# wwPDB EM Validation Summary Report

Nov 3, 2026 – 07:07 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 31OI / pdb_000031oi |
| EMDB ID | : | EMD-58585 |
| Title | : | Yersinia entomophaga holotoxin in its conventional pore state |
| Authors | : | Ng'ang'a, P.N.; Raunser, S.; Bader, R.; Sitsel, O. |
| Deposited on | : | 2026-06-16 |
| Resolution | : | 3.50 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

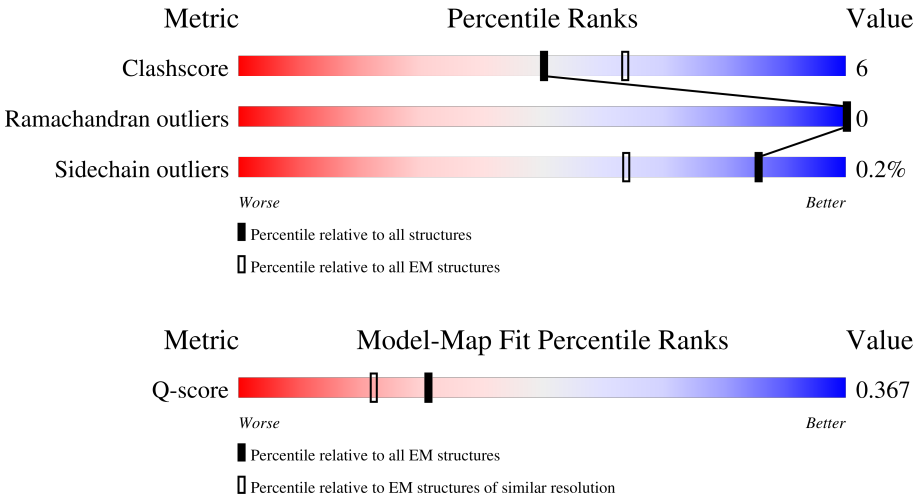
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| MolProbity | : | 4-5-2 with Phenix2.2 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.51 |

# 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 3.50 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.







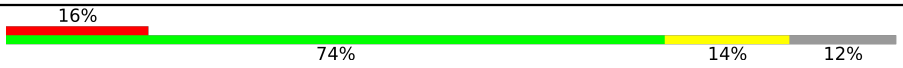
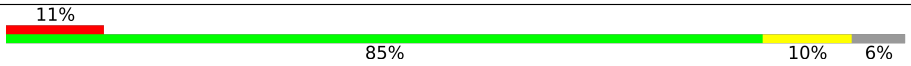
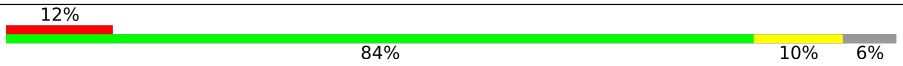
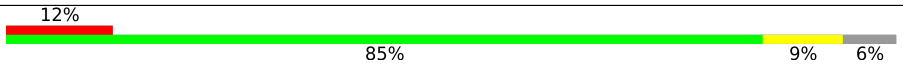
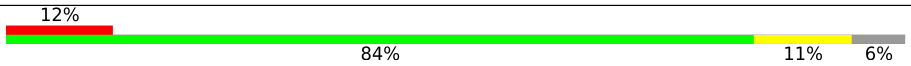
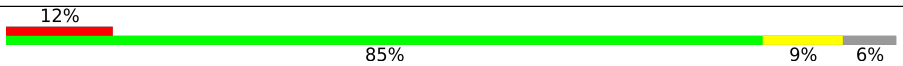
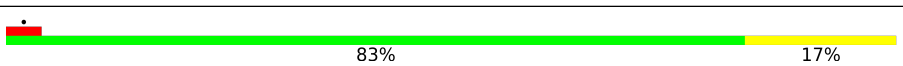
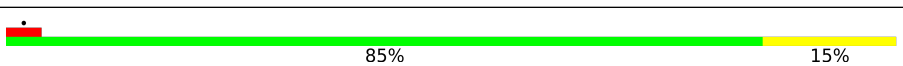
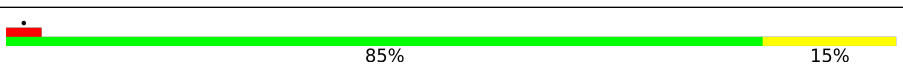
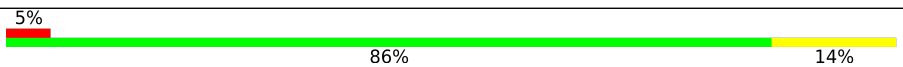
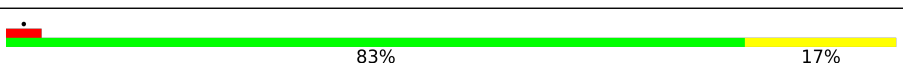
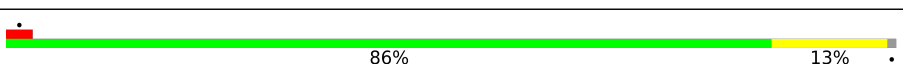
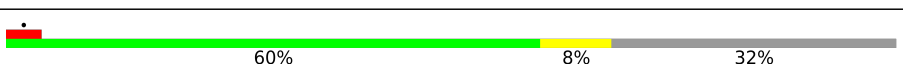
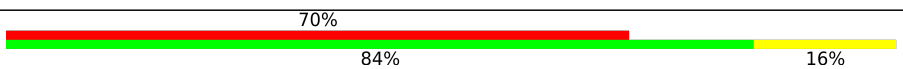
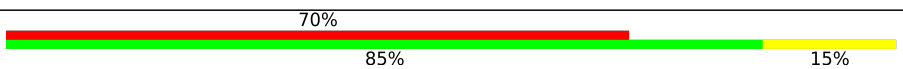
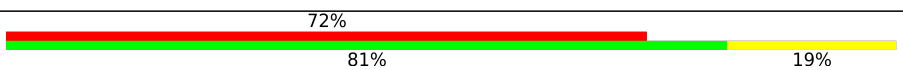
| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 13950 ( 3.00 - 4.00 ) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1164 | 16% 75% 13% 12% |
| 1 | F | 1164 | 16% 73% 15% 12% |
| 1 | I | 1164 | 16% 78% 10% 12% |
| 1 | L | 1164 | 16% 73% 15% 12% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | O | 1164 |   |
| 2 | B | 1365 |   |
| 2 | G | 1365 |   |
| 2 | J | 1365 |   |
| 2 | M | 1365 |   |
| 2 | P | 1365 |   |
| 3 | C | 633 |   |
| 3 | H | 633 |   |
| 3 | K | 633 |   |
| 3 | N | 633 |   |
| 3 | Q | 633 |   |
| 4 | D | 1487 |   |
| 5 | E | 970 |   |
| 6 | R | 542 |   |
| 6 | S | 542 |   |
| 6 | T | 542 |   |
| 6 | U | 542 |   |
| 6 | V | 542 |   |

## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 154987 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 Toxin subunit YenA1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 1026 | Total | C | N | O | S | 0 | 0 |
| | | | 8078 | 5154 | 1327 | 1574 | 23 | | |
| 1 | F | 1026 | Total | C | N | O | S | 0 | 0 |
| | | | 8078 | 5154 | 1327 | 1574 | 23 | | |
| 1 | I | 1026 | Total | C | N | O | S | 0 | 0 |
| | | | 8078 | 5154 | 1327 | 1574 | 23 | | |
| 1 | L | 1026 | Total | C | N | O | S | 0 | 0 |
| | | | 8078 | 5154 | 1327 | 1574 | 23 | | |
| 1 | O | 1026 | Total | C | N | O | S | 0 | 0 |
| | | | 8078 | 5154 | 1327 | 1574 | 23 | | |

- Molecule 2 is a protein called Toxin subunit YenA2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 1286 | Total | C | N | O | S | 0 | 0 |
| | | | 10384 | 6587 | 1744 | 2017 | 36 | | |
| 2 | G | 1286 | Total | C | N | O | S | 0 | 0 |
| | | | 10384 | 6587 | 1744 | 2017 | 36 | | |
| 2 | J | 1286 | Total | C | N | O | S | 0 | 0 |
| | | | 10384 | 6587 | 1744 | 2017 | 36 | | |
| 2 | M | 1286 | Total | C | N | O | S | 0 | 0 |
| | | | 10384 | 6587 | 1744 | 2017 | 36 | | |
| 2 | P | 1286 | Total | C | N | O | S | 0 | 0 |
| | | | 10384 | 6587 | 1744 | 2017 | 36 | | |

There are 15 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 351 | THR | - | insertion | UNP B6A878 |
| B | ? | - | PRO | deletion | UNP B6A878 |
| B | 829 | SER | - | insertion | UNP B6A878 |
| G | 351 | THR | - | insertion | UNP B6A878 |
| G | ? | - | PRO | deletion | UNP B6A878 |
| G | 829 | SER | - | insertion | UNP B6A878 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| J | 351 | THR | - | insertion | UNP B6A878 |
| J | ? | - | PRO | deletion | UNP B6A878 |
| J | 829 | SER | - | insertion | UNP B6A878 |
| M | 351 | THR | - | insertion | UNP B6A878 |
| M | ? | - | PRO | deletion | UNP B6A878 |
| M | 829 | SER | - | insertion | UNP B6A878 |
| P | 351 | THR | - | insertion | UNP B6A878 |
| P | ? | - | PRO | deletion | UNP B6A878 |
| P | 829 | SER | - | insertion | UNP B6A878 |

- Molecule 3 is a protein called Chitinase 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 633 | Total | C | N | O | S | 0 | 0 |
| | | | 4914 | 3107 | 824 | 964 | 19 | | |
| 3 | H | 633 | Total | C | N | O | S | 0 | 0 |
| | | | 4914 | 3107 | 824 | 964 | 19 | | |
| 3 | K | 633 | Total | C | N | O | S | 0 | 0 |
| | | | 4914 | 3107 | 824 | 964 | 19 | | |
| 3 | N | 633 | Total | C | N | O | S | 0 | 0 |
| | | | 4914 | 3107 | 824 | 964 | 19 | | |
| 3 | Q | 633 | Total | C | N | O | S | 0 | 0 |
| | | | 4914 | 3107 | 824 | 964 | 19 | | |

- Molecule 4 is a protein called Toxin subunit YenB.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 1474 | Total | C | N | O | S | 0 | 0 |
| | | | 11696 | 7381 | 2021 | 2258 | 36 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 1484 | ASP | ASN | conflict | UNP B6A880 |

- Molecule 5 is a protein called Toxin subunit YenC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | E | 658 | Total | C | N | O | S | 0 | 0 |
| | | | 5111 | 3187 | 895 | 1017 | 12 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| E | 109 | SER | LYS | conflict | UNP B6A882 |

- Molecule 6 is a protein called Chitinase 1.

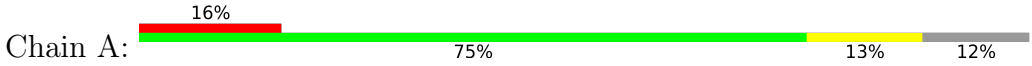
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | R | 542 | Total | C | N | O | S | 0 | 0 |
| | | | 4260 | 2691 | 706 | 850 | 13 | | |
| 6 | S | 542 | Total | C | N | O | S | 0 | 0 |
| | | | 4260 | 2691 | 706 | 850 | 13 | | |
| 6 | T | 542 | Total | C | N | O | S | 0 | 0 |
| | | | 4260 | 2691 | 706 | 850 | 13 | | |
| 6 | U | 542 | Total | C | N | O | S | 0 | 0 |
| | | | 4260 | 2691 | 706 | 850 | 13 | | |
| 6 | V | 542 | Total | C | N | O | S | 0 | 0 |
| | | | 4260 | 2691 | 706 | 850 | 13 | | |

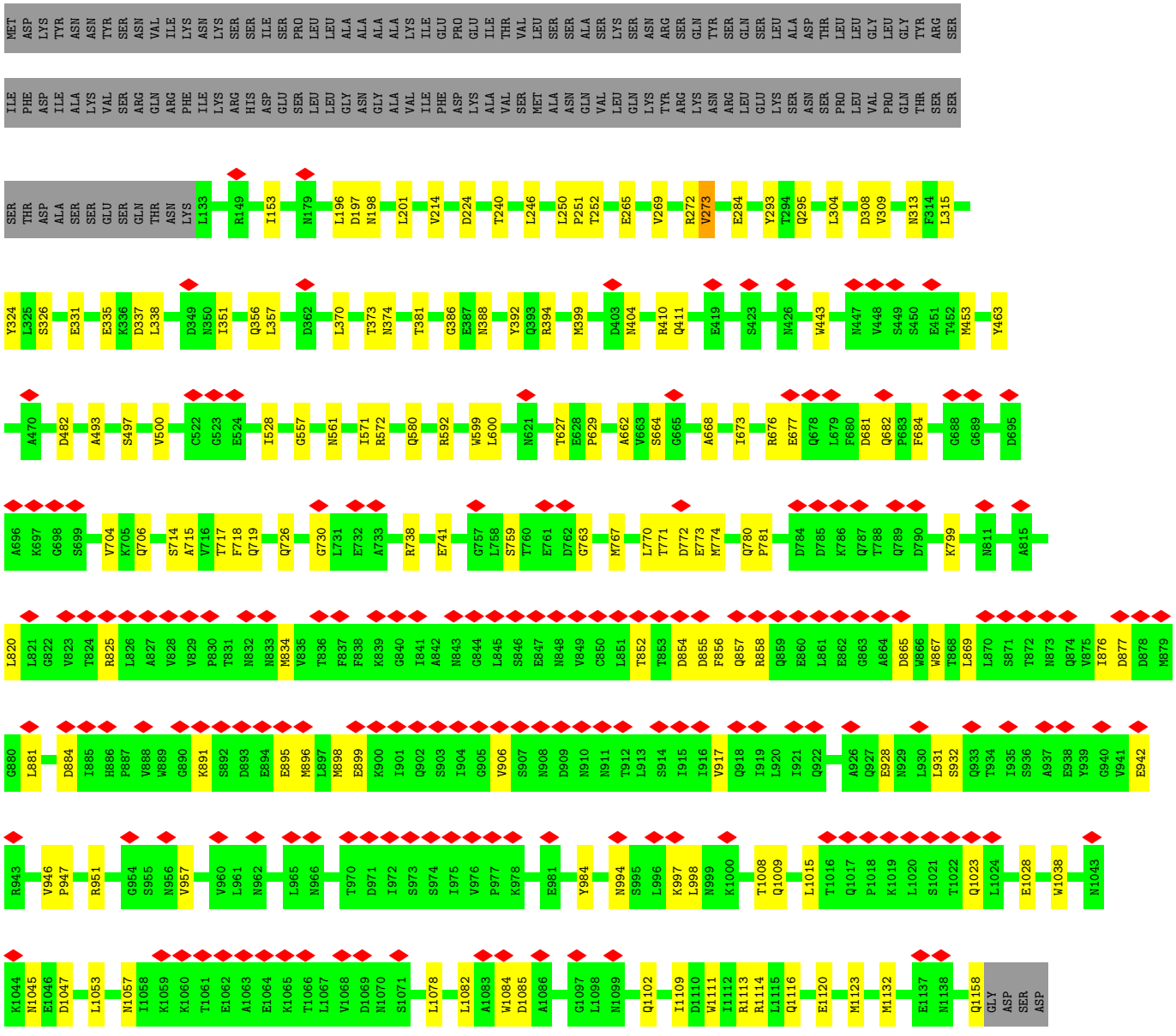
# 3 Residue-property plots (i)

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: Toxin subunit YenA1

Chain A:



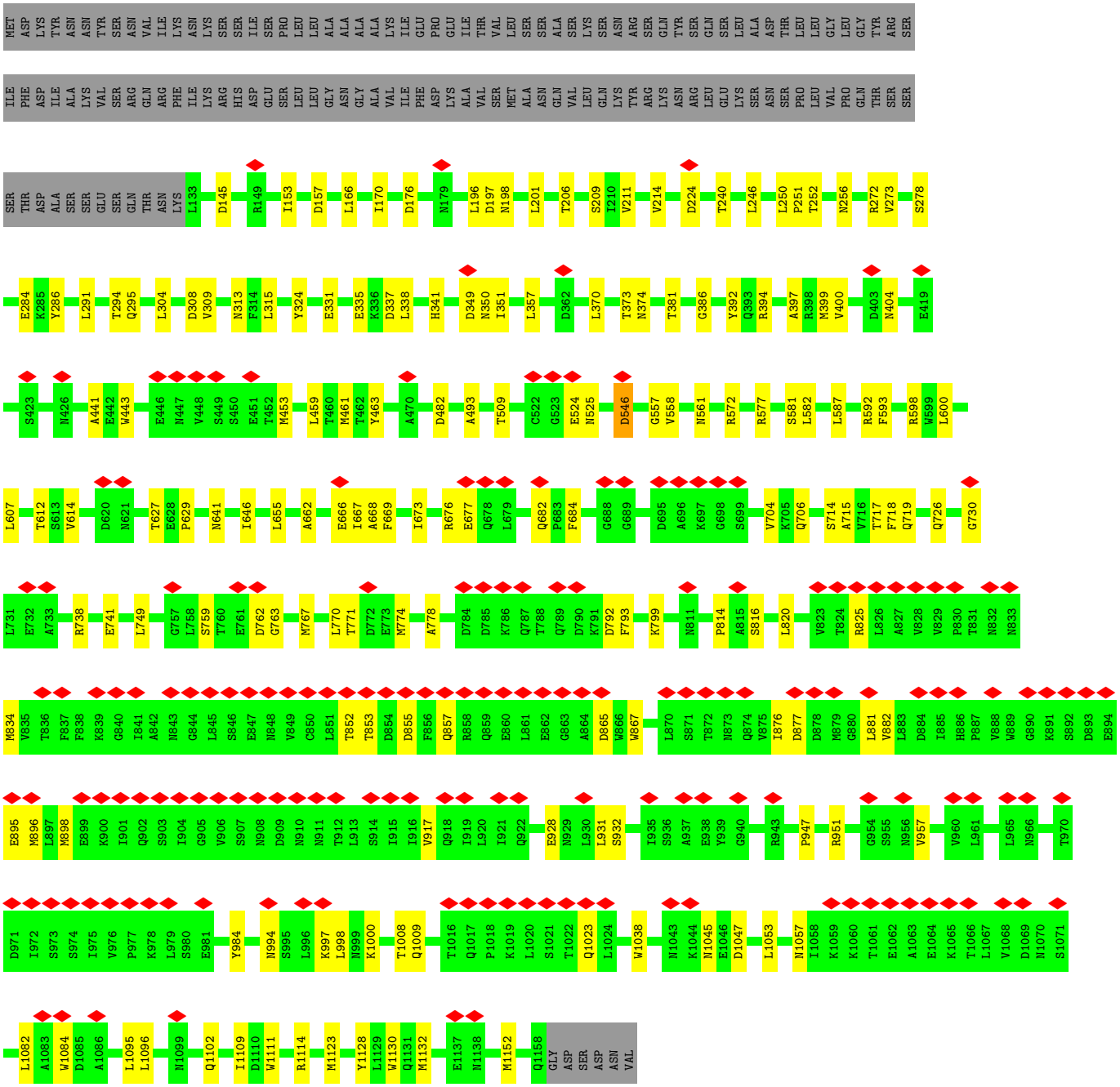






• Molecule 1: Toxin subunit YenA1

Chain F:



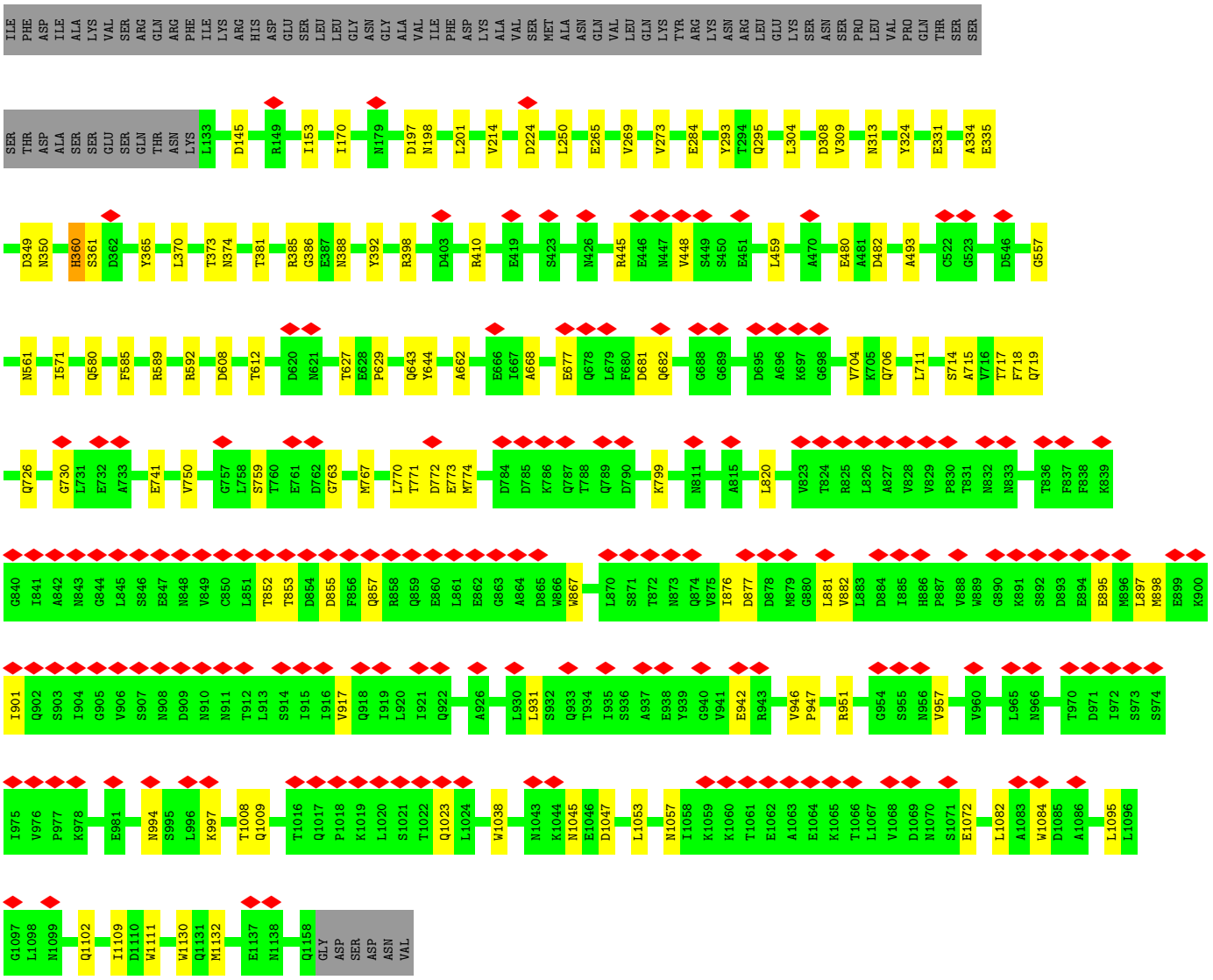




• Molecule 1: Toxin subunit YenA1

Chain I:



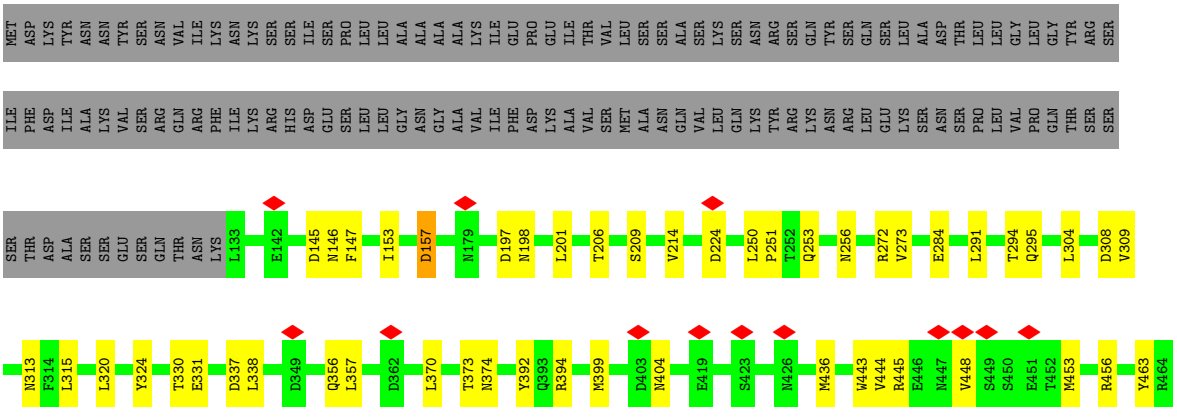


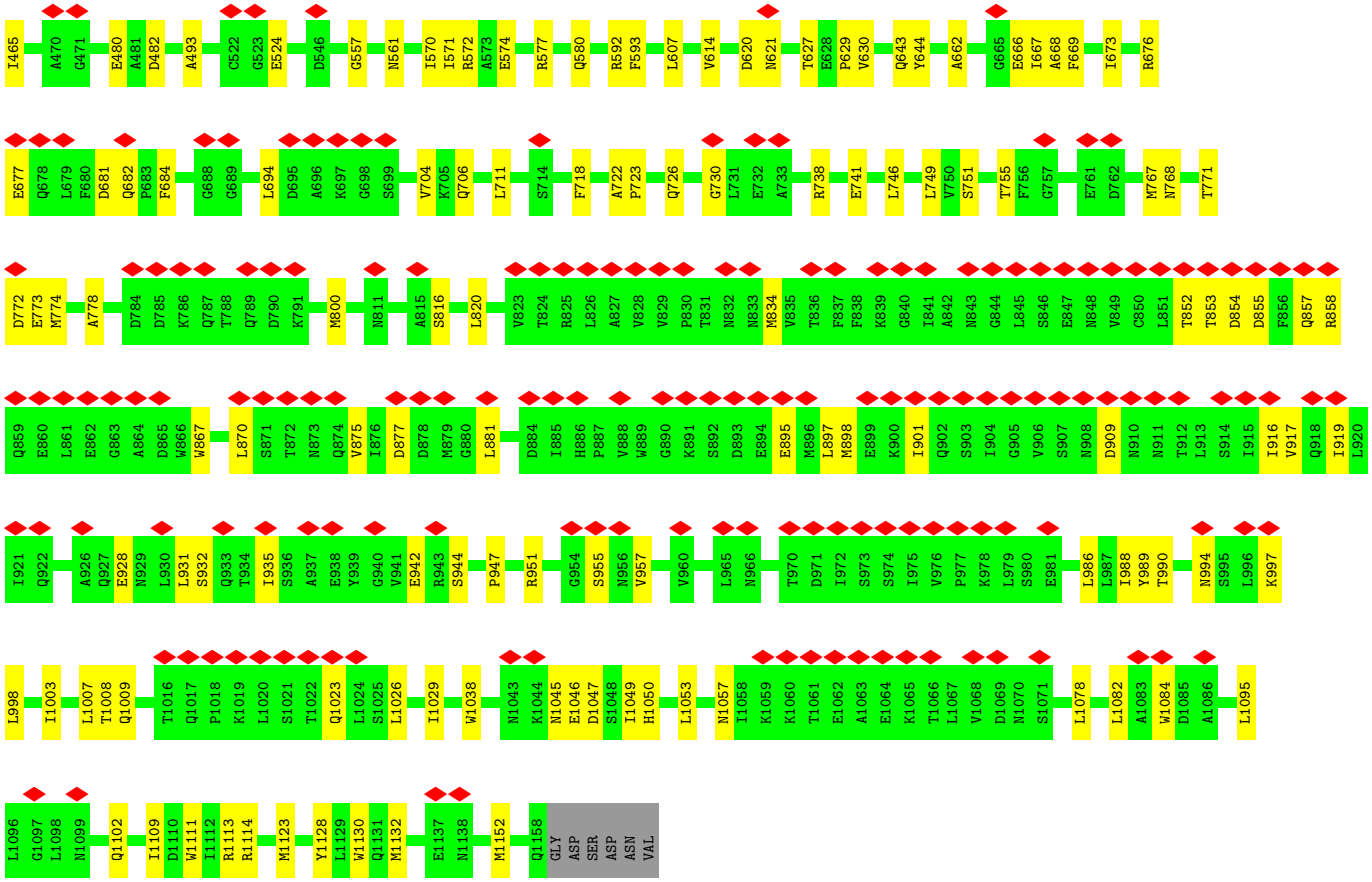



• Molecule 1: Toxin subunit YenA1

Chain L:



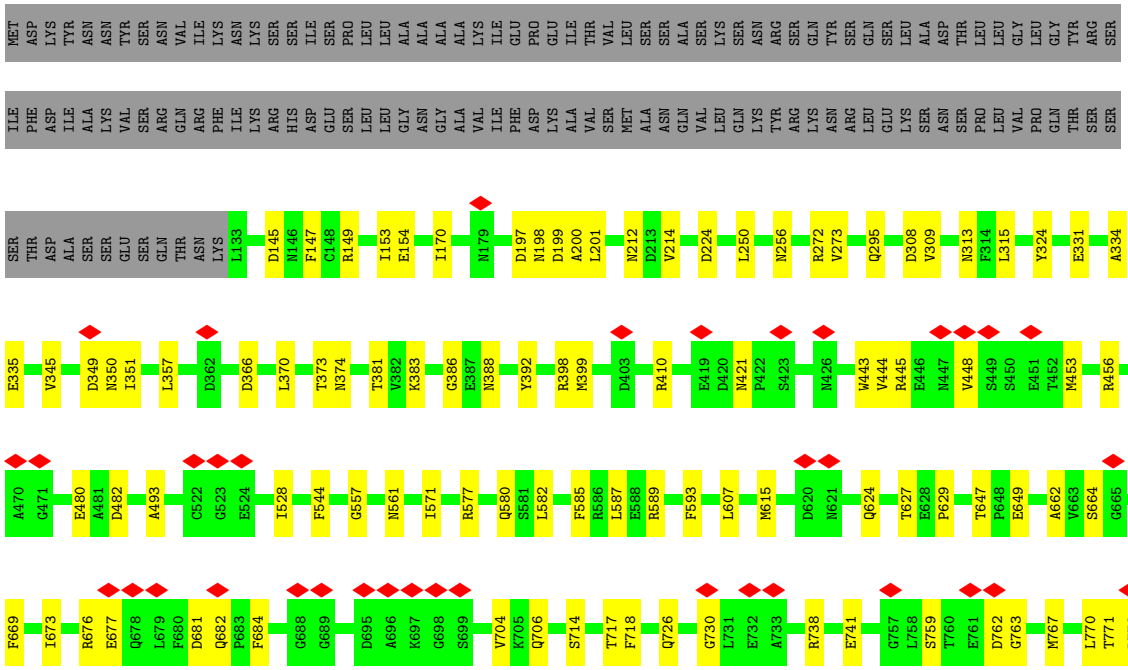



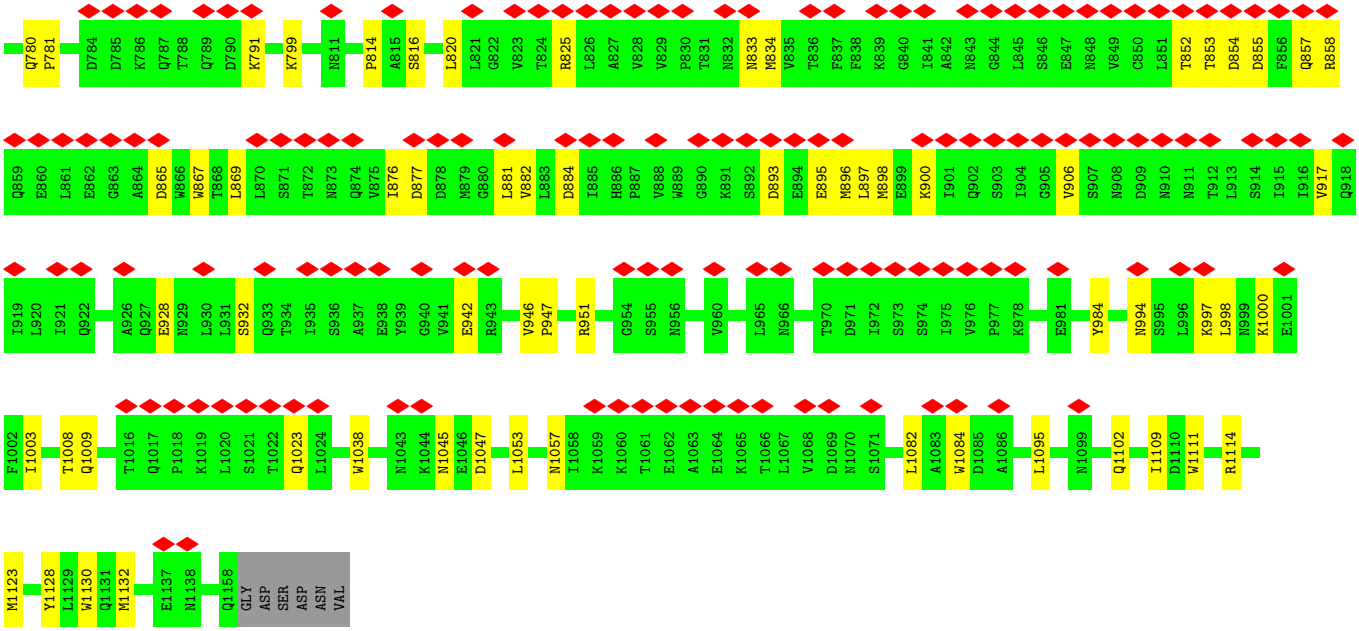


• Molecule 1: Toxin subunit YenA1

Chain O:



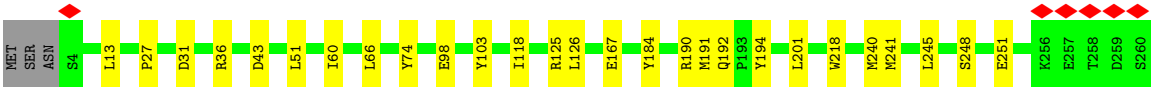






• Molecule 2: Toxin subunit YenA2

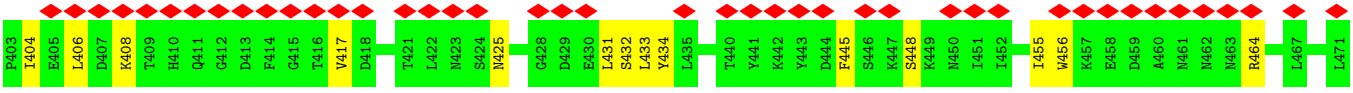
Chain B:

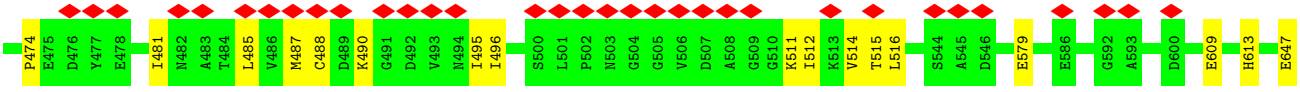


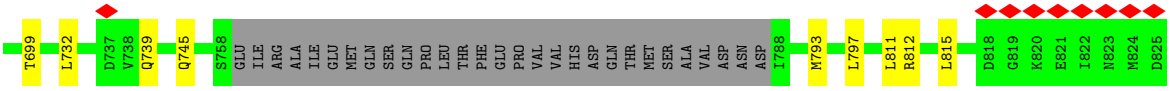



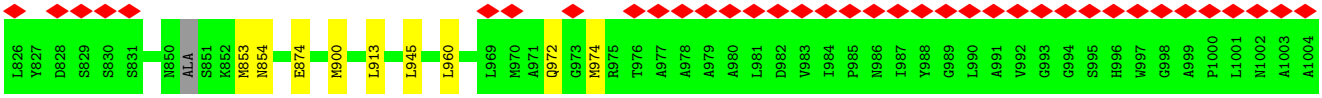


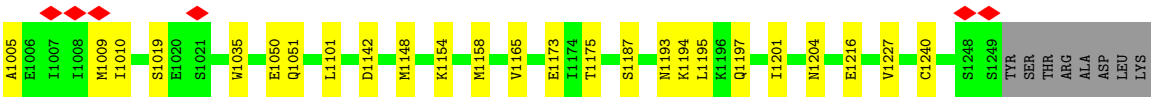




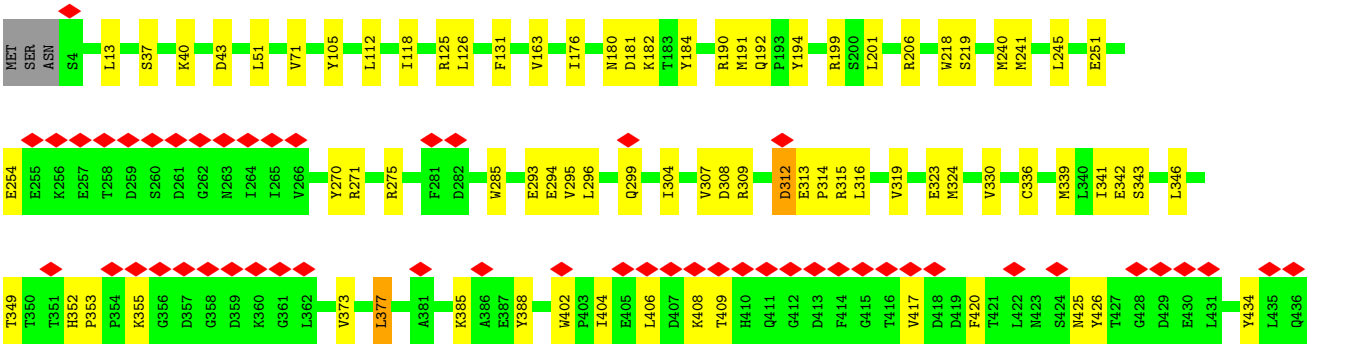





• Molecule 2: Toxin subunit YenA2

Chain G:

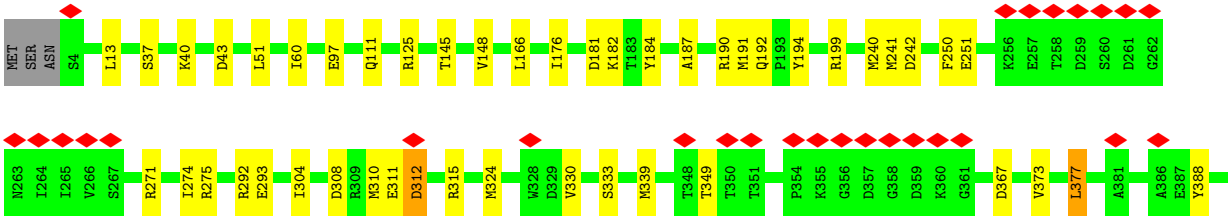


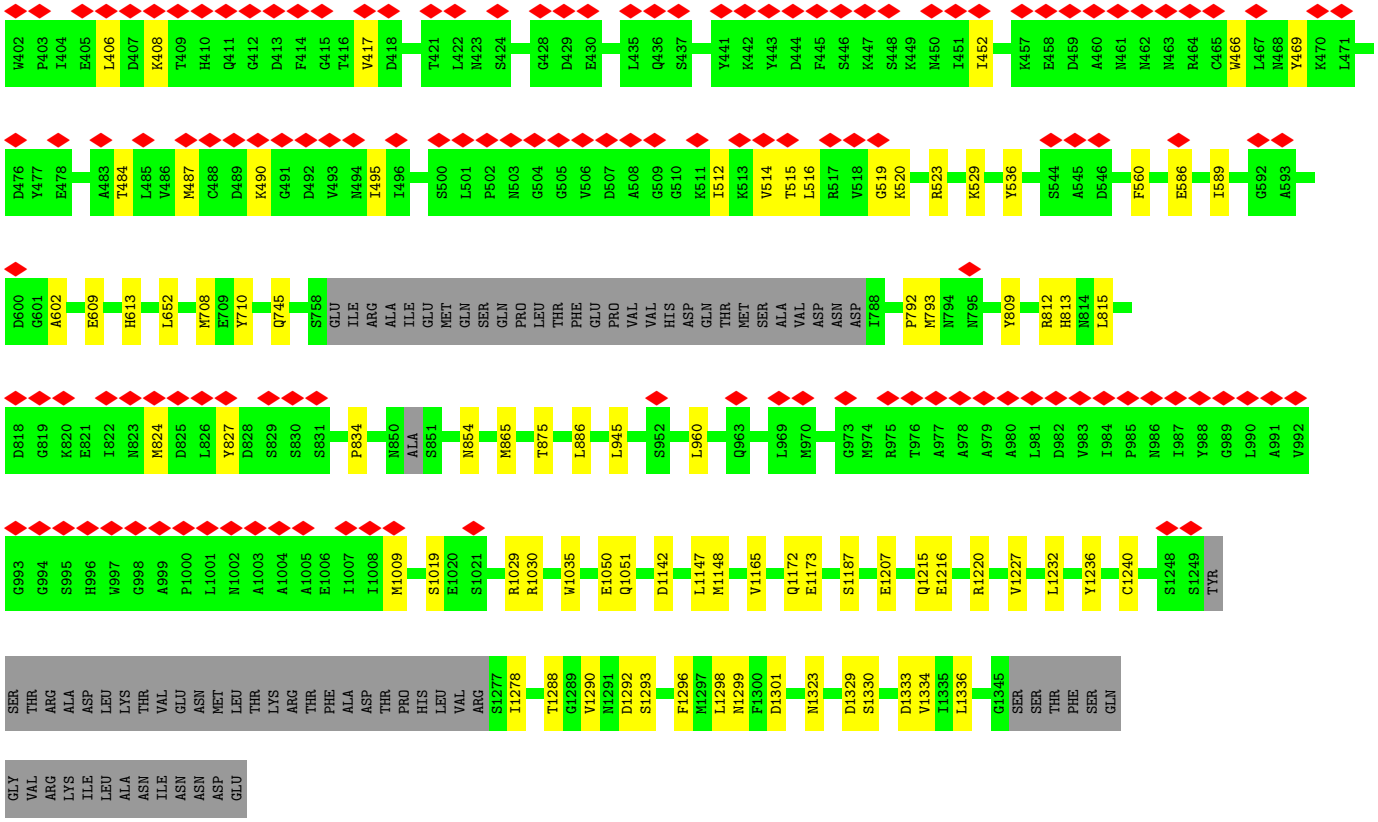



• Molecule 2: Toxin subunit YenA2

Chain J:



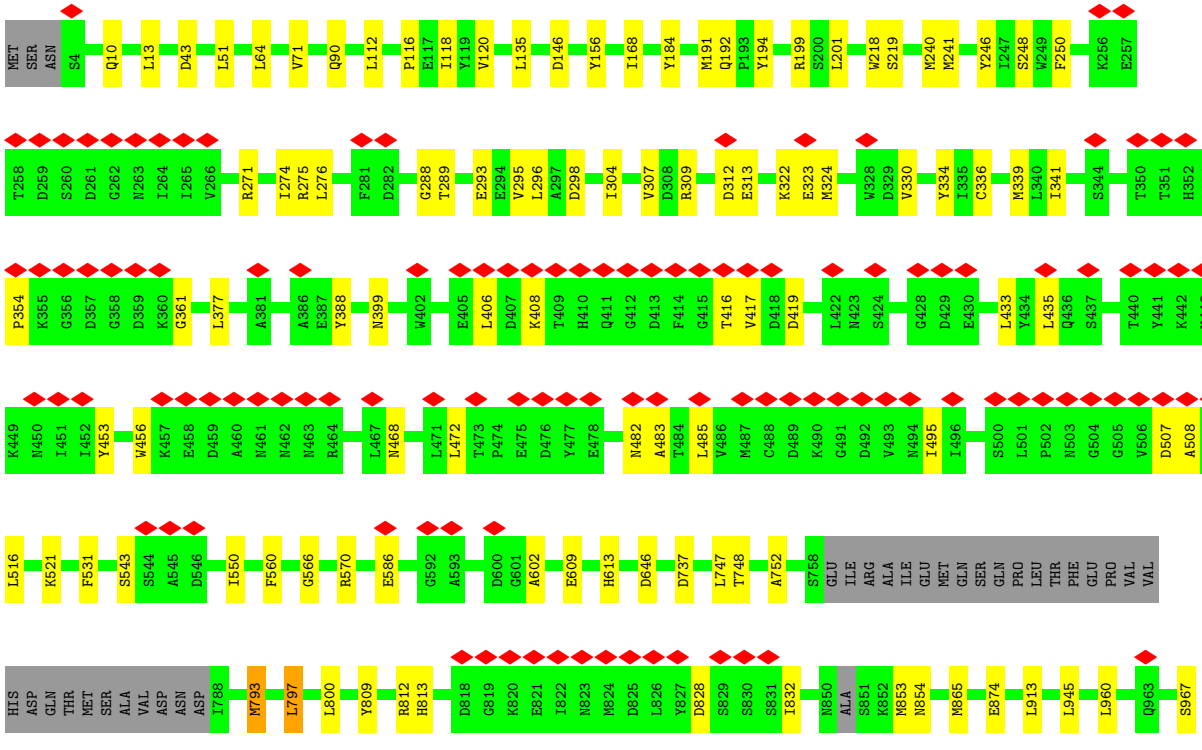



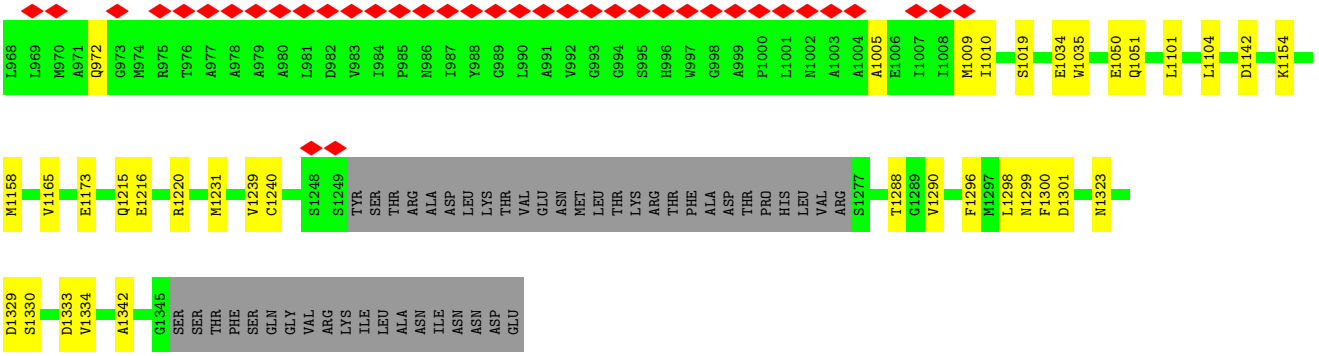


• Molecule 2: Toxin subunit YenA2

Chain M:





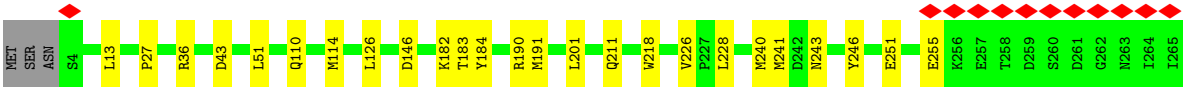


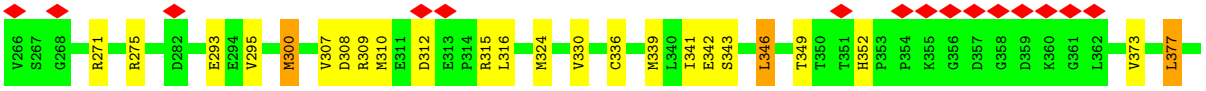


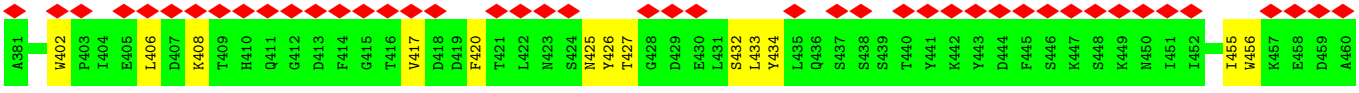
• Molecule 2: Toxin subunit YenA2

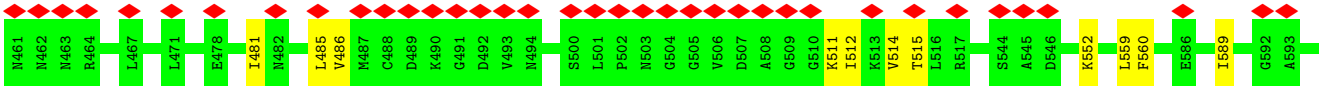
Chain P:

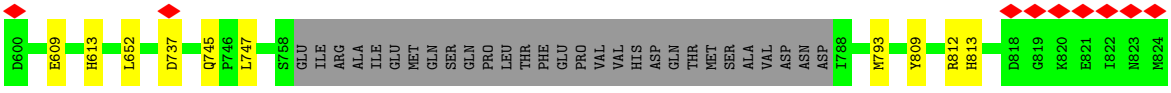


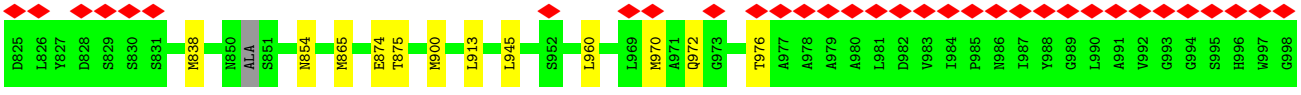









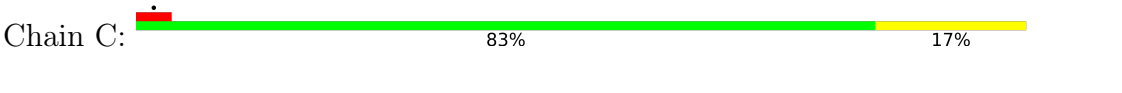








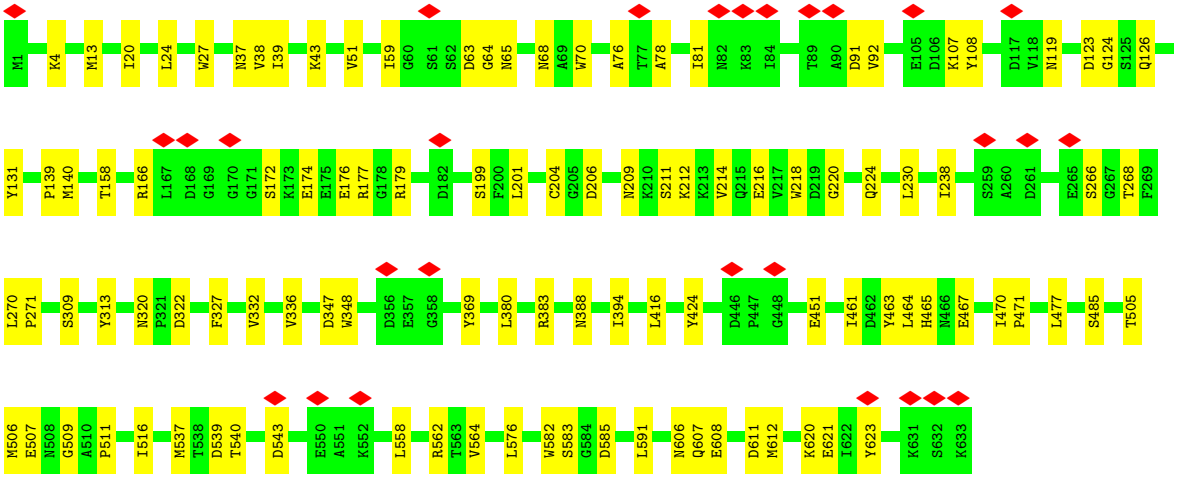






• Molecule 3: Chitinase 2

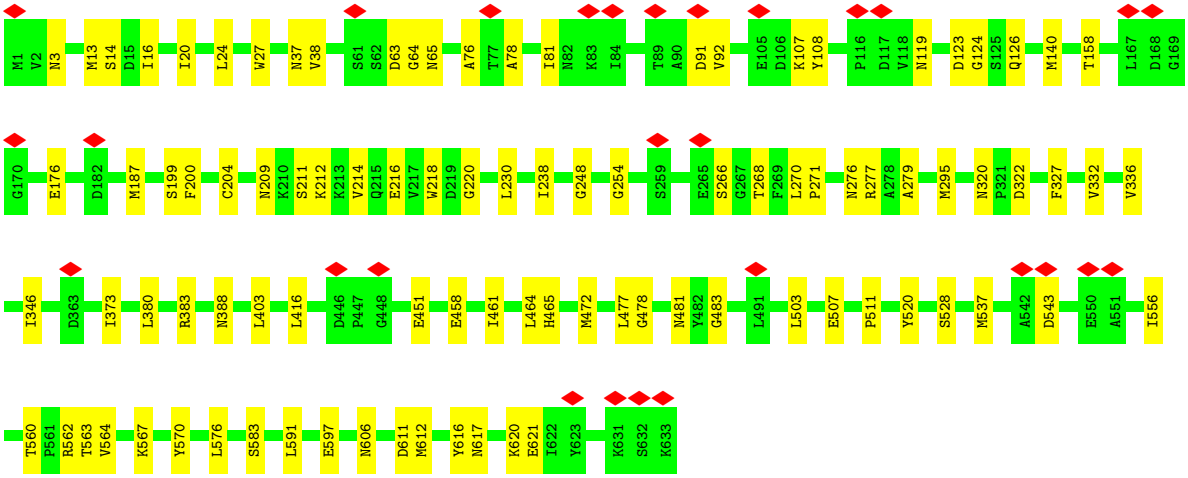
Chain C:




• Molecule 3: Chitinase 2

Chain H:

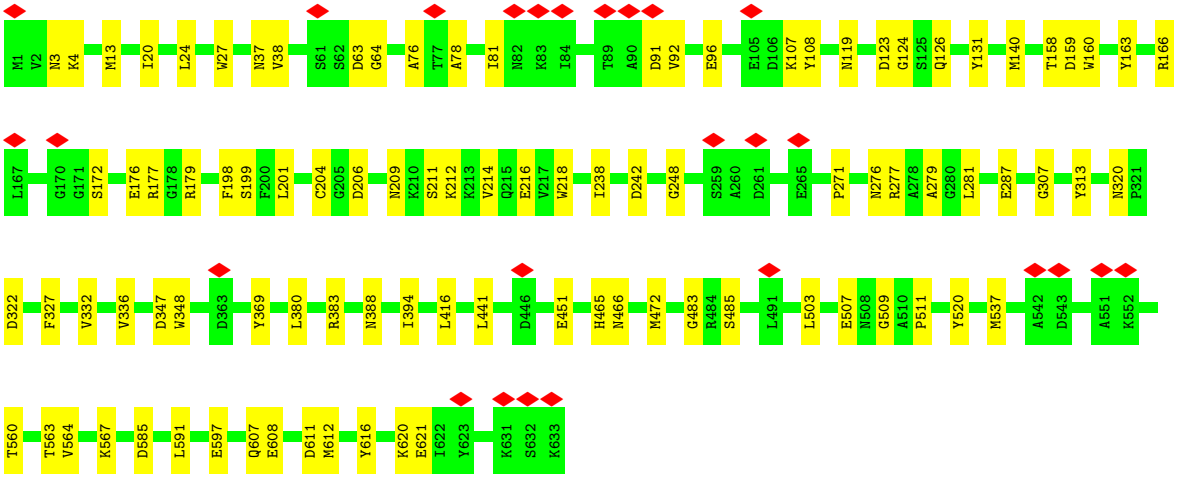



• Molecule 3: Chitinase 2

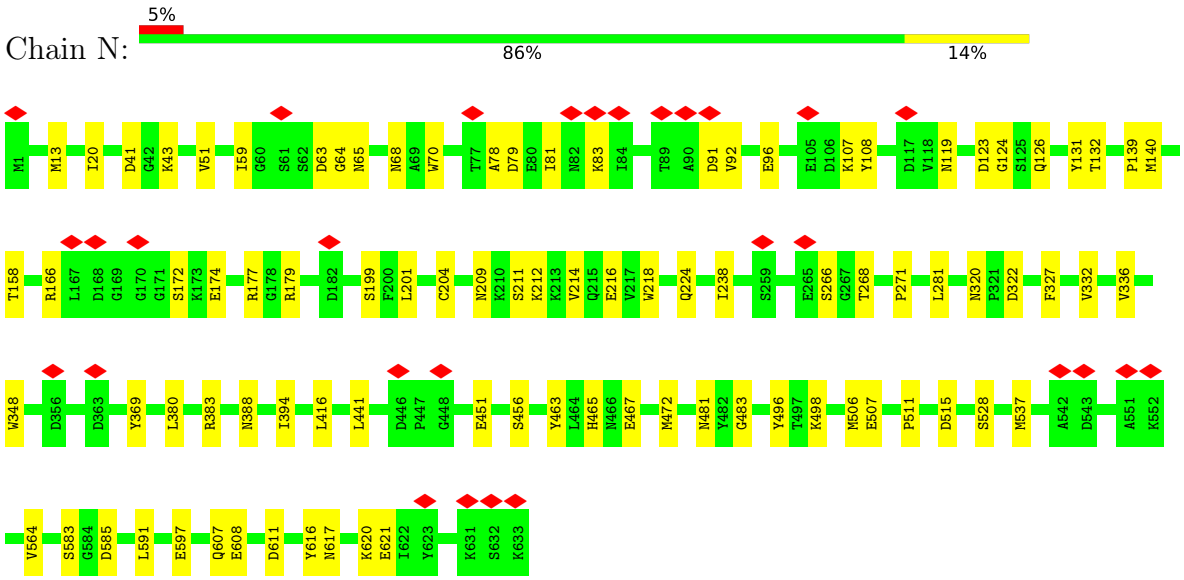
Chain K:



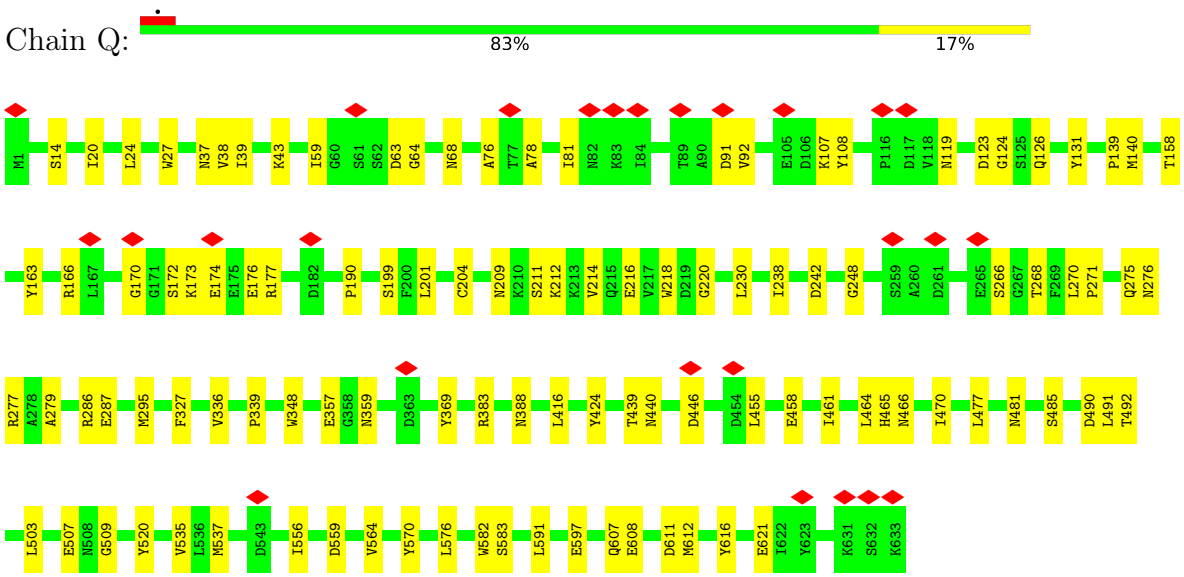
• Molecule 3: Chitinase 2

Chain N:



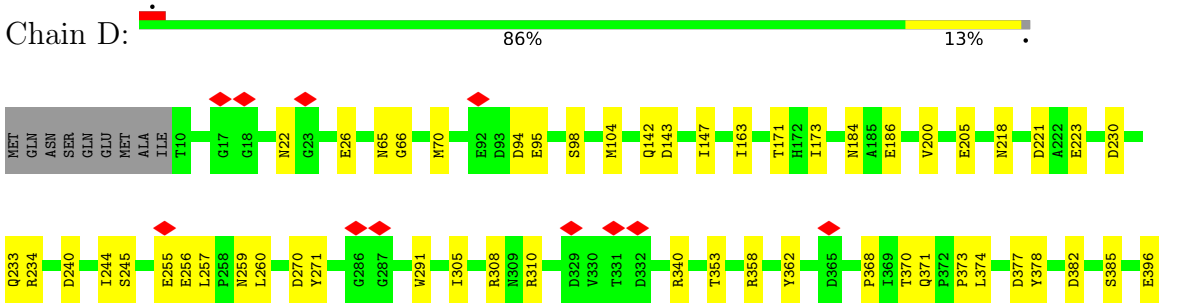

• Molecule 3: Chitinase 2

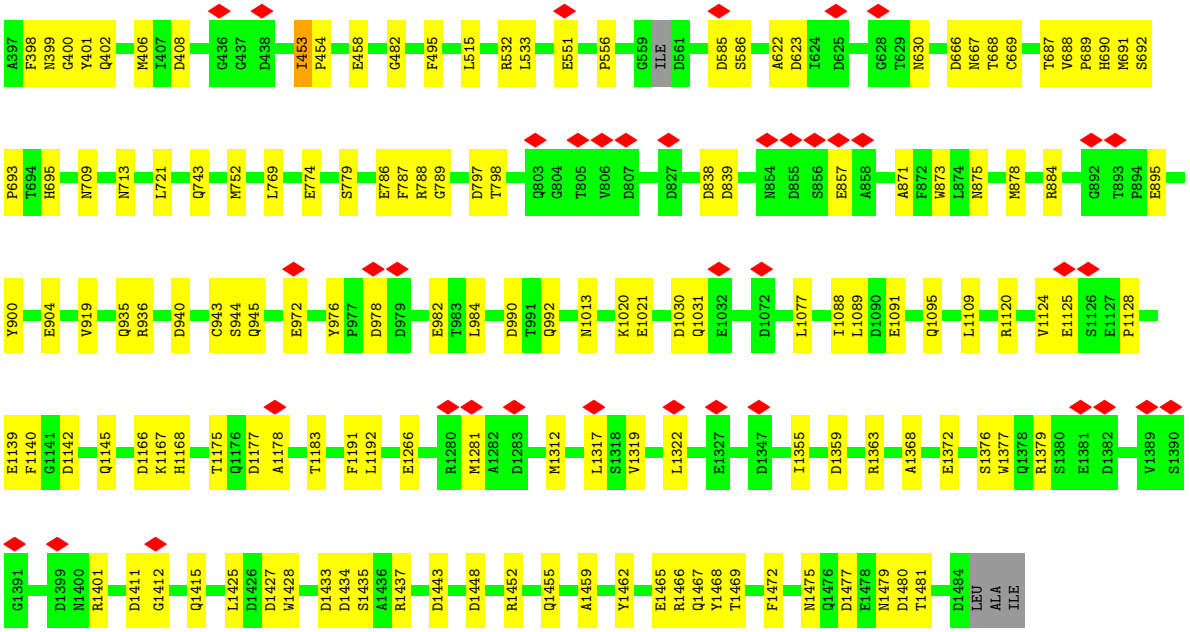
Chain Q:




• Molecule 4: Toxin subunit YenB

Chain D:

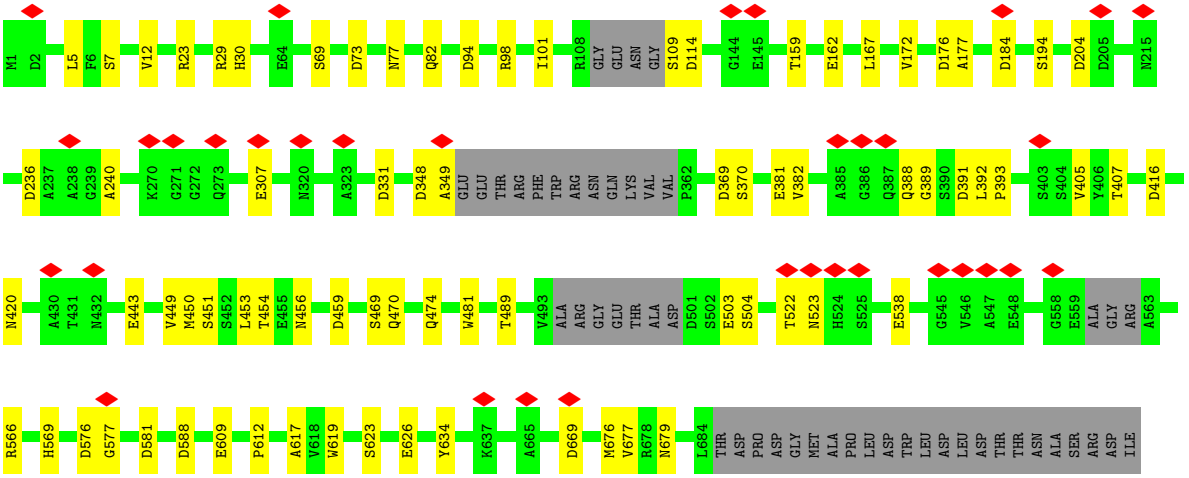





• Molecule 5: Toxin subunit YenC2

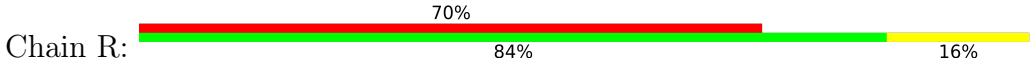
Chain E:

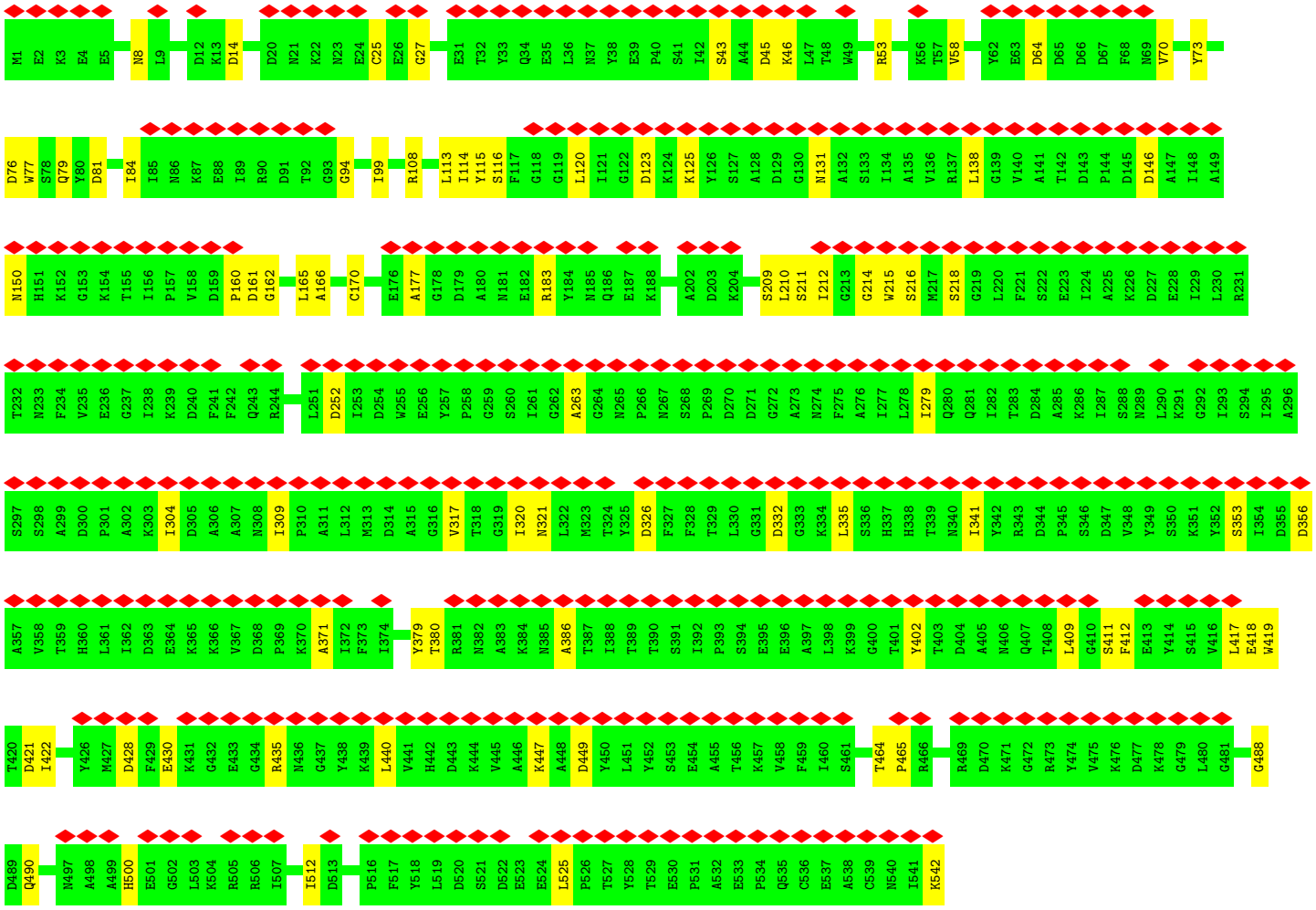



• Molecule 6: Chitinase 1

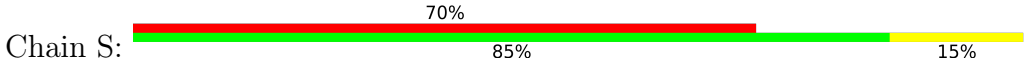
Chain R:

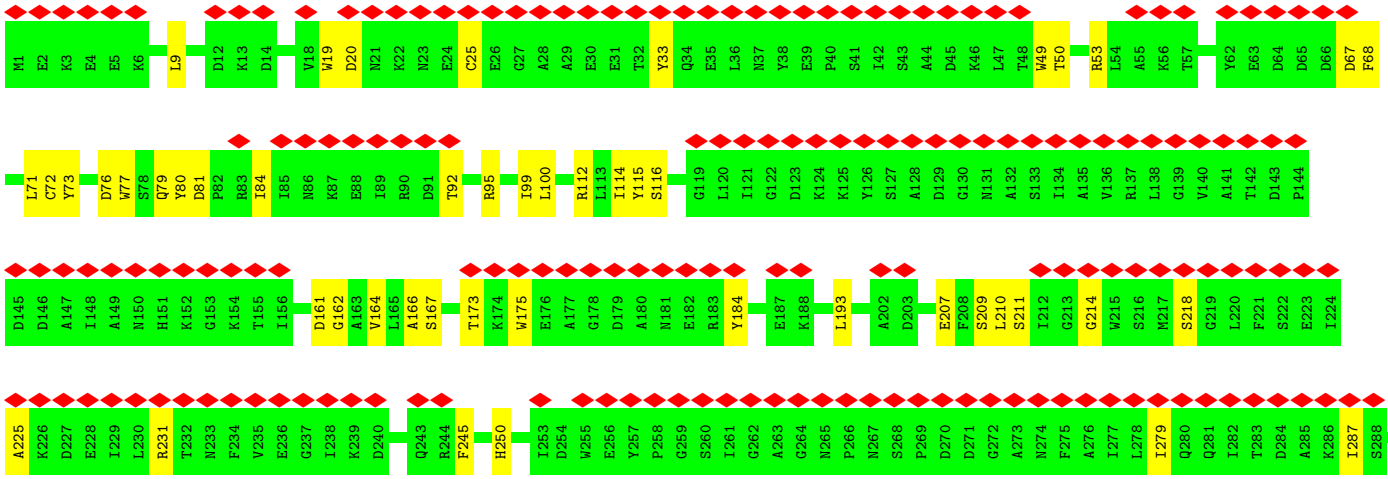


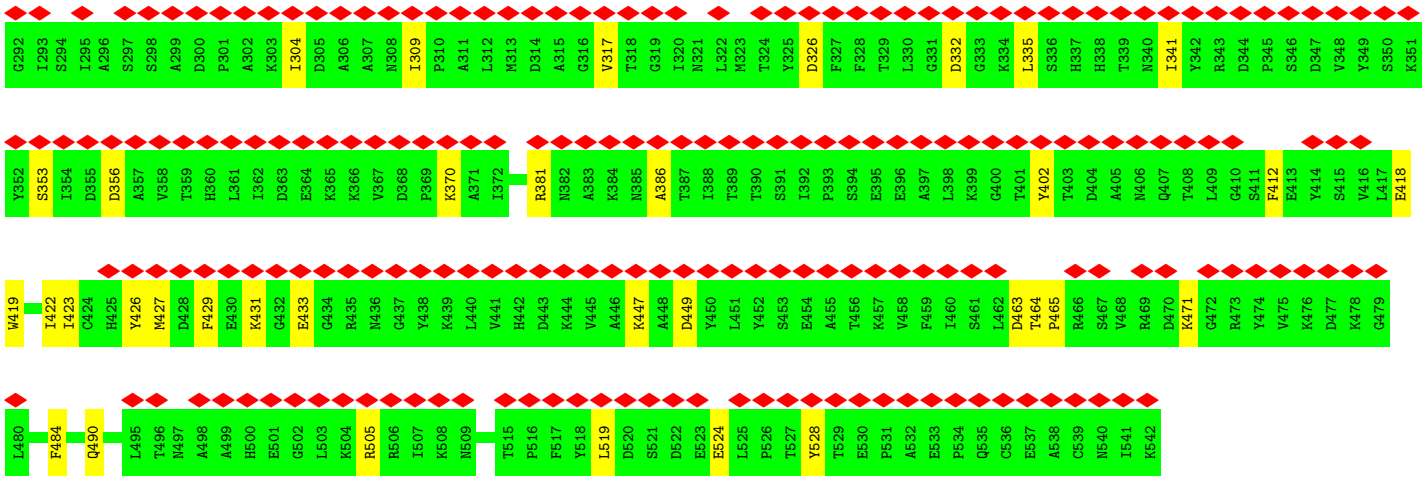




• Molecule 6: Chitinase 1

Chain S:



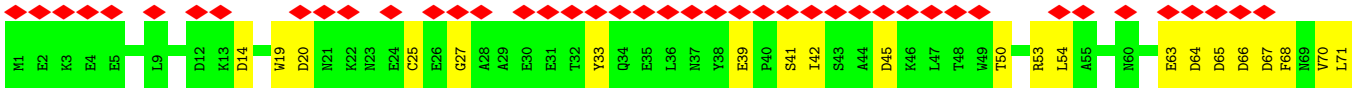



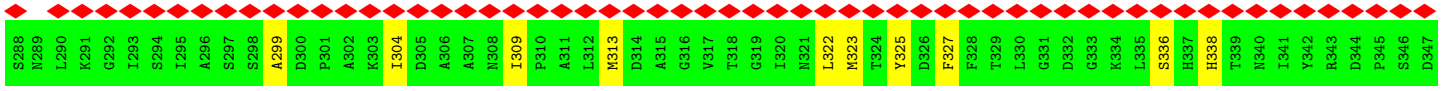



- Molecule 6: Chitinase 1

Chain T:



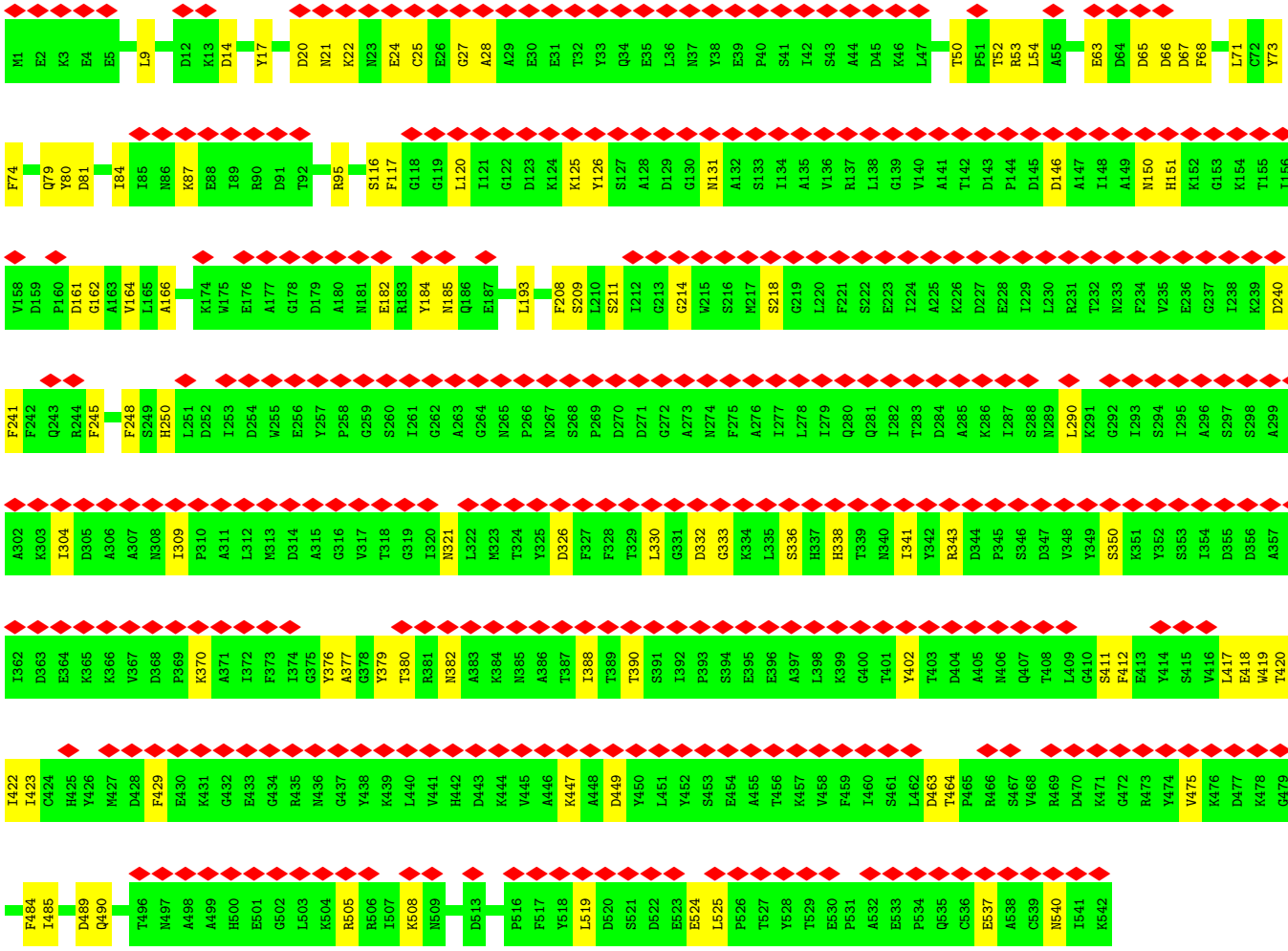




- Molecule 6: Chitinase 1

Chain U:

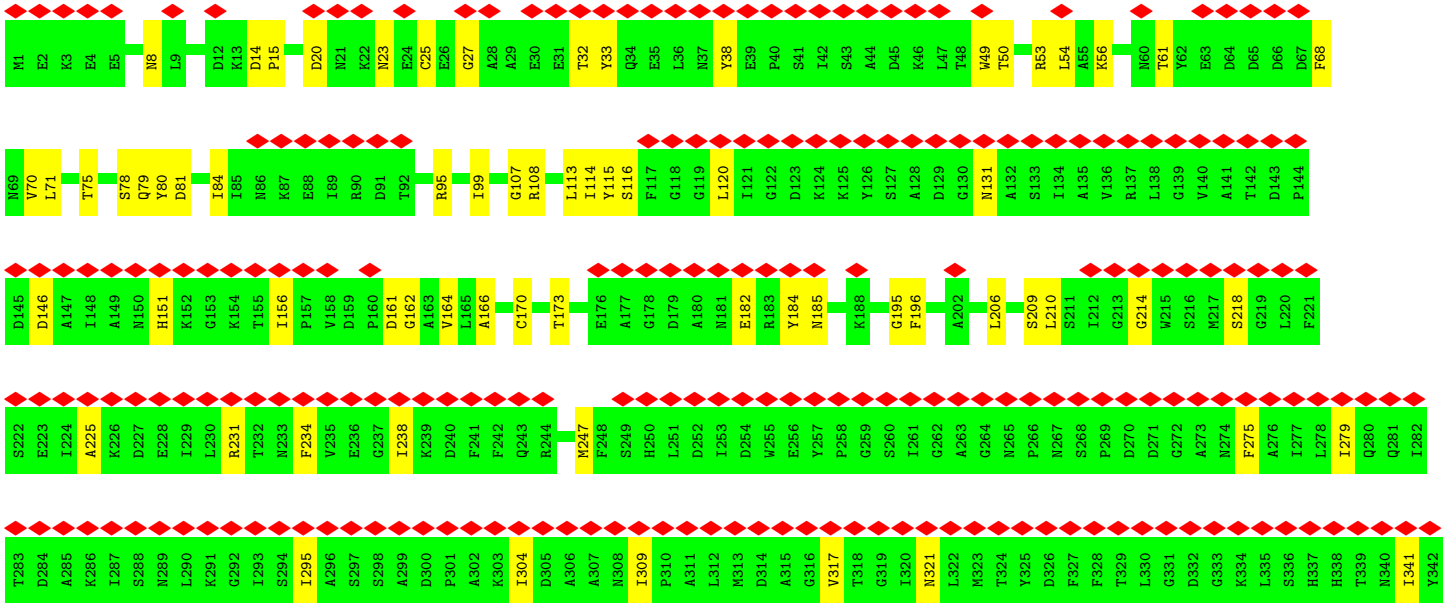


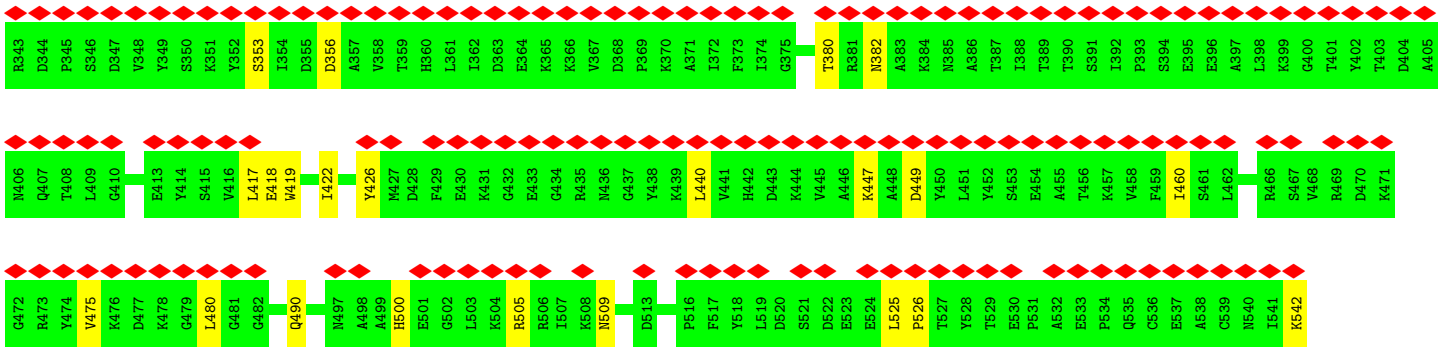


• Molecule 6: Chitinase 1

Chain V:




R343 D344 P345 S346 D347 V348 Y349 S350 K351 Y352 S353 I354 D355 D356 A357 V358 T359 H360 L361 I362 D363 E364 K365 K366 V367 D368 P369 K370 A371 I372 F373 I374 G375 T380 R381 N382 A383 K384 N385 A386 T387 I388 T389 T390 S391 I392 P393 S394 E395 E396 A397 L398 K399 G400 T401 Y402 T403 D404 A405
N406 Q407 T408 L409 G410 E413 Y414 S415 V416 L417 E418 W419 I422 Y426 N427 D428 F429 E430 K431 G432 E433 G434 R435 N436 G437 Y438 K439 L440 V441 H442 D443 K444 V445 A446 K447 A448 D449 Y450 L451 Y452 S453 E454 A455 T456 K457 V458 F459 I460 S461 L462 R466 S467 V468 R469 D470 K471
G472 R473 Y474 V475 K476 D477 K478 G479 L480 G481 G482 Q490 N497 A498 A499 H500 E501 G502 L503 K504 R505 R506 I507 K508 N509 D513 P516 F517 Y518 L519 D520 S521 D522 E523 E524 L525 P526 T527 Y528 T529 E530 P531 A532 E533 P534 Q535 C536 E537 A538 C539 N540 I541 K542

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 122198 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 63 | Depositor |
| Minimum defocus (nm) | 1200 | Depositor |
| Maximum defocus (nm) | 2200 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 1.116 | Depositor |
| Minimum map value | 0.000 | Depositor |
| Average map value | 0.005 | Depositor |
| Map value standard deviation | 0.021 | Depositor |
| Recommended contour level | 0.115 | Depositor |
| Map size (Å) | 528.0, 528.0, 528.0 | wwPDB |
| Map dimensions | 600, 600, 600 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.88, 0.88, 0.88 | 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 | 0.26 | 0/8237 | 0.34 | 0/11204 |
| 1 | F | 0.25 | 0/8237 | 0.33 | 0/11204 |
| 1 | I | 0.26 | 0/8237 | 0.34 | 0/11204 |
| 1 | L | 0.25 | 0/8237 | 0.35 | 0/11204 |
| 1 | O | 0.25 | 0/8237 | 0.33 | 0/11204 |
| 2 | B | 0.43 | 0/10601 | 0.41 | 0/14366 |
| 2 | G | 0.43 | 0/10601 | 0.40 | 0/14366 |
| 2 | J | 0.43 | 0/10601 | 0.41 | 0/14366 |
| 2 | M | 0.43 | 0/10601 | 0.43 | 0/14366 |
| 2 | P | 0.43 | 0/10600 | 0.41 | 0/14363 |
| 3 | C | 0.26 | 0/5033 | 0.33 | 0/6818 |
| 3 | H | 0.27 | 0/5033 | 0.36 | 0/6818 |
| 3 | K | 0.26 | 0/5033 | 0.34 | 0/6818 |
| 3 | N | 0.26 | 0/5033 | 0.34 | 0/6818 |
| 3 | Q | 0.27 | 0/5033 | 0.36 | 0/6818 |
| 4 | D | 0.31 | 0/12010 | 0.34 | 0/16371 |
| 5 | E | 0.23 | 0/5207 | 0.31 | 0/7086 |
| 6 | R | 0.12 | 0/4356 | 0.31 | 0/5900 |
| 6 | S | 0.14 | 0/4356 | 0.32 | 0/5900 |
| 6 | T | 0.12 | 0/4356 | 0.31 | 0/5900 |
| 6 | U | 0.15 | 0/4356 | 0.34 | 0/5900 |
| 6 | V | 0.12 | 0/4356 | 0.29 | 0/5900 |
| All | All | 0.32 | 0/158351 | 0.36 | 0/214894 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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 | 8078 | 0 | 8029 | 100 | 0 |
| 1 | F | 8078 | 0 | 8029 | 115 | 0 |
| 1 | I | 8078 | 0 | 8029 | 79 | 0 |
| 1 | L | 8078 | 0 | 8029 | 120 | 0 |
| 1 | O | 8078 | 0 | 8029 | 112 | 0 |
| 2 | B | 10384 | 0 | 10134 | 100 | 0 |
| 2 | G | 10384 | 0 | 10134 | 104 | 0 |
| 2 | J | 10384 | 0 | 10134 | 89 | 0 |
| 2 | M | 10384 | 0 | 10134 | 102 | 0 |
| 2 | P | 10384 | 0 | 10133 | 97 | 0 |
| 3 | C | 4914 | 0 | 4716 | 76 | 0 |
| 3 | H | 4914 | 0 | 4716 | 63 | 0 |
| 3 | K | 4914 | 0 | 4716 | 60 | 0 |
| 3 | N | 4914 | 0 | 4716 | 57 | 0 |
| 3 | Q | 4914 | 0 | 4716 | 68 | 0 |
| 4 | D | 11696 | 0 | 11142 | 128 | 0 |
| 5 | E | 5111 | 0 | 4959 | 50 | 0 |
| 6 | R | 4260 | 0 | 4098 | 53 | 0 |
| 6 | S | 4260 | 0 | 4098 | 53 | 0 |
| 6 | T | 4260 | 0 | 4098 | 68 | 0 |
| 6 | U | 4260 | 0 | 4098 | 66 | 0 |
| 6 | V | 4260 | 0 | 4098 | 56 | 0 |
| All | All | 154987 | 0 | 150985 | 1712 | 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 6.

The worst 5 of 1712 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) |
|---|---|---|---|
| 4:D:787:PHE:HD2 | 4:D:789:GLY:H | 1.23 | 0.86 |
| 2:M:324:MET:HE1 | 2:M:330:VAL:HG22 | 1.57 | 0.86 |
| 2:B:1005:ALA:HA | 2:B:1009:MET:HE3 | 1.58 | 0.85 |
| 6:U:20:ASP:O | 6:U:22:LYS:NZ | 2.12 | 0.82 |
| 2:M:1005:ALA:HA | 2:M:1009:MET:HE3 | 1.60 | 0.82 |

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 | 1024/1164 (88%) | 993 (97%) | 31 (3%) | 0 | 100 | 100 |
| 1 | F | 1024/1164 (88%) | 992 (97%) | 32 (3%) | 0 | 100 | 100 |
| 1 | I | 1024/1164 (88%) | 1001 (98%) | 23 (2%) | 0 | 100 | 100 |
| 1 | L | 1024/1164 (88%) | 998 (98%) | 26 (2%) | 0 | 100 | 100 |
| 1 | O | 1024/1164 (88%) | 996 (97%) | 28 (3%) | 0 | 100 | 100 |
| 2 | B | 1280/1365 (94%) | 1228 (96%) | 52 (4%) | 0 | 100 | 100 |
| 2 | G | 1280/1365 (94%) | 1223 (96%) | 57 (4%) | 0 | 100 | 100 |
| 2 | J | 1280/1365 (94%) | 1223 (96%) | 57 (4%) | 0 | 100 | 100 |
| 2 | M | 1280/1365 (94%) | 1225 (96%) | 55 (4%) | 0 | 100 | 100 |
| 2 | P | 1278/1365 (94%) | 1229 (96%) | 49 (4%) | 0 | 100 | 100 |
| 3 | C | 631/633 (100%) | 597 (95%) | 34 (5%) | 0 | 100 | 100 |
| 3 | H | 631/633 (100%) | 598 (95%) | 33 (5%) | 0 | 100 | 100 |
| 3 | K | 631/633 (100%) | 597 (95%) | 34 (5%) | 0 | 100 | 100 |
| 3 | N | 631/633 (100%) | 598 (95%) | 33 (5%) | 0 | 100 | 100 |
| 3 | Q | 631/633 (100%) | 598 (95%) | 33 (5%) | 0 | 100 | 100 |
| 4 | D | 1472/1487 (99%) | 1410 (96%) | 62 (4%) | 0 | 100 | 100 |
| 5 | E | 648/970 (67%) | 620 (96%) | 28 (4%) | 0 | 100 | 100 |
| 6 | R | 540/542 (100%) | 523 (97%) | 17 (3%) | 0 | 100 | 100 |
| 6 | S | 540/542 (100%) | 523 (97%) | 17 (3%) | 0 | 100 | 100 |
| 6 | T | 540/542 (100%) | 519 (96%) | 21 (4%) | 0 | 100 | 100 |
| 6 | U | 540/542 (100%) | 528 (98%) | 12 (2%) | 0 | 100 | 100 |
| 6 | V | 540/542 (100%) | 516 (96%) | 24 (4%) | 0 | 100 | 100 |
| All | All | 19493/20977 (93%) | 18735 (96%) | 758 (4%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 898/1022 (88%) | 896 (100%) | 2 (0%) | 87 | 85 |
| 1 | F | 898/1022 (88%) | 896 (100%) | 2 (0%) | 87 | 85 |
| 1 | I | 898/1022 (88%) | 897 (100%) | 1 (0%) | 88 | 87 |
| 1 | L | 898/1022 (88%) | 895 (100%) | 3 (0%) | 86 | 83 |
| 1 | O | 898/1022 (88%) | 897 (100%) | 1 (0%) | 88 | 87 |
| 2 | B | 1136/1210 (94%) | 1131 (100%) | 5 (0%) | 84 | 81 |
| 2 | G | 1136/1210 (94%) | 1132 (100%) | 4 (0%) | 84 | 81 |
| 2 | J | 1136/1210 (94%) | 1131 (100%) | 5 (0%) | 84 | 81 |
| 2 | M | 1136/1210 (94%) | 1132 (100%) | 4 (0%) | 84 | 81 |
| 2 | P | 1136/1210 (94%) | 1132 (100%) | 4 (0%) | 84 | 81 |
| 3 | C | 520/520 (100%) | 520 (100%) | 0 | 100 | 100 |
| 3 | H | 520/520 (100%) | 520 (100%) | 0 | 100 | 100 |
| 3 | K | 520/520 (100%) | 520 (100%) | 0 | 100 | 100 |
| 3 | N | 520/520 (100%) | 520 (100%) | 0 | 100 | 100 |
| 3 | Q | 520/520 (100%) | 519 (100%) | 1 (0%) | 87 | 85 |
| 4 | D | 1255/1266 (99%) | 1252 (100%) | 3 (0%) | 87 | 85 |
| 5 | E | 551/818 (67%) | 551 (100%) | 0 | 100 | 100 |
| 6 | R | 455/455 (100%) | 455 (100%) | 0 | 100 | 100 |
| 6 | S | 455/455 (100%) | 455 (100%) | 0 | 100 | 100 |
| 6 | T | 455/455 (100%) | 454 (100%) | 1 (0%) | 87 | 85 |
| 6 | U | 455/455 (100%) | 455 (100%) | 0 | 100 | 100 |
| 6 | V | 455/455 (100%) | 454 (100%) | 1 (0%) | 87 | 85 |
| All | All | 16851/18119 (93%) | 16814 (100%) | 37 (0%) | 85 | 85 |

5 of 37 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | M | 797 | LEU |
| 6 | T | 313 | MET |
| 1 | O | 544 | PHE |
| 2 | P | 377 | LEU |
| 2 | G | 299 | GLN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | J | 462 | ASN |
| 2 | P | 1332 | ASN |
| 3 | K | 574 | ASN |
| 2 | P | 1283 | GLN |
| 6 | S | 8 | ASN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry

There are no ligands in this entry.

### 5.7 Other polymers

There are no such residues in this entry.

### 5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 5 | E | 1 |
| 2 | P | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | E | 109:SER | C | 114:ASP | N | 5.44 |
| 1 | P | 299:GLN | C | 300:MET | N | 3.27 |

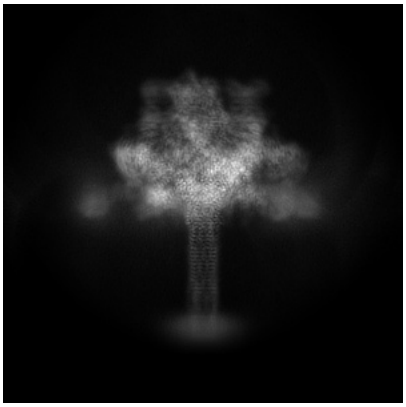
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-58585. These allow visual inspection of the internal detail of the map and identification of artifacts.

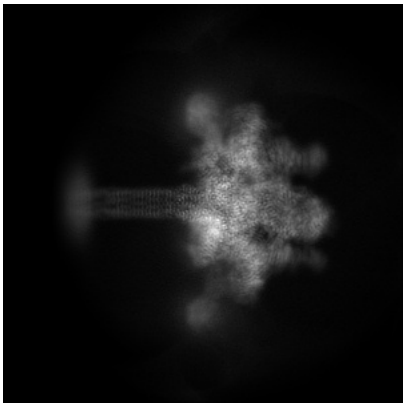
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

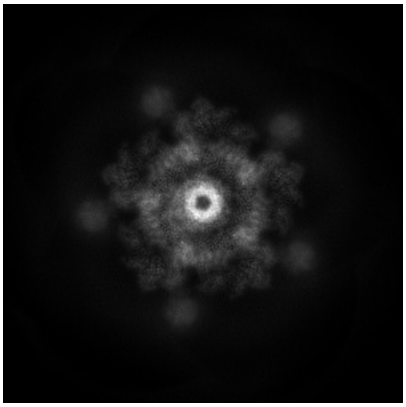
### 6.1.1 Primary map



X



Y



Z

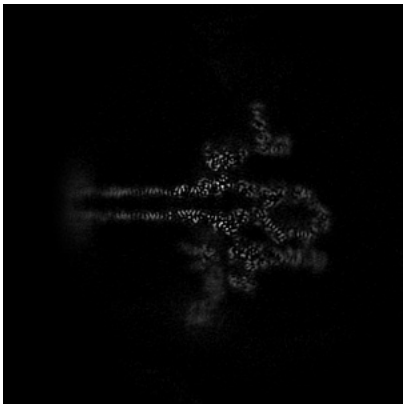
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

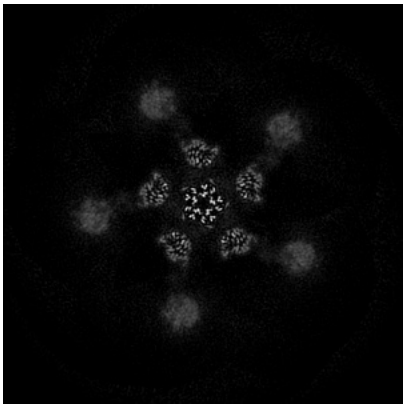
### 6.2.1 Primary map



X Index: 300



Y Index: 300



Z Index: 300

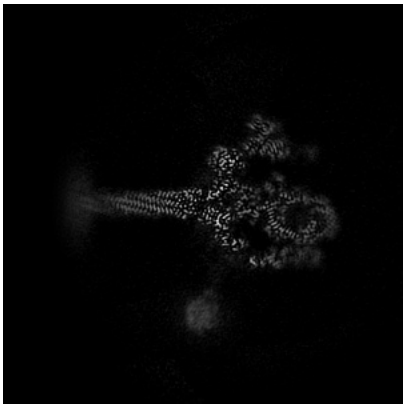
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

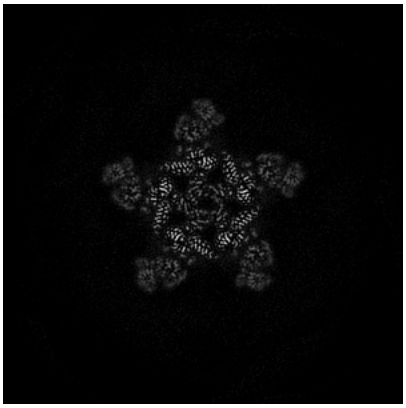
### 6.3.1 Primary map



X Index: 285



Y Index: 283

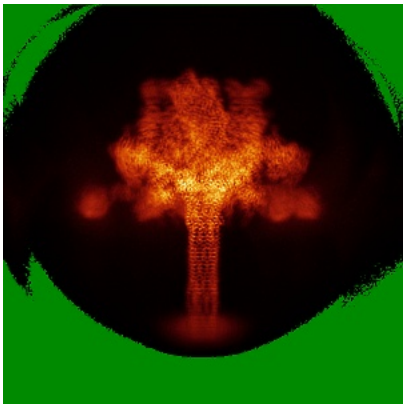


Z Index: 350

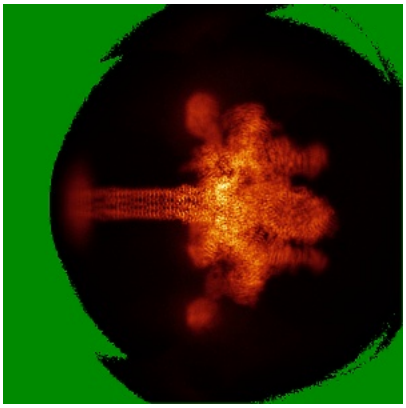
The images above show the largest variance slices of the map in three orthogonal directions.

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

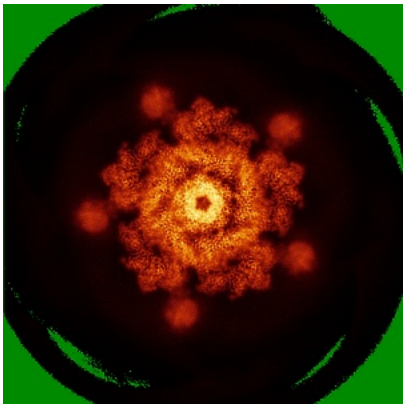
### 6.4.1 Primary map



X



Y

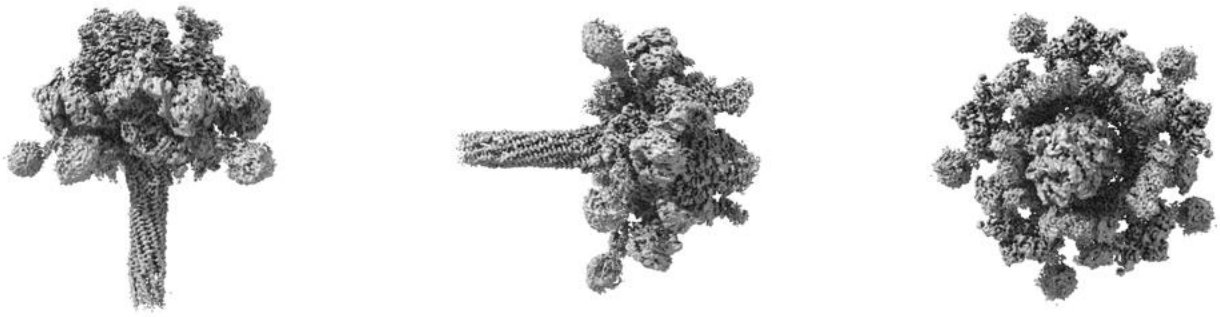


Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.115. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

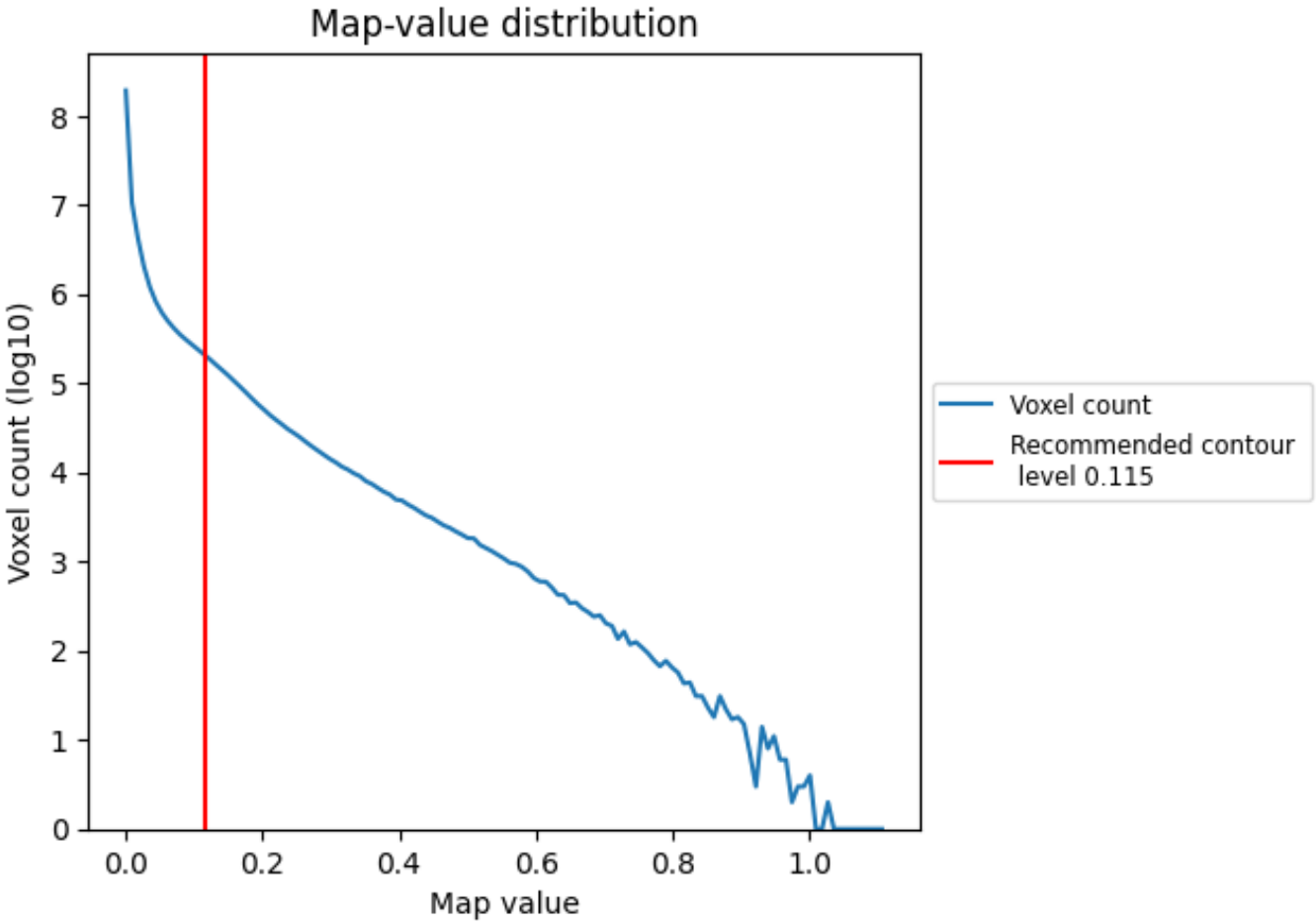
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

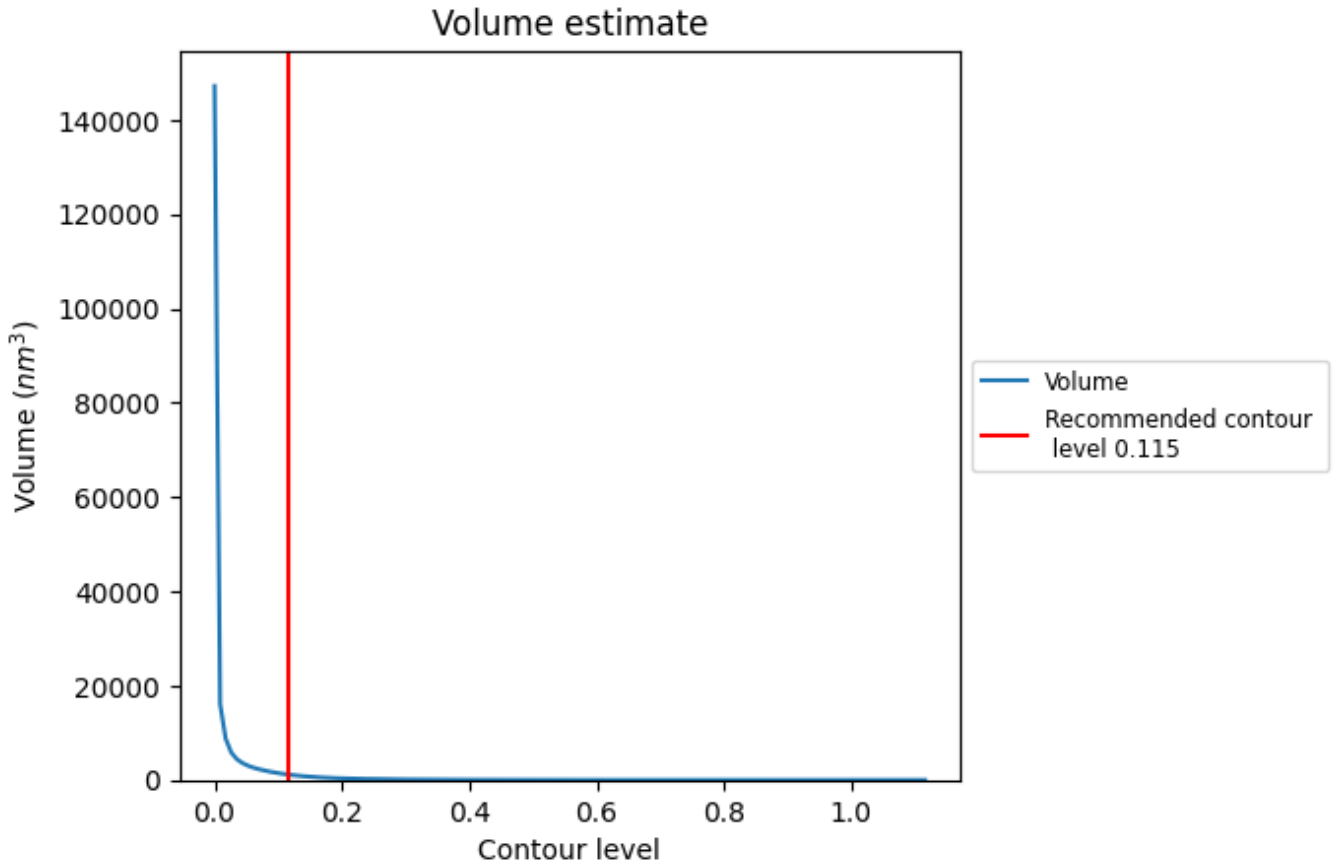
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

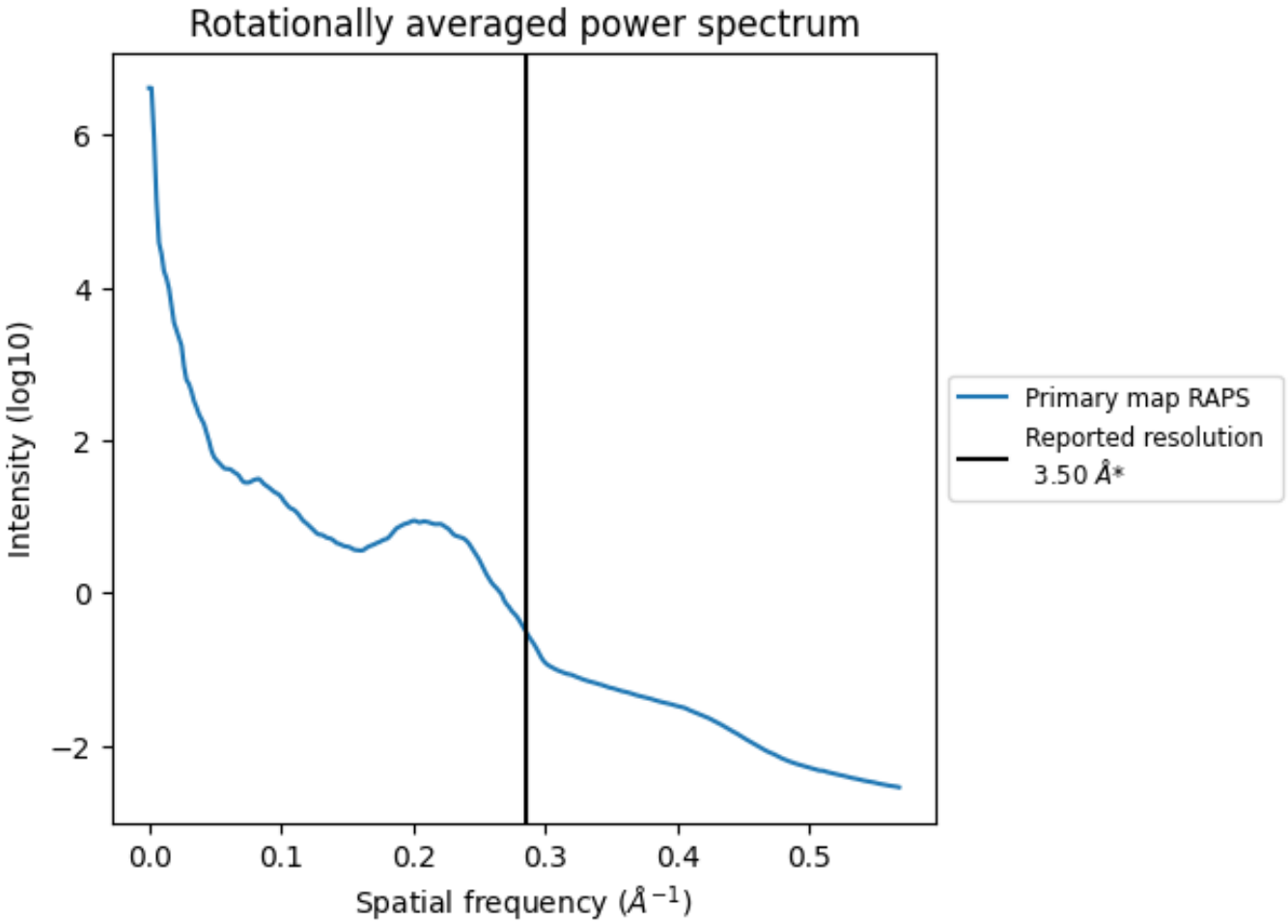
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 1157 $nm^3$; this corresponds to an approximate mass of 1046 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 0.286 Å$^{-1}$

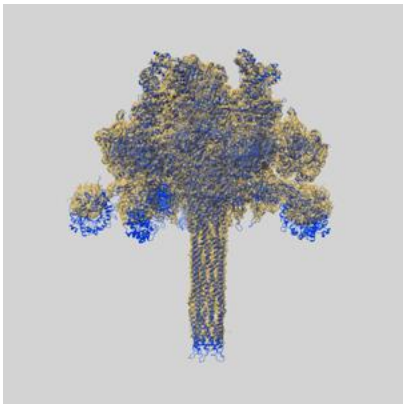
# 8 Fourier-Shell correlation (i)

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

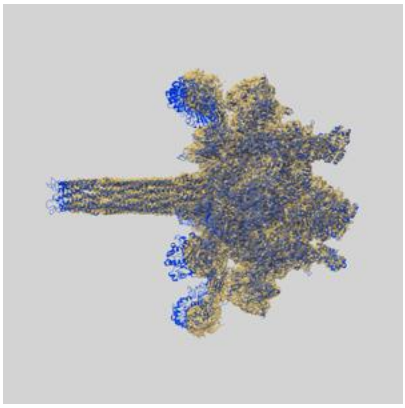
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-58585 and PDB model 31OI. Per-residue inclusion information can be found in section 3 on page 7.

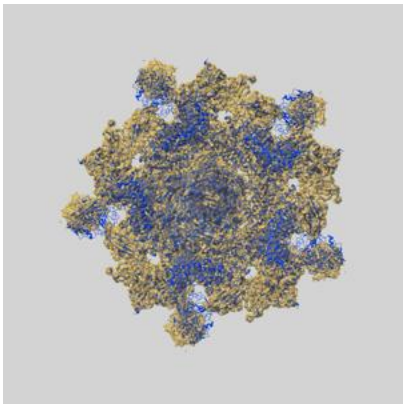
## 9.1 Map-model overlay



X



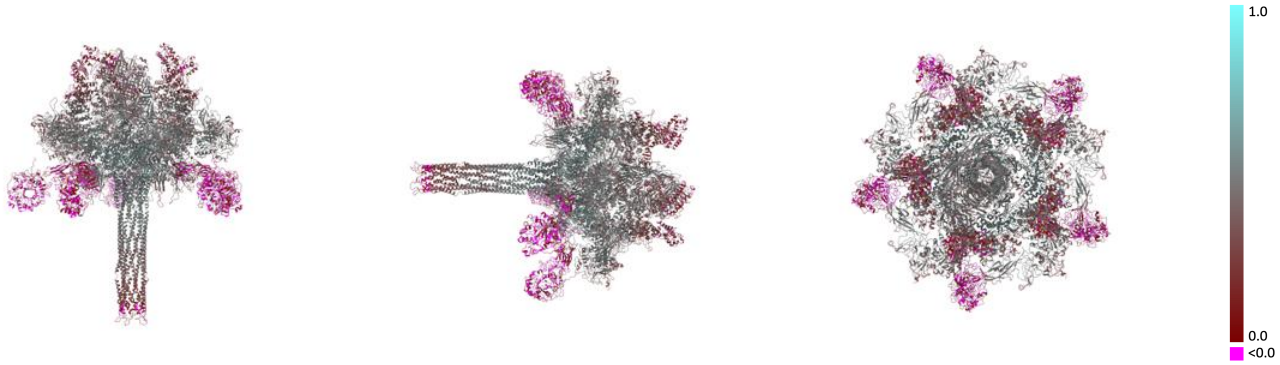
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.115 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.

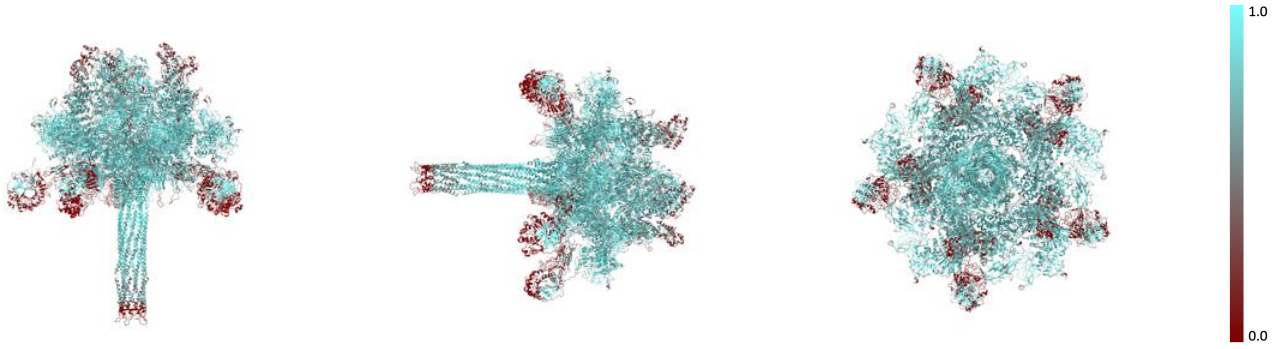
## 9.2 Q-score mapped to coordinate model (i)




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.

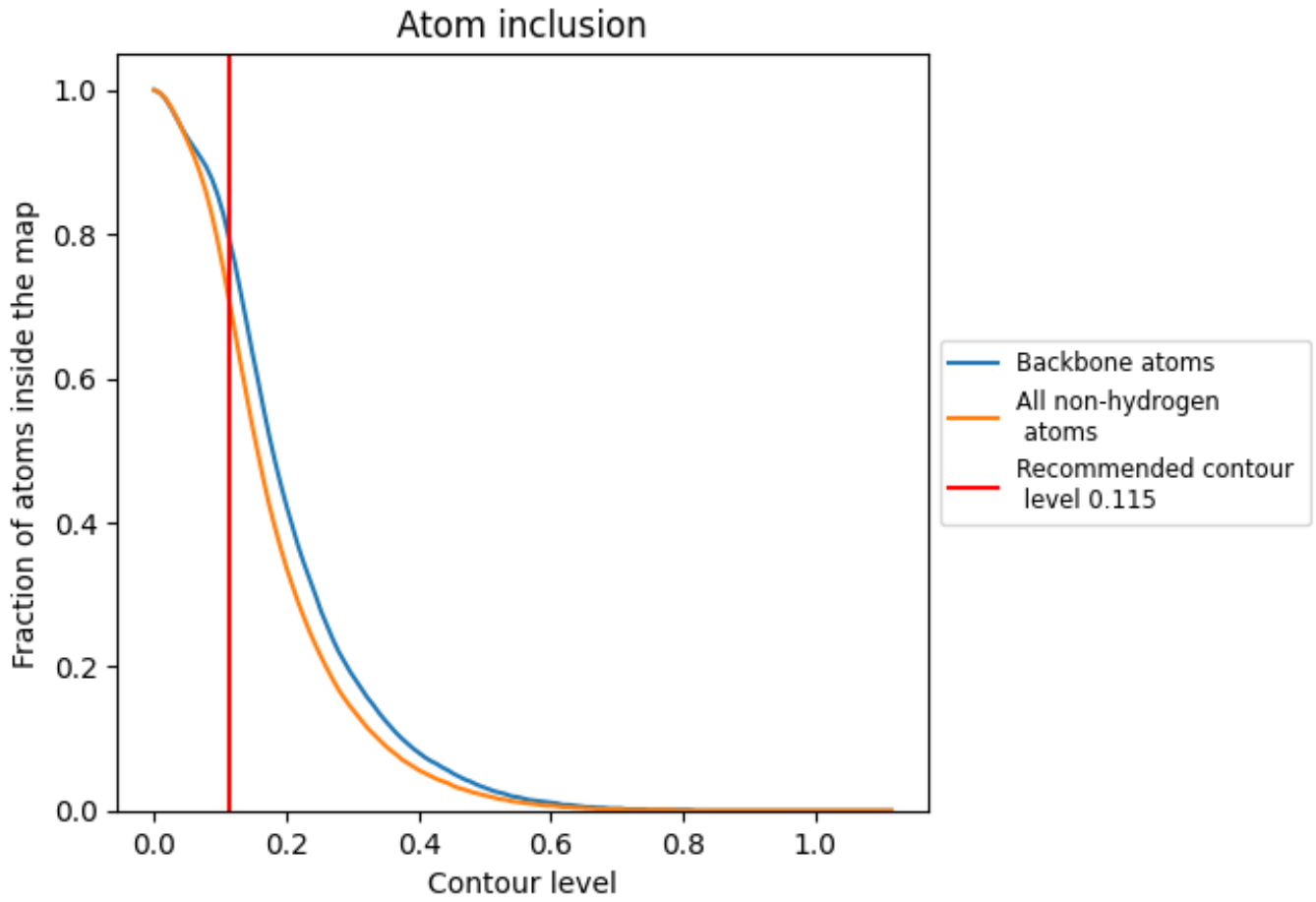
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.115).

## 9.4 Atom inclusion (i)




At the recommended contour level, 79% of all backbone atoms, 70% 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 (0.115) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7000 | 0.3670 |
| A | 0.6940 | 0.3680 |
| B | 0.7840 | 0.4430 |
| C | 0.8220 | 0.4260 |
| D | 0.8210 | 0.4580 |
| E | 0.8070 | 0.4170 |
| F | 0.6950 | 0.3720 |
| G | 0.7780 | 0.4420 |
| H | 0.8200 | 0.4240 |
| I | 0.6940 | 0.3710 |
| J | 0.7770 | 0.4400 |
| K | 0.8260 | 0.4230 |
| L | 0.6940 | 0.3720 |
| M | 0.7780 | 0.4380 |
| N | 0.8250 | 0.4270 |
| O | 0.6950 | 0.3680 |
| P | 0.7800 | 0.4370 |
| Q | 0.8230 | 0.4250 |
| R | 0.2830 | 0.0690 |
| S | 0.2840 | 0.0500 |
| T | 0.2740 | 0.0430 |
| U | 0.2870 | 0.0520 |
| V | 0.2770 | 0.0420 |

