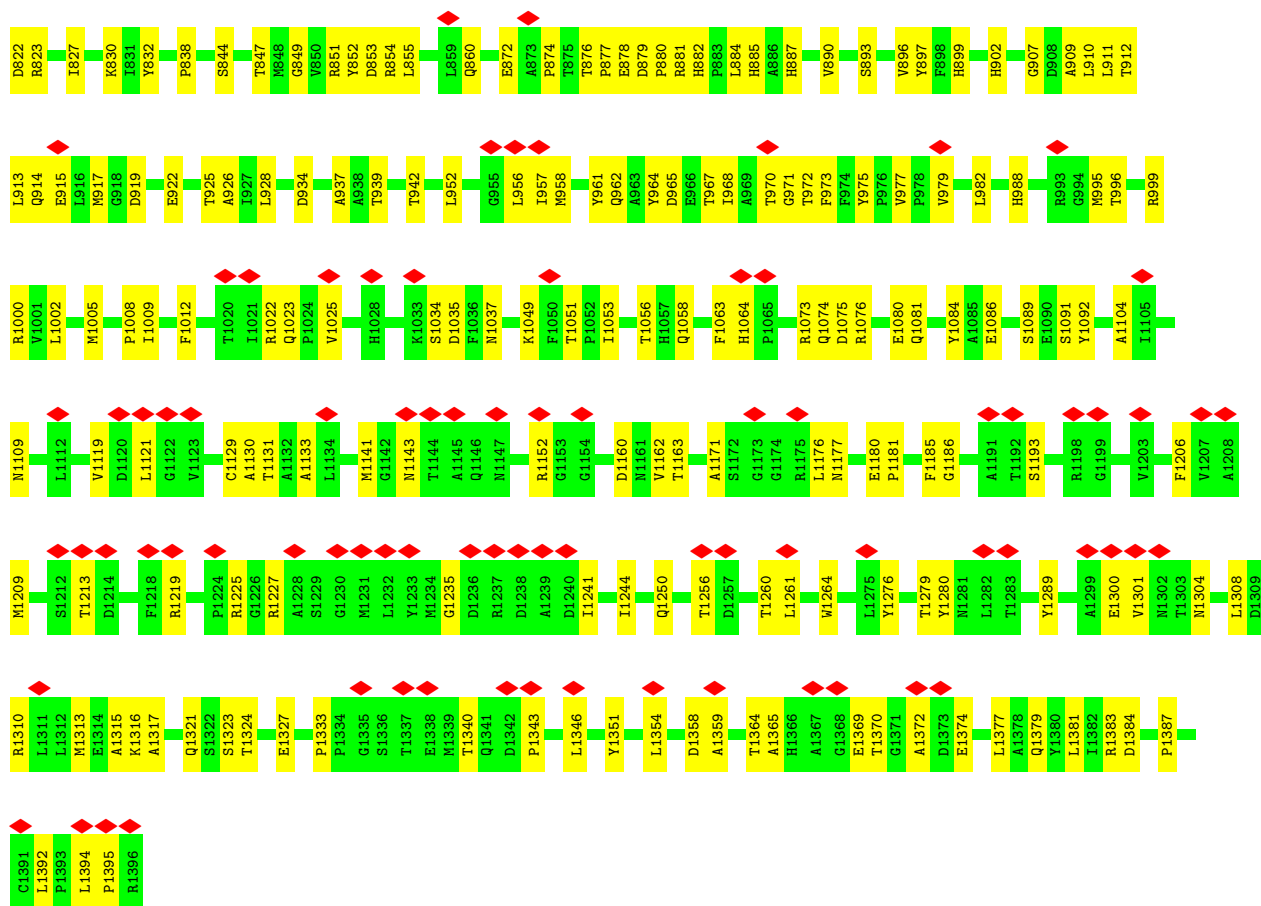


• Molecule 1: Major capsid protein

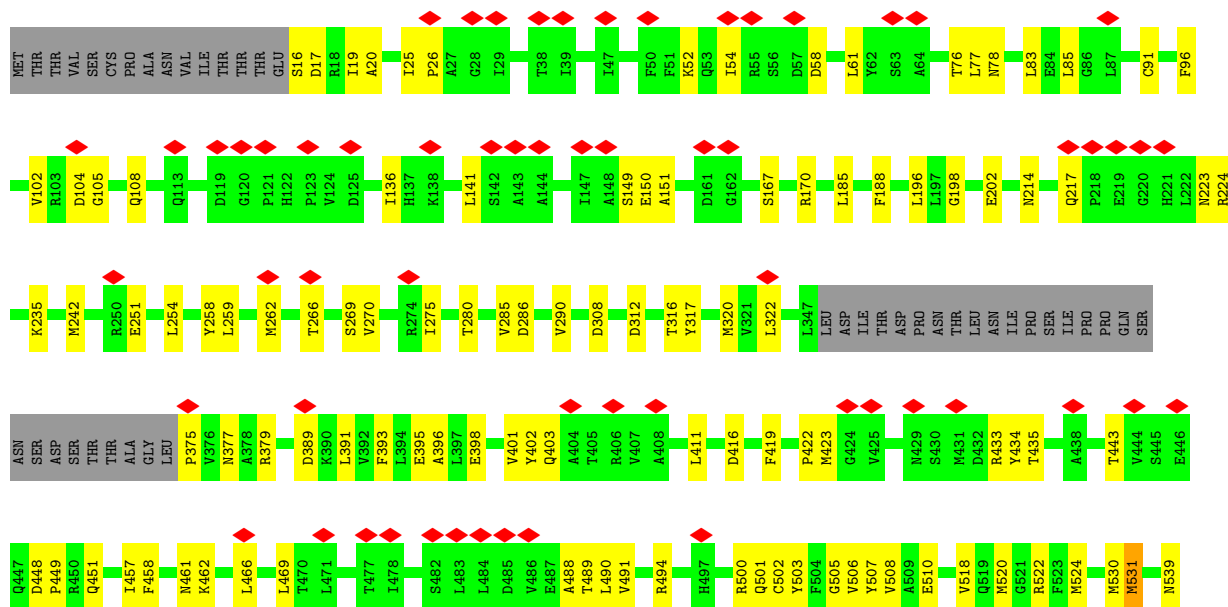


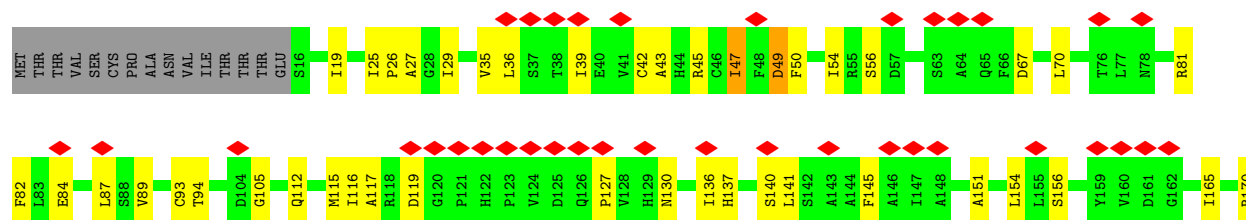




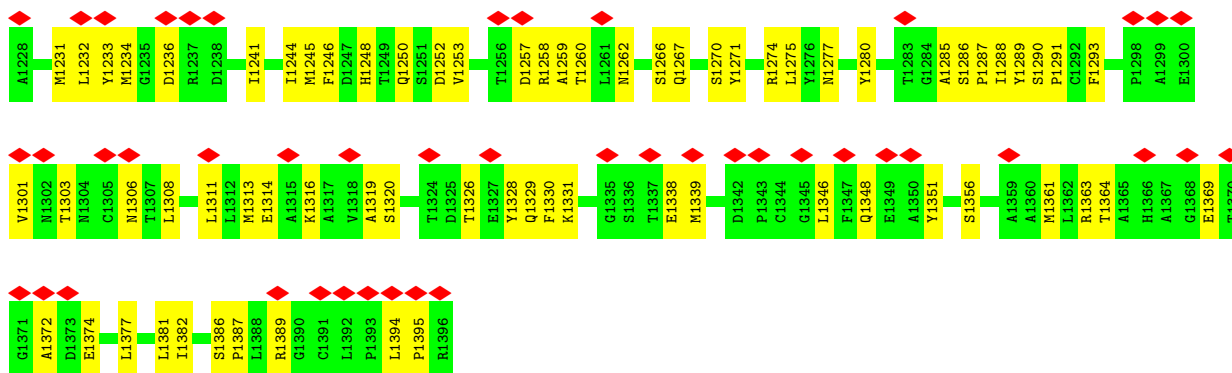


• Molecule 1: Major capsid protein

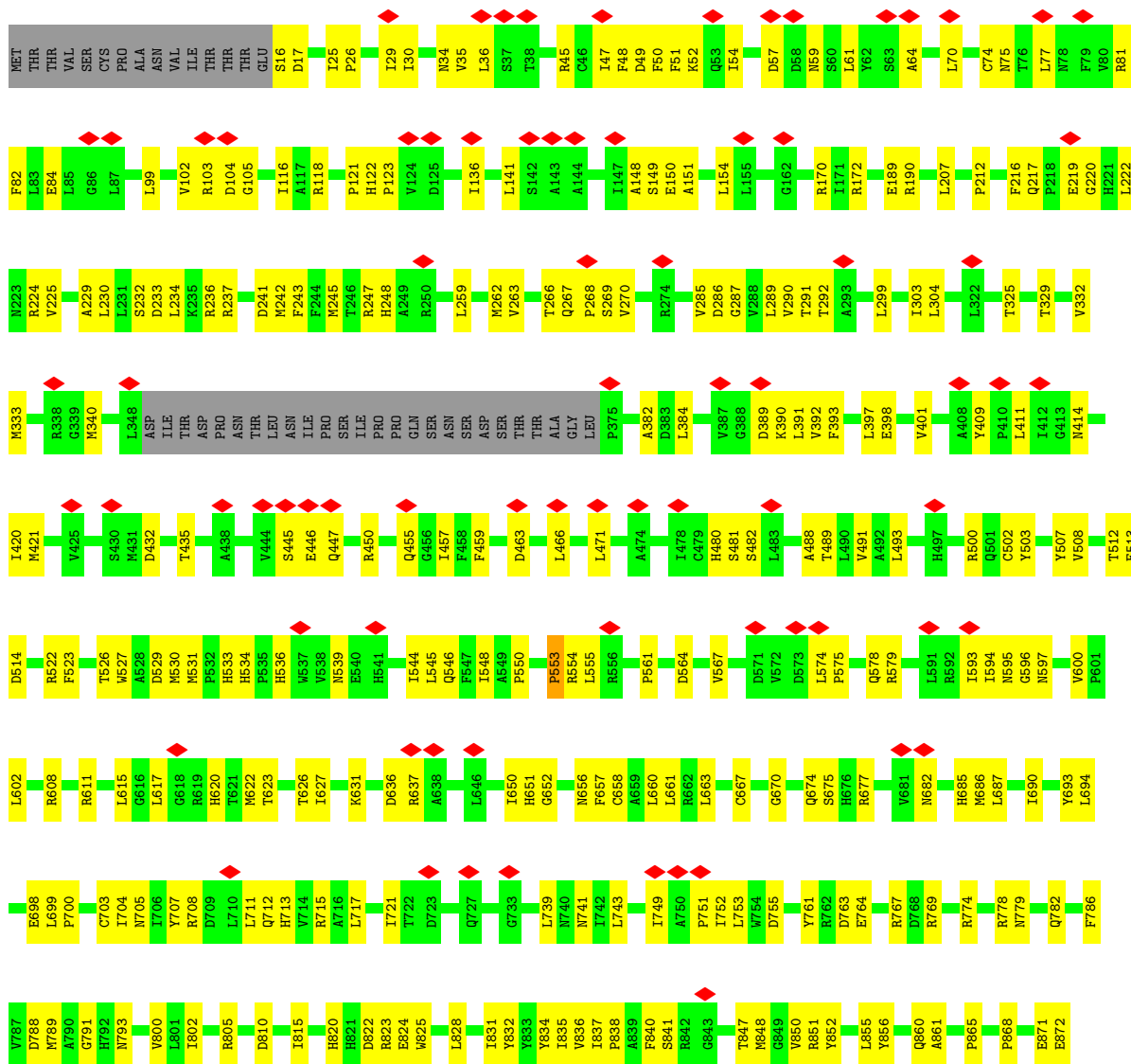


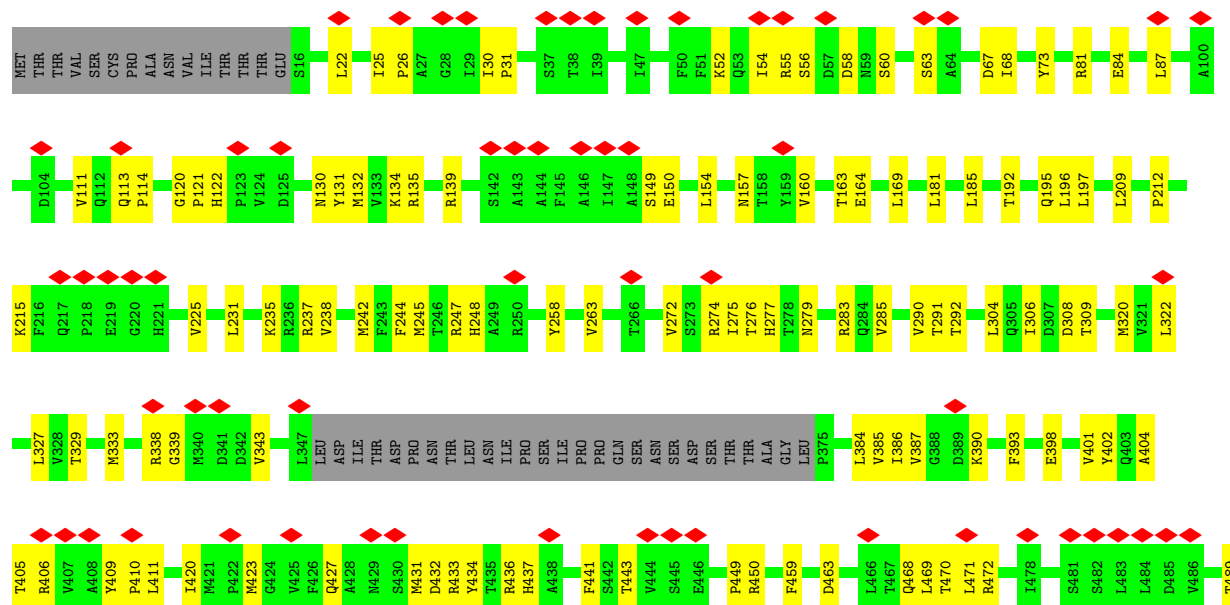


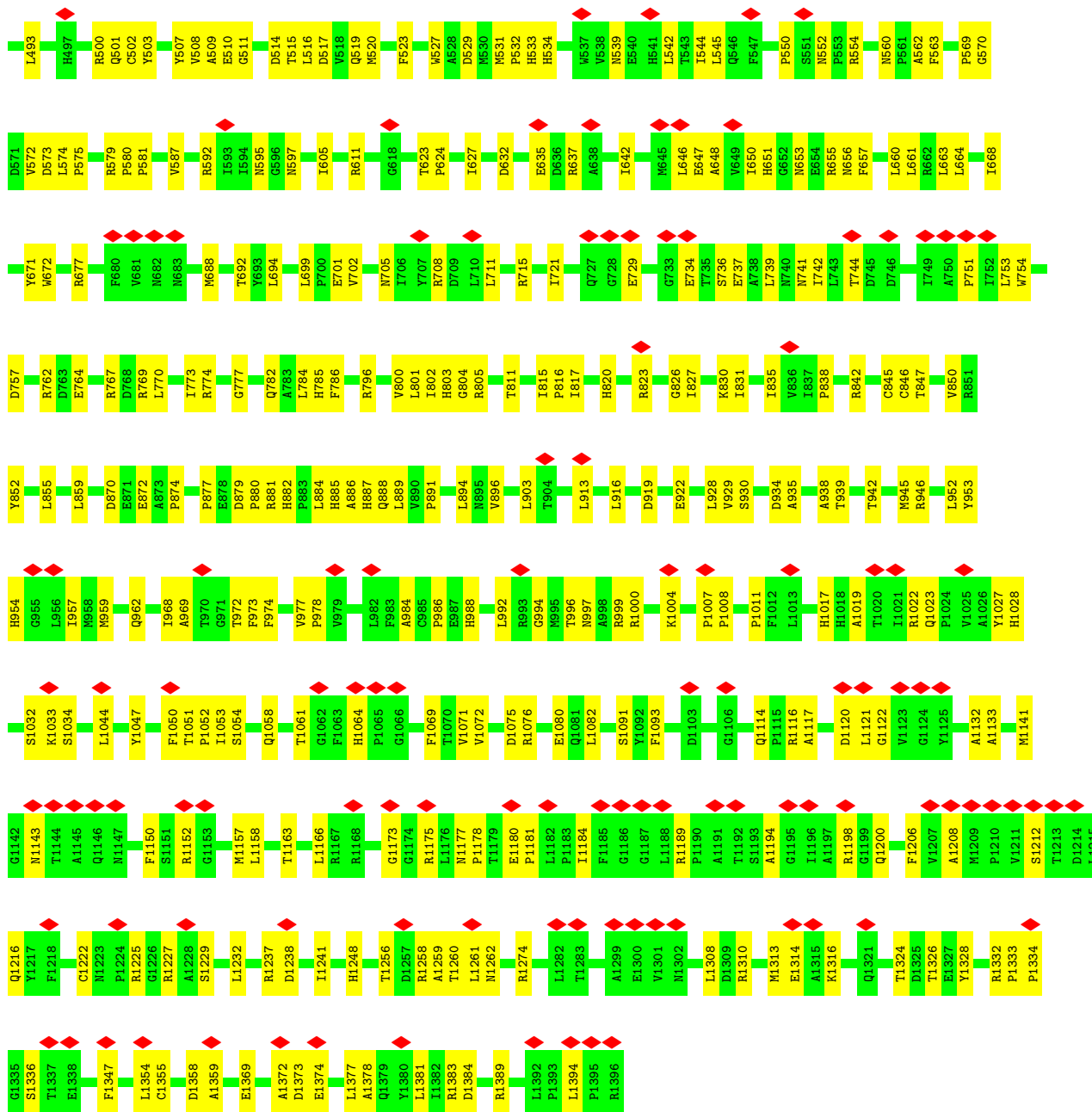
|       |       |       |      |      |      |      |      |      |      |      |
|-------|-------|-------|------|------|------|------|------|------|------|------|
| G154  | L1158 | F1077 | V807 | V649 | F557 | D473 | K390 | G324 | A349 | I171 |
| H159  | L1082 | A1078 | T811 | L650 | E558 | A474 | L391 | THR  | R250 | R172 |
| D160  | L1083 | L1083 | R823 | N653 | L559 | M475 | V392 | ASN  | E251 | A173 |
| N161  | Y1084 | E921  | E824 | R654 | F563 | T477 | F393 | LEU  | P251 | I174 |
| E164  | R1087 | R922  | I827 | N656 | D571 | I478 | L397 | THR  | R253 | Q175 |
| S1165 | A1088 | R923  | S736 | L660 | V572 | C479 | E398 | ALA  | I255 | M177 |
| L1166 | S1089 | A926  | L739 | L661 | D573 | H480 | R399 | LEU  | S256 | M180 |
| I1169 | E1090 | T927  | L743 | L664 | L574 | S482 | R400 | MET  | L259 | V184 |
| T1170 | S1091 | L928  | T744 | C667 | P577 | L483 | Y402 | LYS  | M262 | L185 |
| F1093 | Y1092 | S930  | D745 | S675 | Q578 | L484 | Q403 | ALA  | C265 | E189 |
| V1094 | F1093 | S931  | D746 | S676 | R579 | A404 | T405 | VAL  | T266 | E190 |
| G1095 | Y1094 | P933  | F748 | S677 | P580 | D485 | R406 | ARG  | Q267 | G191 |
| Q1098 | Q1098 | D934  | H676 | V678 | P581 | V486 | V407 | GLY  | P268 | T192 |
| V1099 | V1099 | R837  | L749 | R677 | E582 | L490 | A408 | ASP  | S269 | L197 |
| H1100 | H1100 | P838  | A750 | F680 | V587 | L493 | Y409 | VAL  | V270 | L200 |
| A1104 | A1104 | A937  | L752 | V681 | N588 | R494 | P410 | ALA  | R274 | L201 |
| T1111 | T1111 | A938  | L753 | V682 | A589 | Q495 | L411 | ARG  | I275 | E202 |
| L1112 | L1112 | N944  | W754 | N683 | T590 | Q496 | L412 | HIS  | T276 | K203 |
| F1185 | F1185 | N945  | A758 | F684 | L591 | H497 | P422 | LEU  | H277 | A204 |
| G1186 | G1186 | R946  | A766 | F685 | L592 | C502 | M423 | LEU  | T278 | P205 |
| G1187 | G1187 | T947  | A768 | N686 | L593 | Y503 | G424 | ASP  | N279 | P206 |
| L1188 | L1188 | Y948  | R769 | N687 | N595 | Q495 | V425 | THR  | T280 | L207 |
| R1189 | R1189 | D949  | L770 | N688 | G596 | Y507 | F426 | ASP  | R281 | S208 |
| P1190 | P1190 | A951  | P771 | N689 | N597 | V508 | Q427 | PRO  | G282 | L209 |
| A1191 | A1191 | L952  | A772 | L690 | P604 | E513 | A428 | ASN  | R283 | I213 |
| T1192 | T1192 | Y953  | I773 | T691 | D609 | D514 | N429 | THR  | Q284 | N214 |
| S1193 | S1193 | R954  | R774 | T692 | C510 | T515 | M430 | ASN  | V288 | I217 |
| A1194 | A1194 | G955  | V775 | Y693 | R611 | L516 | M431 | ILE  | L289 | P218 |
| G1195 | G1195 | L956  | S776 | L694 | Q614 | G521 | D432 | PRO  | A293 | H221 |
| I1196 | I1196 | Y957  | G777 | L697 | L615 | R222 | T435 | PRO  | K296 | L222 |
| A1197 | A1197 | N958  | R778 | L699 | G616 | F523 | A438 | GLN  | R297 | N223 |
| R1198 | R1198 | Y961  | Q782 | E698 | L617 | M524 | V444 | SER  | Q298 | R224 |
| G1199 | G1199 | Q962  | L783 | L699 | G618 | E525 | S445 | ASN  | L299 | R227 |
| Q1200 | Q1200 | A963  | H785 | T704 | R619 | T526 | E445 | SER  | L300 | L230 |
| F1206 | F1206 | Y964  | D788 | N705 | T627 | M530 | Q447 | ASP  | Q301 | L231 |
| V1207 | V1207 | R881  | M789 | R708 | R628 | M531 | D448 | SER  | G302 | S232 |
| A1208 | A1208 | H882  | L789 | L709 | A629 | H536 | P449 | THR  | I303 | D233 |
| M1209 | M1209 | R883  | H792 | L711 | V630 | H537 | R450 | ALA  | L304 | L234 |
| P1210 | P1210 | L884  | F793 | Q712 | T633 | T643 | Q451 | GLY  | Q305 | D234 |
| T1211 | T1211 | H885  | F794 | H713 | T637 | I544 | Q455 | LEU  | I306 | K235 |
| S1212 | S1212 | Q888  | Q795 | V714 | R637 | F547 | F458 | P376 | D307 | R236 |
| D1214 | D1214 | L889  | R796 | R715 | T641 | F547 | N461 | V376 | D308 | R237 |
| L1215 | L1215 | L890  | R797 | A716 | I642 | P550 | K462 | N377 | D312 | V238 |
| Q1216 | Q1216 | L891  | D798 | L717 | G643 | S551 | R462 | L384 | G318 | C239 |
| V1217 | V1217 | I911  | D799 | R718 | Y644 | N552 | L466 | V385 | E319 | D241 |
| F1218 | F1218 | T912  | L801 | D723 | R645 | P553 | T467 | I386 | M320 | T246 |
| R1219 | R1219 | L913  | I802 | F724 | L646 | R554 | Q468 | D389 | V321 | R247 |
| N1223 | N1223 | L913  | R805 | T726 | E647 | R555 | L471 | L322 | L322 | H248 |
| P1224 | P1224 | L913  | F806 | T727 | A648 | R556 | R472 | Q323 | Q323 |      |
| R1225 | R1225 |       |      |      |      |      |      |      |      |      |
| G1226 | G1226 |       |      |      |      |      |      |      |      |      |
| R1227 | R1227 |       |      |      |      |      |      |      |      |      |



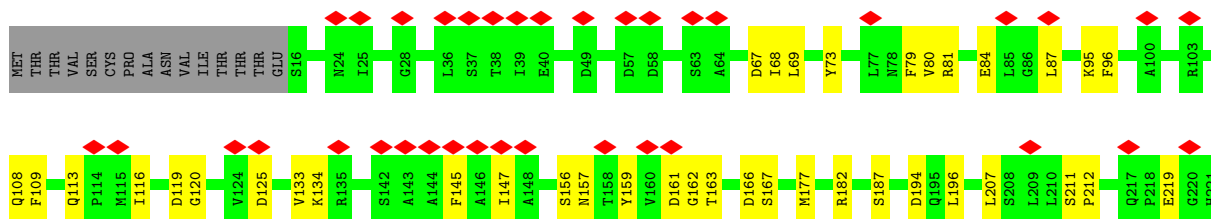
• Molecule 1: Major capsid protein

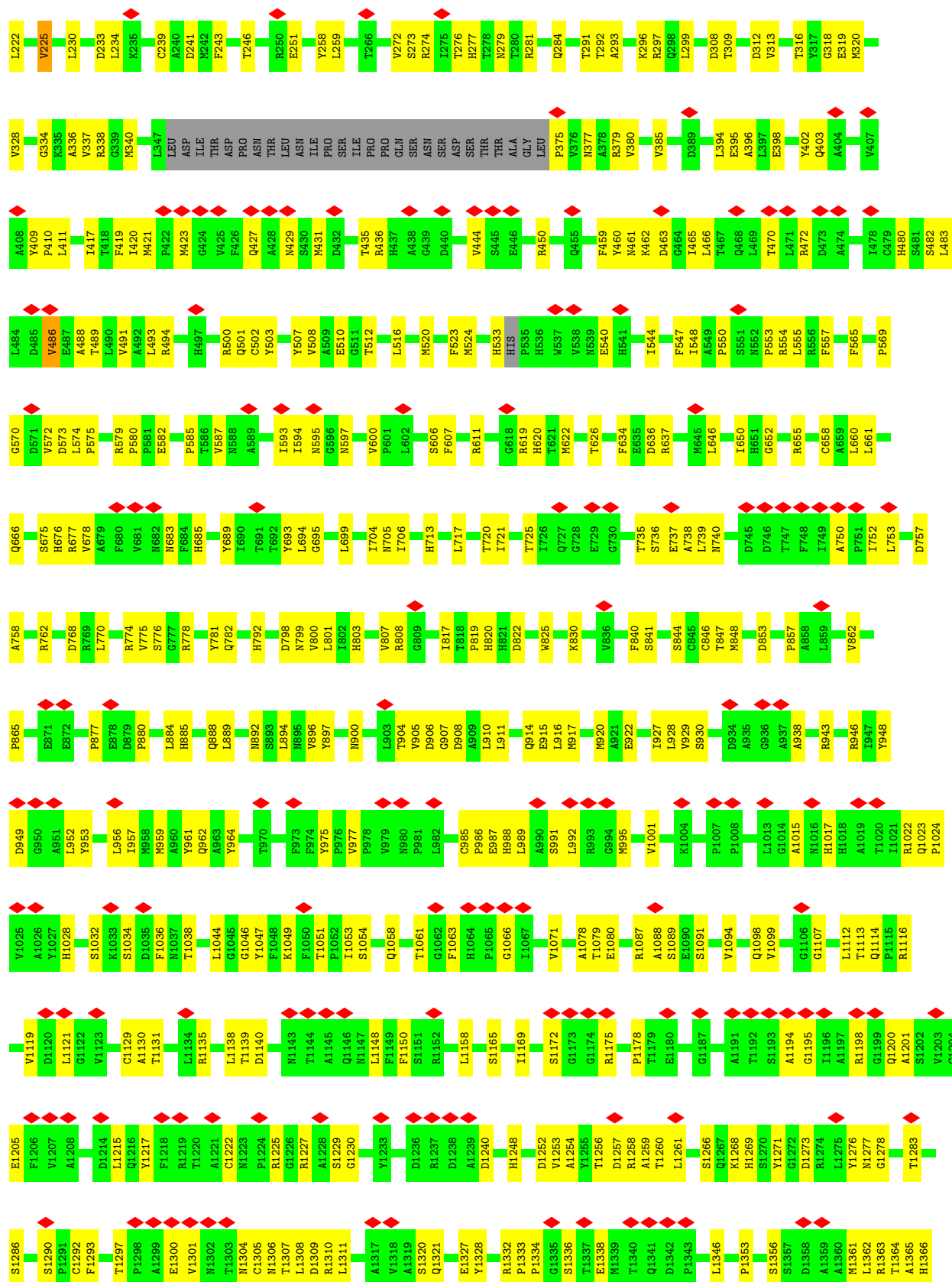


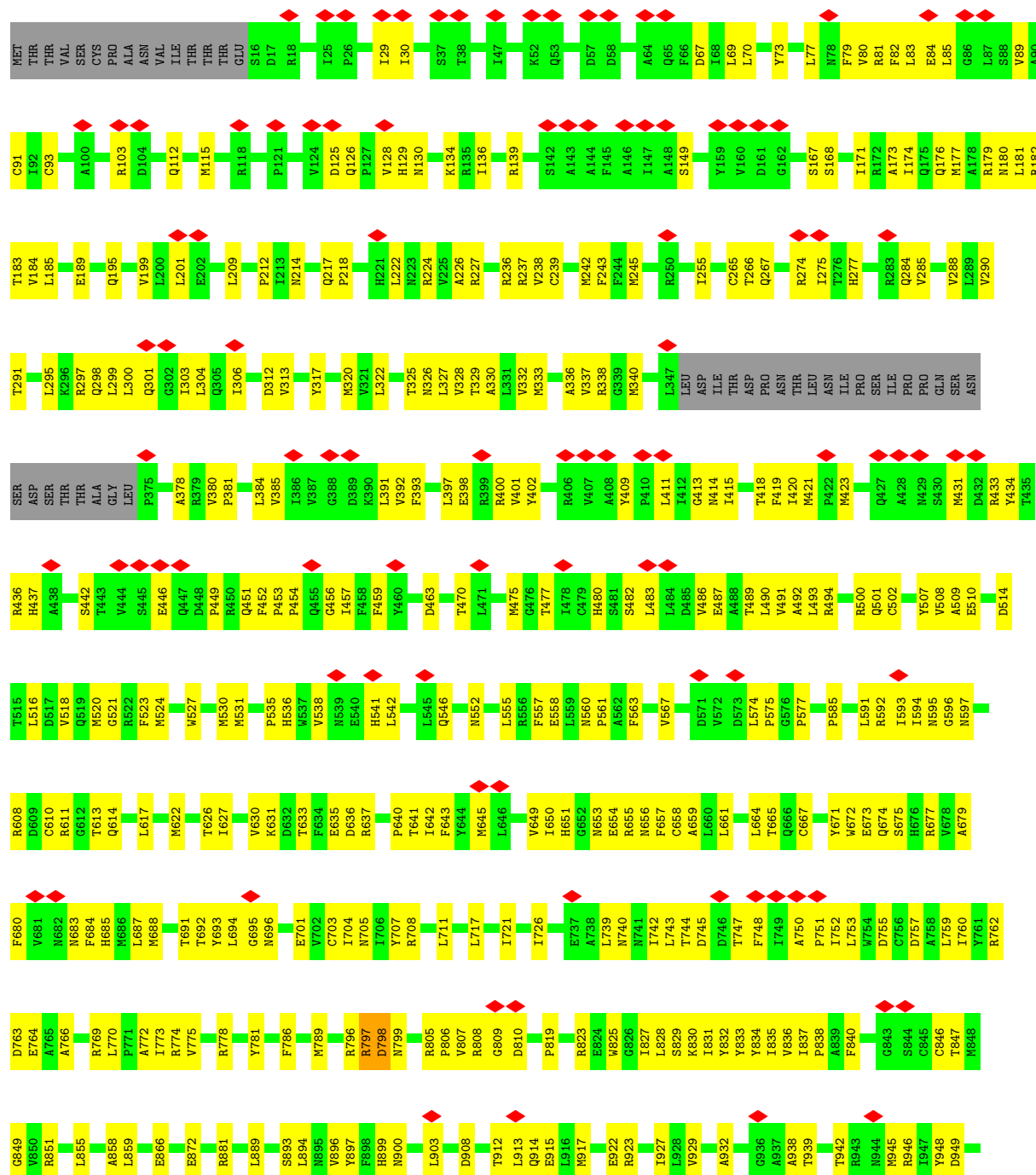




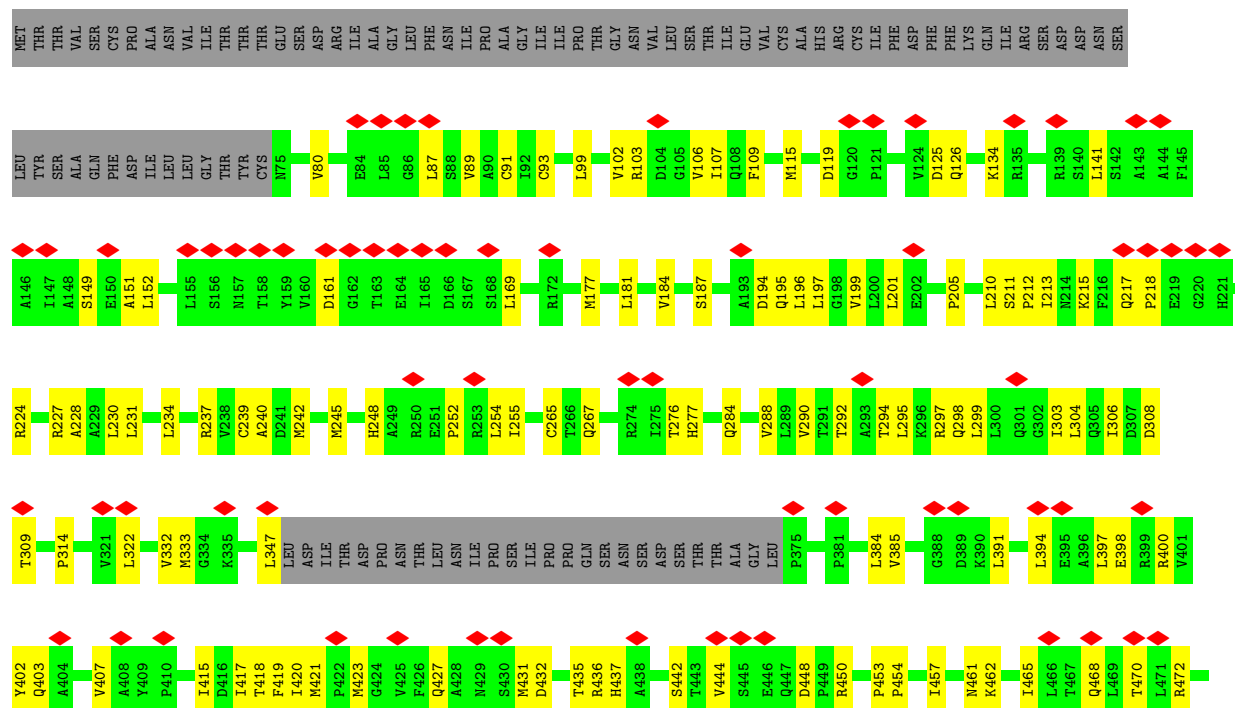
• Molecule 1: Major capsid protein





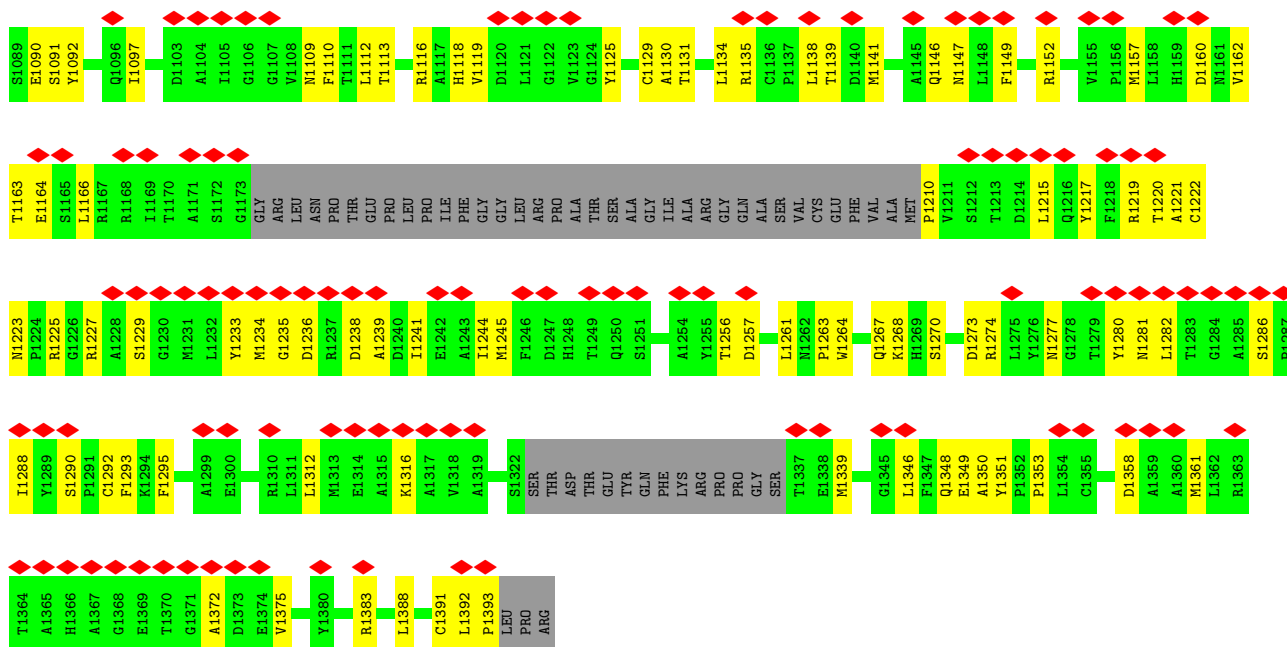




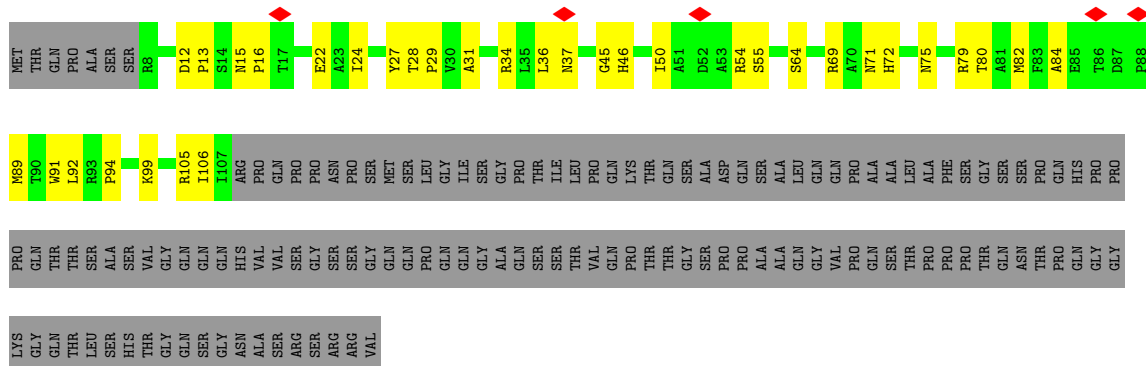




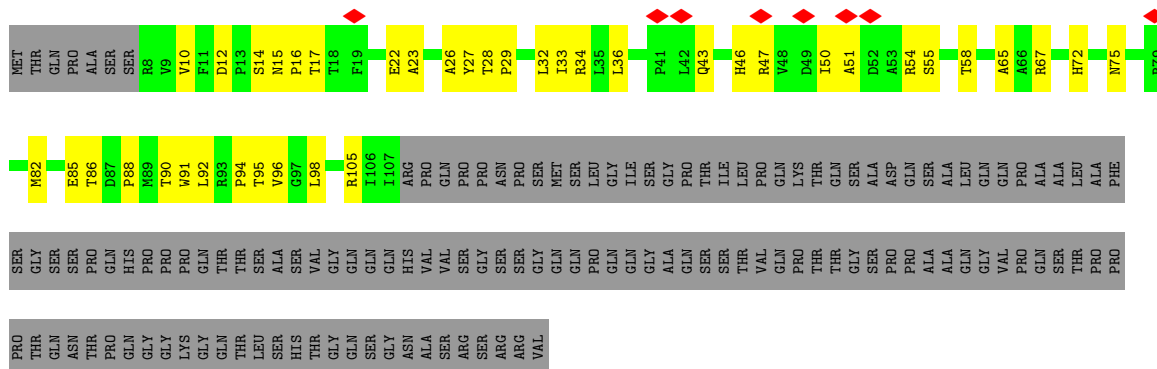




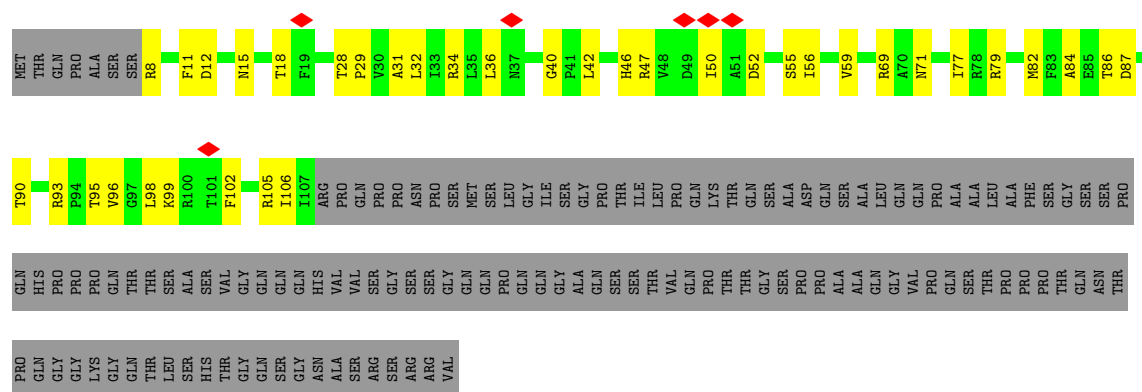
• Molecule 2: Small capsomere-interacting protein



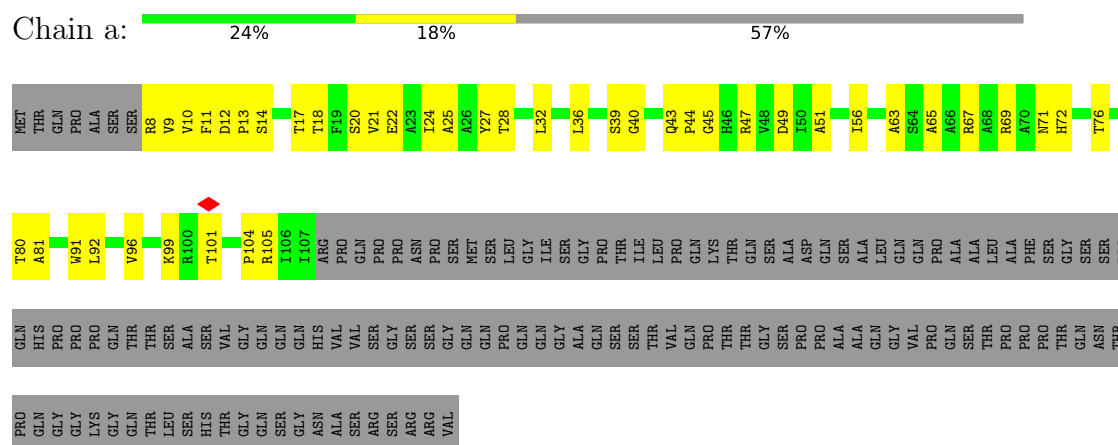
• Molecule 2: Small capsomere-interacting protein



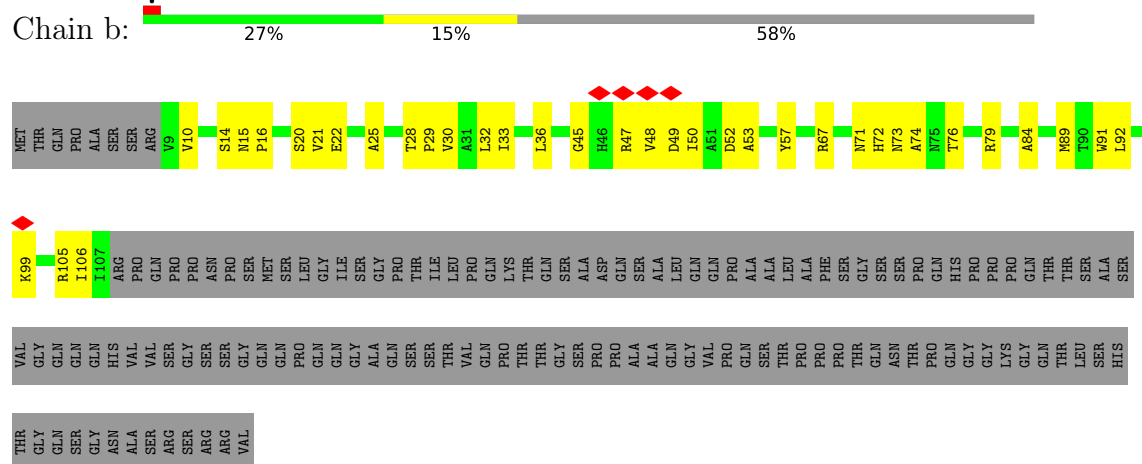




• Molecule 2: Small capsomere-interacting protein

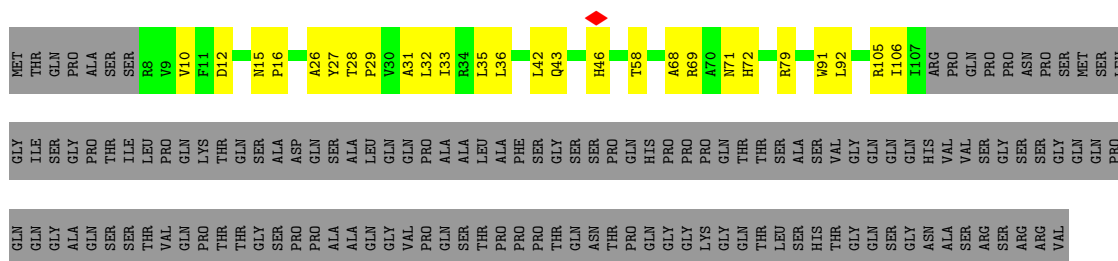


• Molecule 2: Small capsomere-interacting protein

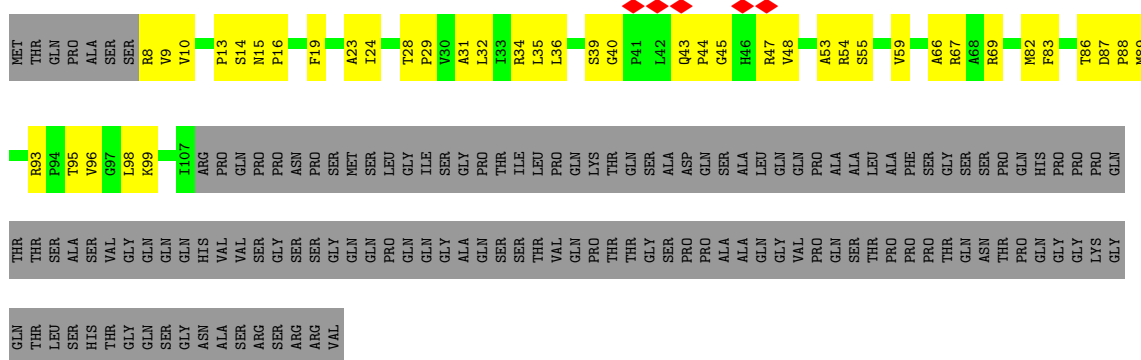


• Molecule 2: Small capsomere-interacting protein

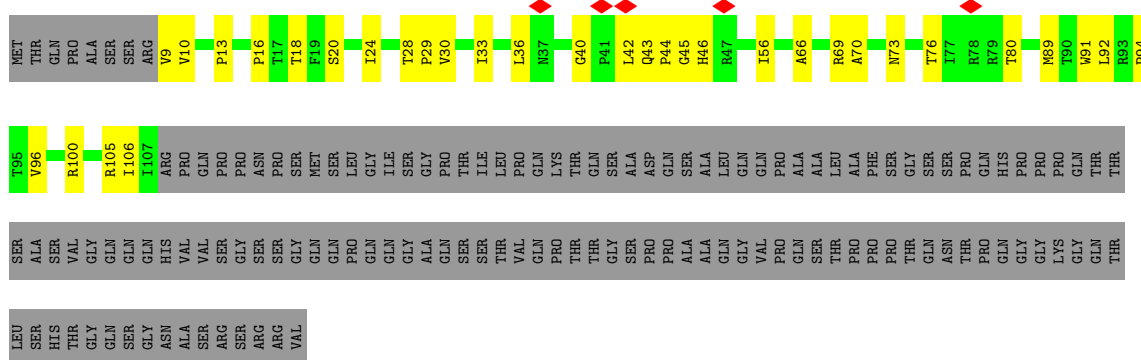




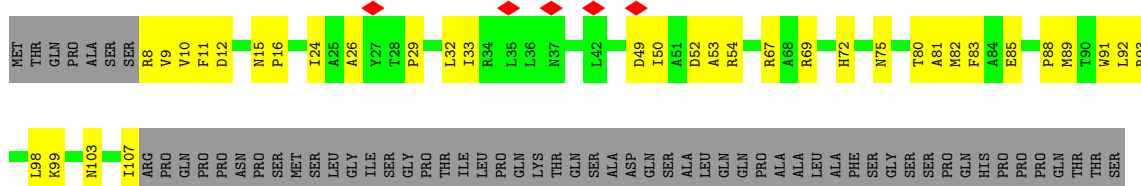
• Molecule 2: Small capsomere-interacting protein



• Molecule 2: Small capsomere-interacting protein



• Molecule 2: Small capsomere-interacting protein

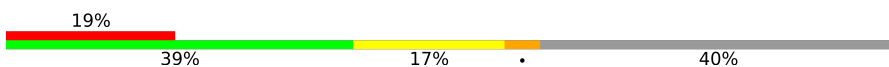






GLY  
GLN  
THR  
LEU  
SER  
HIS  
THR  
GLY  
GLN  
SER  
GLY  
ASN  
ALA  
SER  
SER  
SER  
ARG  
ARG  
VAL

• Molecule 3: Triplex capsid protein 1

Chain e: 

MET GLY SER GLN PRO THR ASN HIS PHE THR LEU ASN GLU GLN THR LEU CYS GLY THR ASN PHE MET ILE GLN ILE GLY ASN GLY LEU HIS MET THR TYR ALA PRO GLY PHE PHE GLY ASN TRP SER ARG ASP LEU THR ILE GLY PRO ARG PHE GLY

GLY LEU ASN LYS GLN PRO THR HIS VAL F130 F131 E136 H137 A138 V142 L145 R146 H147 P148 S149 D150 M151 E154 A155 R230 M231 T157 L158 T159 Q160 A161 I162 G162 R163 D164 L168 L172 R173 M174 M177 A178 C179 T180 A181 P182 W183 THR VAL T118 T119 Q120

L121 Q124 V125 S126 L127 T128 D129 F130 E136 H137 A138 V142 L145 R146 H147 P148 S149 D150 M151 E154 A155 R230 M231 T157 L158 T159 Q160 A161 I162 G162 R163 D164 L168 L172 R173 M174 M177 A178 C179 T180 A181 P182 W183 THR VAL T118 T119 Q120

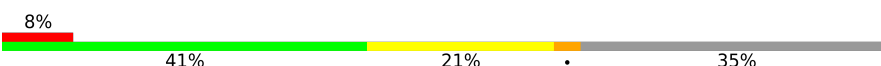
Y194 V195 S197 L198 S199 F200 L201 A202 A203 C204 R205 T210 D211 D216 T220 R221 A221 T222 V223 Y226 G227 C228 S229 R230 M231 T232 T233 R234 L235 I236 R237 L318 K319 H320 V321 L242 M245 V246 Q247 F251 F255 I256 S257 F258 F259 G260 S261 L262 T266 T267 Q268 D269 H270 N273

I274 T275 A276 V277 Q282 A284 A285 R286 T287 D288 K289 T290 S291 T292 R293 R294 V295 T296 V307 D308 H312 L313 S314 A315 D316 G317 L318 K319 H320 V321 L242 M245 V246 Q247 F251 F255 I256 S257 F258 F259 G260 S261 L262 T266 T267 Q268 D269 H270 N273

ALA GLU ASN ALA TRP GLY THR GLU VAL ALA ASN THR HIS GLN PRO TYR ASN THR ARG ALA THR VAL GLN LEU VAL GLN LEU SER ASN ASP THR PRO SER PRO ARG CYS SER ILE GLY GLU THR GLY THR VAL ASN TRP TRP LEU ALA ARG GLN ARG LEU TYR GLN TRP THR ASP

PHE ARG GLY GLN THR TRP L430 S431 T438 L439 T442 L443 P444 S445 E446 S447 V448 R449 Y450 T451 R452 R453 M454 G458 G459 L467 E468 G469 G474 T475 N476 T477 V478 N479 Y482 TYR

• Molecule 3: Triplex capsid protein 1

Chain f: 

MET GLY SER GLN PRO THR ASN HIS PHE THR LEU ASN GLU GLN THR LEU CYS GLY THR ASN PHE MET ILE GLN ILE GLY ASN GLY LEU HIS MET THR TYR ALA PRO GLY PHE PHE GLY ASN TRP SER ARG ASP LEU THR ILE GLY PRO ARG PHE GLY

GLY LEU ASN LYS GLN PRO THR HIS VAL F130 F131 E136 H137 A138 V142 L145 R146 H147 P148 S149 D150 M151 E154 A155 R230 M231 T232 T233 R234 L235 I236 R237 L318 K319 H320 V321 L242 M245 V246 Q247 F251 F255 I256 S257 F258 F259 G260 S261 L262 T266 T267 Q268 D269 H270 N273

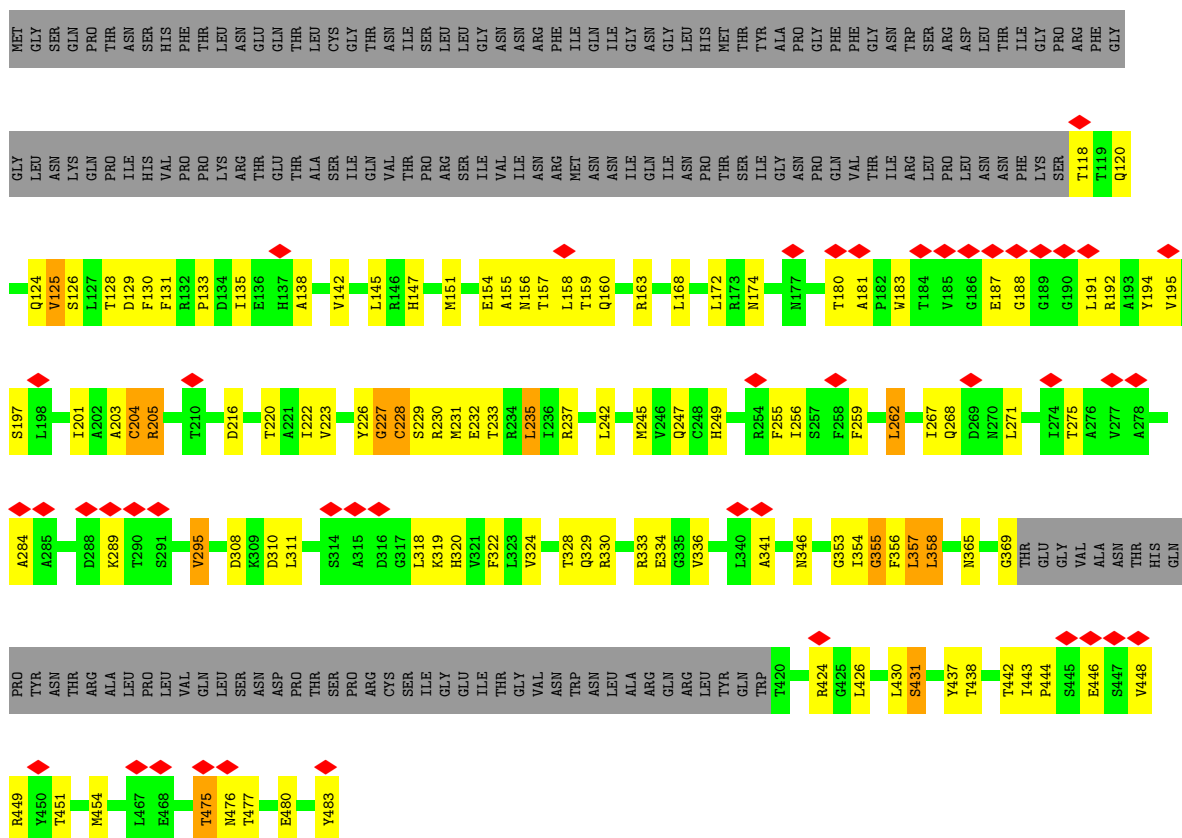
L121 I122 Q123 Q124 V125 S126 L127 T128 D129 F130 F131 E136 H137 A138 V142 L145 R146 H147 P148 S149 D150 M151 E154 A155 R230 M231 T232 T233 R234 L235 I236 R237 L318 K319 H320 V321 L242 M245 V246 Q247 F251 F255 I256 S257 F258 F259 G260 S261 L262 T266 T267 Q268 D269 H270 N273

T201 A202 C204 R205 A206 E207 T210 D216 T220 A221 T222 V223 Y226 G227 C228 S229 R230 M231 T232 T233 R234 L235 I236 R237 L318 K319 H320 V321 L242 M245 V246 Q247 F251 F255 I256 S257 F258 F259 G260 S261 L262 T266 T267 Q268 D269 H270 N273

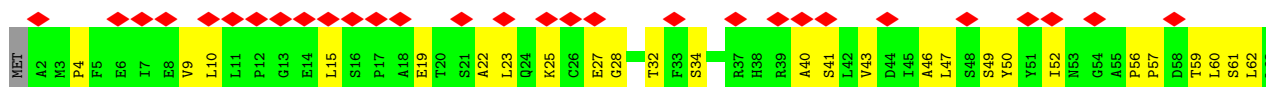
I274 T275 R286 T287 D288 K289 T290 V295 L299 F304 W305 D306 V307 D308 R309 R310 D310 L311 H312 L313 A315 D316 G317 L318 K319 H320 V321 L242 M245 V246 Q247 F251 F255 I256 S257 F258 F259 G260 S261 L262 T266 T267 Q268 D269 H270 N273

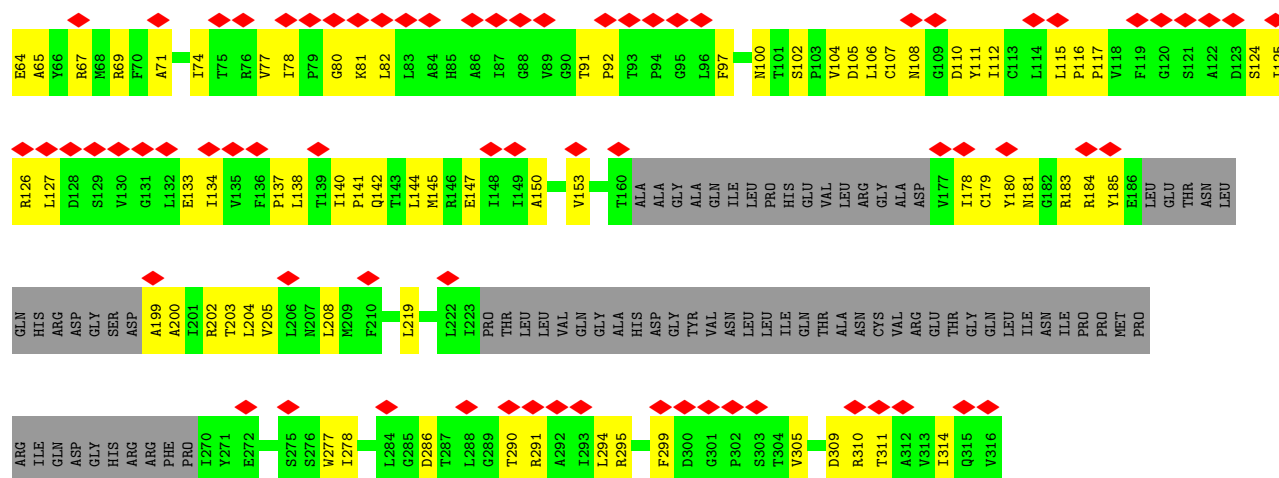


- Molecule 3: Triplex capsid protein 1

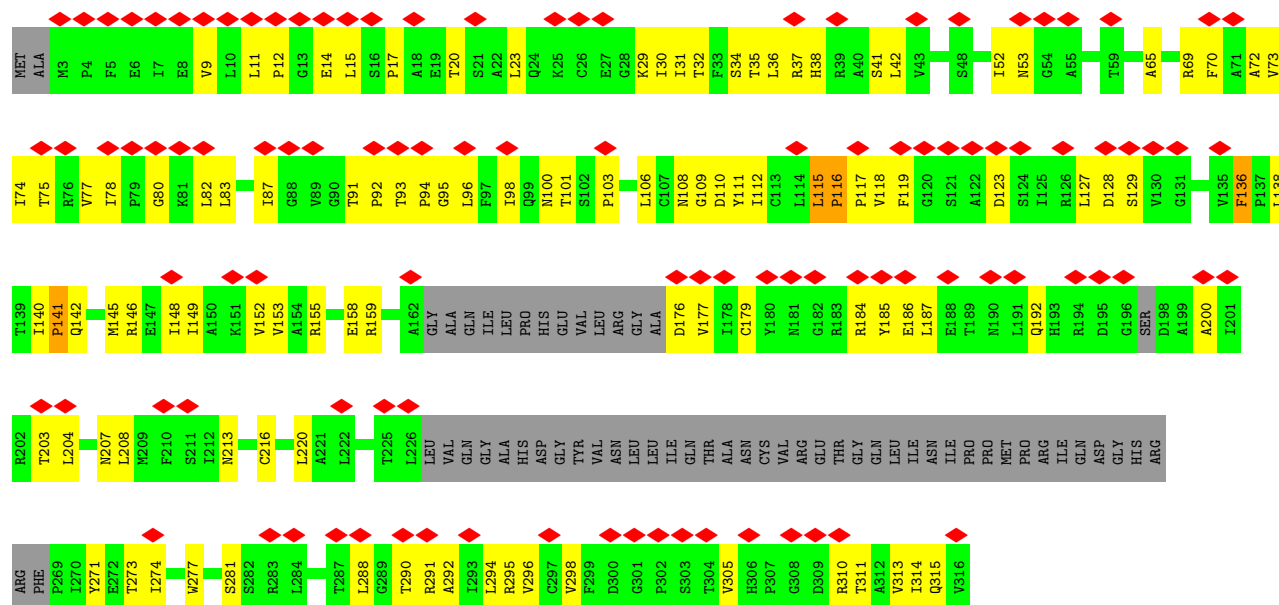


- Molecule 4: Triplex capsid protein 2

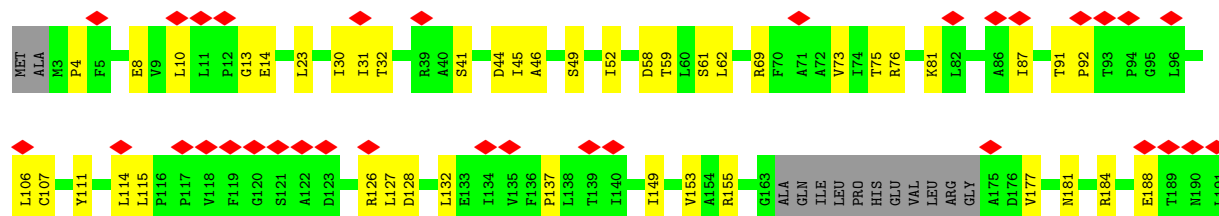


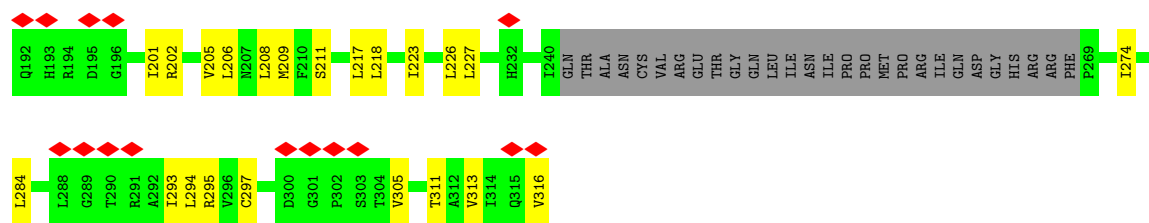


• Molecule 4: Triplex capsid protein 2

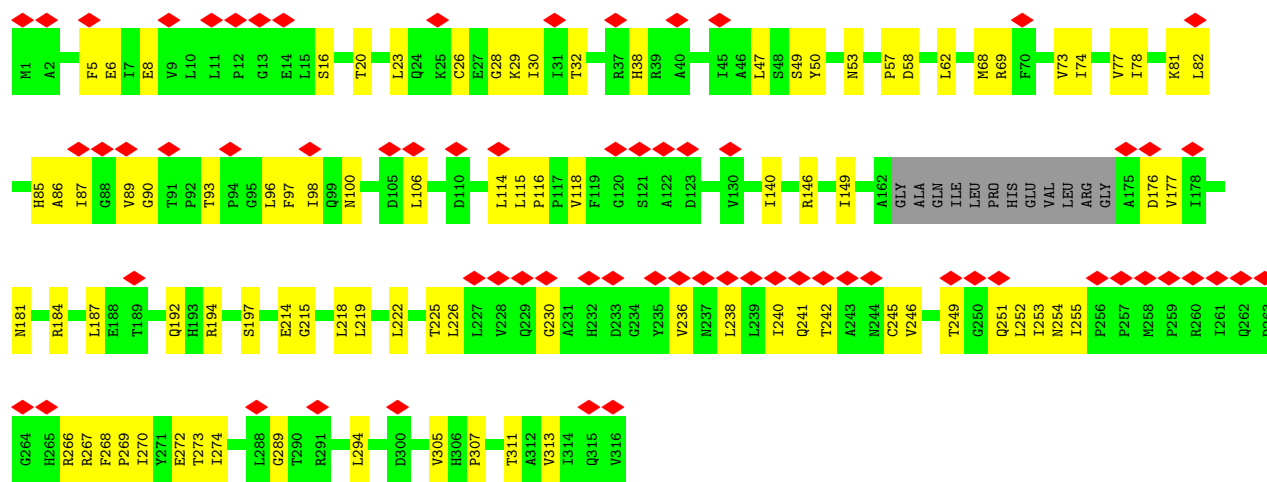


• Molecule 4: Triplex capsid protein 2

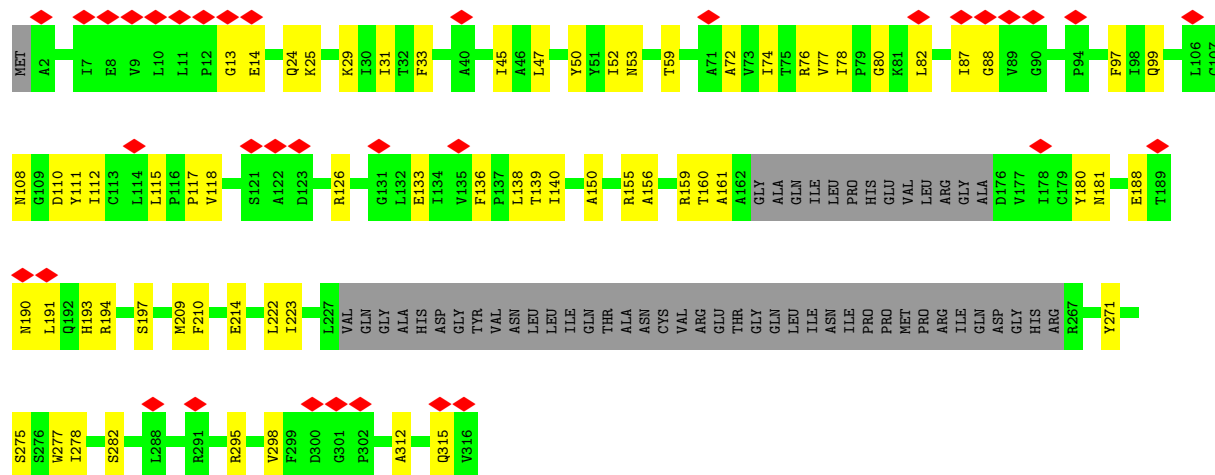




• Molecule 4: Triplex capsid protein 2

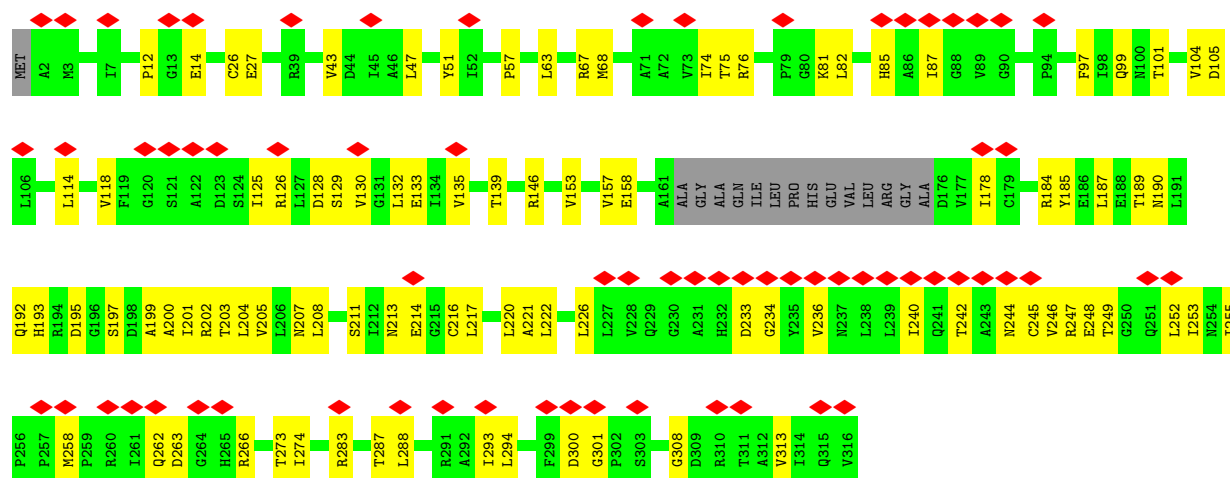


• Molecule 4: Triplex capsid protein 2

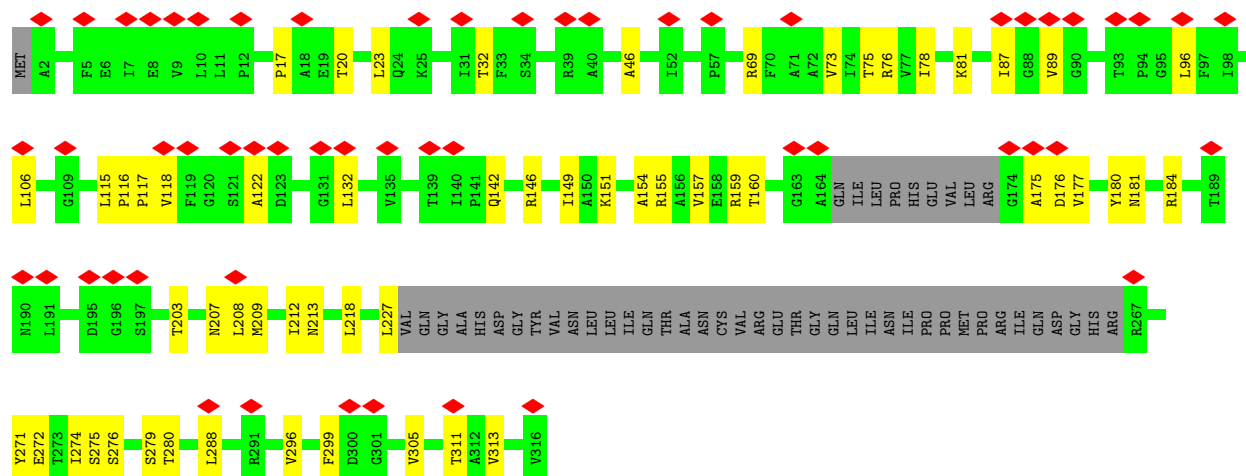


• Molecule 4: Triplex capsid protein 2

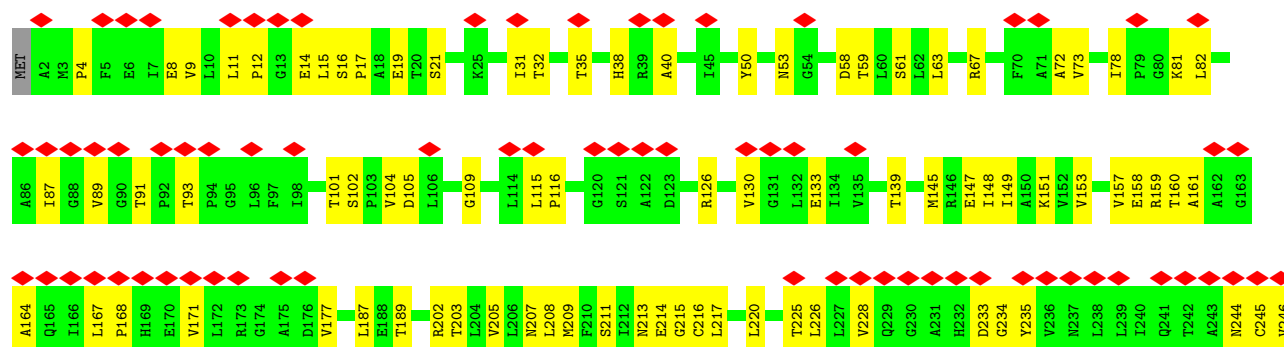




• Molecule 4: Triplex capsid protein 2

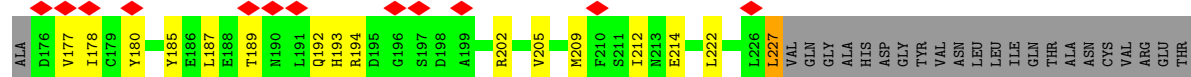
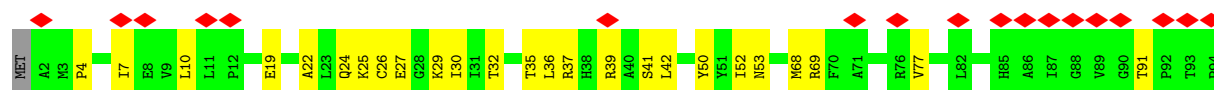


• Molecule 4: Triplex capsid protein 2

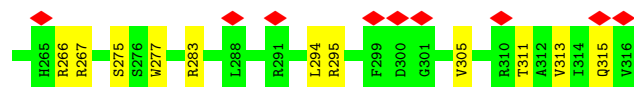
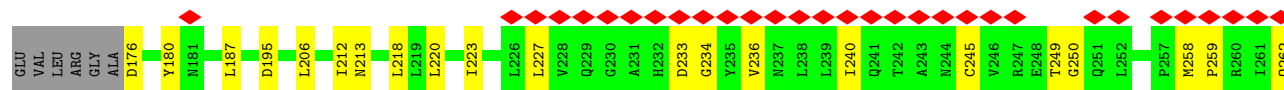
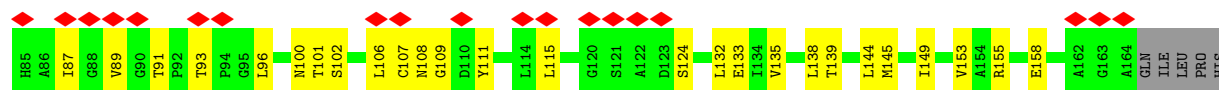




• Molecule 4: Triplex capsid protein 2



• Molecule 4: Triplex capsid protein 2



## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, Not provided             |           |
| Number of particles used             | 2838                            | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY             | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 56                              | 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                    | 13.818                          | Depositor |
| Minimum map value                    | -12.706                         | Depositor |
| Average map value                    | -0.004                          | Depositor |
| Map value standard deviation         | 1.495                           | Depositor |
| Recommended contour level            | 3                               | Depositor |
| Map size ( $\text{\AA}$ )            | 1672.9601, 1672.9601, 1672.9601 | wwPDB     |
| Map dimensions                       | 1280, 1280, 1280                | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.307, 1.307, 1.307             | Depositor |



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 1   | A     | 0.30         | 0/10846        | 0.43        | 0/14767        |
| 1   | B     | 0.25         | 0/10854        | 0.43        | 2/14778 (0.0%) |
| 1   | C     | 0.27         | 0/10846        | 0.43        | 1/14767 (0.0%) |
| 1   | E     | 0.26         | 1/10834 (0.0%) | 0.43        | 5/14748 (0.0%) |
| 1   | F     | 0.23         | 1/10846 (0.0%) | 0.44        | 3/14767 (0.0%) |
| 1   | G     | 0.22         | 0/10377        | 0.44        | 1/14130 (0.0%) |
| 1   | M     | 0.30         | 0/10835        | 0.43        | 2/14752 (0.0%) |
| 1   | N     | 0.30         | 0/10835        | 0.42        | 1/14752 (0.0%) |
| 1   | O     | 0.30         | 0/10854        | 0.42        | 1/14778 (0.0%) |
| 1   | P     | 0.30         | 0/10854        | 0.43        | 0/14778        |
| 1   | Q     | 0.30         | 0/10846        | 0.43        | 1/14767 (0.0%) |
| 1   | R     | 0.29         | 0/10835        | 0.45        | 2/14752 (0.0%) |
| 1   | S     | 0.30         | 0/10854        | 0.42        | 0/14778        |
| 1   | T     | 0.30         | 0/10846        | 0.43        | 0/14767        |
| 1   | U     | 0.23         | 0/10675        | 0.44        | 3/14536 (0.0%) |
| 1   | z     | 0.18         | 0/4800         | 0.43        | 0/6517         |
| 2   | D     | 0.20         | 0/782          | 0.48        | 0/1069         |
| 2   | H     | 0.21         | 0/771          | 0.49        | 0/1055         |
| 2   | I     | 0.21         | 0/782          | 0.47        | 0/1069         |
| 2   | J     | 0.20         | 0/782          | 0.43        | 0/1069         |
| 2   | K     | 0.20         | 0/782          | 0.47        | 0/1069         |
| 2   | L     | 0.19         | 0/782          | 0.49        | 0/1069         |
| 2   | V     | 0.20         | 0/782          | 0.46        | 0/1069         |
| 2   | W     | 0.21         | 0/782          | 0.46        | 0/1069         |
| 2   | X     | 0.21         | 0/782          | 0.45        | 0/1069         |
| 2   | Y     | 0.21         | 0/782          | 0.45        | 0/1069         |
| 2   | Z     | 0.23         | 0/782          | 0.46        | 0/1069         |
| 2   | a     | 0.22         | 0/782          | 0.48        | 0/1069         |
| 2   | b     | 0.21         | 0/771          | 0.46        | 0/1055         |
| 2   | c     | 0.23         | 0/782          | 0.49        | 0/1069         |
| 2   | d     | 0.21         | 0/782          | 0.49        | 0/1069         |
| 3   | e     | 0.46         | 5/2342 (0.2%)  | 1.03        | 31/3175 (1.0%) |
| 3   | f     | 0.41         | 3/2547 (0.1%)  | 0.92        | 21/3456 (0.6%) |
| 3   | g     | 0.46         | 3/2551 (0.1%)  | 0.87        | 19/3461 (0.5%) |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 3   | h     | 0.42         | 2/2550 (0.1%)    | 0.87        | 19/3459 (0.5%)    |
| 3   | i     | 0.43         | 3/2544 (0.1%)    | 0.91        | 24/3451 (0.7%)    |
| 4   | j     | 0.20         | 0/1868           | 0.43        | 0/2542            |
| 4   | k     | 0.28         | 0/2127           | 0.41        | 0/2898            |
| 4   | l     | 0.24         | 0/2046           | 0.38        | 0/2787            |
| 4   | m     | 0.27         | 0/2064           | 0.40        | 0/2811            |
| 4   | n     | 0.29         | 0/2055           | 0.47        | 2/2799 (0.1%)     |
| 4   | o     | 0.28         | 2/2003 (0.1%)    | 0.59        | 7/2727 (0.3%)     |
| 4   | p     | 0.26         | 0/2368           | 0.41        | 0/3227            |
| 4   | q     | 0.25         | 0/2350           | 0.40        | 0/3203            |
| 4   | r     | 0.26         | 0/2453           | 0.43        | 1/3345 (0.0%)     |
| 4   | s     | 0.27         | 0/2364           | 0.41        | 1/3222 (0.0%)     |
| All | All   | 0.28         | 20/212777 (0.0%) | 0.48        | 147/289704 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | C     | 0                   | 1                   |
| 1   | F     | 0                   | 1                   |
| 1   | G     | 0                   | 1                   |
| 1   | Q     | 0                   | 1                   |
| 1   | T     | 0                   | 2                   |
| 3   | g     | 0                   | 1                   |
| All | All   | 0                   | 7                   |

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

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | g     | 133 | PRO  | N-CD  | 11.23 | 1.63        | 1.47     |
| 3   | h     | 228 | CYS  | CA-C  | 8.32  | 1.64        | 1.52     |
| 3   | f     | 228 | CYS  | CA-C  | 8.30  | 1.63        | 1.52     |
| 3   | e     | 228 | CYS  | CA-C  | 8.13  | 1.63        | 1.52     |
| 3   | i     | 228 | CYS  | CA-C  | 7.62  | 1.62        | 1.52     |

The worst 5 of 147 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | R     | 22  | LEU  | N-CA-C | -10.80 | 99.51       | 111.28   |
| 3   | f     | 308 | ASP  | N-CA-C | 10.52  | 122.32      | 111.07   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | e     | 333 | ARG  | N-CA-C | 10.18 | 122.65      | 110.44   |
| 3   | e     | 284 | ALA  | N-CA-C | 9.77  | 123.87      | 112.93   |
| 1   | F     | 798 | ASP  | N-CA-C | 9.72  | 122.87      | 110.33   |

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | C     | 1394 | LEU  | Mainchain |
| 1   | F     | 1394 | LEU  | Mainchain |
| 1   | Q     | 1394 | LEU  | Mainchain |
| 1   | T     | 1394 | LEU  | Mainchain |
| 1   | T     | 531  | MET  | Peptide   |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 10592 | 0        | 10438    | 256     | 0            |
| 1   | B     | 10600 | 0        | 10449    | 363     | 0            |
| 1   | C     | 10592 | 0        | 10438    | 304     | 0            |
| 1   | E     | 10582 | 0        | 10431    | 317     | 0            |
| 1   | F     | 10592 | 0        | 10438    | 419     | 0            |
| 1   | G     | 10133 | 0        | 9988     | 423     | 0            |
| 1   | M     | 10582 | 0        | 10429    | 270     | 0            |
| 1   | N     | 10582 | 0        | 10429    | 298     | 0            |
| 1   | O     | 10600 | 0        | 10449    | 255     | 0            |
| 1   | P     | 10600 | 0        | 10449    | 275     | 0            |
| 1   | Q     | 10592 | 0        | 10438    | 238     | 0            |
| 1   | R     | 10582 | 0        | 10429    | 281     | 0            |
| 1   | S     | 10600 | 0        | 10449    | 245     | 0            |
| 1   | T     | 10592 | 0        | 10438    | 250     | 0            |
| 1   | U     | 10422 | 0        | 10256    | 418     | 0            |
| 1   | z     | 4709  | 0        | 4688     | 159     | 0            |
| 2   | D     | 765   | 0        | 777      | 33      | 0            |
| 2   | H     | 754   | 0        | 764      | 29      | 0            |
| 2   | I     | 765   | 0        | 777      | 33      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 2   | J     | 765    | 0        | 777      | 33      | 0            |
| 2   | K     | 765    | 0        | 777      | 41      | 0            |
| 2   | L     | 765    | 0        | 777      | 37      | 0            |
| 2   | V     | 765    | 0        | 777      | 37      | 0            |
| 2   | W     | 765    | 0        | 777      | 39      | 0            |
| 2   | X     | 765    | 0        | 777      | 29      | 0            |
| 2   | Y     | 765    | 0        | 777      | 34      | 0            |
| 2   | Z     | 765    | 0        | 777      | 36      | 0            |
| 2   | a     | 765    | 0        | 777      | 35      | 0            |
| 2   | b     | 754    | 0        | 764      | 33      | 0            |
| 2   | c     | 765    | 0        | 777      | 22      | 0            |
| 2   | d     | 765    | 0        | 777      | 32      | 0            |
| 3   | e     | 2294   | 0        | 2262     | 79      | 0            |
| 3   | f     | 2492   | 0        | 2443     | 96      | 0            |
| 3   | g     | 2497   | 0        | 2449     | 92      | 0            |
| 3   | h     | 2496   | 0        | 2447     | 106     | 0            |
| 3   | i     | 2490   | 0        | 2442     | 82      | 0            |
| 4   | j     | 1837   | 0        | 1909     | 82      | 0            |
| 4   | k     | 2090   | 0        | 2152     | 47      | 0            |
| 4   | l     | 2010   | 0        | 2074     | 46      | 0            |
| 4   | m     | 2028   | 0        | 2090     | 45      | 0            |
| 4   | n     | 2019   | 0        | 2082     | 53      | 0            |
| 4   | o     | 1969   | 0        | 2031     | 103     | 0            |
| 4   | p     | 2325   | 0        | 2393     | 65      | 0            |
| 4   | q     | 2307   | 0        | 2371     | 74      | 0            |
| 4   | r     | 2407   | 0        | 2476     | 85      | 0            |
| 4   | s     | 2321   | 0        | 2384     | 58      | 0            |
| All | All   | 207987 | 0        | 206270   | 5915    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 5915 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:523:PHE:CD1  | 1:G:1011:PRO:HD3 | 1.46                     | 1.49              |
| 1:G:523:PHE:CE1  | 1:G:1011:PRO:HD3 | 1.53                     | 1.40              |
| 4:o:115:LEU:HD12 | 4:o:116:PRO:CD   | 1.51                     | 1.40              |
| 3:e:357:LEU:CD1  | 3:e:358:LEU:HD12 | 1.57                     | 1.35              |
| 3:h:357:LEU:CD1  | 3:h:358:LEU:HD12 | 1.57                     | 1.33              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 1350/1396 (97%) | 1184 (88%) | 165 (12%) | 1 (0%)   | 48          | 82  |
| 1   | B     | 1351/1396 (97%) | 1191 (88%) | 160 (12%) | 0        | 100         | 100 |
| 1   | C     | 1350/1396 (97%) | 1194 (88%) | 156 (12%) | 0        | 100         | 100 |
| 1   | E     | 1347/1396 (96%) | 1185 (88%) | 162 (12%) | 0        | 100         | 100 |
| 1   | F     | 1350/1396 (97%) | 1191 (88%) | 159 (12%) | 0        | 100         | 100 |
| 1   | G     | 1291/1396 (92%) | 1135 (88%) | 155 (12%) | 1 (0%)   | 48          | 82  |
| 1   | M     | 1349/1396 (97%) | 1206 (89%) | 143 (11%) | 0        | 100         | 100 |
| 1   | N     | 1349/1396 (97%) | 1207 (90%) | 142 (10%) | 0        | 100         | 100 |
| 1   | O     | 1351/1396 (97%) | 1201 (89%) | 150 (11%) | 0        | 100         | 100 |
| 1   | P     | 1351/1396 (97%) | 1221 (90%) | 129 (10%) | 1 (0%)   | 48          | 82  |
| 1   | Q     | 1350/1396 (97%) | 1210 (90%) | 140 (10%) | 0        | 100         | 100 |
| 1   | R     | 1349/1396 (97%) | 1194 (88%) | 154 (11%) | 1 (0%)   | 48          | 82  |
| 1   | S     | 1351/1396 (97%) | 1206 (89%) | 145 (11%) | 0        | 100         | 100 |
| 1   | T     | 1350/1396 (97%) | 1194 (88%) | 155 (12%) | 1 (0%)   | 48          | 82  |
| 1   | U     | 1327/1396 (95%) | 1167 (88%) | 160 (12%) | 0        | 100         | 100 |
| 1   | z     | 595/1396 (43%)  | 505 (85%)  | 90 (15%)  | 0        | 100         | 100 |
| 2   | D     | 98/235 (42%)    | 79 (81%)   | 19 (19%)  | 0        | 100         | 100 |
| 2   | H     | 97/235 (41%)    | 78 (80%)   | 19 (20%)  | 0        | 100         | 100 |
| 2   | I     | 98/235 (42%)    | 79 (81%)   | 19 (19%)  | 0        | 100         | 100 |
| 2   | J     | 98/235 (42%)    | 79 (81%)   | 19 (19%)  | 0        | 100         | 100 |
| 2   | K     | 98/235 (42%)    | 82 (84%)   | 16 (16%)  | 0        | 100         | 100 |
| 2   | L     | 98/235 (42%)    | 76 (78%)   | 22 (22%)  | 0        | 100         | 100 |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 2   | V     | 98/235 (42%)      | 75 (76%)    | 23 (24%)   | 0        | 100         | 100 |
| 2   | W     | 98/235 (42%)      | 79 (81%)    | 19 (19%)   | 0        | 100         | 100 |
| 2   | X     | 98/235 (42%)      | 84 (86%)    | 14 (14%)   | 0        | 100         | 100 |
| 2   | Y     | 98/235 (42%)      | 76 (78%)    | 22 (22%)   | 0        | 100         | 100 |
| 2   | Z     | 98/235 (42%)      | 80 (82%)    | 18 (18%)   | 0        | 100         | 100 |
| 2   | a     | 98/235 (42%)      | 78 (80%)    | 20 (20%)   | 0        | 100         | 100 |
| 2   | b     | 97/235 (41%)      | 82 (84%)    | 15 (16%)   | 0        | 100         | 100 |
| 2   | c     | 98/235 (42%)      | 78 (80%)    | 20 (20%)   | 0        | 100         | 100 |
| 2   | d     | 98/235 (42%)      | 77 (79%)    | 20 (20%)   | 1 (1%)   | 12          | 47  |
| 3   | e     | 283/483 (59%)     | 261 (92%)   | 19 (7%)    | 3 (1%)   | 11          | 45  |
| 3   | f     | 312/483 (65%)     | 289 (93%)   | 19 (6%)    | 4 (1%)   | 9           | 40  |
| 3   | g     | 313/483 (65%)     | 289 (92%)   | 23 (7%)    | 1 (0%)   | 36          | 71  |
| 3   | h     | 313/483 (65%)     | 290 (93%)   | 20 (6%)    | 3 (1%)   | 12          | 47  |
| 3   | i     | 312/483 (65%)     | 290 (93%)   | 20 (6%)    | 2 (1%)   | 21          | 58  |
| 4   | j     | 233/316 (74%)     | 213 (91%)   | 20 (9%)    | 0        | 100         | 100 |
| 4   | k     | 269/316 (85%)     | 238 (88%)   | 31 (12%)   | 0        | 100         | 100 |
| 4   | l     | 257/316 (81%)     | 225 (88%)   | 32 (12%)   | 0        | 100         | 100 |
| 4   | m     | 261/316 (83%)     | 229 (88%)   | 32 (12%)   | 0        | 100         | 100 |
| 4   | n     | 259/316 (82%)     | 231 (89%)   | 28 (11%)   | 0        | 100         | 100 |
| 4   | o     | 250/316 (79%)     | 226 (90%)   | 24 (10%)   | 0        | 100         | 100 |
| 4   | p     | 300/316 (95%)     | 278 (93%)   | 22 (7%)    | 0        | 100         | 100 |
| 4   | q     | 297/316 (94%)     | 266 (90%)   | 31 (10%)   | 0        | 100         | 100 |
| 4   | r     | 313/316 (99%)     | 289 (92%)   | 24 (8%)    | 0        | 100         | 100 |
| 4   | s     | 300/316 (95%)     | 275 (92%)   | 25 (8%)    | 0        | 100         | 100 |
| All | All   | 26501/31436 (84%) | 23462 (88%) | 3020 (11%) | 19 (0%)  | 49          | 82  |

5 of 19 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 48  | PHE  |
| 3   | e     | 227 | GLY  |
| 3   | f     | 227 | GLY  |
| 3   | g     | 227 | GLY  |
| 3   | h     | 227 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | A     | 1143/1182 (97%) | 1143 (100%) | 0        | 100         | 100 |
| 1   | B     | 1144/1182 (97%) | 1144 (100%) | 0        | 100         | 100 |
| 1   | C     | 1143/1182 (97%) | 1143 (100%) | 0        | 100         | 100 |
| 1   | E     | 1142/1182 (97%) | 1141 (100%) | 1 (0%)   | 88          | 88  |
| 1   | F     | 1143/1182 (97%) | 1143 (100%) | 0        | 100         | 100 |
| 1   | G     | 1092/1182 (92%) | 1092 (100%) | 0        | 100         | 100 |
| 1   | M     | 1142/1182 (97%) | 1141 (100%) | 1 (0%)   | 88          | 88  |
| 1   | N     | 1142/1182 (97%) | 1142 (100%) | 0        | 100         | 100 |
| 1   | O     | 1144/1182 (97%) | 1144 (100%) | 0        | 100         | 100 |
| 1   | P     | 1144/1182 (97%) | 1143 (100%) | 1 (0%)   | 88          | 88  |
| 1   | Q     | 1143/1182 (97%) | 1142 (100%) | 1 (0%)   | 88          | 88  |
| 1   | R     | 1142/1182 (97%) | 1140 (100%) | 2 (0%)   | 87          | 85  |
| 1   | S     | 1144/1182 (97%) | 1144 (100%) | 0        | 100         | 100 |
| 1   | T     | 1143/1182 (97%) | 1143 (100%) | 0        | 100         | 100 |
| 1   | U     | 1125/1182 (95%) | 1122 (100%) | 3 (0%)   | 86          | 84  |
| 1   | z     | 511/1182 (43%)  | 510 (100%)  | 1 (0%)   | 87          | 85  |
| 2   | D     | 79/189 (42%)    | 79 (100%)   | 0        | 100         | 100 |
| 2   | H     | 78/189 (41%)    | 78 (100%)   | 0        | 100         | 100 |
| 2   | I     | 79/189 (42%)    | 79 (100%)   | 0        | 100         | 100 |
| 2   | J     | 79/189 (42%)    | 79 (100%)   | 0        | 100         | 100 |
| 2   | K     | 79/189 (42%)    | 79 (100%)   | 0        | 100         | 100 |
| 2   | L     | 79/189 (42%)    | 79 (100%)   | 0        | 100         | 100 |
| 2   | V     | 79/189 (42%)    | 79 (100%)   | 0        | 100         | 100 |
| 2   | W     | 79/189 (42%)    | 79 (100%)   | 0        | 100         | 100 |
| 2   | X     | 79/189 (42%)    | 79 (100%)   | 0        | 100         | 100 |
| 2   | Y     | 79/189 (42%)    | 79 (100%)   | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 2   | Z     | 79/189 (42%)      | 79 (100%)    | 0        | 100         | 100 |
| 2   | a     | 79/189 (42%)      | 79 (100%)    | 0        | 100         | 100 |
| 2   | b     | 78/189 (41%)      | 78 (100%)    | 0        | 100         | 100 |
| 2   | c     | 79/189 (42%)      | 79 (100%)    | 0        | 100         | 100 |
| 2   | d     | 79/189 (42%)      | 79 (100%)    | 0        | 100         | 100 |
| 3   | e     | 245/410 (60%)     | 232 (95%)    | 13 (5%)  | 20          | 41  |
| 3   | f     | 262/410 (64%)     | 244 (93%)    | 18 (7%)  | 14          | 36  |
| 3   | g     | 263/410 (64%)     | 247 (94%)    | 16 (6%)  | 17          | 38  |
| 3   | h     | 263/410 (64%)     | 247 (94%)    | 16 (6%)  | 17          | 38  |
| 3   | i     | 262/410 (64%)     | 247 (94%)    | 15 (6%)  | 18          | 39  |
| 4   | j     | 205/267 (77%)     | 205 (100%)   | 0        | 100         | 100 |
| 4   | k     | 232/267 (87%)     | 232 (100%)   | 0        | 100         | 100 |
| 4   | l     | 224/267 (84%)     | 224 (100%)   | 0        | 100         | 100 |
| 4   | m     | 224/267 (84%)     | 224 (100%)   | 0        | 100         | 100 |
| 4   | n     | 224/267 (84%)     | 224 (100%)   | 0        | 100         | 100 |
| 4   | o     | 220/267 (82%)     | 219 (100%)   | 1 (0%)   | 81          | 82  |
| 4   | p     | 258/267 (97%)     | 258 (100%)   | 0        | 100         | 100 |
| 4   | q     | 257/267 (96%)     | 257 (100%)   | 0        | 100         | 100 |
| 4   | r     | 266/267 (100%)    | 266 (100%)   | 0        | 100         | 100 |
| 4   | s     | 257/267 (96%)     | 257 (100%)   | 0        | 100         | 100 |
| All | All   | 22432/26467 (85%) | 22343 (100%) | 89 (0%)  | 81          | 83  |

5 of 89 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | h     | 118 | THR  |
| 3   | h     | 451 | THR  |
| 3   | h     | 125 | VAL  |
| 3   | h     | 245 | MET  |
| 3   | i     | 125 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 485 such sidechains are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 656 | ASN  |
| 4   | l     | 315 | GLN  |
| 1   | B     | 713 | HIS  |
| 3   | g     | 344 | GLN  |
| 1   | z     | 113 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

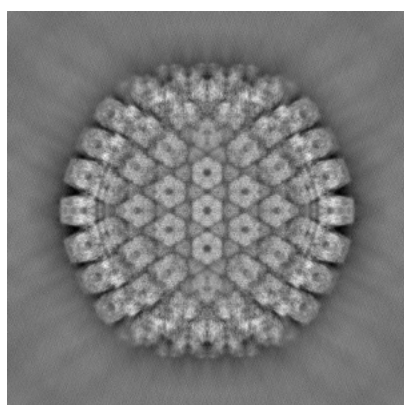
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0881. These allow visual inspection of the internal detail of the map and identification of artifacts.

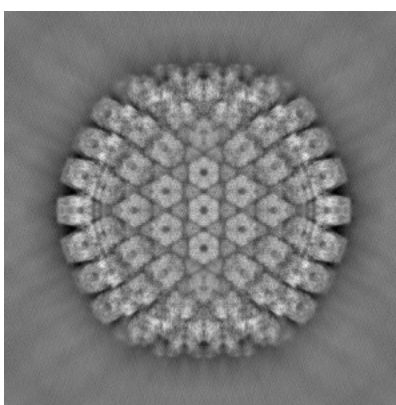
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

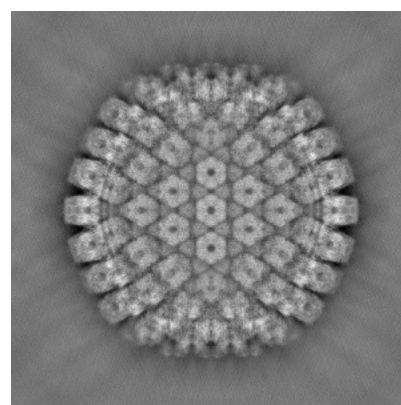
#### 6.1.1 Primary map



X



Y

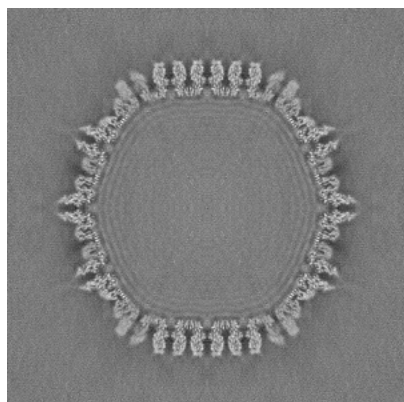


Z

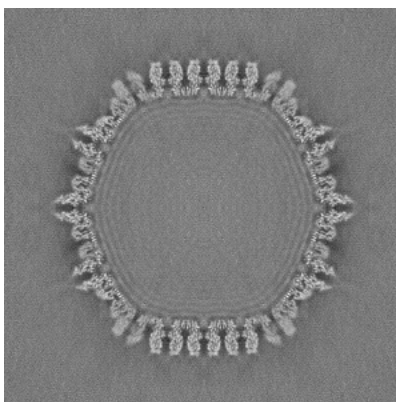
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

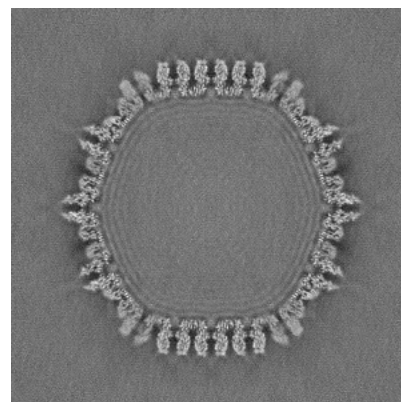
#### 6.2.1 Primary map



X Index: 640



Y Index: 640

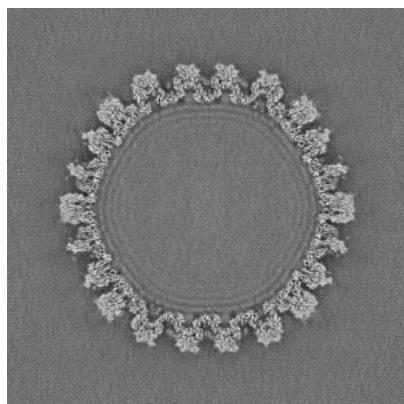


Z Index: 640

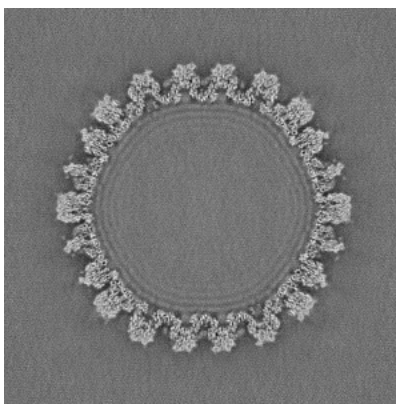
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

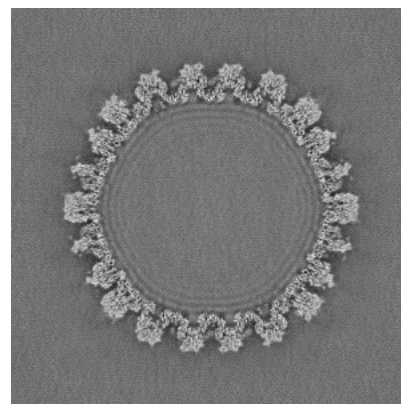
### 6.3.1 Primary map



X Index: 742



Y Index: 538

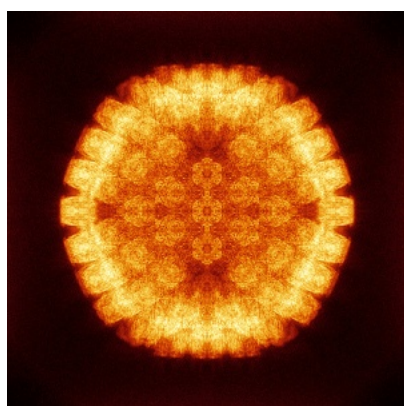


Z Index: 537

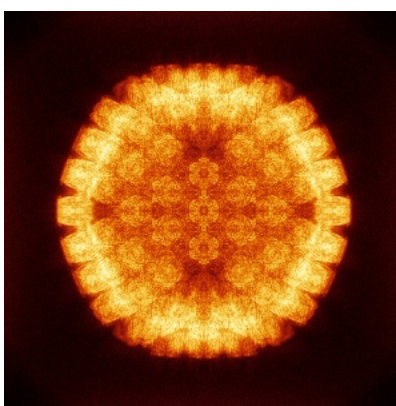
The images above show the largest variance slices of the map in three orthogonal directions.

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

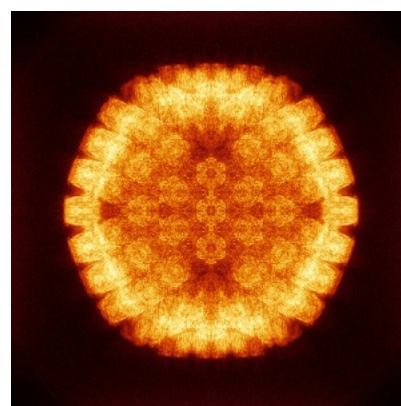
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views

This section was not generated.

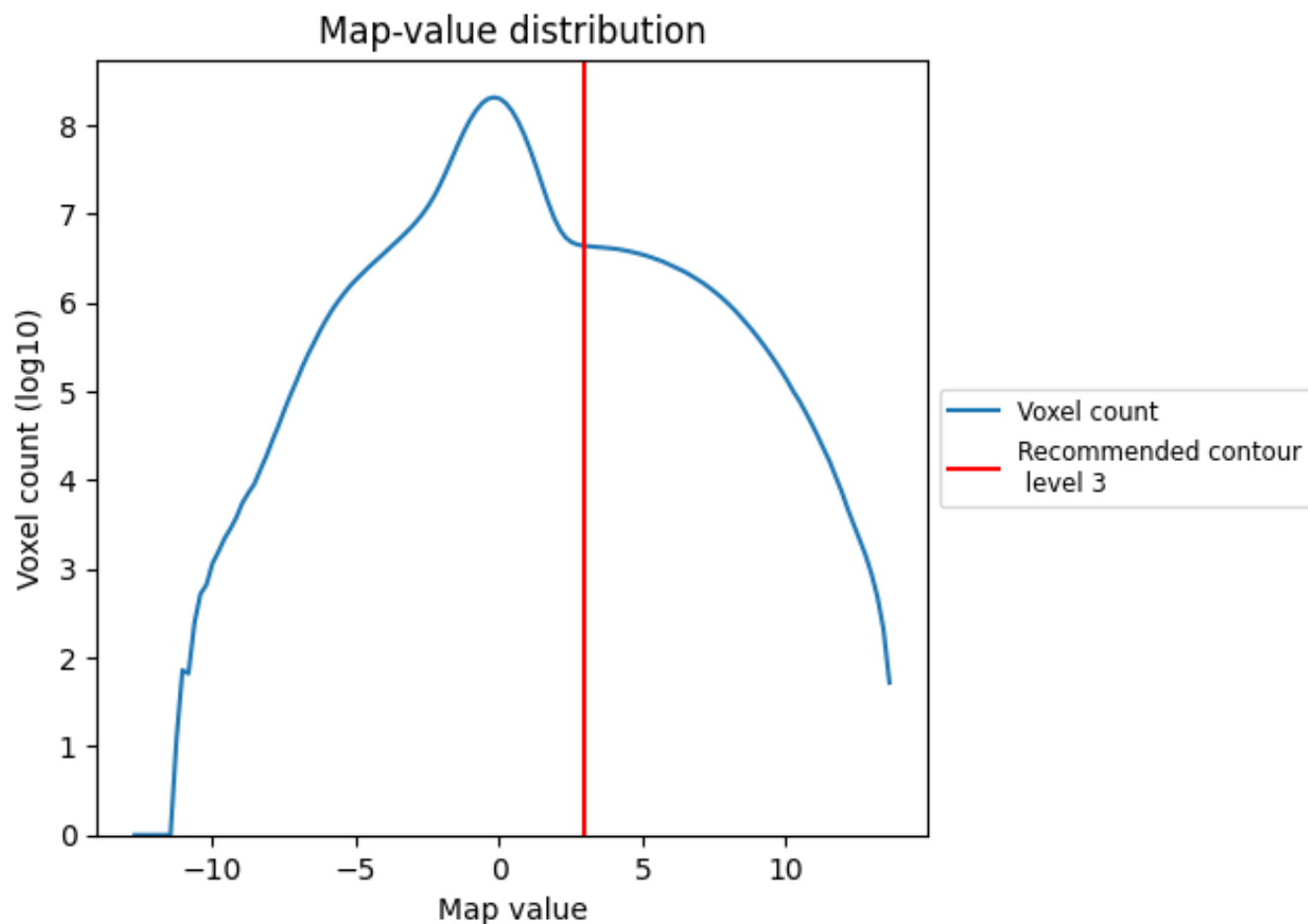
## 6.6 Mask visualisation

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

## 7 Map analysis [i](#)

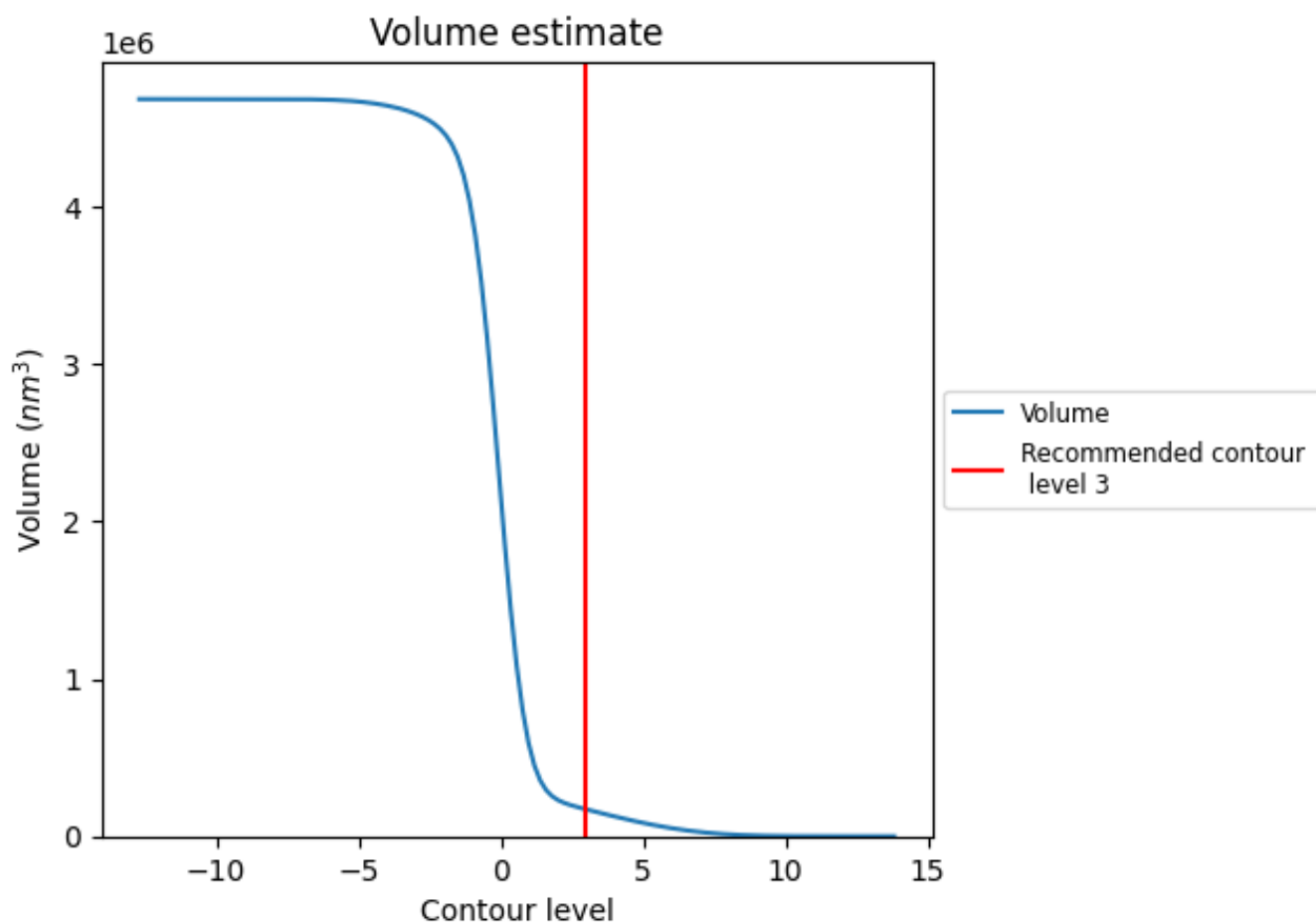
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

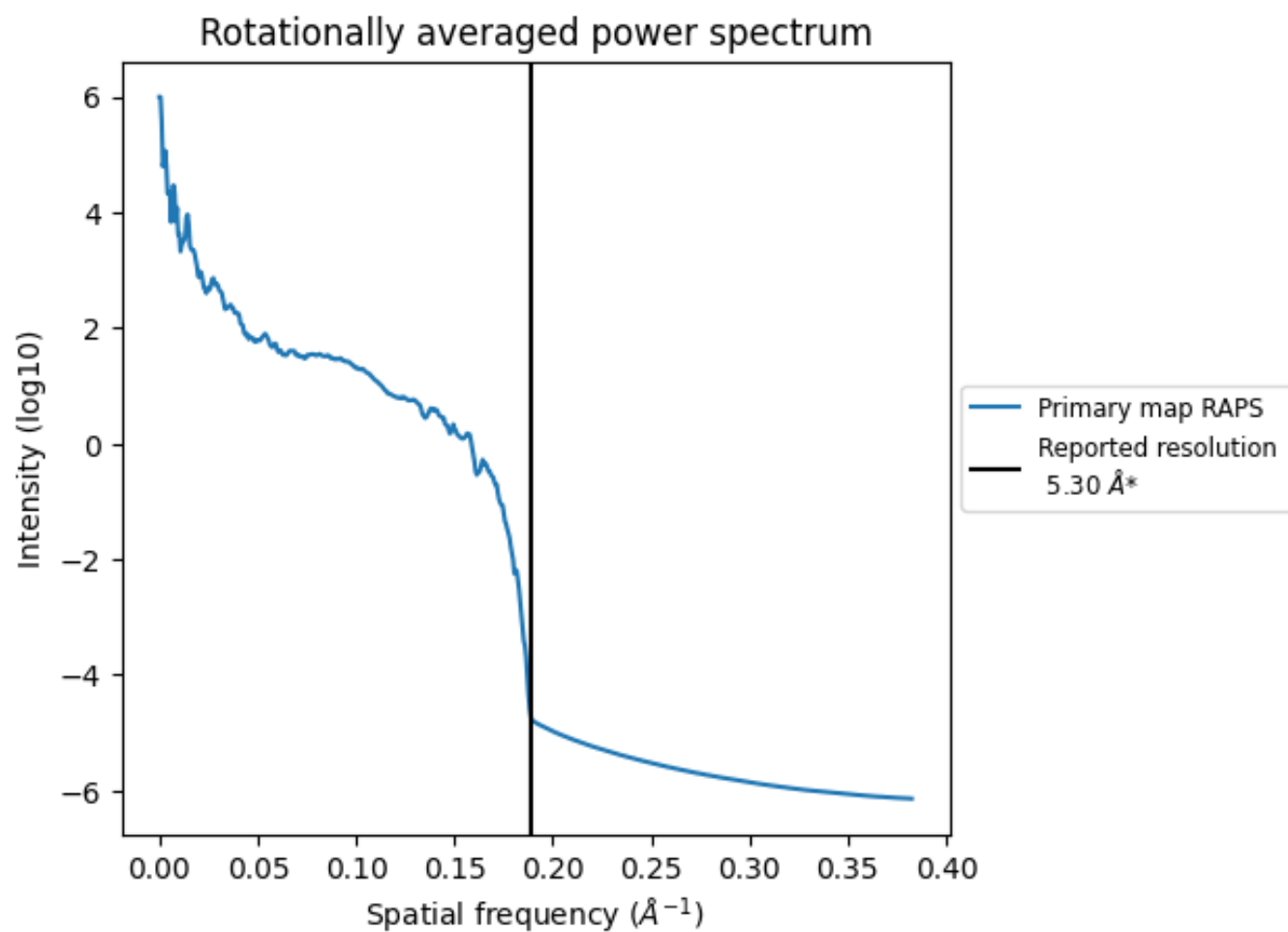
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 170845 nm<sup>3</sup>; this corresponds to an approximate mass of 154328 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.189 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

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

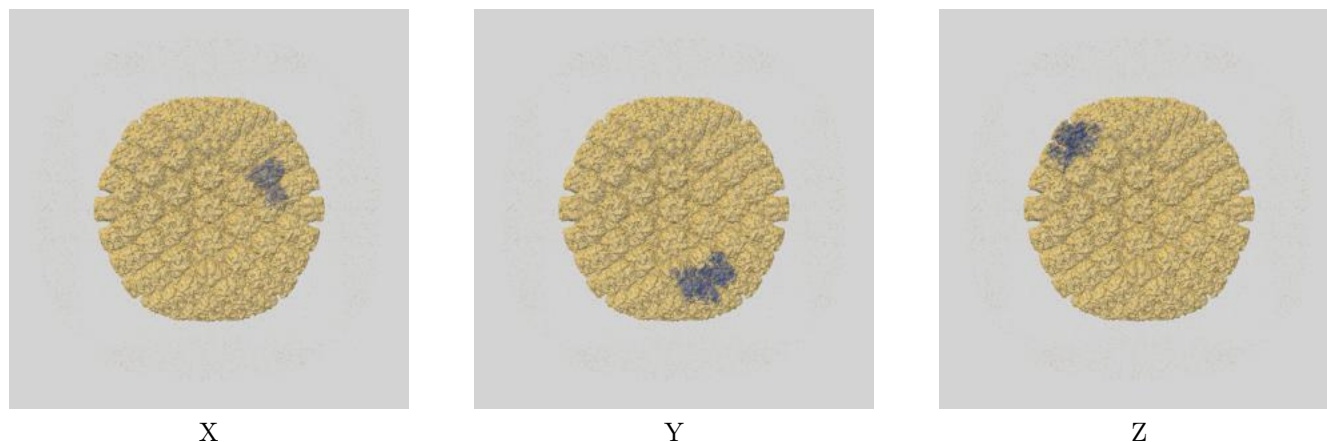


## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0881 and PDB model 6LGN. Per-residue inclusion information can be found in section 3 on page 8.

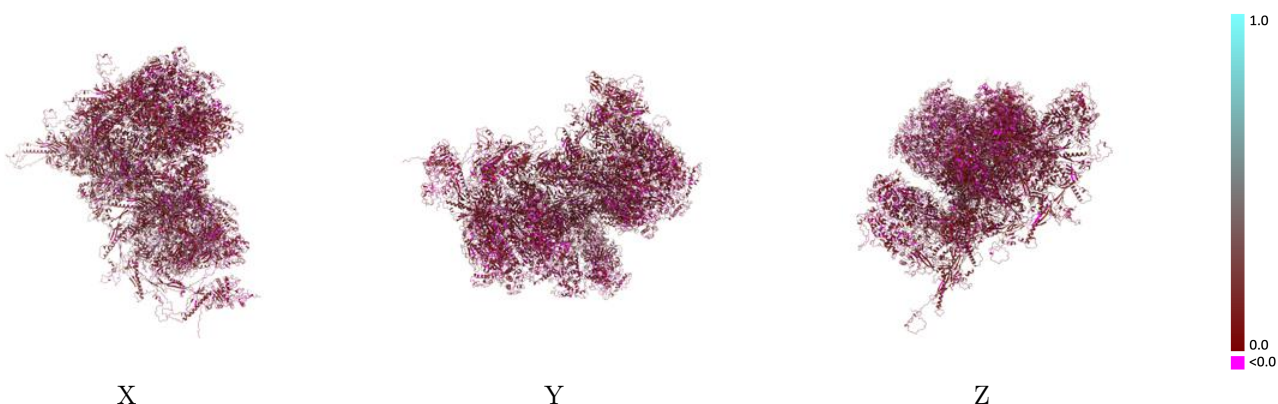
### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

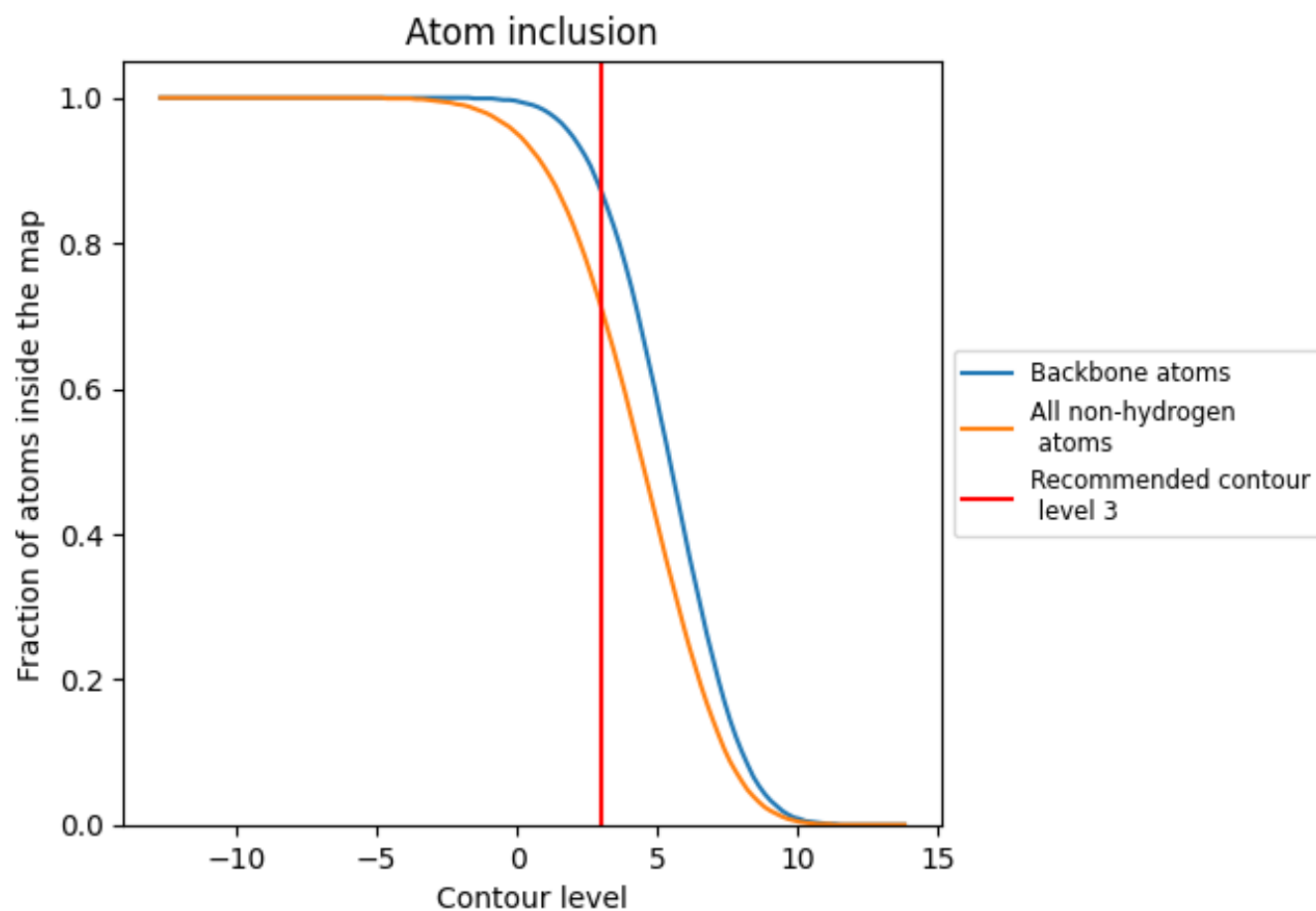


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 71% 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 (3) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7120   |  0.1190   |
| A     |  0.6990   |  0.1210   |
| B     |  0.7370   |  0.1130   |
| C     |  0.7210   |  0.1170   |
| D     |  0.8800   |  0.1070   |
| E     |  0.7020   |  0.1160   |
| F     |  0.7280   |  0.1190   |
| G     |  0.7360   |  0.1160   |
| H     |  0.8860   |  0.1060   |
| I     |  0.9130   |  0.1090   |
| J     |  0.9050   |  0.1100   |
| K     |  0.8960   |  0.1230   |
| L     |  0.8570   |  0.1010   |
| M     |  0.7010   |  0.1190   |
| N     |  0.7350  |  0.1200  |
| O     |  0.7310 |  0.1210 |
| P     |  0.7340 |  0.1220 |
| Q     |  0.7240 |  0.1200 |
| R     |  0.7070 |  0.1180 |
| S     |  0.7300 |  0.1200 |
| T     |  0.7230 |  0.1180 |
| U     |  0.7100 |  0.1160 |
| V     |  0.8420 |  0.0970 |
| W     |  0.8990 |  0.1030 |
| X     |  0.8810 |  0.1050 |
| Y     |  0.8900 |  0.0780 |
| Z     |  0.8770 |  0.0950 |
| a     |  0.9040 |  0.0980 |
| b     |  0.8780 |  0.0990 |
| c     |  0.9160 |  0.1090 |
| d     |  0.8770 |  0.0910 |
| e     |  0.5570 |  0.1220 |
| f     |  0.7060 |  0.1310 |
| g     |  0.7200 |  0.1240 |
| h     |  0.7060 |  0.1300 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| i     |  0.6880 |  0.1310 |
| j     |  0.5190 |  0.1260 |
| k     |  0.6540 |  0.1310 |
| l     |  0.6970 |  0.1430 |
| m     |  0.6500 |  0.1410 |
| n     |  0.6260 |  0.1440 |
| o     |  0.4990 |  0.1220 |
| p     |  0.6270 |  0.1310 |
| q     |  0.6450 |  0.1380 |
| r     |  0.5940 |  0.1380 |
| s     |  0.6040 |  0.1370 |
| z     |  0.5410 |  0.1000 |