# Full wwPDB EM Validation Report

Oct 13, 2024 – 05:33 pm BST

| | | |
|---|---|---|
| PDB ID | : | 7NVG |
| EMDB ID | : | EMD-12603 |
| Title | : | Salmonella flagellar basal body refined in C1 map |
| Authors | : | Johnson, S.; Furlong, E.; Lea, S.M. |
| Deposited on | : | 2021-03-15 |
| Resolution | : | 3.70 Å(reported) |

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

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

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

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

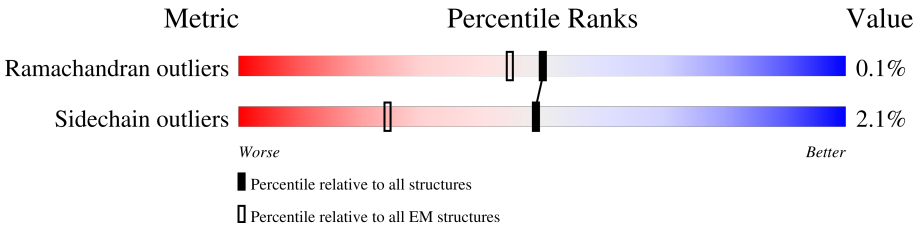
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev113 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA,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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A1 | 560 | 12% 27% 73% |
| 1 | B1 | 560 | 20% 44% 55% |
| 1 | C1 | 560 | 16% 44% 55% |
| 1 | D1 | 560 | 12% 27% 73% |
| 1 | E1 | 560 | 18% 44% 55% |
| 1 | F1 | 560 | 12% 27% 73% |
| 1 | G1 | 560 | 18% 44% 55% |
| 1 | H1 | 560 | 19% 44% 55% |
| 1 | I1 | 560 | 19% 44% 55% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | J1 | 560 | 13% 26% 73% |
| 1 | K1 | 560 | 22% 44% 55% |
| 1 | L1 | 560 | 23% 44% 55% |
| 1 | M1 | 560 | 13% 27% 73% |
| 1 | N1 | 560 | 22% 44% 55% |
| 1 | O1 | 560 | 22% 44% 55% |
| 1 | P1 | 560 | 13% 26% 73% |
| 1 | Q1 | 560 | 25% 44% 55% |
| 1 | R1 | 560 | 29% 44% 55% |
| 1 | S1 | 560 | 15% 27% 73% |
| 1 | T1 | 560 | 31% 44% 55% |
| 1 | U1 | 560 | 33% 44% 55% |
| 1 | V1 | 560 | 16% 27% 73% |
| 1 | W1 | 560 | 30% 44% 55% |
| 1 | X1 | 560 | 28% 44% 55% |
| 1 | Y1 | 560 | 25% 44% 55% |
| 1 | Z1 | 560 | 14% 27% 73% |
| 1 | a1 | 560 | 21% 44% 55% |
| 1 | b1 | 560 | 12% 27% 73% |
| 1 | c1 | 560 | 20% 44% 55% |
| 1 | d1 | 560 | 18% 44% 55% |
| 1 | e1 | 560 | 10% 27% 73% |
| 1 | f1 | 560 | 17% 44% 55% |
| 1 | g1 | 560 | 17% 44% 55% |
| 1 | h1 | 560 | 18% 44% 55% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | A2 | 245 | 18% 84% 15% |
| 2 | B2 | 245 | 11% 84% 15% |
| 2 | C2 | 245 | 9% 84% 15% |
| 2 | D2 | 245 | 10% 84% 15% |
| 2 | E2 | 245 | 21% 84% 15% |
| 3 | F2 | 264 | 29% 97% |
| 4 | G2 | 89 | 20% 99% |
| 4 | H2 | 89 | 11% 99% |
| 4 | I2 | 89 | 12% 99% |
| 4 | J2 | 89 | 25% 98% |
| 5 | K2 | 104 | 7% 37% 62% |
| 5 | L2 | 104 | 13% 72% 28% |
| 5 | M2 | 104 | 8% 72% 28% |
| 5 | N2 | 104 | 9% 72% 28% |
| 5 | O2 | 104 | 12% 72% 28% |
| 5 | P2 | 104 | 9% 72% 28% |
| 6 | Q2 | 138 | 32% 96% |
| 6 | R2 | 138 | 14% 87% 13% |
| 6 | S2 | 138 | 17% 88% 12% |
| 6 | T2 | 138 | 9% 76% 23% |
| 6 | U2 | 138 | 20% 84% 14% |
| 7 | V2 | 134 | 23% 98% |
| 7 | W2 | 134 | 12% 99% |
| 7 | X2 | 134 | 10% 98% |
| 7 | Y2 | 134 | 7% 99% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 7 | Z2 | 134 | 10% 98% |
| 7 | a2 | 134 | 14% 99% |
| 8 | b2 | 251 | 14% 98% |
| 8 | c2 | 251 | 6% 98% |
| 8 | d2 | 251 | 99% |
| 8 | e2 | 251 | 7% 98% |
| 8 | f2 | 251 | 7% 98% |
| 9 | 12 | 260 | 19% 100% |
| 9 | 22 | 260 | 19% 100% |
| 9 | 32 | 260 | 23% 100% |
| 9 | 42 | 260 | 72% 99% |
| 9 | g2 | 260 | 7% 100% |
| 9 | h2 | 260 | 7% 100% |
| 9 | i2 | 260 | 5% 100% |
| 9 | j2 | 260 | 6% 100% |
| 9 | k2 | 260 | 6% 100% |
| 9 | l2 | 260 | 5% 96% |
| 9 | m2 | 260 | 96% |
| 9 | n2 | 260 | 5% 95% |
| 9 | o2 | 260 | 5% 96% |
| 9 | p2 | 260 | 5% 96% |
| 9 | q2 | 260 | 96% |
| 9 | r2 | 260 | 100% |
| 9 | s2 | 260 | 7% 100% |
| 9 | t2 | 260 | 6% 99% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | u2 | 260 | 7% 100% |
| 9 | v2 | 260 | 6% 100% |
| 9 | w2 | 260 | 5% 100% |
| 9 | x2 | 260 | 9% 100% |
| 9 | y2 | 260 | 19% 100% |
| 9 | z2 | 260 | 27% 99% |
| 10 | A3 | 232 | 85% 88% 9% |
| 10 | B3 | 232 | 85% 88% 9% |
| 10 | C3 | 232 | 85% 88% 9% |
| 10 | D3 | 232 | 86% 88% 9% |
| 10 | E3 | 232 | 85% 88% 9% |
| 10 | F3 | 232 | 84% 88% 9% |
| 10 | G3 | 232 | 86% 88% 9% |
| 10 | H3 | 232 | 86% 88% 9% |
| 10 | I3 | 232 | 87% 88% 9% |
| 10 | J3 | 232 | 85% 88% 9% |
| 10 | K3 | 232 | 85% 88% 9% |
| 10 | L3 | 232 | 85% 88% 9% |
| 10 | M3 | 232 | 86% 88% 9% |
| 10 | N3 | 232 | 85% 88% 9% |
| 10 | O3 | 232 | 86% 88% 9% |
| 10 | P3 | 232 | 87% 88% 9% |
| 10 | Q3 | 232 | 88% 88% 9% |
| 10 | R3 | 232 | 86% 88% 9% |
| 10 | S3 | 232 | 88% 88% 9% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 10 | T3 | 232 | 87% 88% 9% |
| 10 | U3 | 232 | 87% 88% 9% |
| 10 | V3 | 232 | 87% 88% 9% |
| 10 | W3 | 232 | 86% 88% 9% |
| 10 | X3 | 232 | 88% 88% 9% |
| 10 | Y3 | 232 | 87% 88% 9% |
| 10 | Z3 | 232 | 84% 88% 9% |
| 11 | a3 | 365 | 83% 80% 16% |
| 11 | b3 | 365 | 83% 80% 16% |
| 11 | c3 | 365 | 84% 80% 16% |
| 11 | d3 | 365 | 83% 80% 16% |
| 11 | e3 | 365 | 83% 80% 16% |
| 11 | f3 | 365 | 84% 80% 16% |
| 11 | g3 | 365 | 83% 80% 16% |
| 11 | h3 | 365 | 84% 80% 16% |
| 11 | i3 | 365 | 83% 80% 16% |
| 11 | j3 | 365 | 84% 80% 16% |
| 11 | k3 | 365 | 84% 80% 16% |
| 11 | l3 | 365 | 84% 80% 16% |
| 11 | m3 | 365 | 84% 80% 16% |
| 11 | n3 | 365 | 83% 80% 16% |
| 11 | o3 | 365 | 84% 80% 16% |
| 11 | p3 | 365 | 84% 80% 16% |
| 11 | q3 | 365 | 84% 80% 16% |
| 11 | r3 | 365 | 84% 80% 16% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 11 | s3 | 365 | 84% 80% 16% |
| 11 | t3 | 365 | 84% 80% 16% |
| 11 | u3 | 365 | 84% 80% 16% |
| 11 | v3 | 365 | 84% 80% 16% |
| 11 | w3 | 365 | 84% 80% 16% |
| 11 | x3 | 365 | 84% 80% 16% |
| 11 | y3 | 365 | 84% 80% 16% |
| 11 | z3 | 365 | 83% 80% 16% |
| 12 | A4 | 232 | 76% 86% 13% |
| 12 | B4 | 232 | 76% 88% 12% |
| 12 | C4 | 232 | 79% 86% 14% |
| 12 | D4 | 232 | 79% 87% 13% |
| 12 | E4 | 232 | 79% 88% 12% |

# 2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 246311 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 Flagellar M-ring protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A1 | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 726 | 223 | 241 | 3 | | |
| 1 | B1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | C1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | D1 | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 726 | 223 | 241 | 3 | | |
| 1 | E1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | F1 | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 726 | 223 | 241 | 3 | | |
| 1 | G1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | H1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | I1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | J1 | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 726 | 223 | 241 | 3 | | |
| 1 | K1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | L1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | M1 | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 726 | 223 | 241 | 3 | | |
| 1 | N1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | O1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | P1 | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 726 | 223 | 241 | 3 | | |
| 1 | Q1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | R1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | S1 | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 726 | 223 | 241 | 3 | | |
| 1 | T1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | U1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | V1 | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 726 | 223 | 241 | 3 | | |
| 1 | W1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | X1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | Y1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | Z1 | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 726 | 223 | 241 | 3 | | |
| 1 | a1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | b1 | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 726 | 223 | 241 | 3 | | |
| 1 | c1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | d1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | e1 | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 726 | 223 | 241 | 3 | | |
| 1 | f1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | g1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |
| 1 | h1 | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 1931 | 1187 | 355 | 385 | 4 | | |

- Molecule 2 is a protein called Flagellar biosynthetic protein FliP.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | A2 | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1623 | 1084 | 251 | 276 | 12 | | |
| 2 | B2 | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1623 | 1084 | 251 | 276 | 12 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | C2 | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1623 | 1084 | 251 | 276 | 12 | | |
| 2 | D2 | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1623 | 1084 | 251 | 276 | 12 | | |
| 2 | E2 | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1623 | 1084 | 251 | 276 | 12 | | |

- Molecule 3 is a protein called Flagellar biosynthetic protein FliR.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | F2 | 258 | Total | C | N | O | S | 0 | 0 |
| | | | 1986 | 1329 | 314 | 327 | 16 | | |

- Molecule 4 is a protein called Flagellar biosynthetic protein FliQ.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | G2 | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 670 | 449 | 100 | 114 | 7 | | |
| 4 | H2 | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 670 | 449 | 100 | 114 | 7 | | |
| 4 | I2 | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 670 | 449 | 100 | 114 | 7 | | |
| 4 | J2 | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 670 | 449 | 100 | 114 | 7 | | |

- Molecule 5 is a protein called Flagellar hook-basal body complex protein FliE.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | K2 | 39 | Total | C | N | O | S | 0 | 0 |
| | | | 296 | 183 | 51 | 56 | 6 | | |
| 5 | L2 | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 563 | 347 | 102 | 108 | 6 | | |
| 5 | M2 | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 563 | 347 | 102 | 108 | 6 | | |
| 5 | N2 | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 563 | 347 | 102 | 108 | 6 | | |
| 5 | O2 | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 563 | 347 | 102 | 108 | 6 | | |
| 5 | P2 | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 563 | 347 | 102 | 108 | 6 | | |

- Molecule 6 is a protein called Flagellar basal body rod protein FlgB.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | Q2 | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 1023 | 630 | 188 | 200 | 5 | | |
| 6 | R2 | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 932 | 578 | 169 | 180 | 5 | | |
| 6 | S2 | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 942 | 583 | 173 | 181 | 5 | | |
| 6 | T2 | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 835 | 516 | 153 | 161 | 5 | | |
| 6 | U2 | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 925 | 573 | 168 | 179 | 5 | | |

- Molecule 7 is a protein called Flagellar basal-body rod protein FlgC.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | V2 | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 969 | 604 | 167 | 193 | 5 | | |
| 7 | W2 | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 964 | 601 | 166 | 192 | 5 | | |
| 7 | X2 | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 964 | 601 | 166 | 192 | 5 | | |
| 7 | Y2 | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 964 | 601 | 166 | 192 | 5 | | |
| 7 | Z2 | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 964 | 601 | 166 | 192 | 5 | | |
| 7 | a2 | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 964 | 601 | 166 | 192 | 5 | | |

- Molecule 8 is a protein called Flagellar basal body protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | b2 | 249 | Total | C | N | O | S | 0 | 0 |
| | | | 1812 | 1111 | 325 | 368 | 8 | | |
| 8 | c2 | 249 | Total | C | N | O | S | 0 | 0 |
| | | | 1812 | 1111 | 325 | 368 | 8 | | |
| 8 | d2 | 249 | Total | C | N | O | S | 0 | 0 |
| | | | 1812 | 1111 | 325 | 368 | 8 | | |
| 8 | e2 | 249 | Total | C | N | O | S | 0 | 0 |
| | | | 1812 | 1111 | 325 | 368 | 8 | | |
| 8 | f2 | 249 | Total | C | N | O | S | 0 | 0 |
| | | | 1812 | 1111 | 325 | 368 | 8 | | |

- Molecule 9 is a protein called Flagellar basal-body rod protein FlgG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | g2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | h2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | i2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | j2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | k2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | l2 | 249 | Total | C | N | O | S | 0 | 0 |
| | | | 1871 | 1157 | 328 | 381 | 5 | | |
| 9 | m2 | 249 | Total | C | N | O | S | 0 | 0 |
| | | | 1871 | 1157 | 328 | 381 | 5 | | |
| 9 | n2 | 249 | Total | C | N | O | S | 0 | 0 |
| | | | 1871 | 1157 | 328 | 381 | 5 | | |
| 9 | o2 | 249 | Total | C | N | O | S | 0 | 0 |
| | | | 1871 | 1157 | 328 | 381 | 5 | | |
| 9 | p2 | 249 | Total | C | N | O | S | 0 | 0 |
| | | | 1871 | 1157 | 328 | 381 | 5 | | |
| 9 | q2 | 251 | Total | C | N | O | S | 0 | 0 |
| | | | 1885 | 1166 | 330 | 384 | 5 | | |
| 9 | r2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | s2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | t2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | u2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | v2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | w2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | x2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | y2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | z2 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | 12 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |
| 9 | 22 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | 32 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1948 | 1202 | 340 | 400 | 6 | | |
| 9 | 42 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1949 | 1202 | 341 | 400 | 6 | | |

- Molecule 10 is a protein called Flagellar L-ring protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | A3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | B3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | C3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | D3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | E3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | F3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | G3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | H3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | I3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | J3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | K3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | L3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | M3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | N3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | O3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | P3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | Q3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | R3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | S3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | T3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | U3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | V3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | W3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1580 | 984 | 282 | 310 | 4 | | |
| 10 | X3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | Y3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 10 | Z3 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |

- Molecule 11 is a protein called Flagellar P-ring protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | a3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | b3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | c3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | d3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | e3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | f3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | g3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | h3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1379 | 408 | 451 | 13 | | |
| 11 | i3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | j3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | k3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | l3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | m3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | n3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | o3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | p3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | q3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | r3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 11 | s3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | t3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | u3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | v3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | w3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | x3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | y3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |
| 11 | z3 | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2252 | 1379 | 409 | 451 | 13 | | |

- Molecule 12 is a protein called Basal-body rod modification protein FlgD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | A4 | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1475 | 914 | 253 | 307 | 1 | | |
| 12 | B4 | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1493 | 924 | 256 | 312 | 1 | | |
| 12 | C4 | 199 | Total | C | N | O | S | 0 | 0 |
| | | | 1458 | 903 | 250 | 304 | 1 | | |

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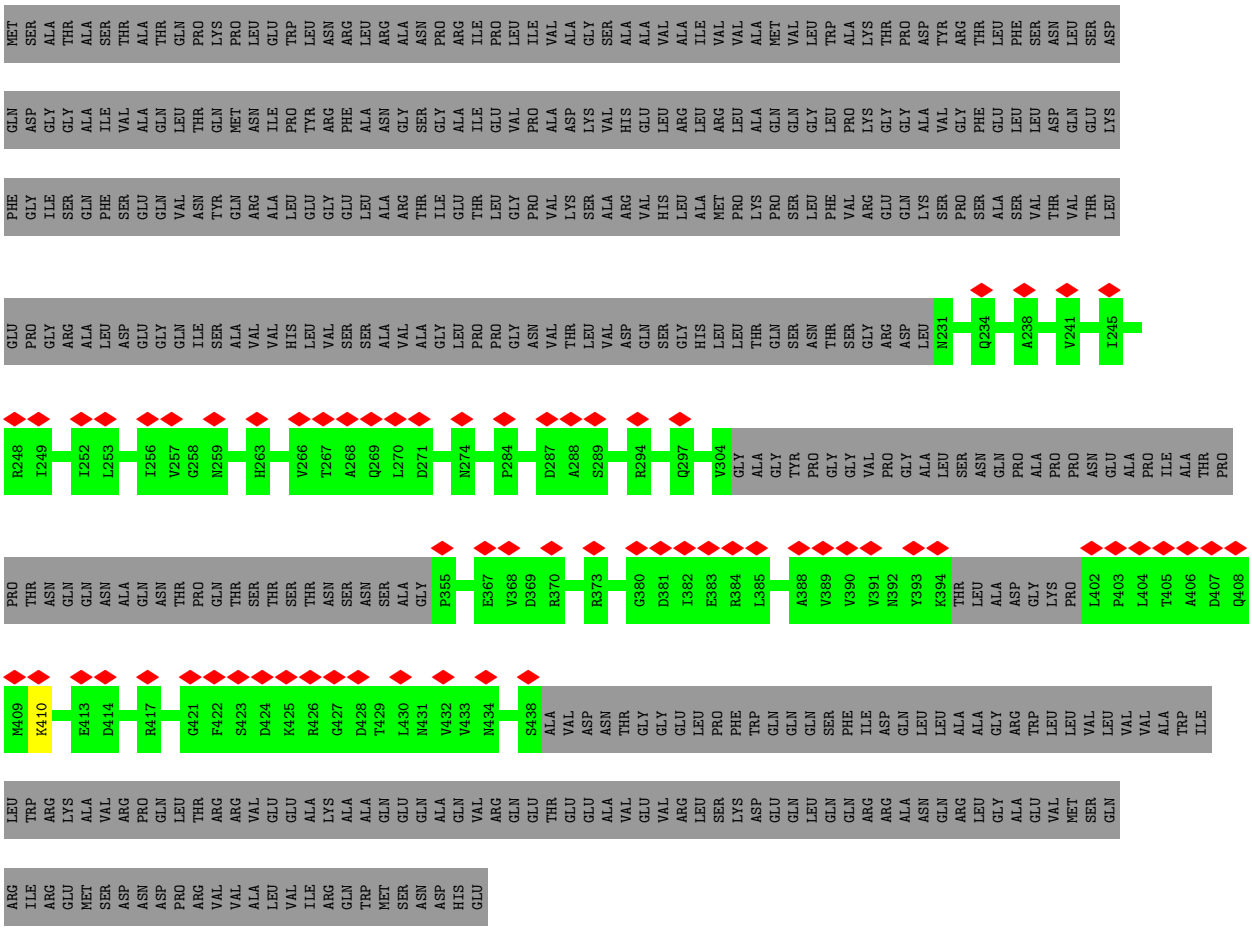
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | D4 | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1482 | 917 | 254 | 310 | 1 | | |
| 12 | E4 | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1493 | 924 | 256 | 312 | 1 | | |

# 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.

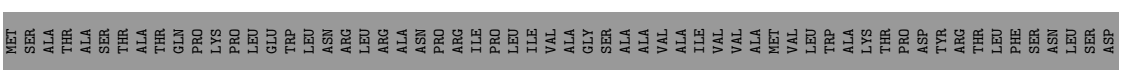
• Molecule 1: Flagellar M-ring protein

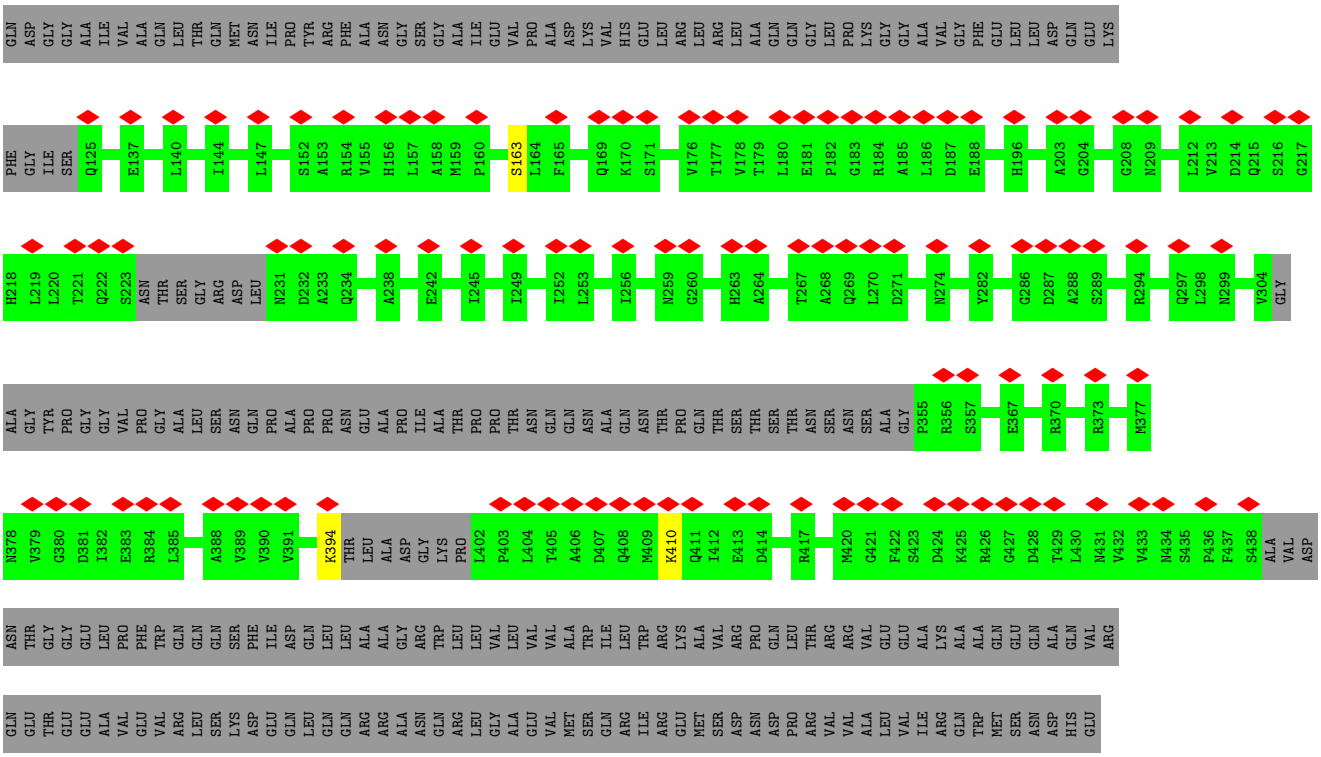
Chain A1:




• Molecule 1: Flagellar M-ring protein

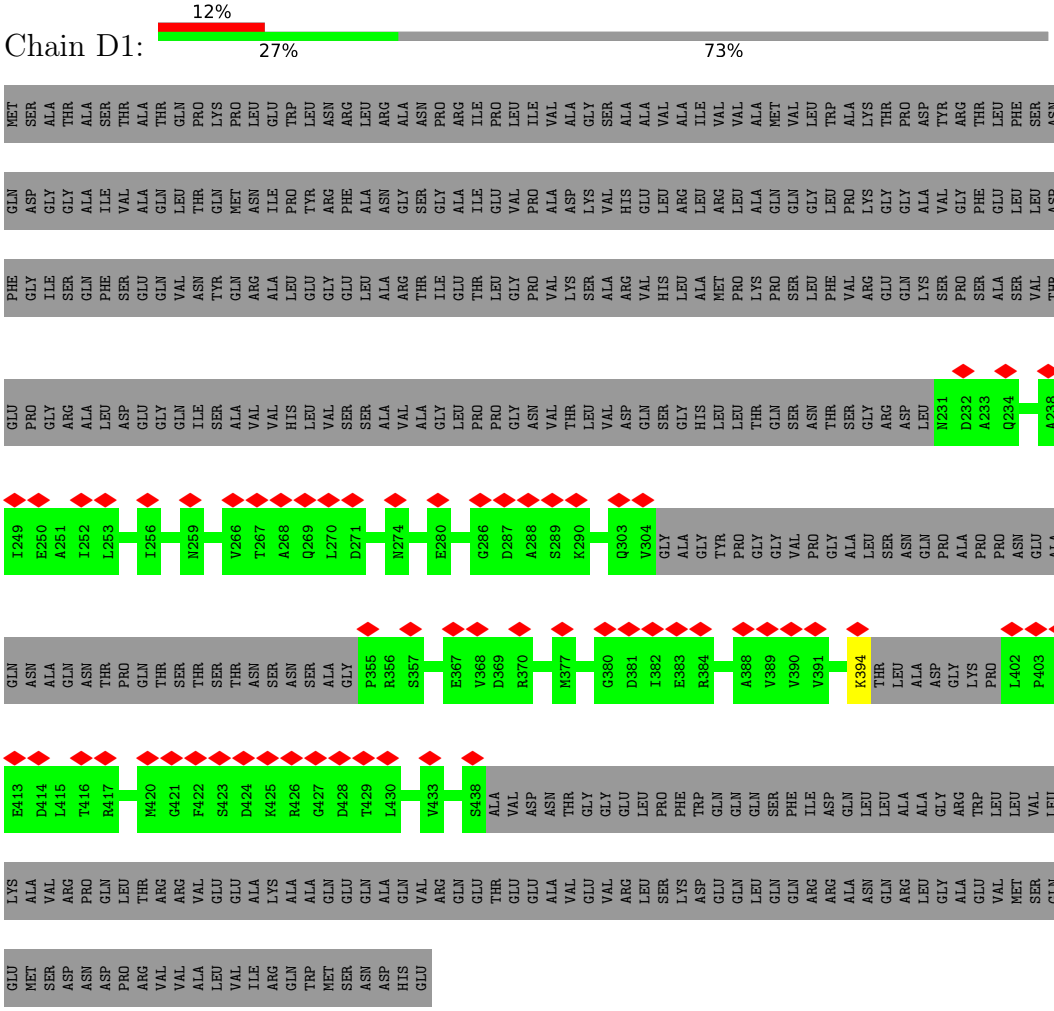
Chain B1:





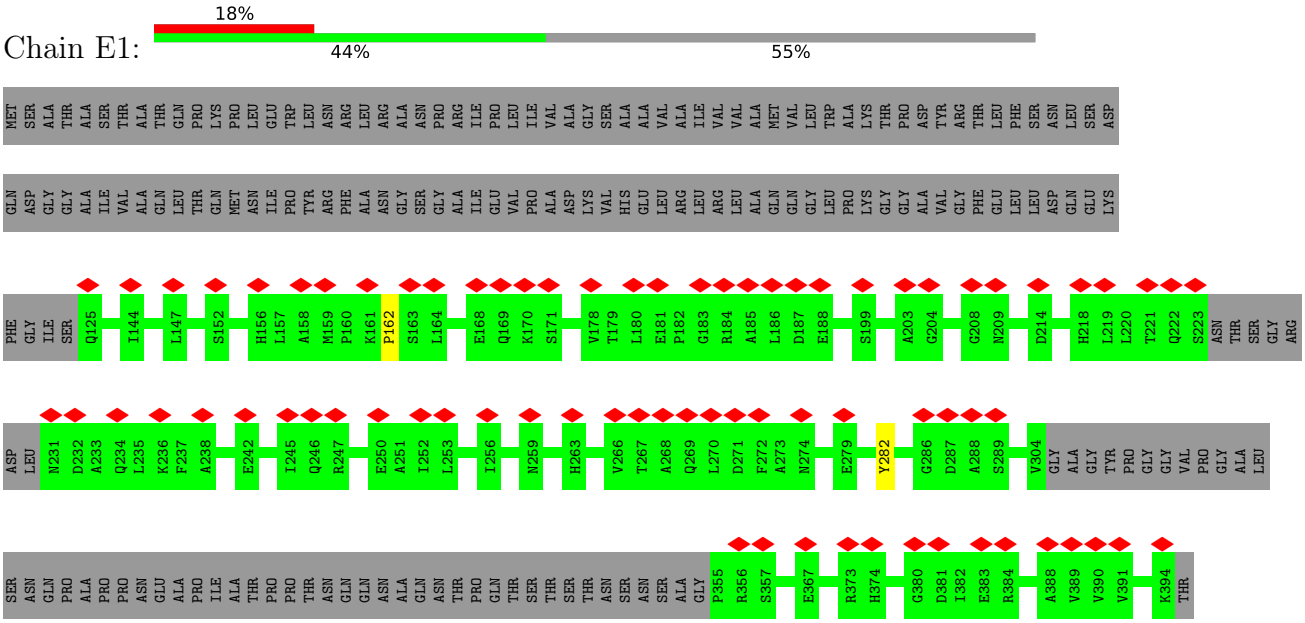
• Molecule 1: Flagellar M-ring protein

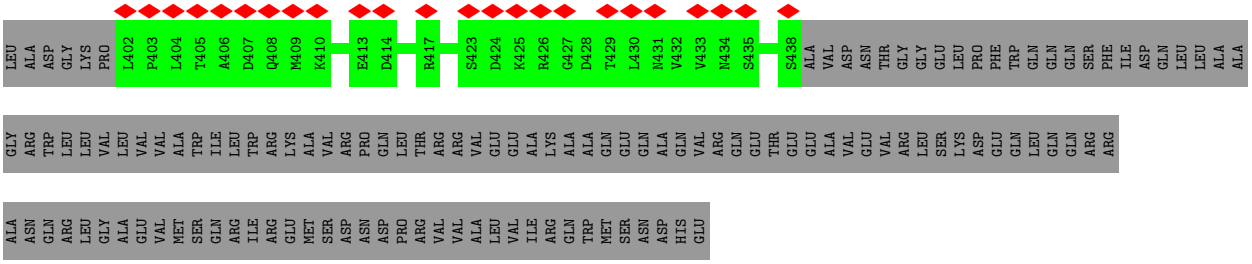
Chain D1:




• Molecule 1: Flagellar M-ring protein

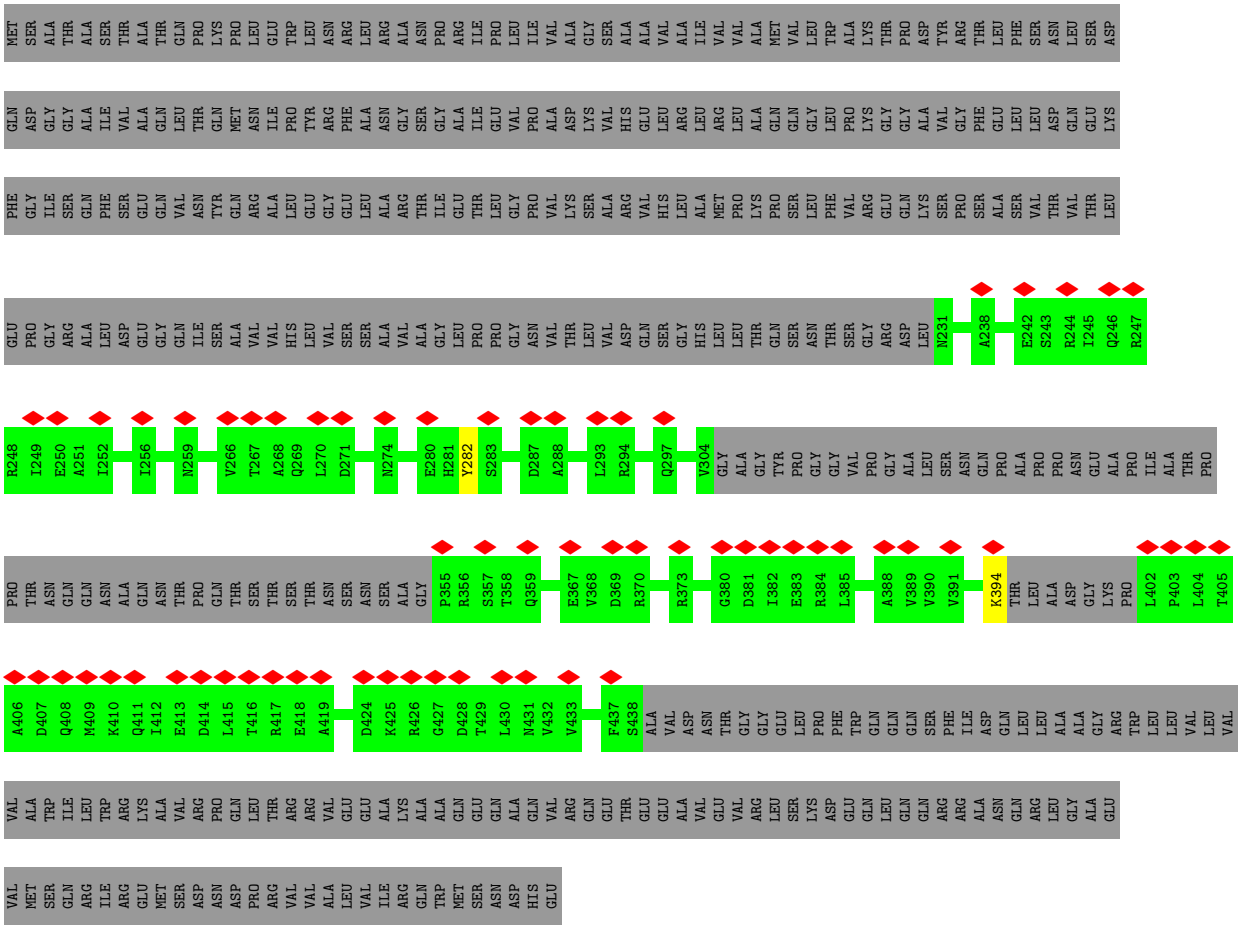
Chain E1:





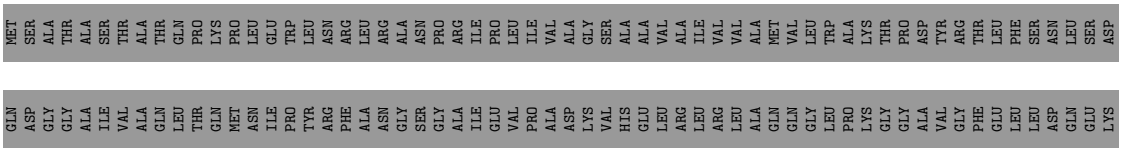
• Molecule 1: Flagellar M-ring protein

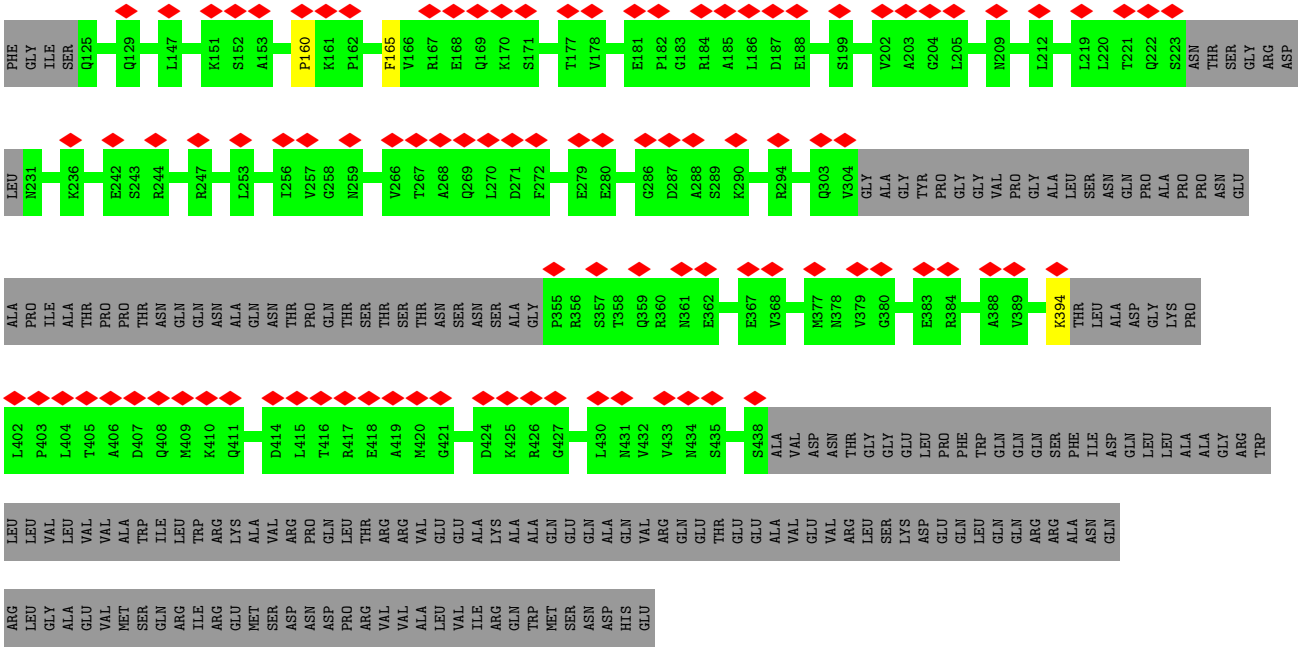
Chain F1:



• Molecule 1: Flagellar M-ring protein

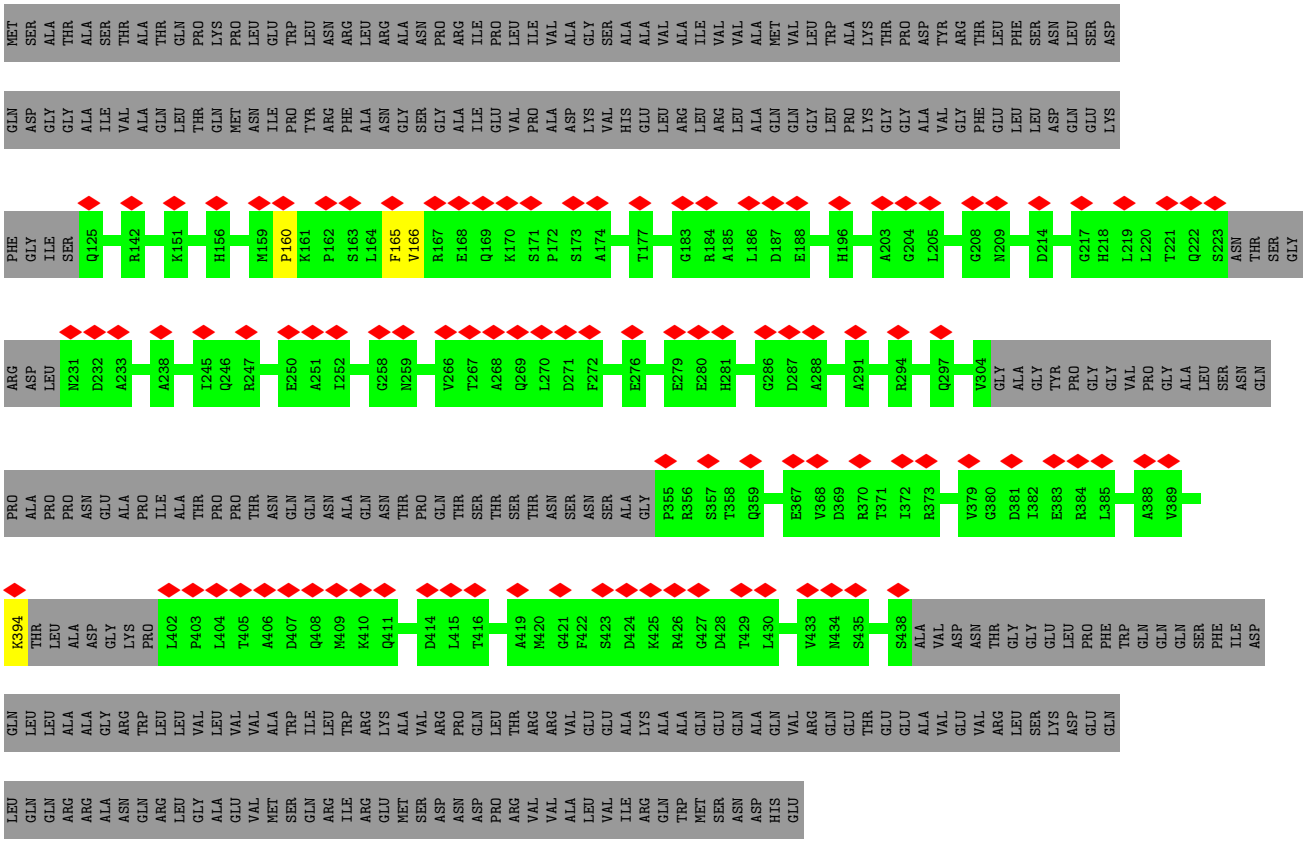
Chain G1:





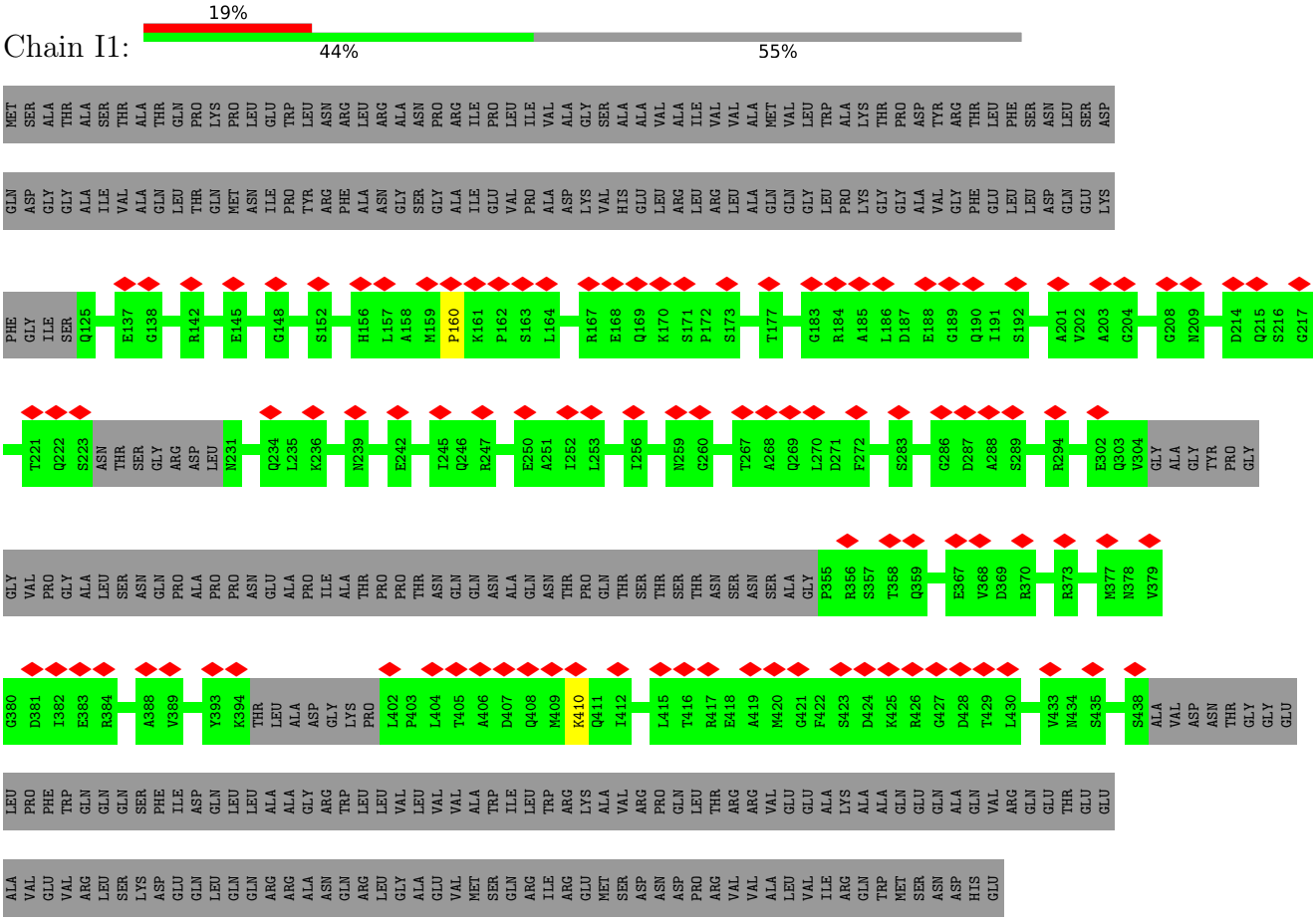
• Molecule 1: Flagellar M-ring protein

Chain H1:



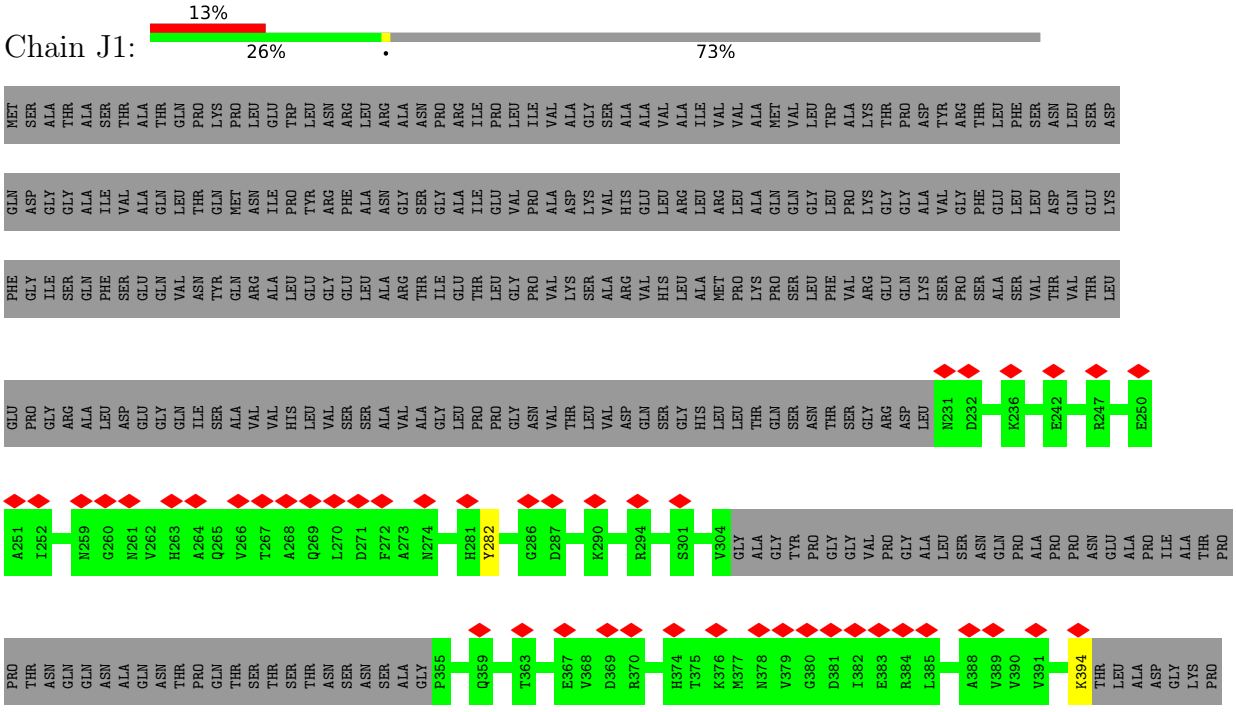
• Molecule 1: Flagellar M-ring protein

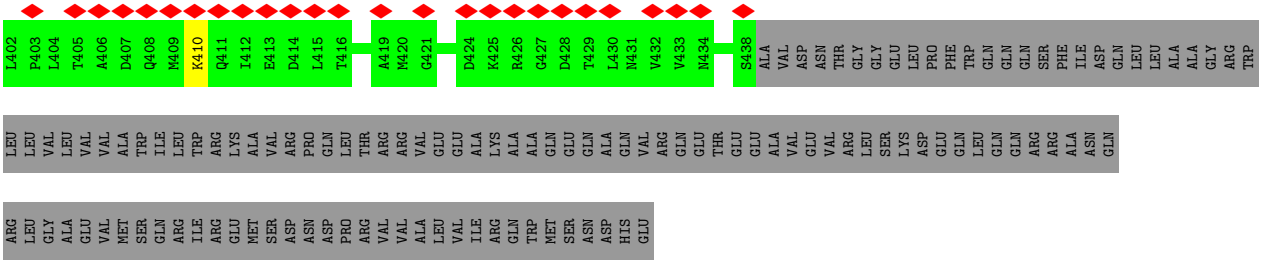
Chain I1:




• Molecule 1: Flagellar M-ring protein

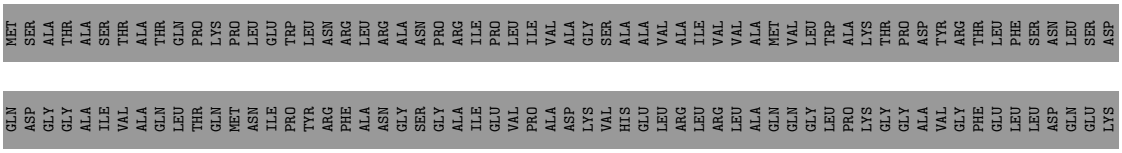
Chain J1:

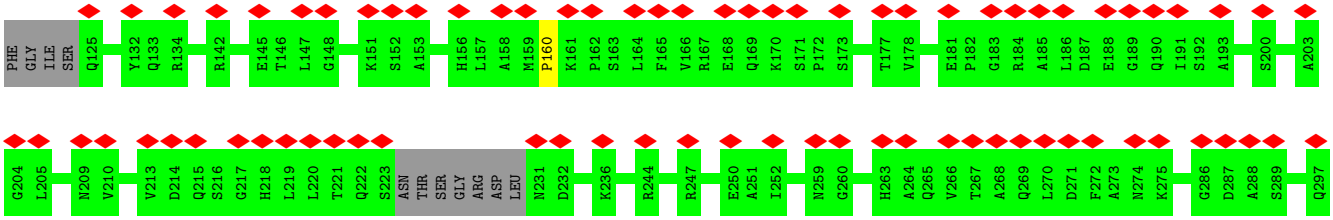


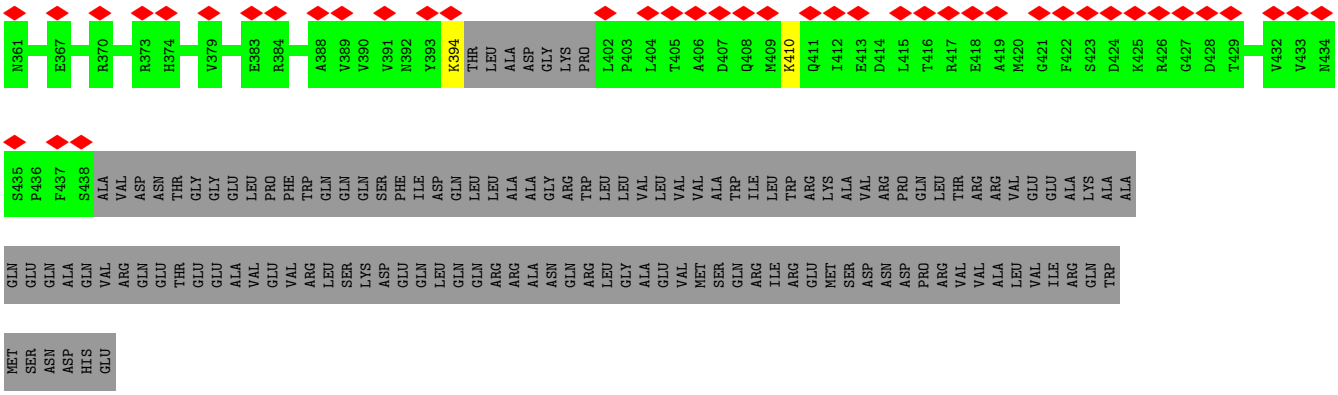



• Molecule 1: Flagellar M-ring protein

Chain K1:

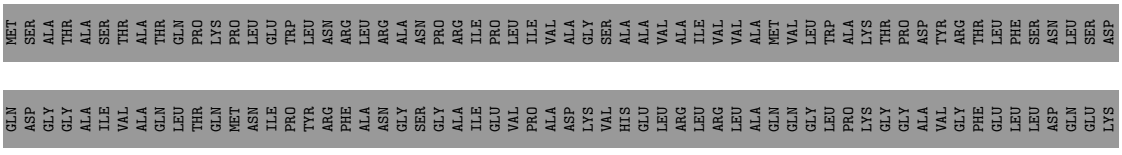


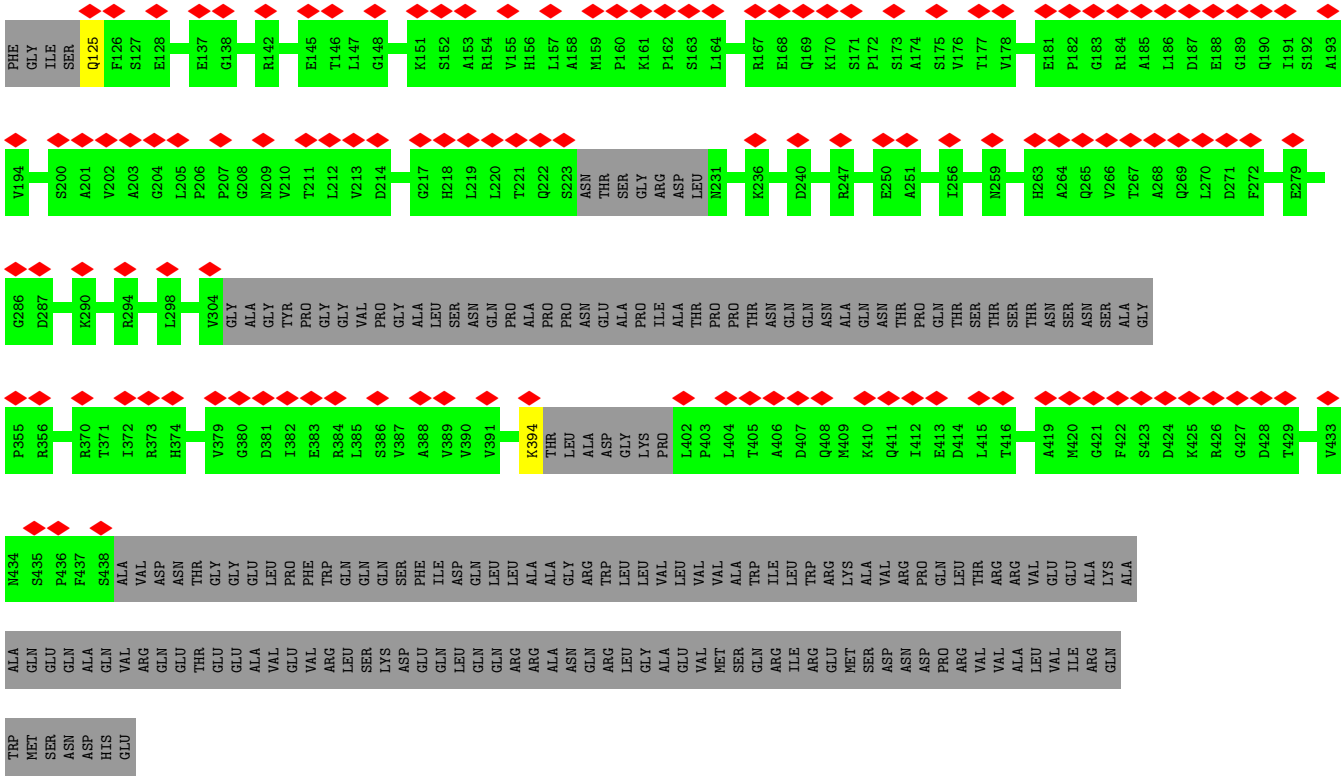




• Molecule 1: Flagellar M-ring protein

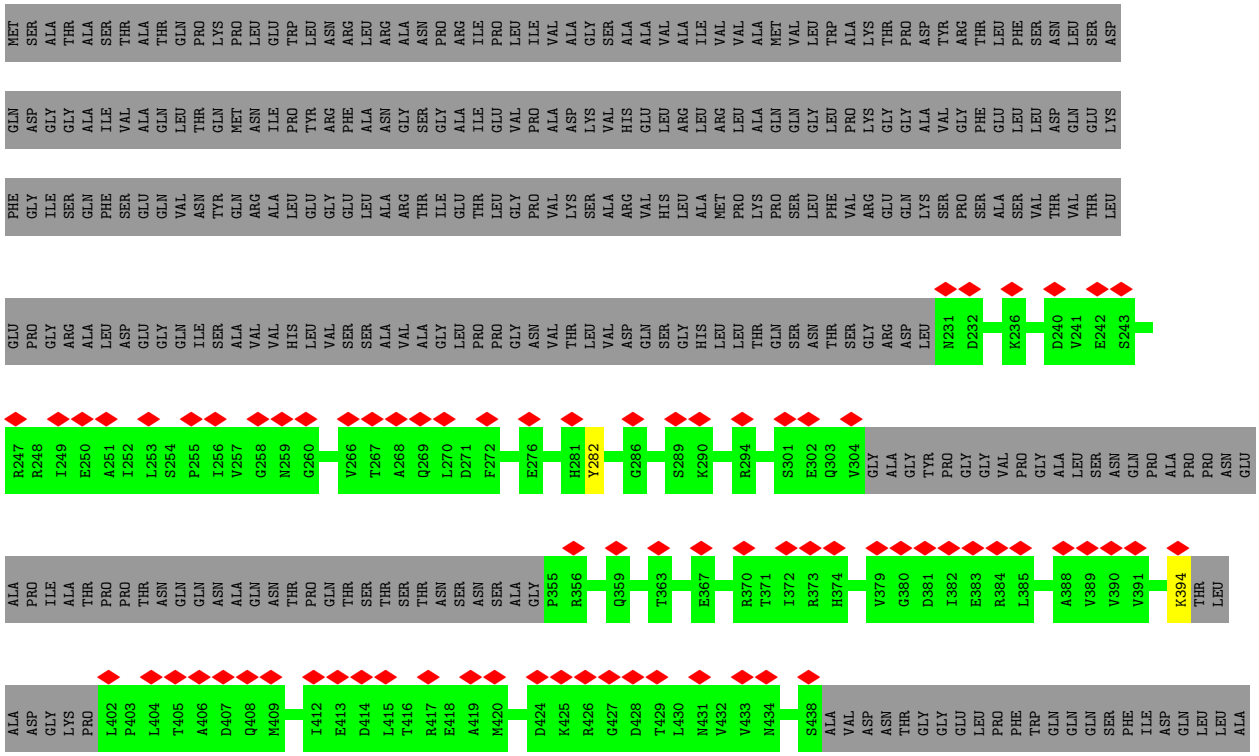
Chain L1:

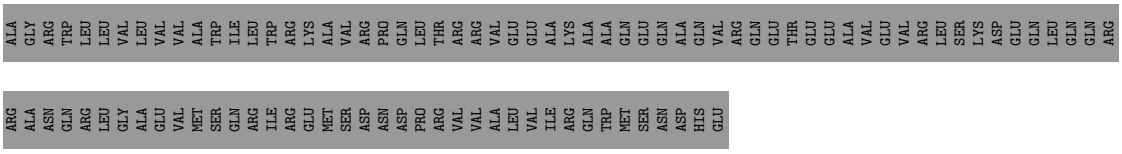




• Molecule 1: Flagellar M-ring protein

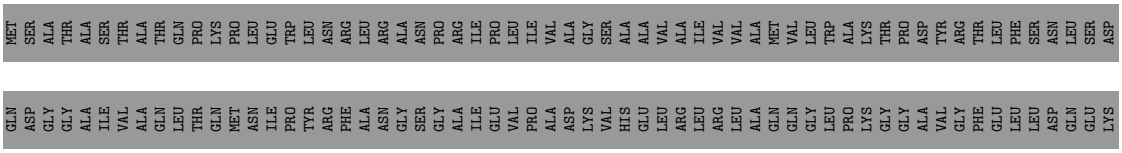
Chain M1:

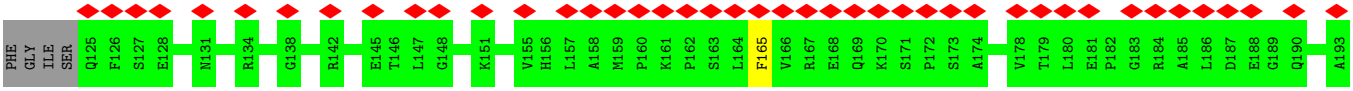


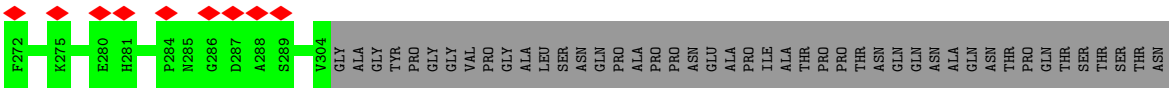


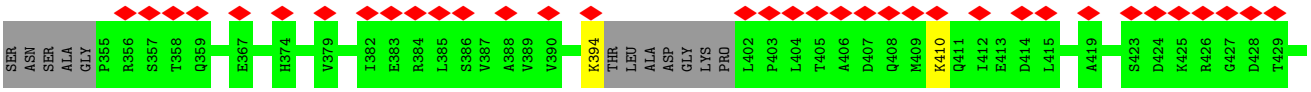

• Molecule 1: Flagellar M-ring protein

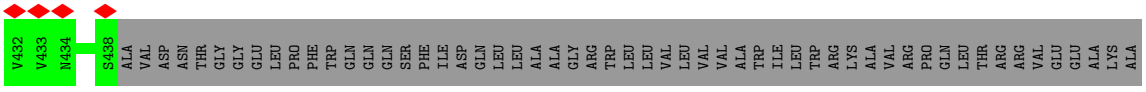
Chain N1:



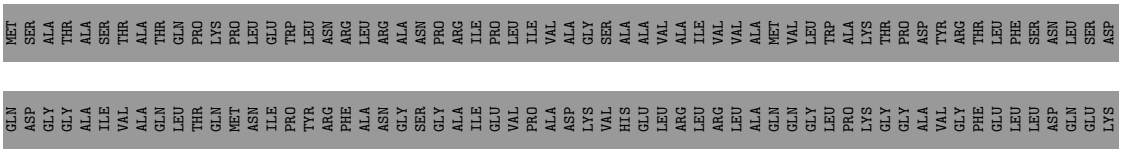


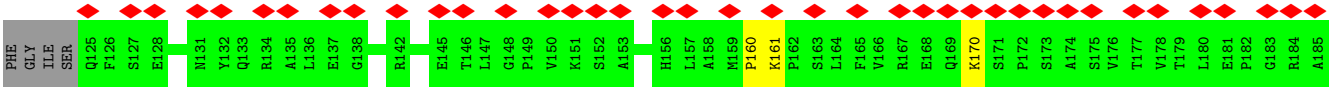



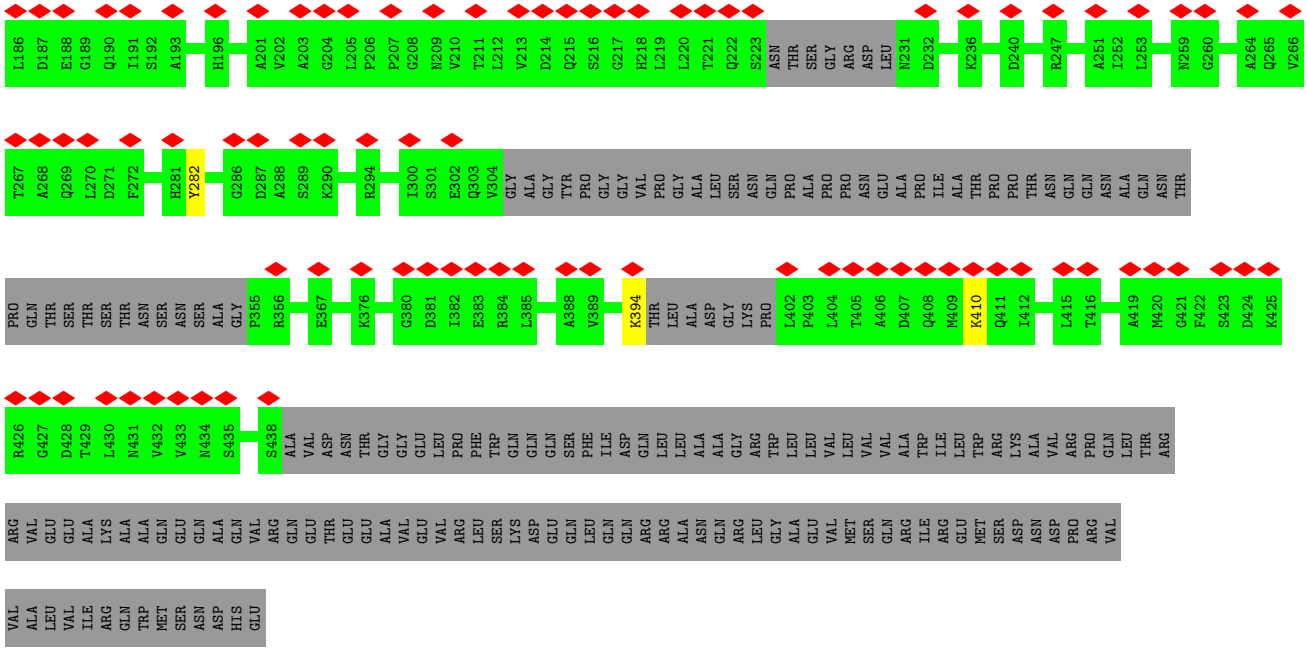



• Molecule 1: Flagellar M-ring protein

Chain O1:

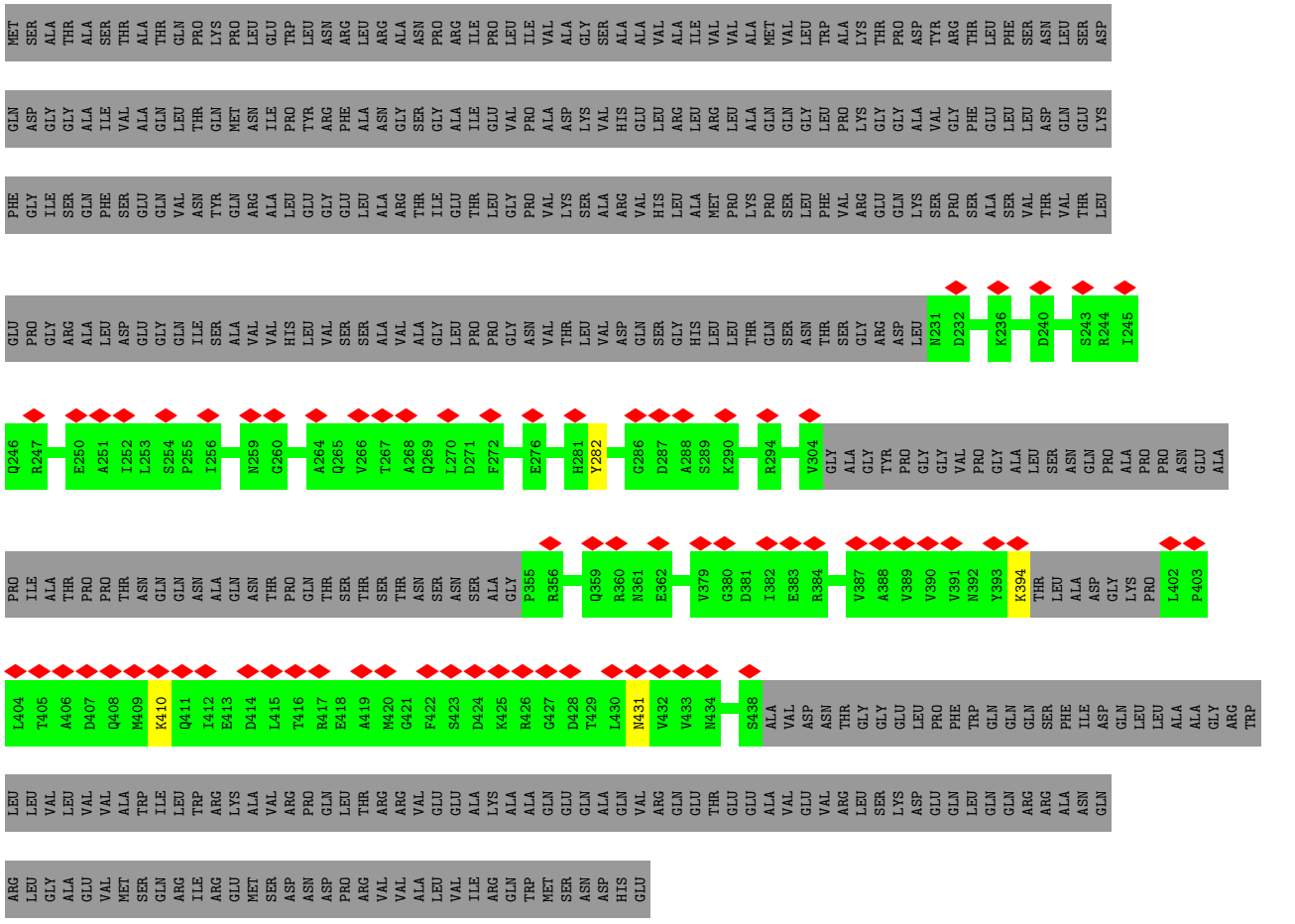




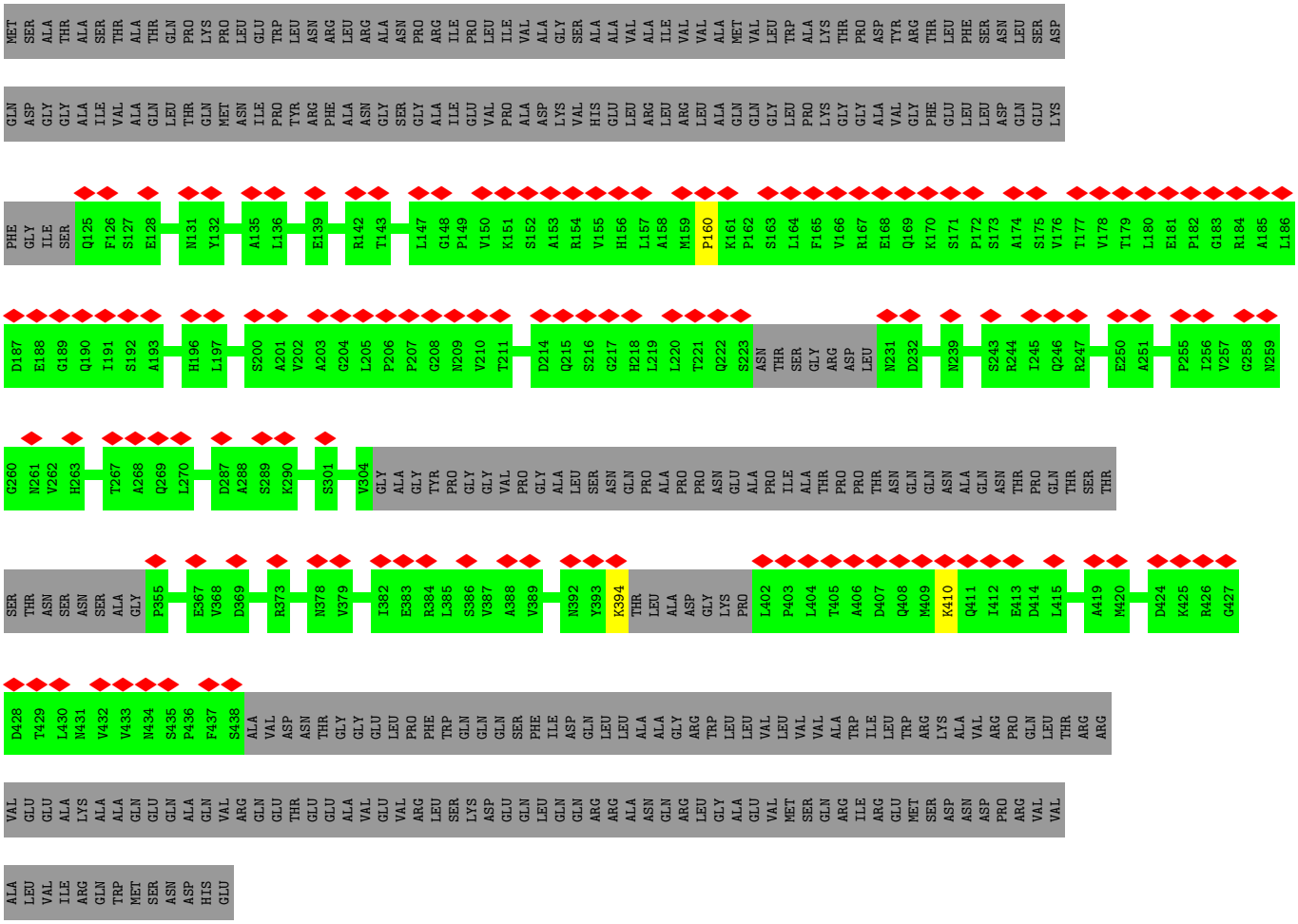

- Molecule 1: Flagellar M-ring protein

Chain P1:



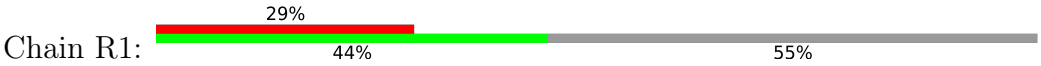
• Molecule 1: Flagellar M-ring protein

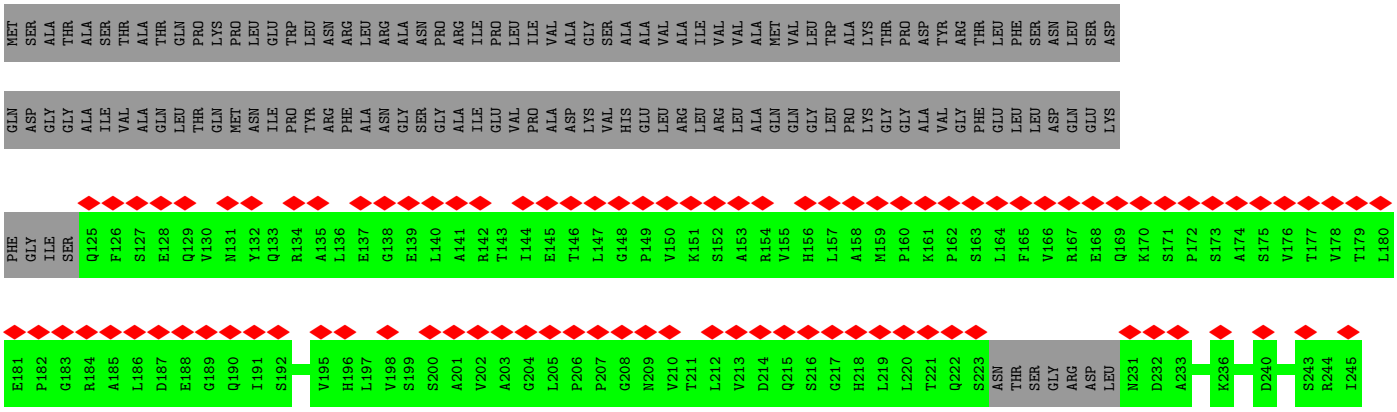
Chain Q1:

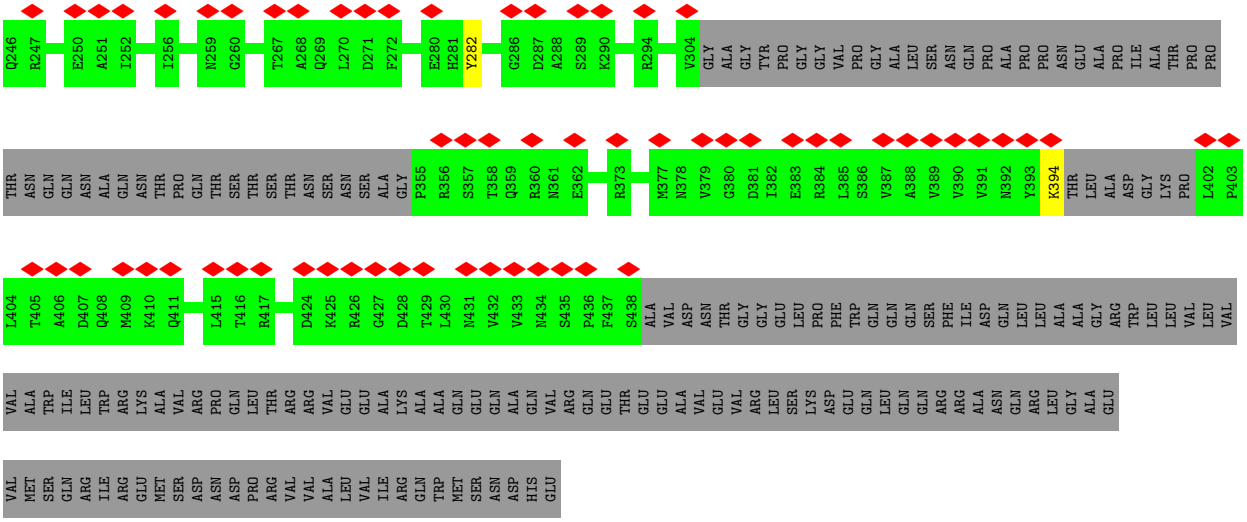



• Molecule 1: Flagellar M-ring protein

Chain R1:

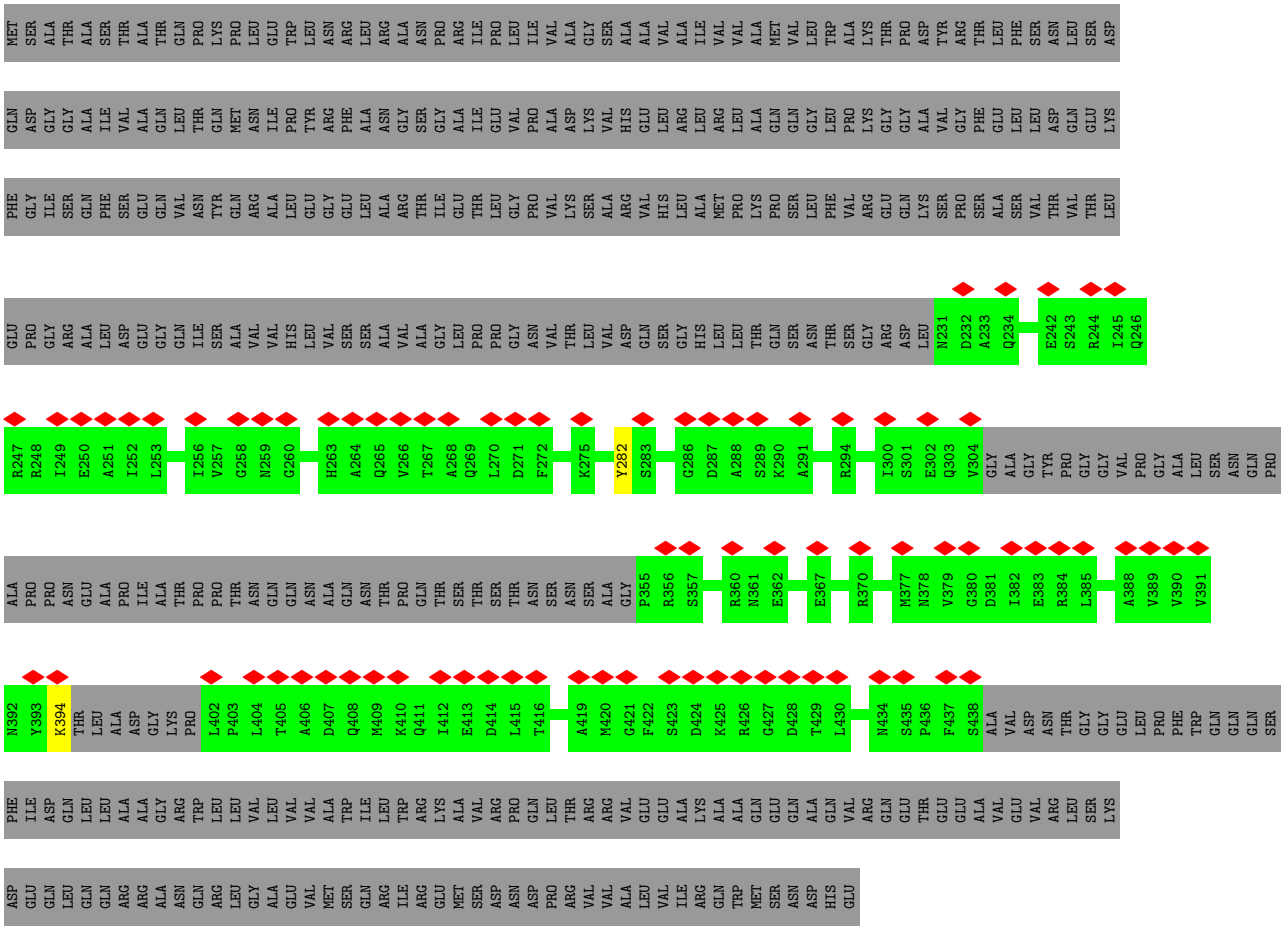




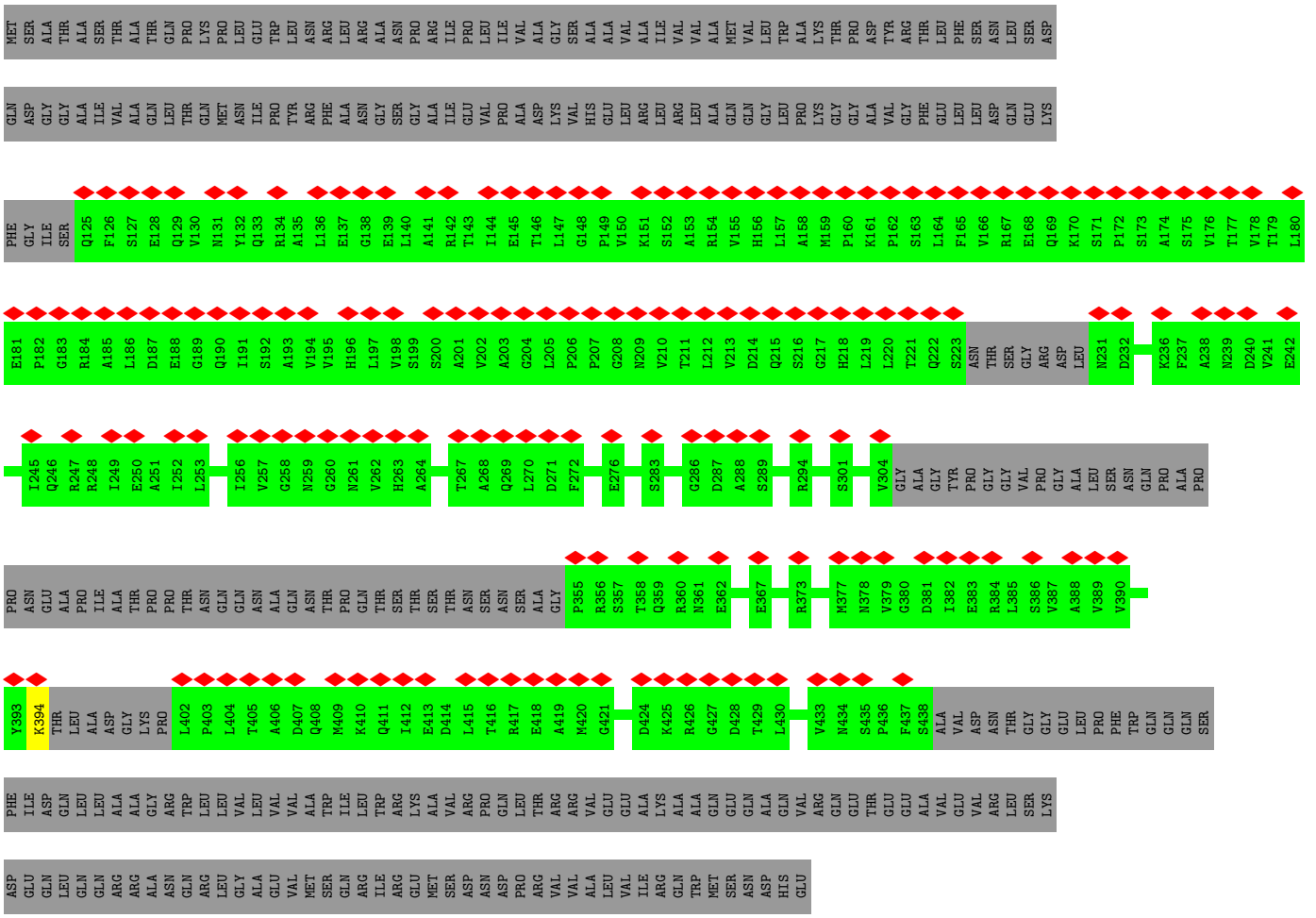
• Molecule 1: Flagellar M-ring protein

Chain S1:



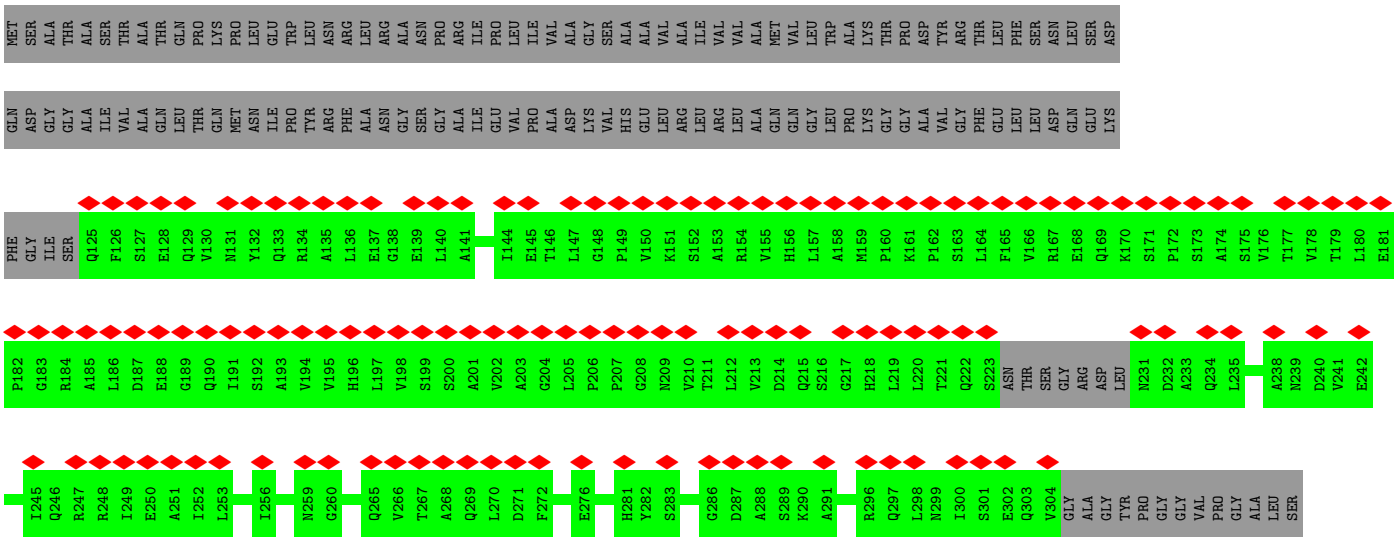
• Molecule 1: Flagellar M-ring protein

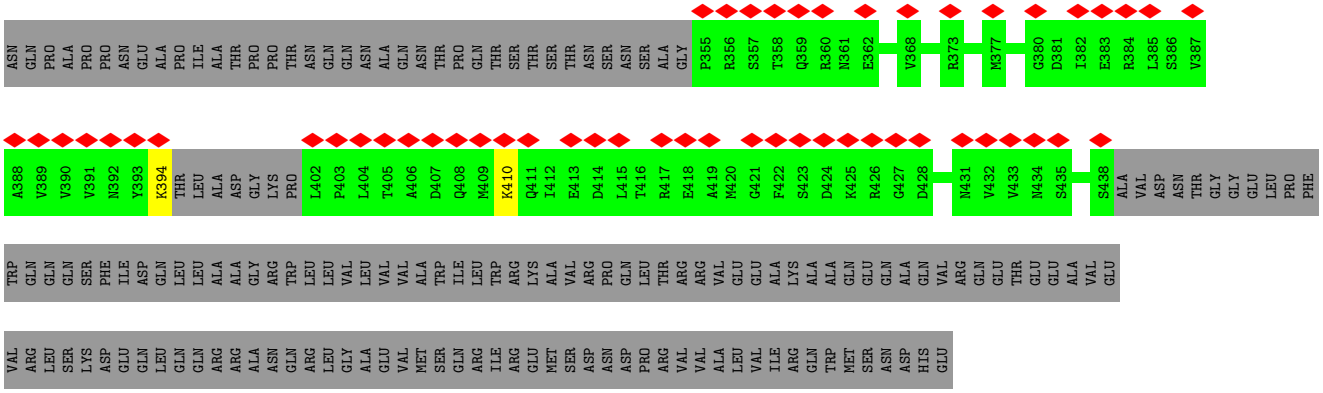
Chain T1:



• Molecule 1: Flagellar M-ring protein

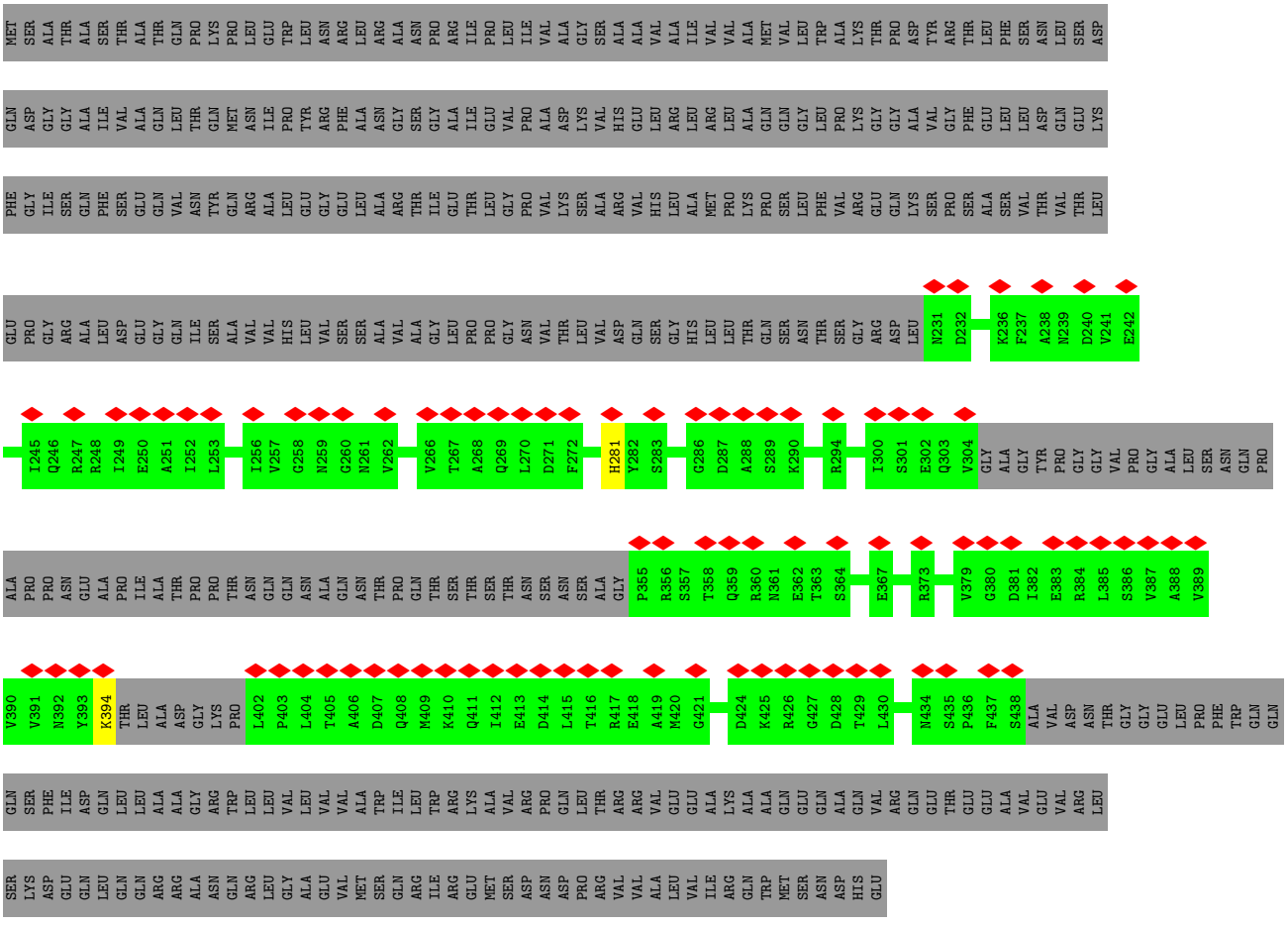
Chain U1:





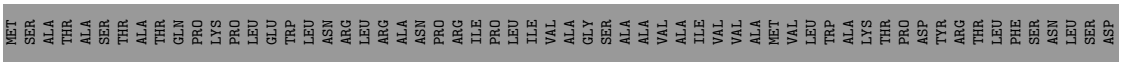
• Molecule 1: Flagellar M-ring protein

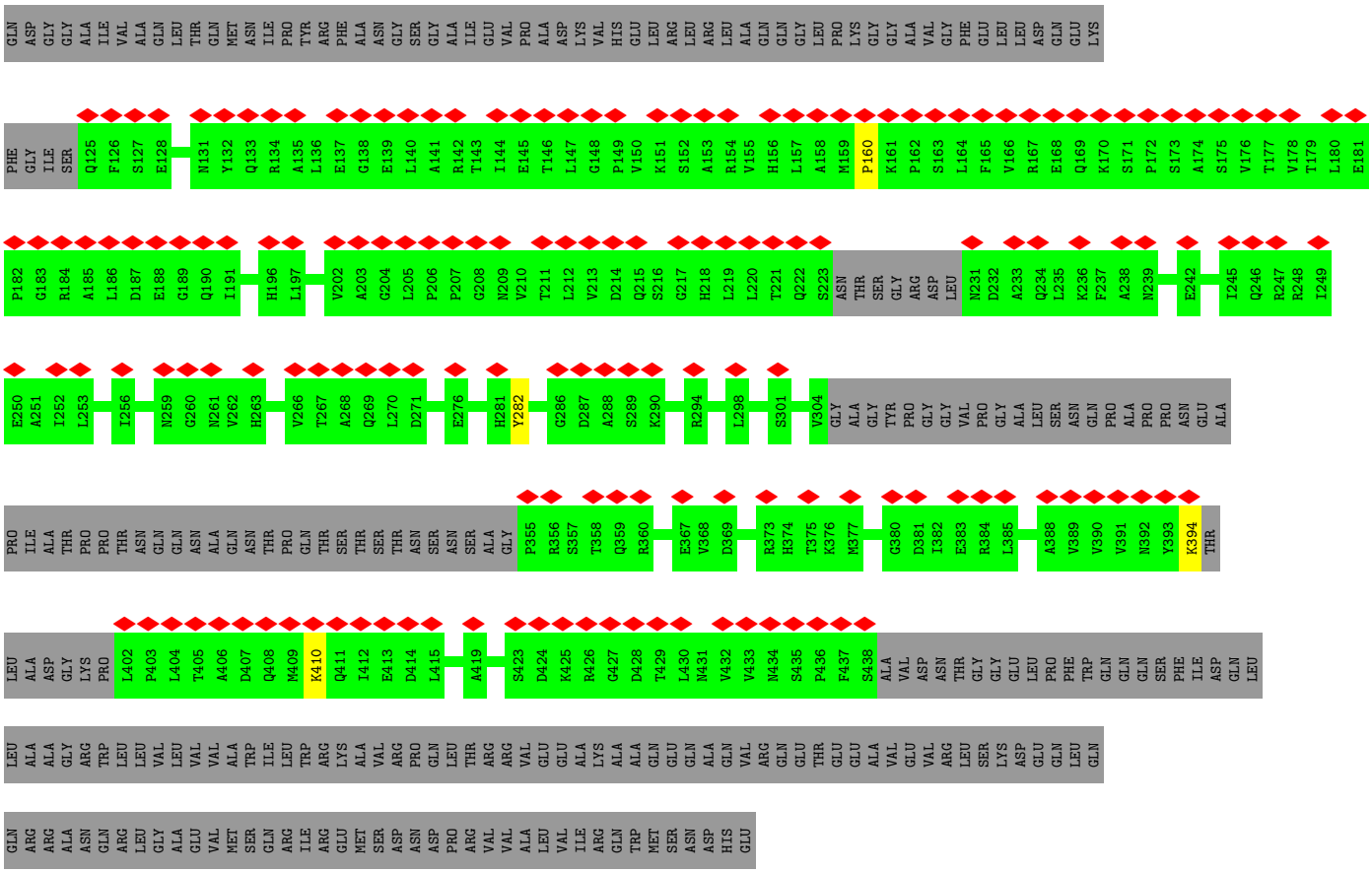
Chain V1:



• Molecule 1: Flagellar M-ring protein

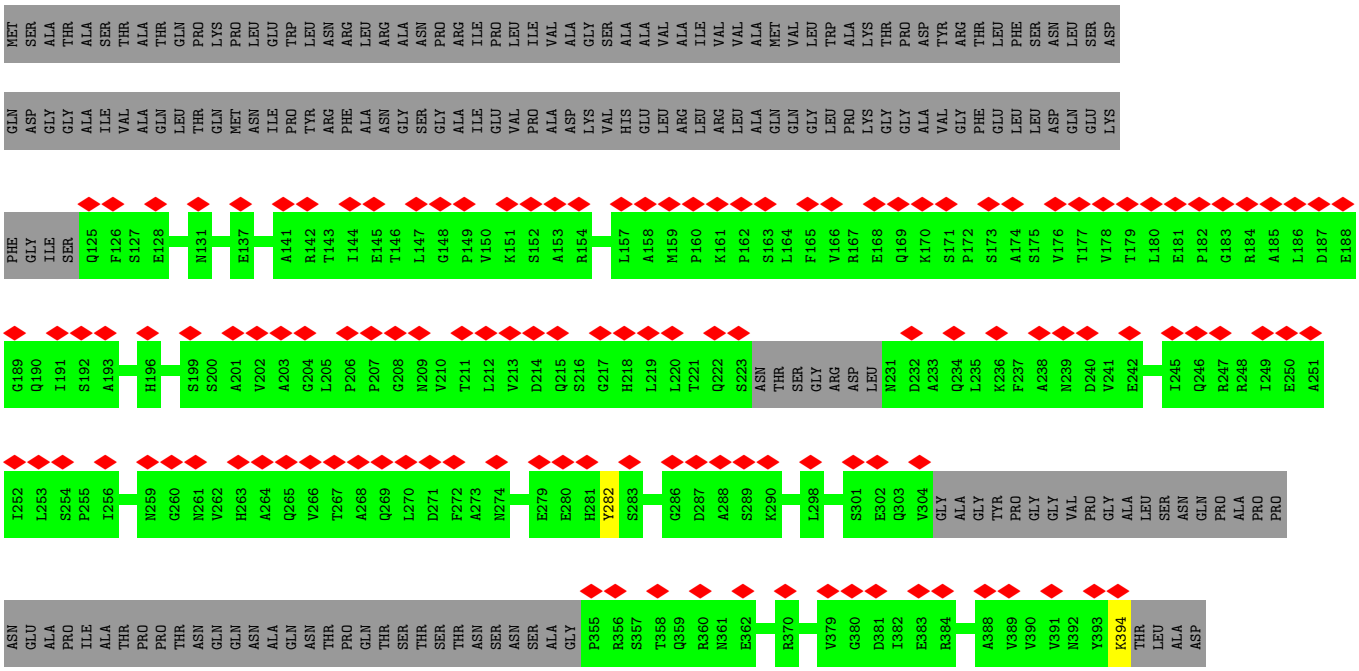
Chain W1:

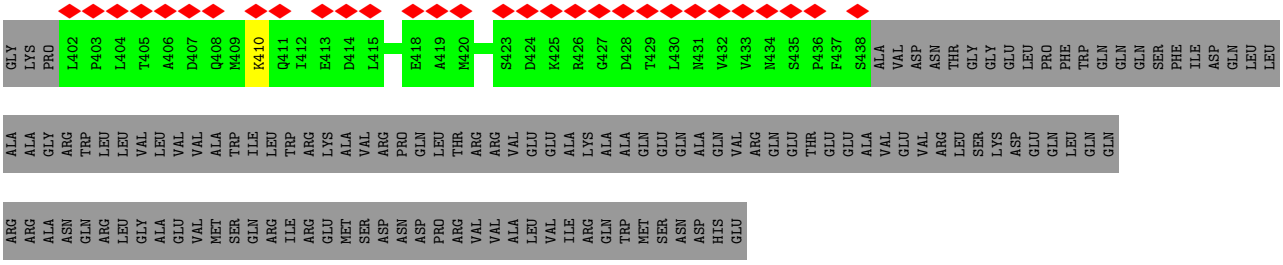




• Molecule 1: Flagellar M-ring protein

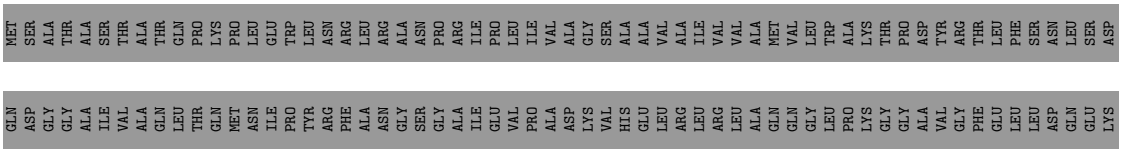
Chain X1:

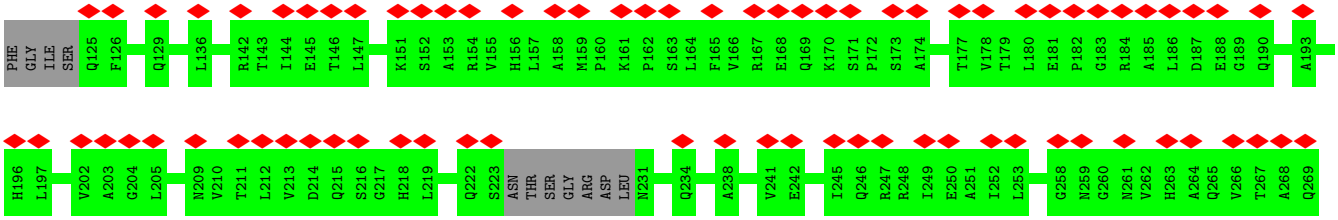


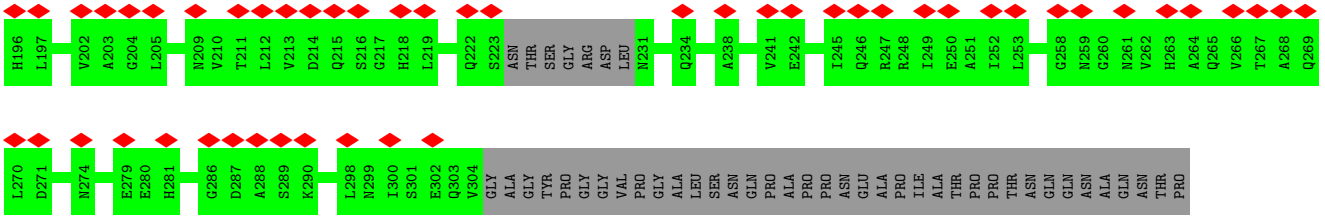


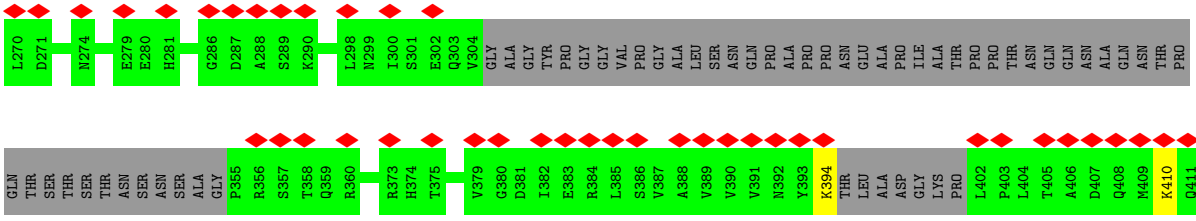
• Molecule 1: Flagellar M-ring protein

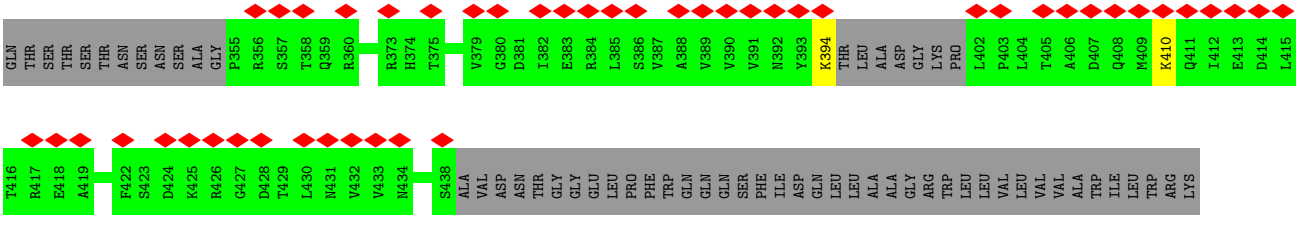
Chain Y1:

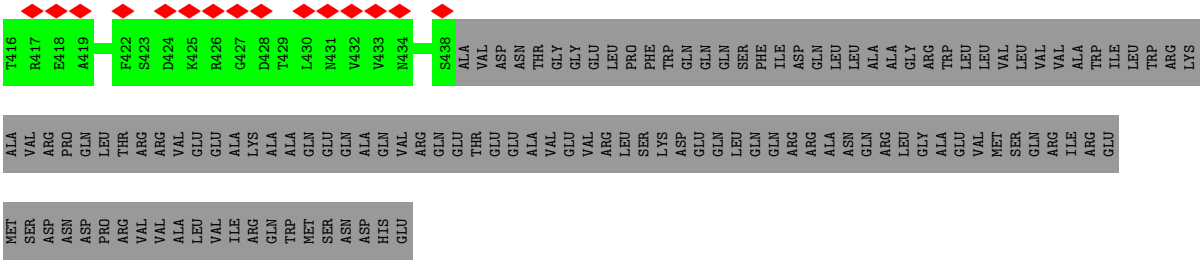








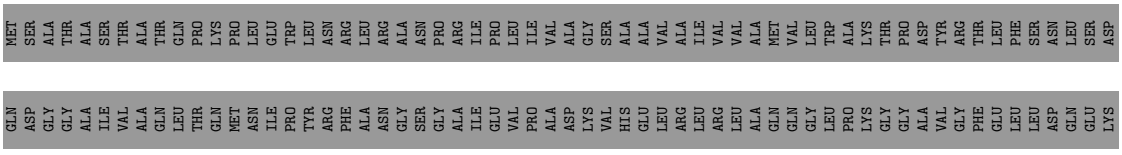


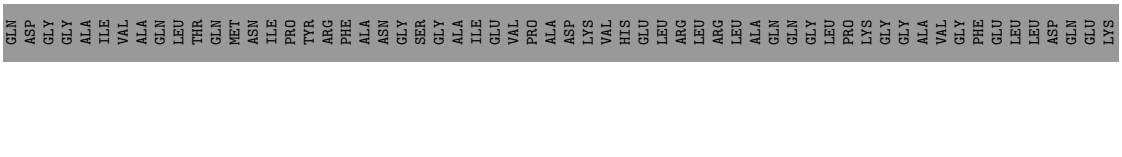


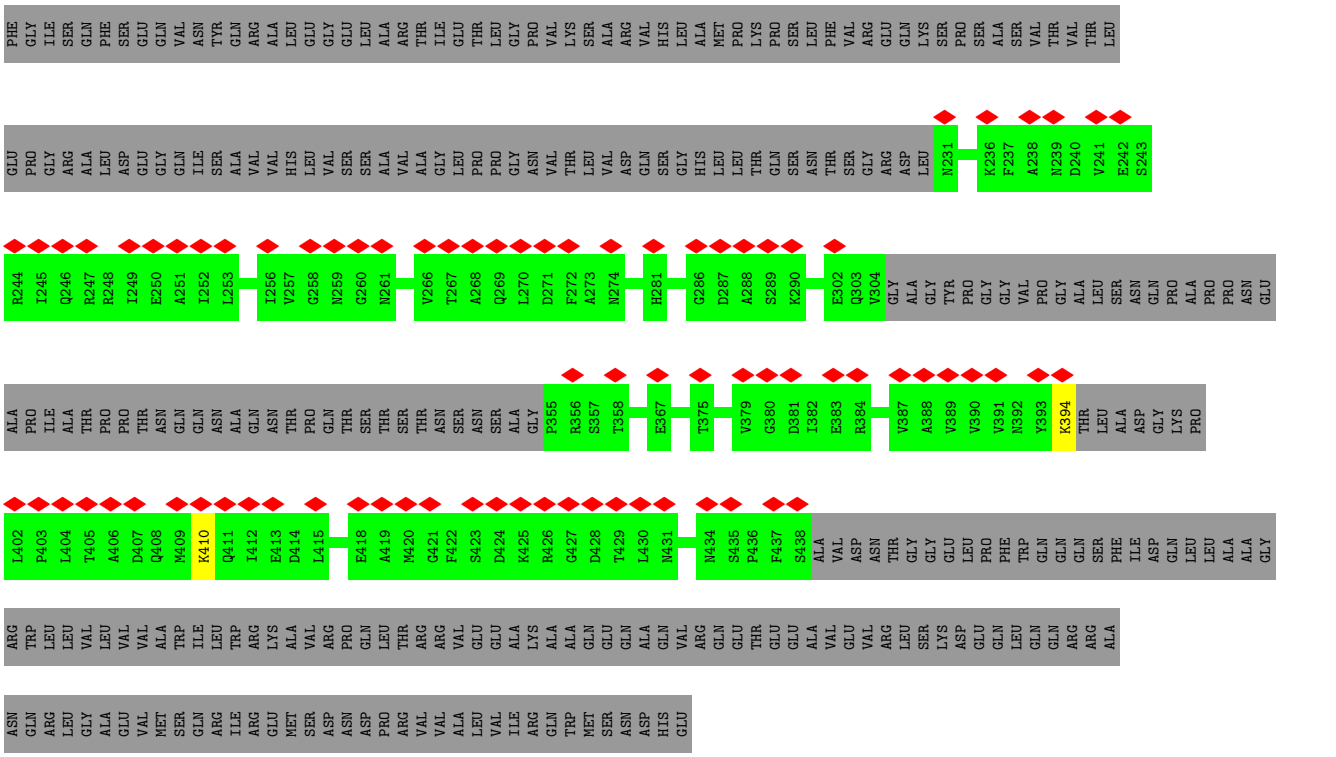


• Molecule 1: Flagellar M-ring protein

Chain Z1:

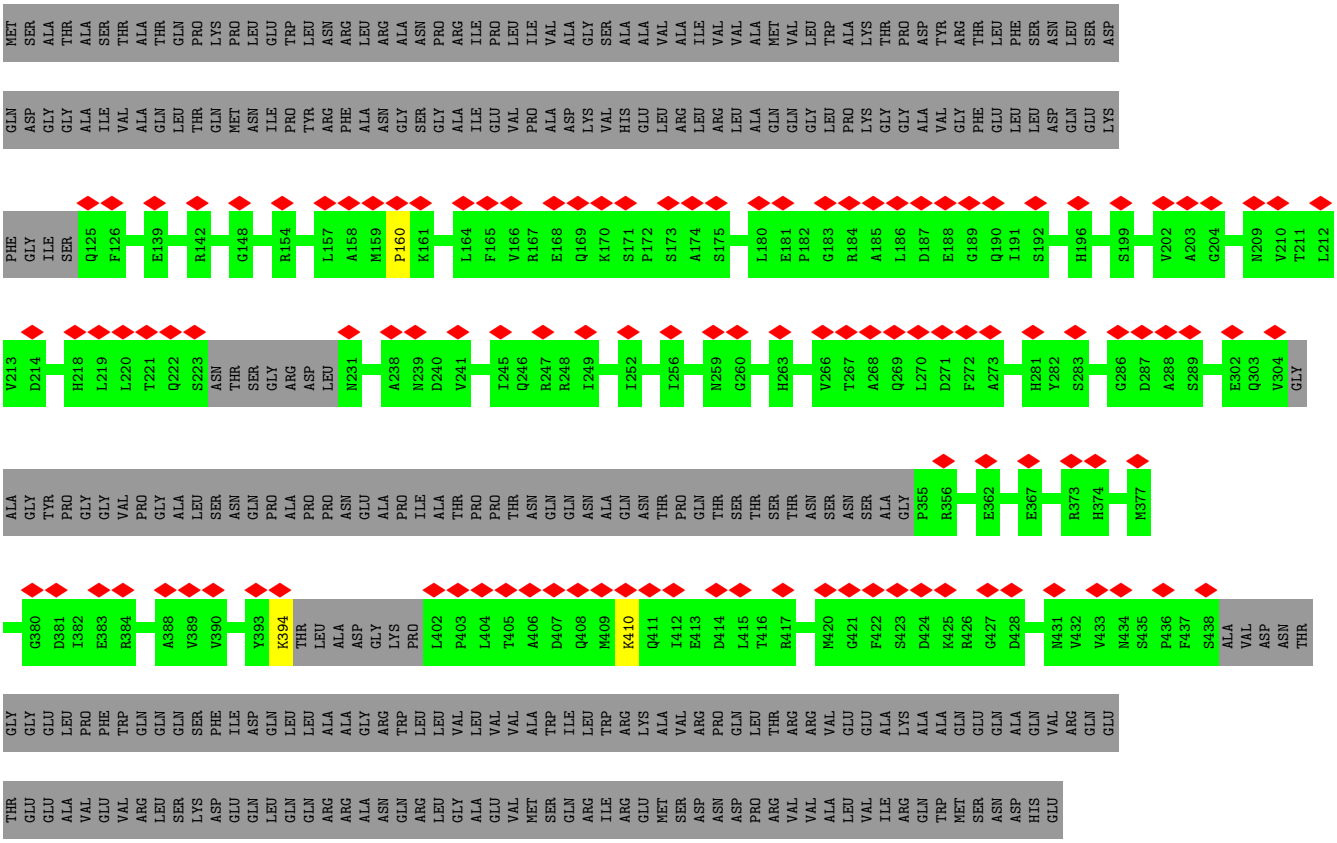






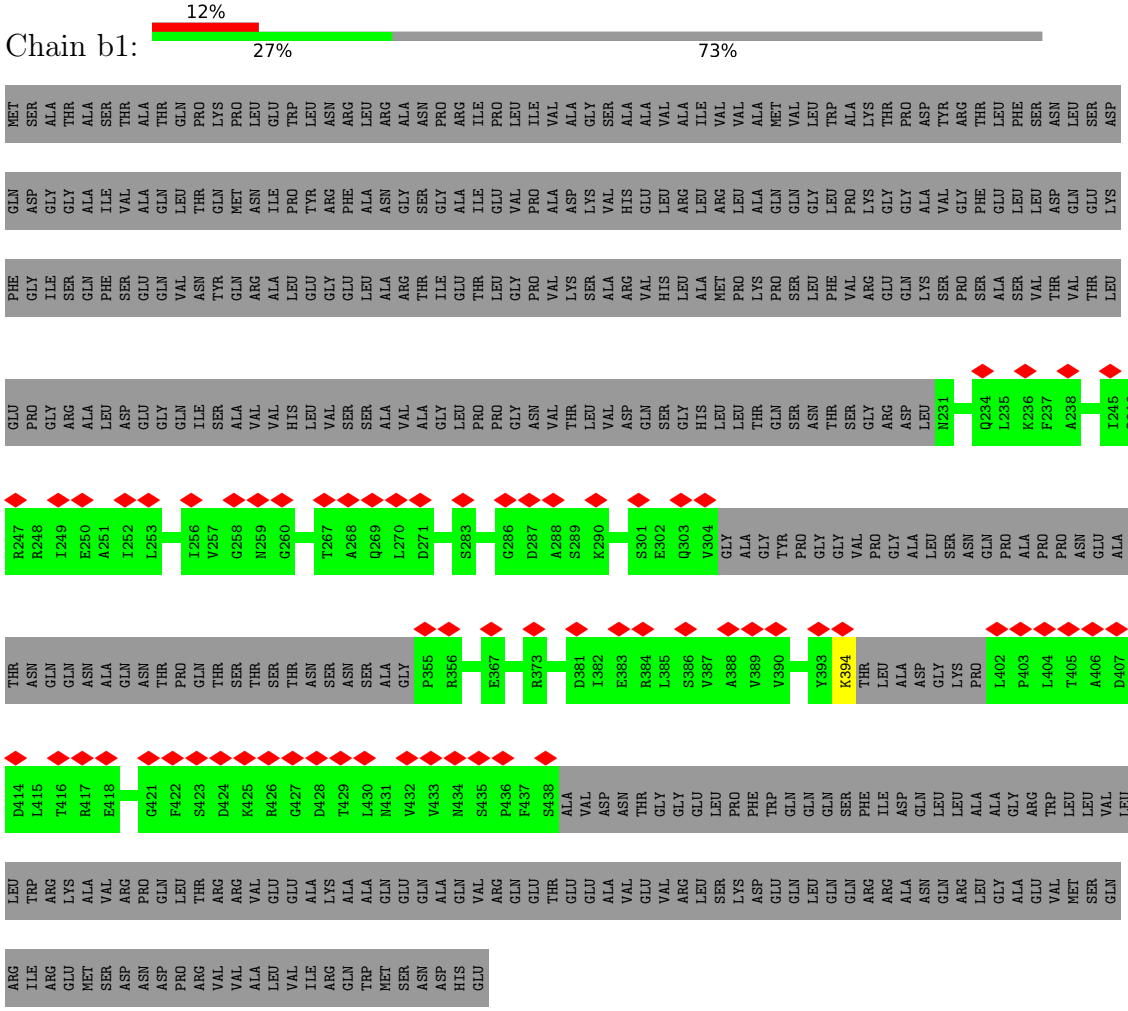
• Molecule 1: Flagellar M-ring protein

Chain a1:



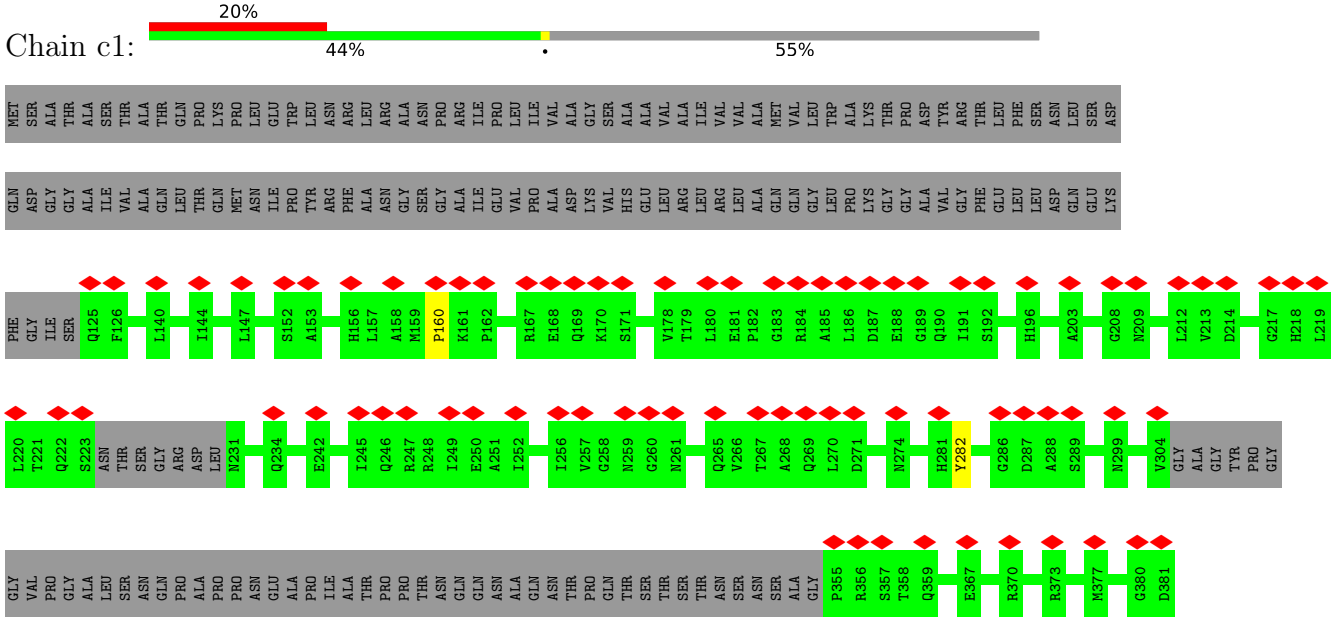
• Molecule 1: Flagellar M-ring protein

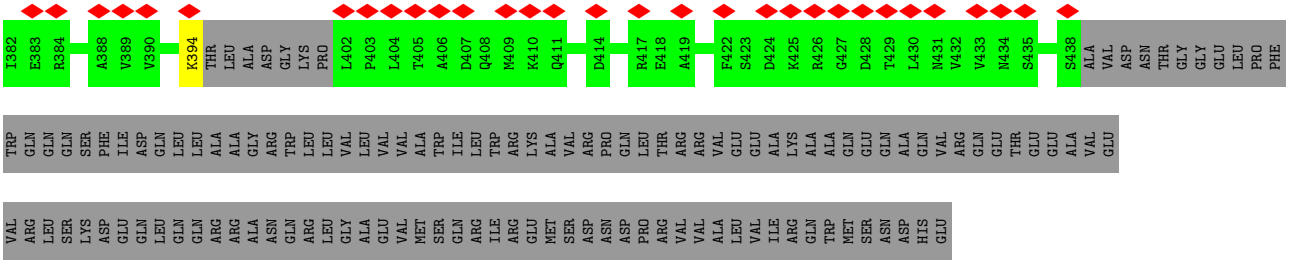
Chain b1:




• Molecule 1: Flagellar M-ring protein

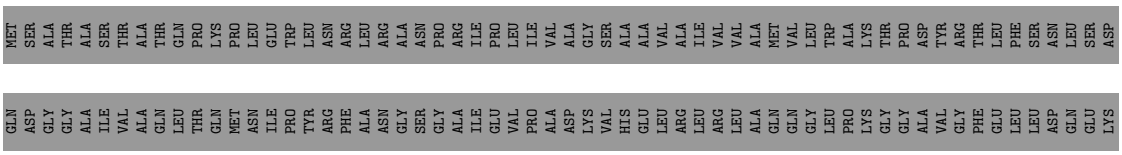
Chain c1:

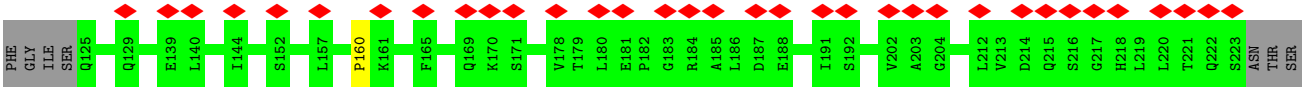


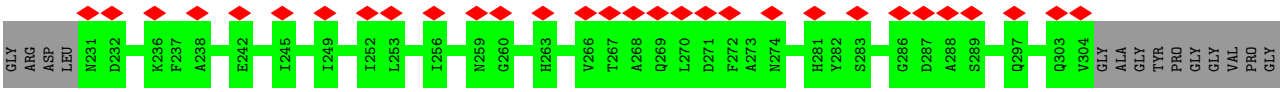


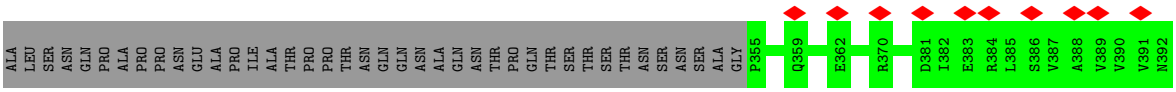
• Molecule 1: Flagellar M-ring protein

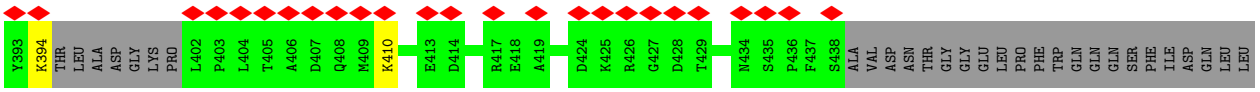
Chain d1:

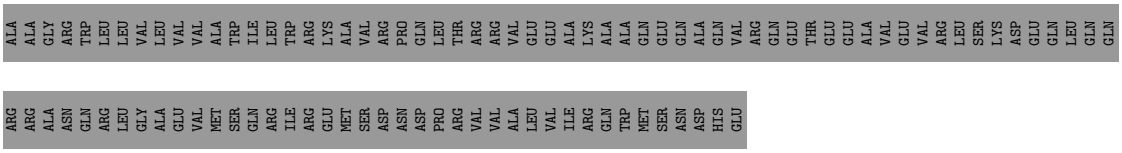






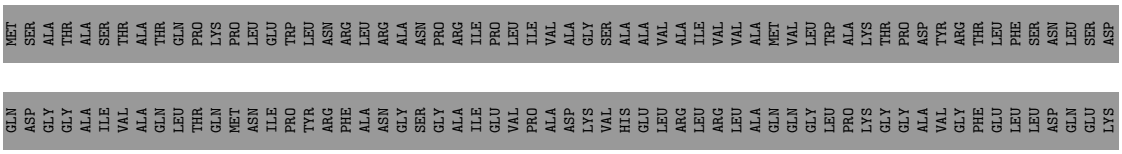


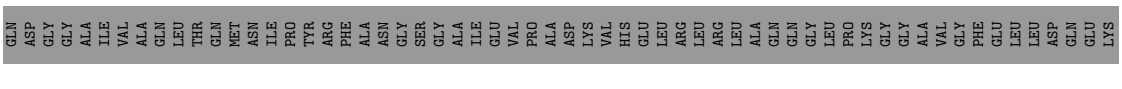


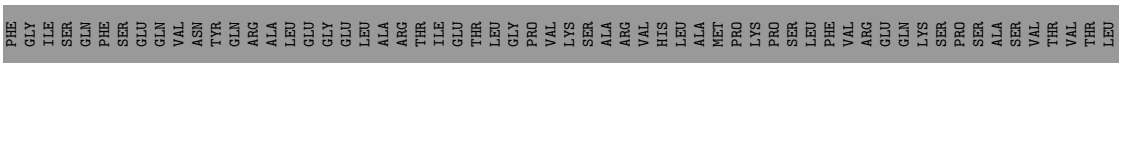


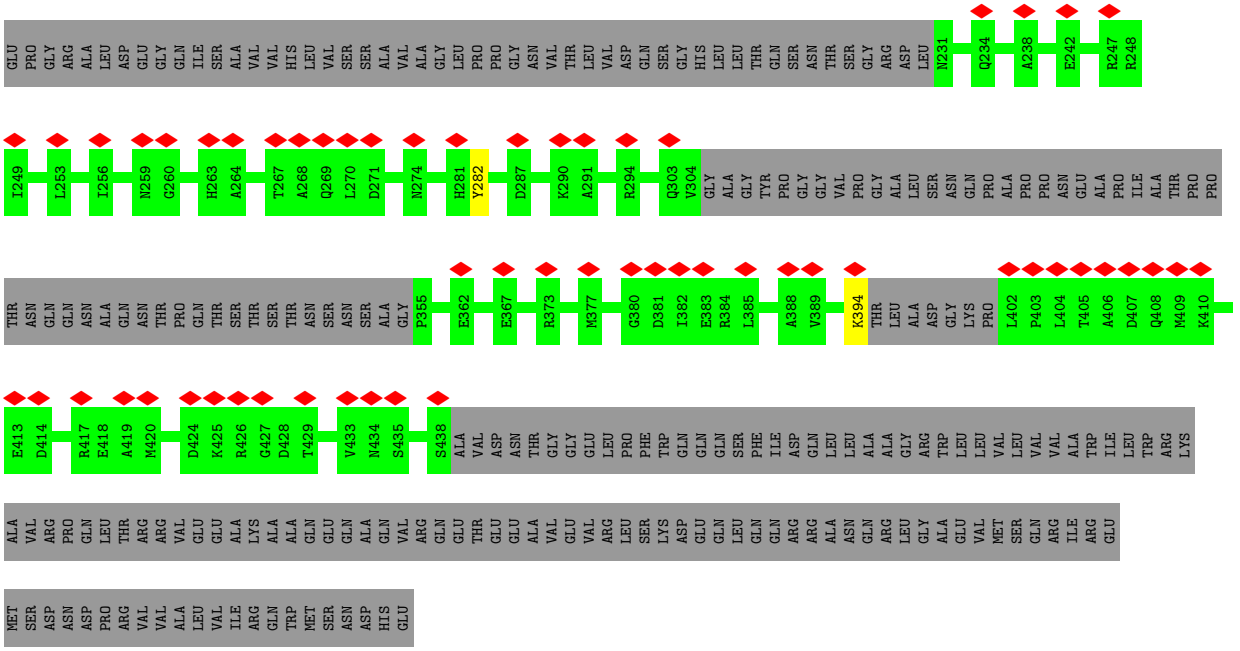
• Molecule 1: Flagellar M-ring protein

Chain e1:



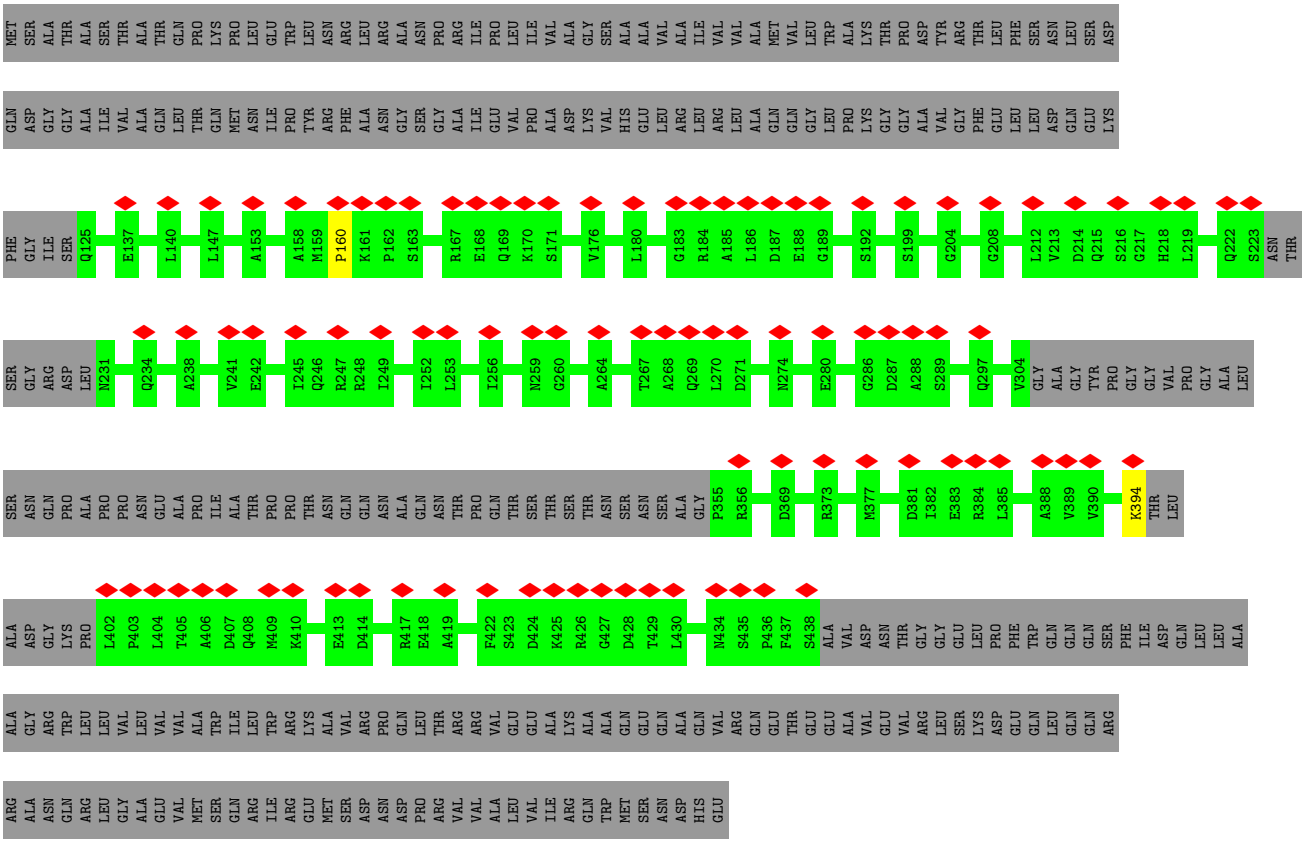






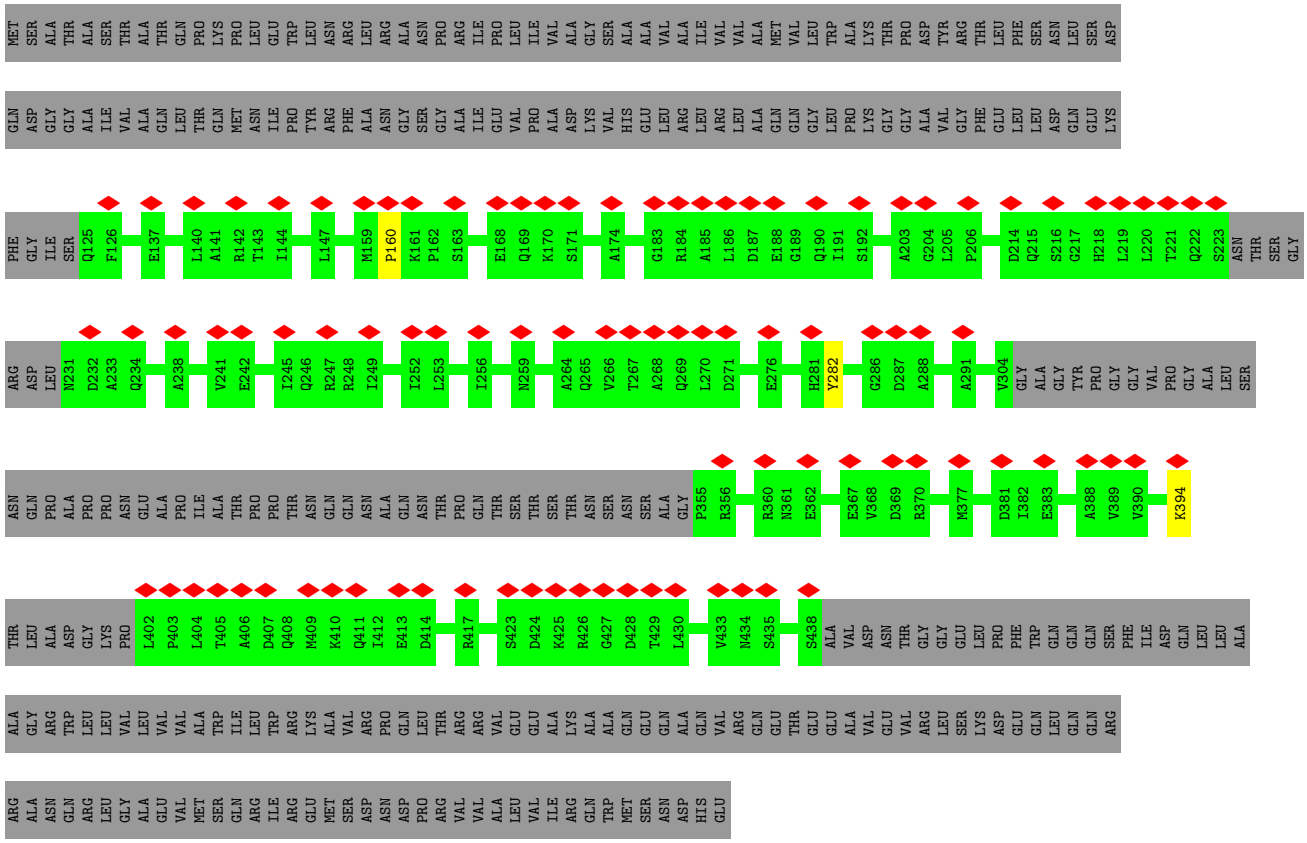
• Molecule 1: Flagellar M-ring protein

Chain f1:



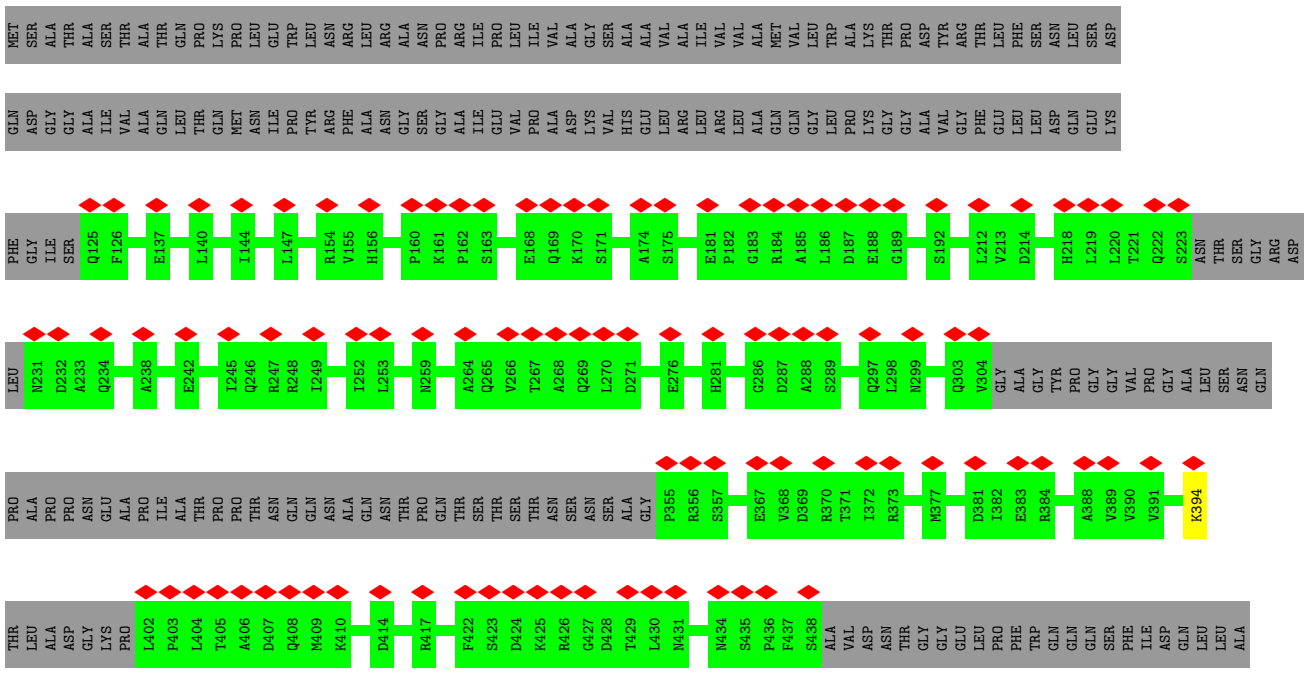
• Molecule 1: Flagellar M-ring protein

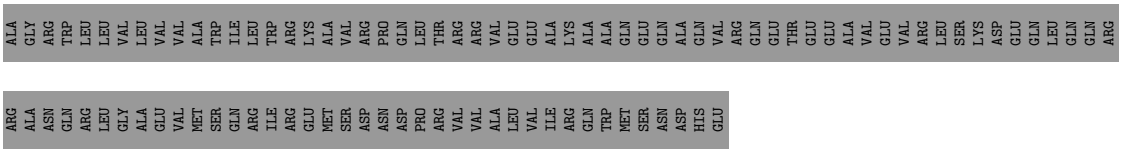
Chain g1:



• Molecule 1: Flagellar M-ring protein

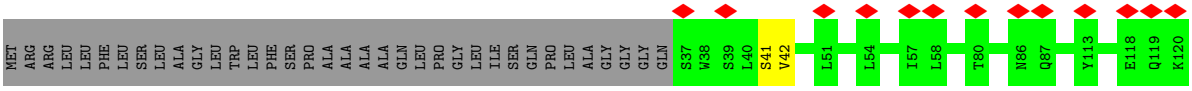
Chain h1:

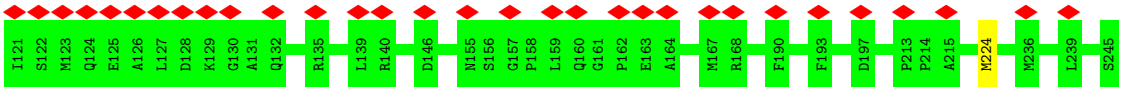





• Molecule 2: Flagellar biosynthetic protein FliP

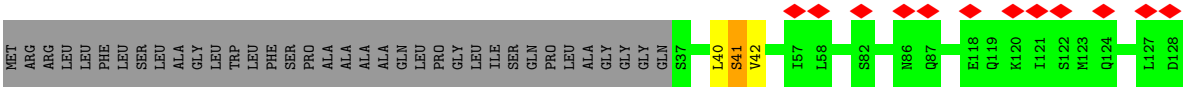
Chain A2:

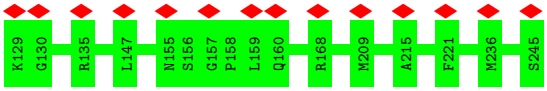



• Molecule 2: Flagellar biosynthetic protein FliP

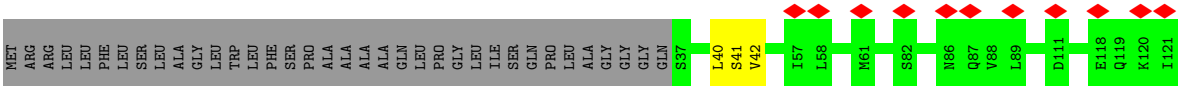
Chain B2:

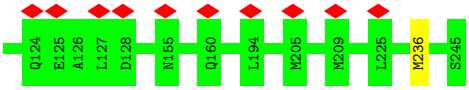



• Molecule 2: Flagellar biosynthetic protein FliP

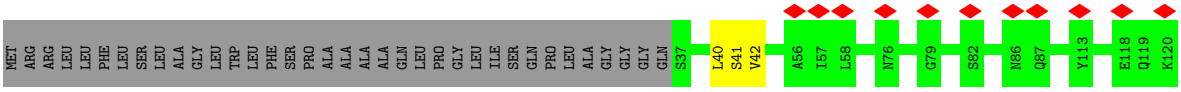
Chain C2:

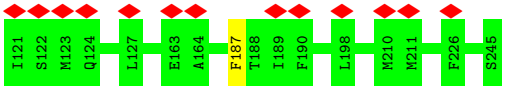



• Molecule 2: Flagellar biosynthetic protein FliP

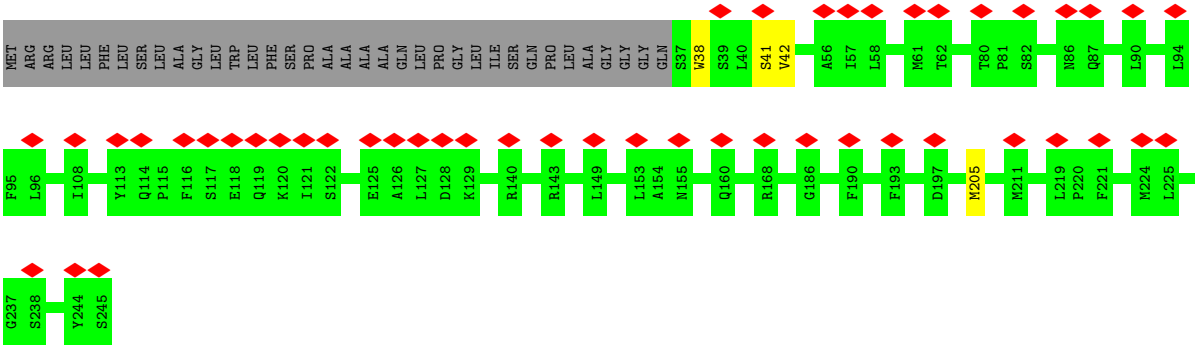
Chain D2:



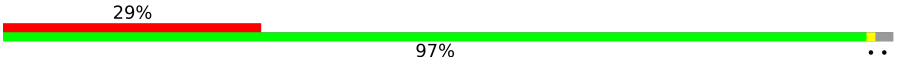
• Molecule 2: Flagellar biosynthetic protein FliP

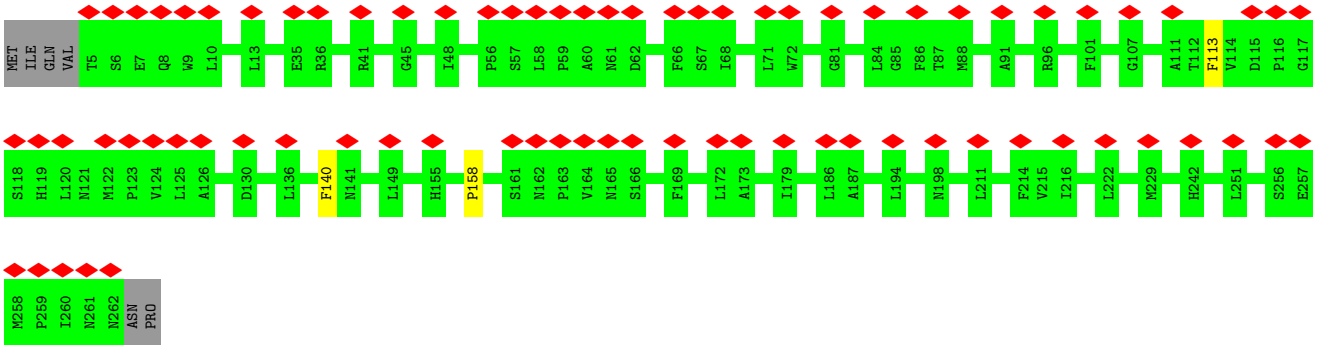
Chain E2:




• Molecule 3: Flagellar biosynthetic protein FliR

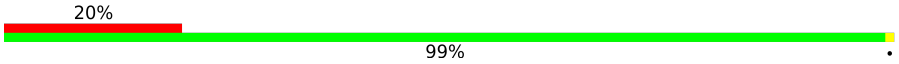
Chain F2:

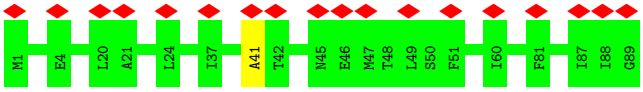



• Molecule 4: Flagellar biosynthetic protein FliQ

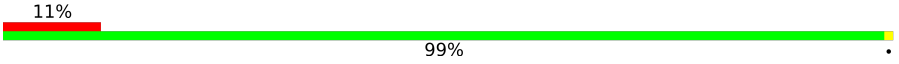
Chain G2:

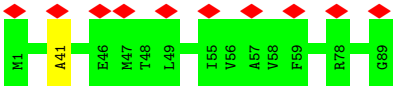



• Molecule 4: Flagellar biosynthetic protein FliQ

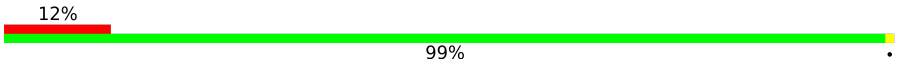
Chain H2:

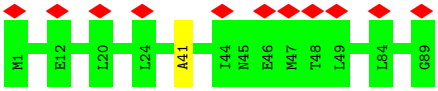



• Molecule 4: Flagellar biosynthetic protein FliQ

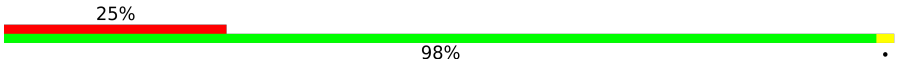
Chain I2:

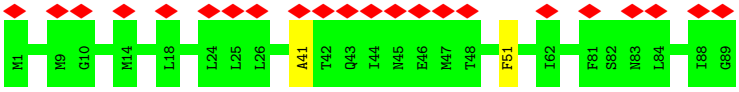





• Molecule 4: Flagellar biosynthetic protein FliQ

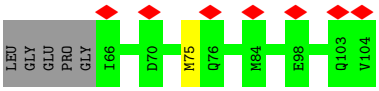
Chain J2:



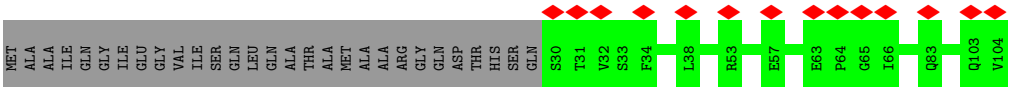

• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain K2:



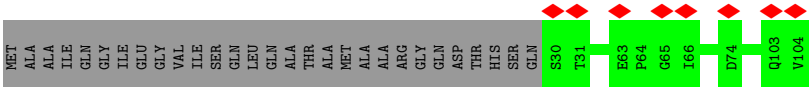

• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain L2:




• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain M2:




• Molecule 5: Flagellar hook-basal body complex protein FliE

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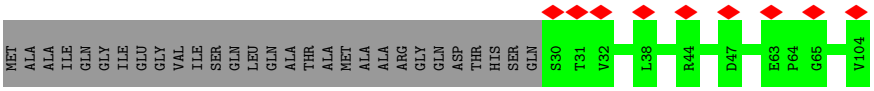
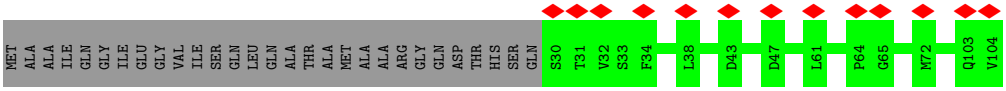
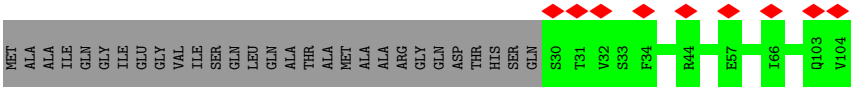



• Molecule 5: Flagellar hook-basal body complex protein FliE

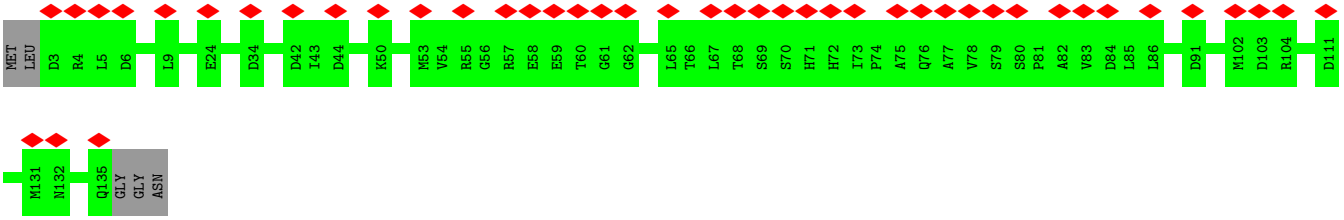
Chain O2:



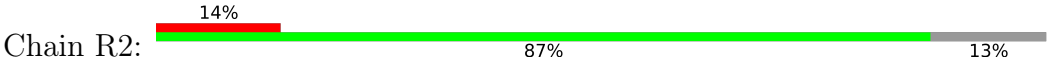

• Molecule 5: Flagellar hook-basal body complex protein FliE

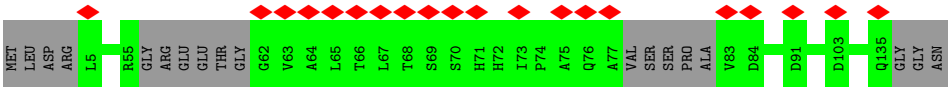



• Molecule 6: Flagellar basal body rod protein FlgB

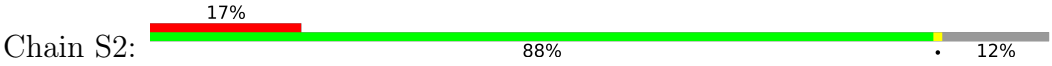


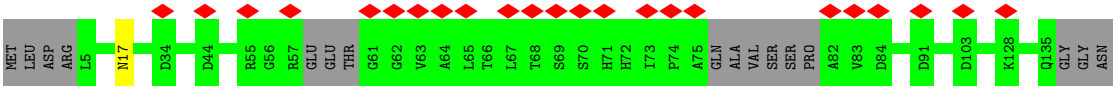

• Molecule 6: Flagellar basal body rod protein FlgB



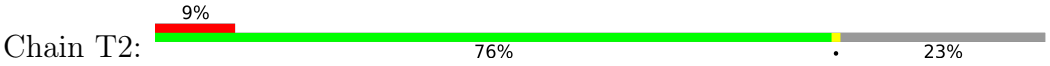



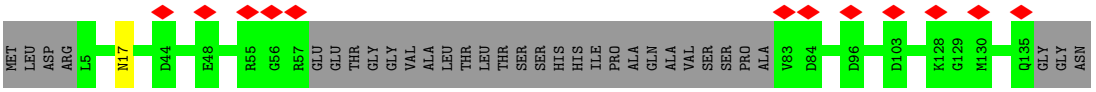

• Molecule 6: Flagellar basal body rod protein FlgB



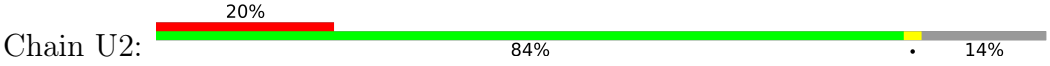



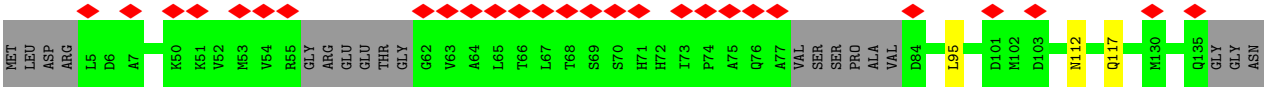

• Molecule 6: Flagellar basal body rod protein FlgB



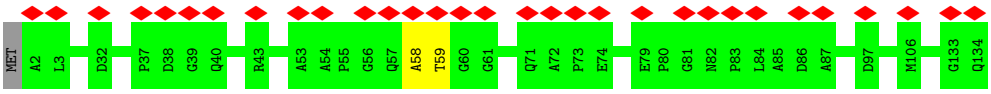




• Molecule 6: Flagellar basal body rod protein FlgB

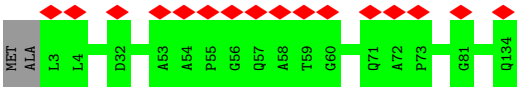




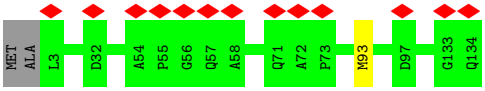

• Molecule 7: Flagellar basal-body rod protein FlgC



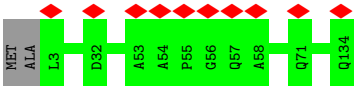

• Molecule 7: Flagellar basal-body rod protein FlgC



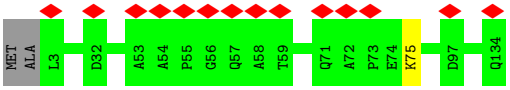

• Molecule 7: Flagellar basal-body rod protein FlgC



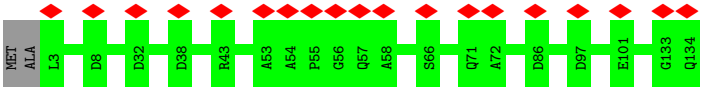

• Molecule 7: Flagellar basal-body rod protein FlgC




• Molecule 7: Flagellar basal-body rod protein FlgC

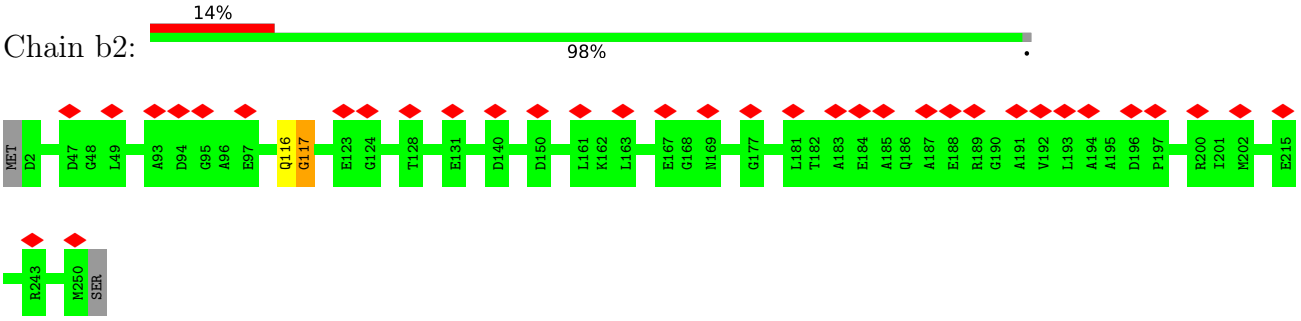



• Molecule 7: Flagellar basal-body rod protein FlgC



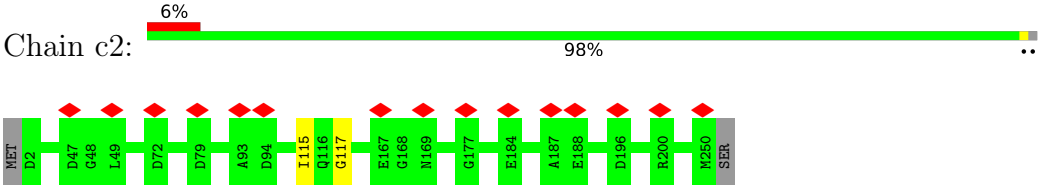

• Molecule 8: Flagellar basal body protein

Chain b2:



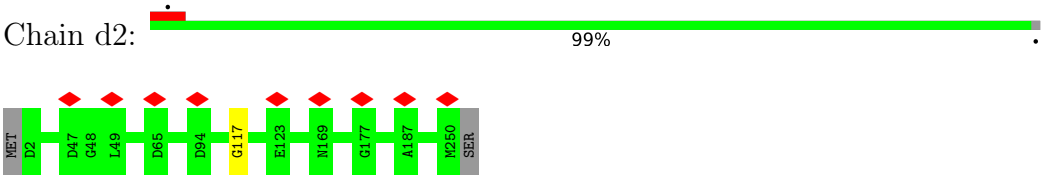

• Molecule 8: Flagellar basal body protein

Chain c2:



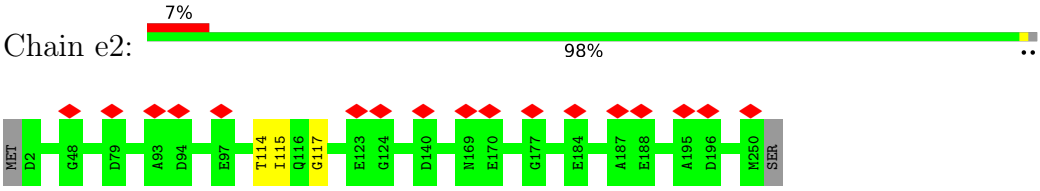

• Molecule 8: Flagellar basal body protein

Chain d2:



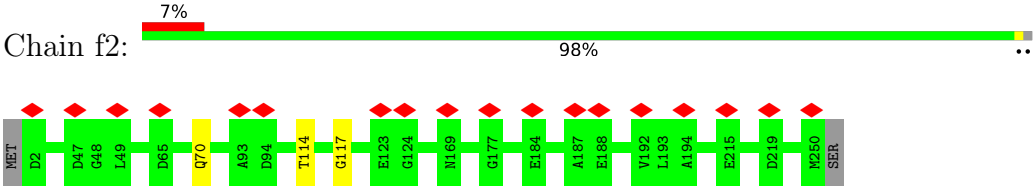

• Molecule 8: Flagellar basal body protein

Chain e2:



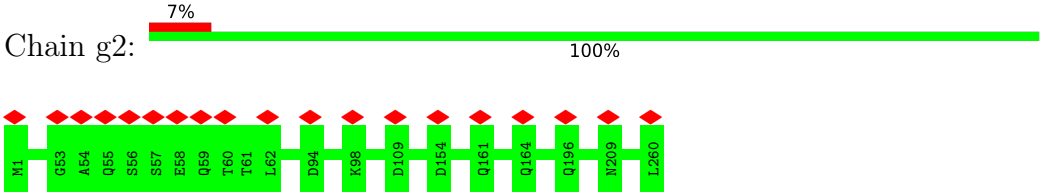

• Molecule 8: Flagellar basal body protein

Chain f2:



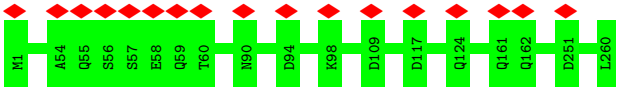

• Molecule 9: Flagellar basal-body rod protein FlgG

Chain g2:



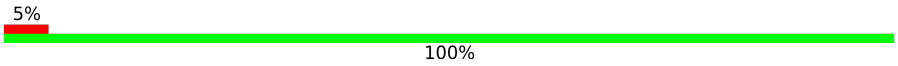

• Molecule 9: Flagellar basal-body rod protein FlgG

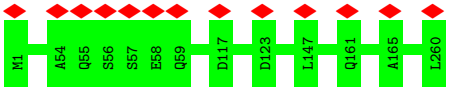
Chain h2:




• Molecule 9: Flagellar basal-body rod protein FlgG

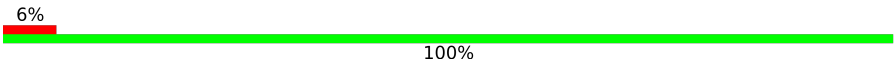
Chain i2:

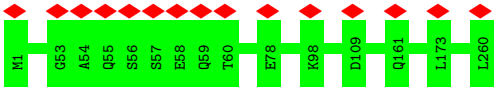



• Molecule 9: Flagellar basal-body rod protein FlgG

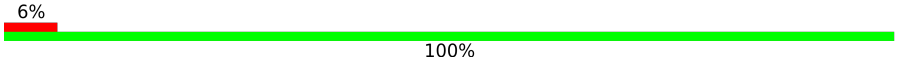
Chain j2:

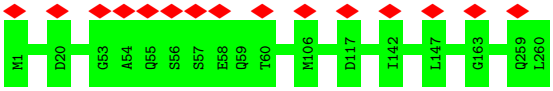



• Molecule 9: Flagellar basal-body rod protein FlgG

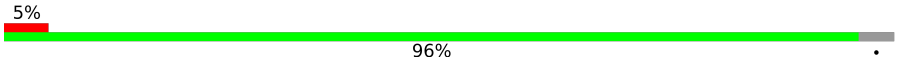
Chain k2:

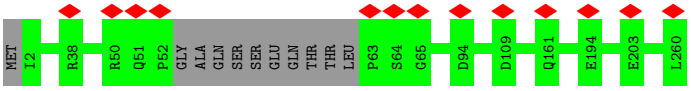



• Molecule 9: Flagellar basal-body rod protein FlgG

Chain l2:




• Molecule 9: Flagellar basal-body rod protein FlgG

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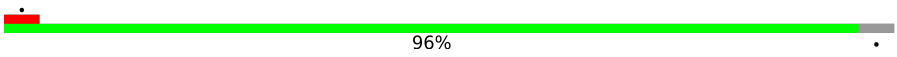
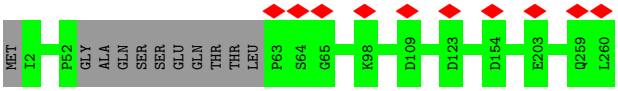
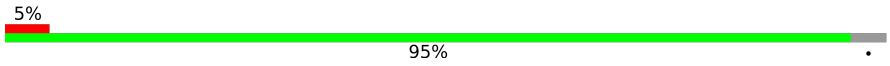
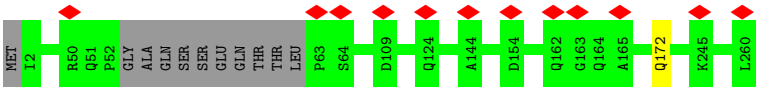



• Molecule 9: Flagellar basal-body rod protein FlgG

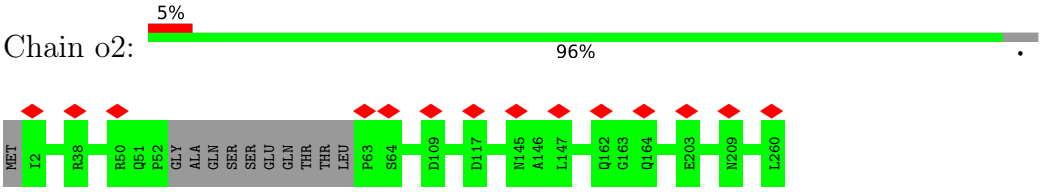
Chain n2:




• Molecule 9: Flagellar basal-body rod protein FlgG

Chain o2:




• Molecule 9: Flagellar basal-body rod protein FlgG

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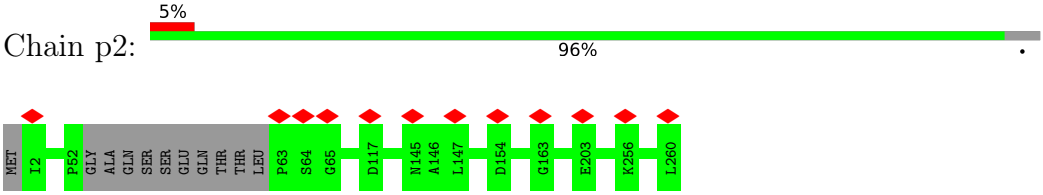
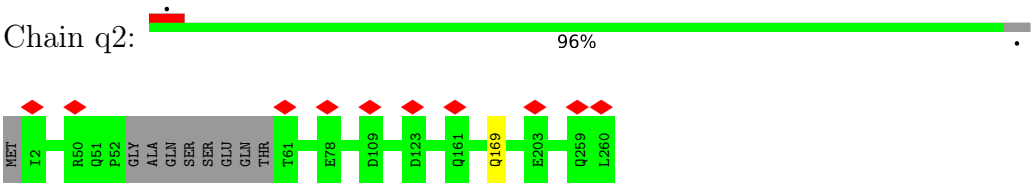


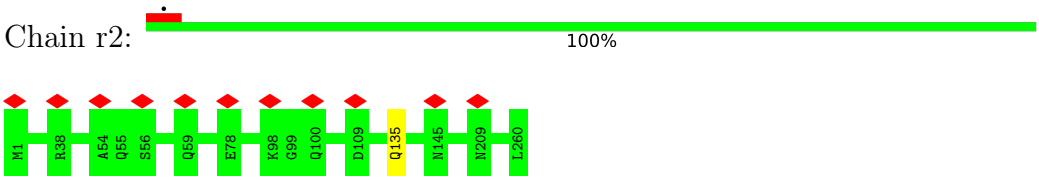

• Molecule 9: Flagellar basal-body rod protein FlgG

Chain q2:



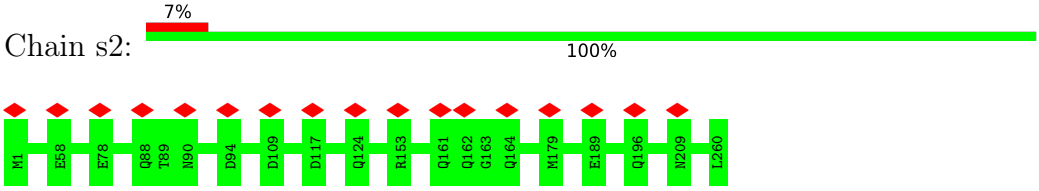

• Molecule 9: Flagellar basal-body rod protein FlgG

Chain r2:




• Molecule 9: Flagellar basal-body rod protein FlgG

Chain s2:




• Molecule 9: Flagellar basal-body rod protein FlgG

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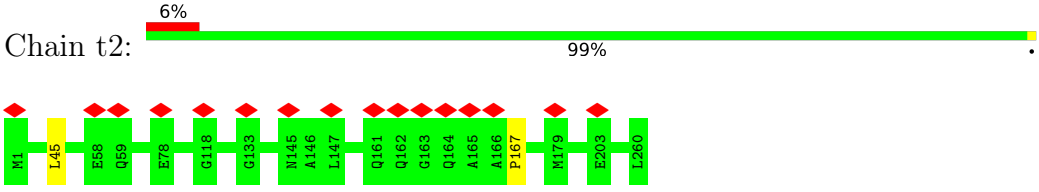
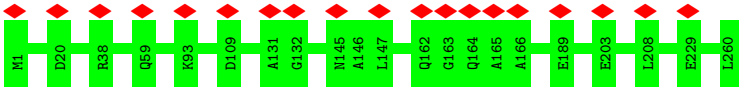


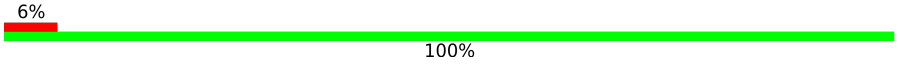

• Molecule 9: Flagellar basal-body rod protein FlgG

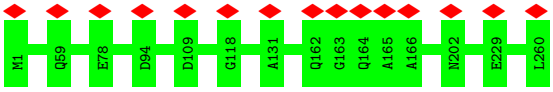
Chain u2:




• Molecule 9: Flagellar basal-body rod protein FlgG

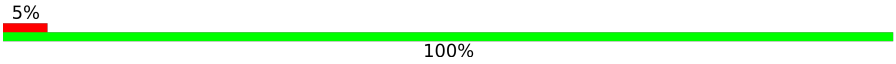
Chain v2:

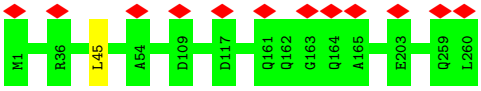



• Molecule 9: Flagellar basal-body rod protein FlgG

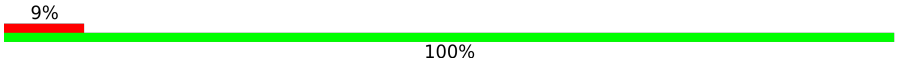
Chain w2:

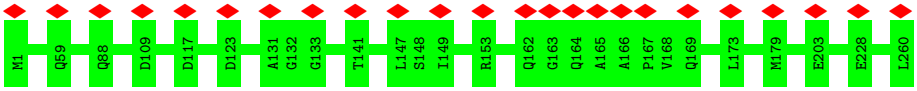



• Molecule 9: Flagellar basal-body rod protein FlgG

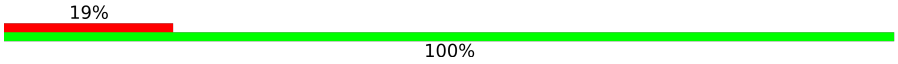
Chain x2:

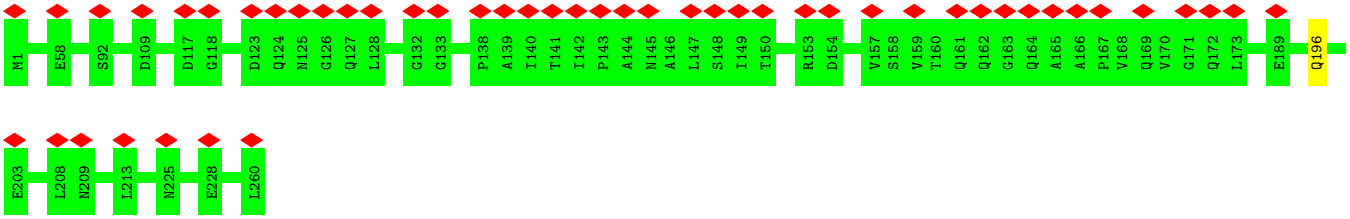



• Molecule 9: Flagellar basal-body rod protein FlgG

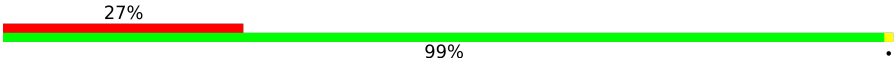
Chain y2:

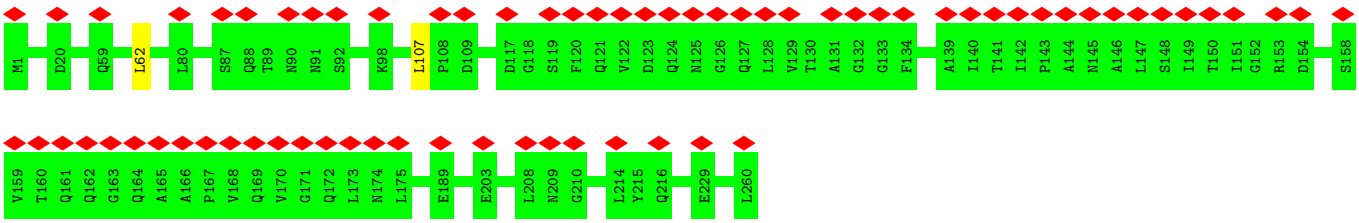



• Molecule 9: Flagellar basal-body rod protein FlgG

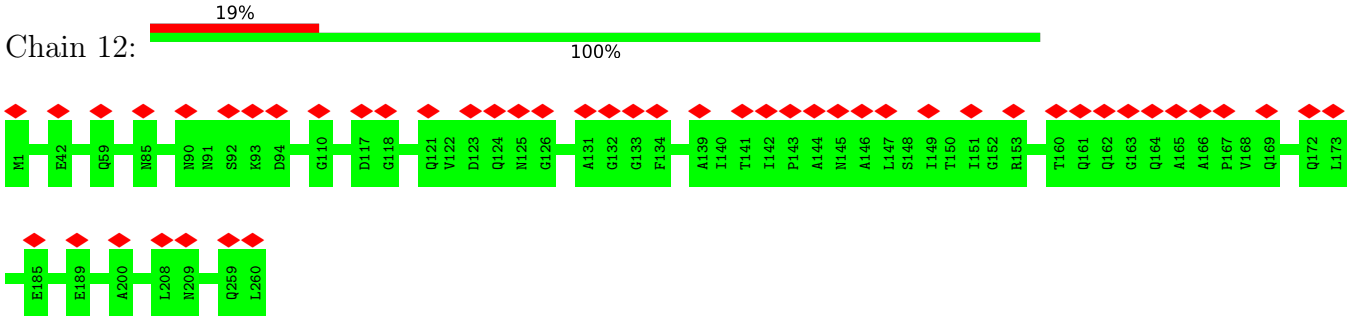
Chain z2:



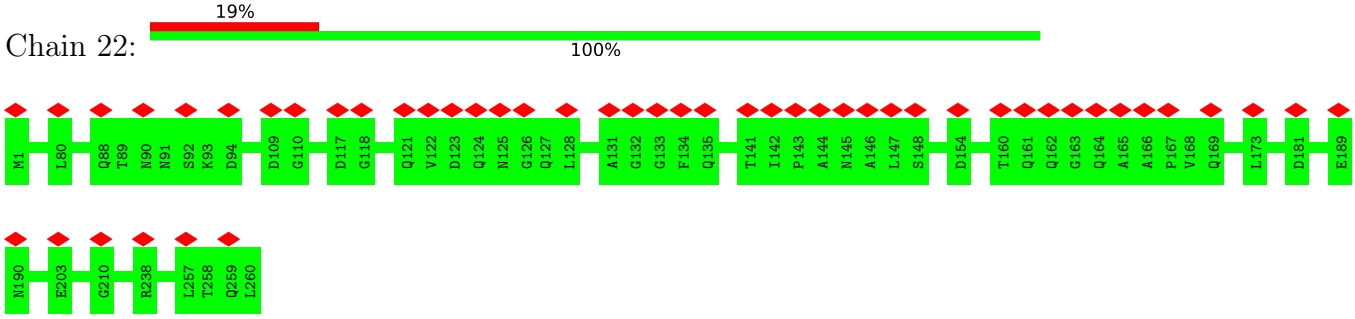

• Molecule 9: Flagellar basal-body rod protein FlgG

Chain 12:



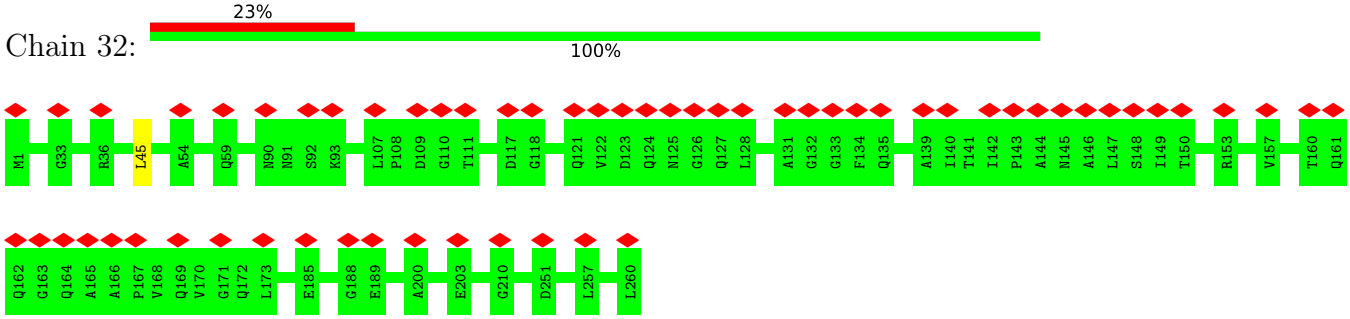

• Molecule 9: Flagellar basal-body rod protein FlgG

Chain 22:



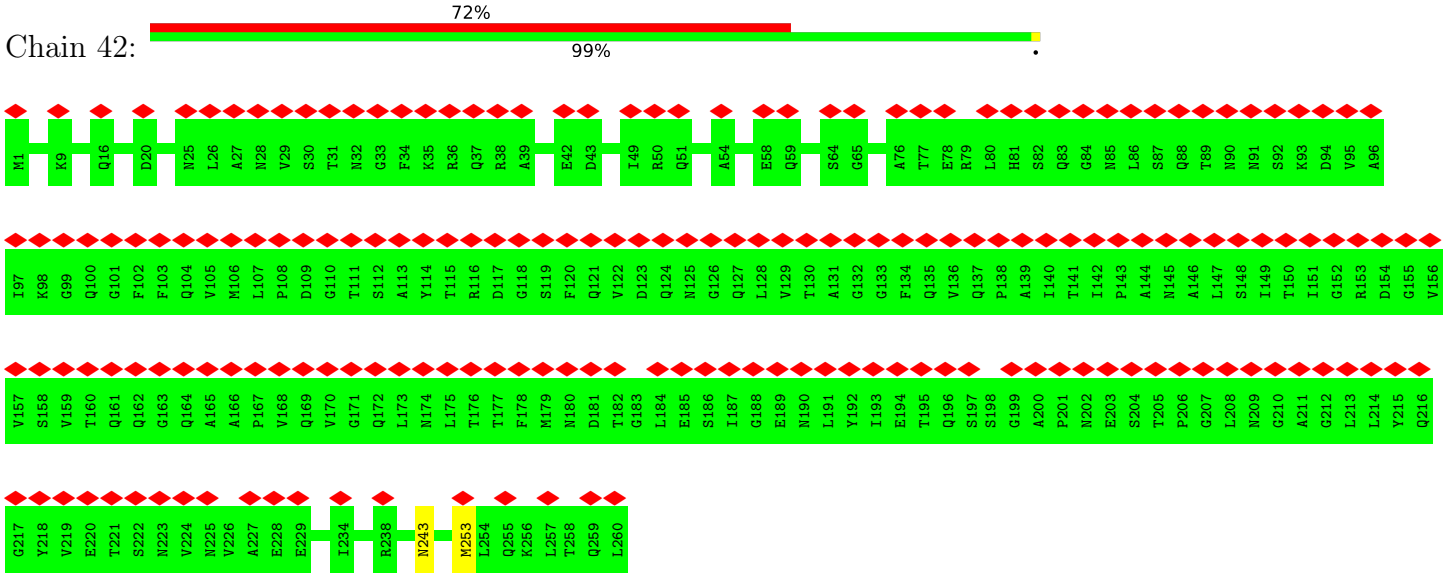

• Molecule 9: Flagellar basal-body rod protein FlgG

Chain 32:



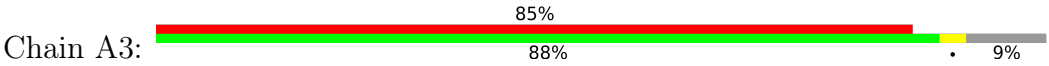

• Molecule 9: Flagellar basal-body rod protein FlgG

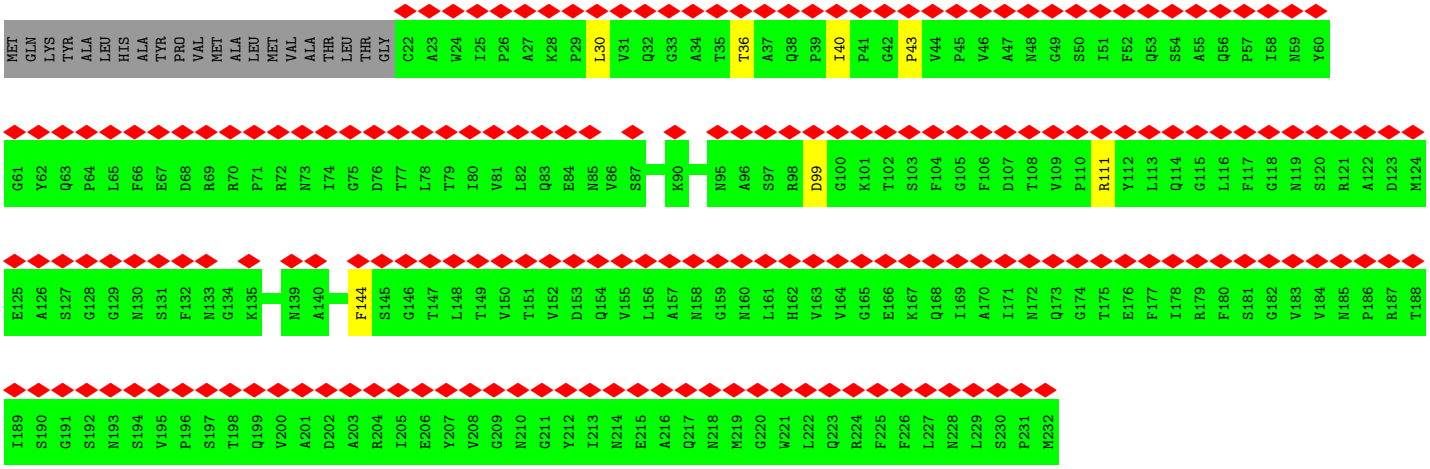
Chain 42:



• Molecule 10: Flagellar L-ring protein

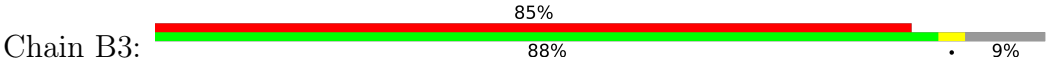
Chain A3:

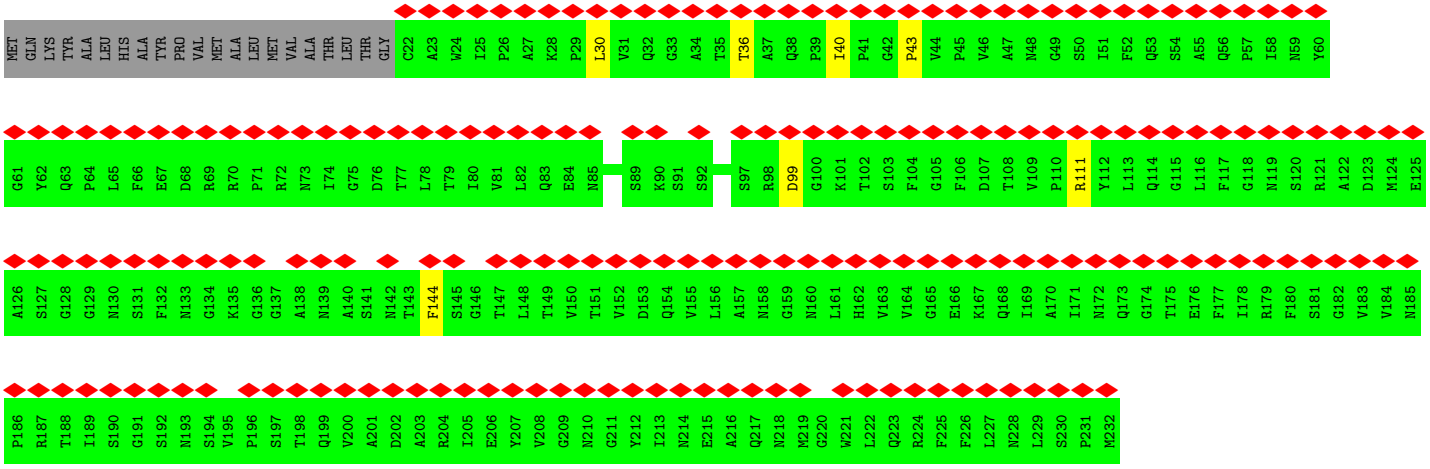



• Molecule 10: Flagellar L-ring protein

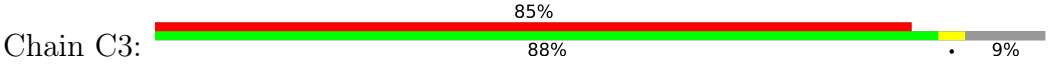
Chain B3:

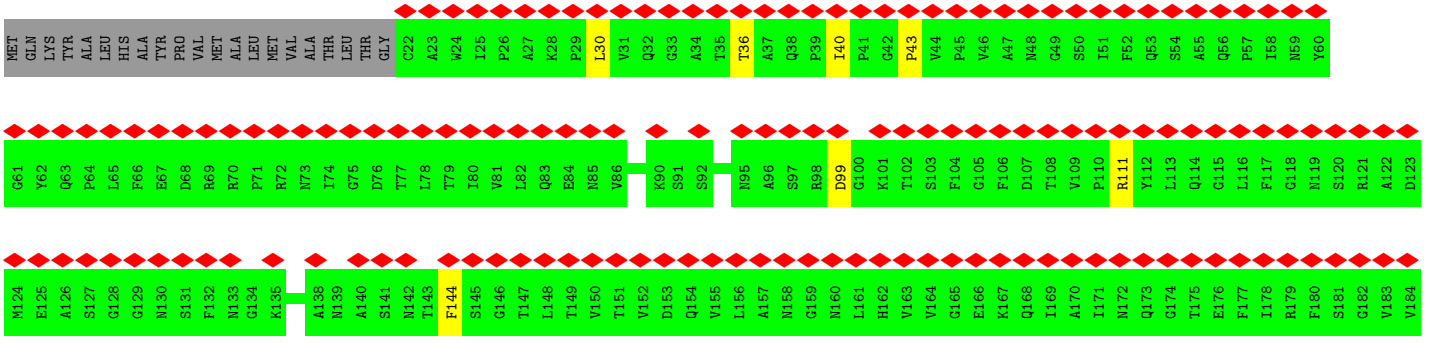



• Molecule 10: Flagellar L-ring protein

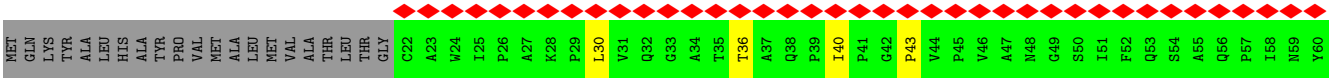
Chain C3:

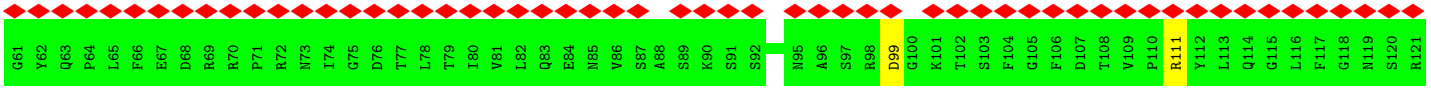


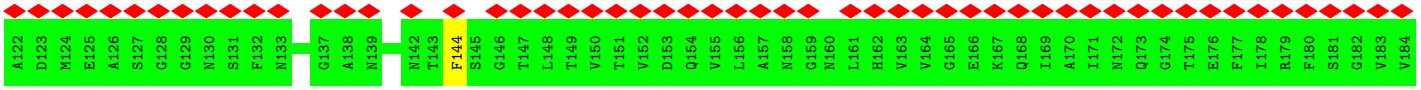



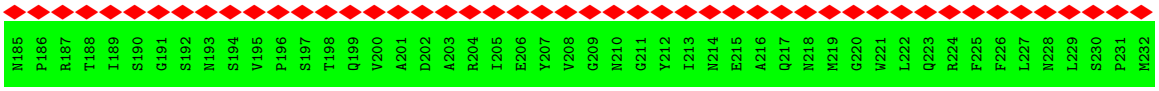
• Molecule 10: Flagellar L-ring protein

Chain D3:



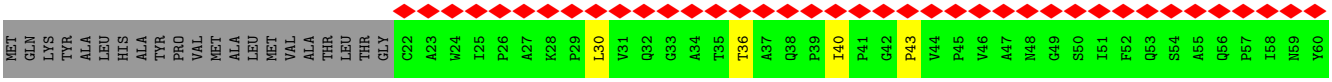



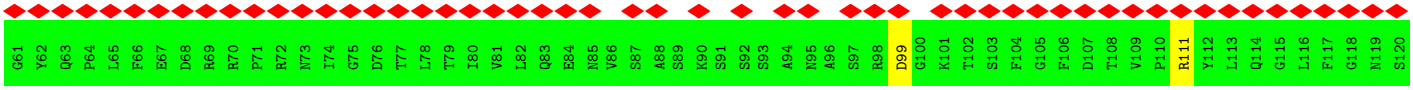



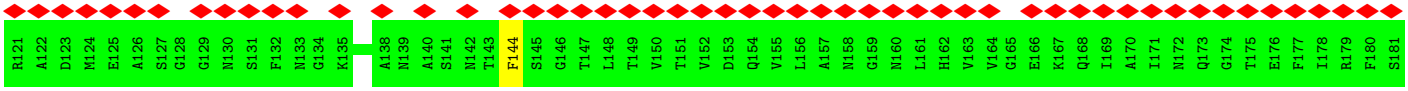



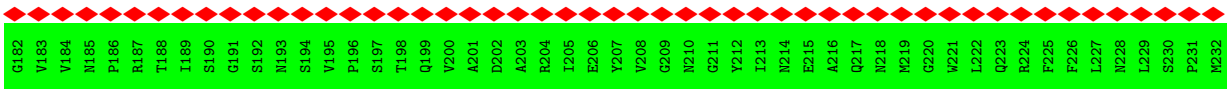

• Molecule 10: Flagellar L-ring protein

Chain E3:



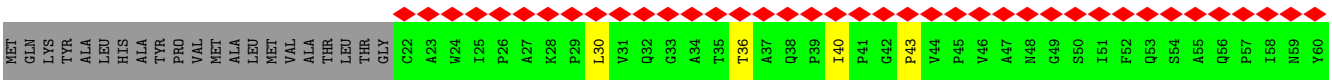



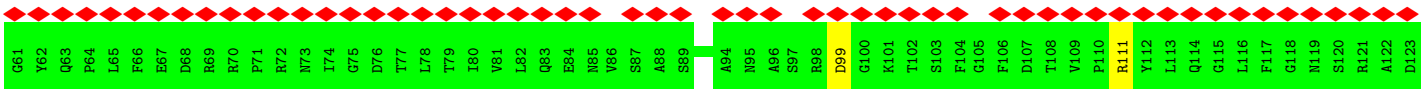



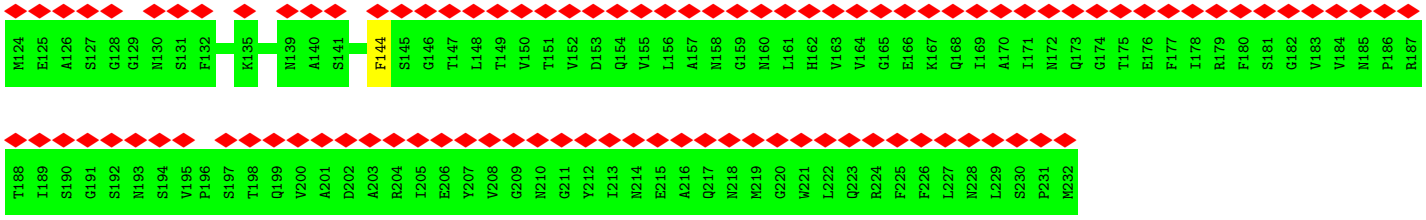




• Molecule 10: Flagellar L-ring protein

Chain F3:

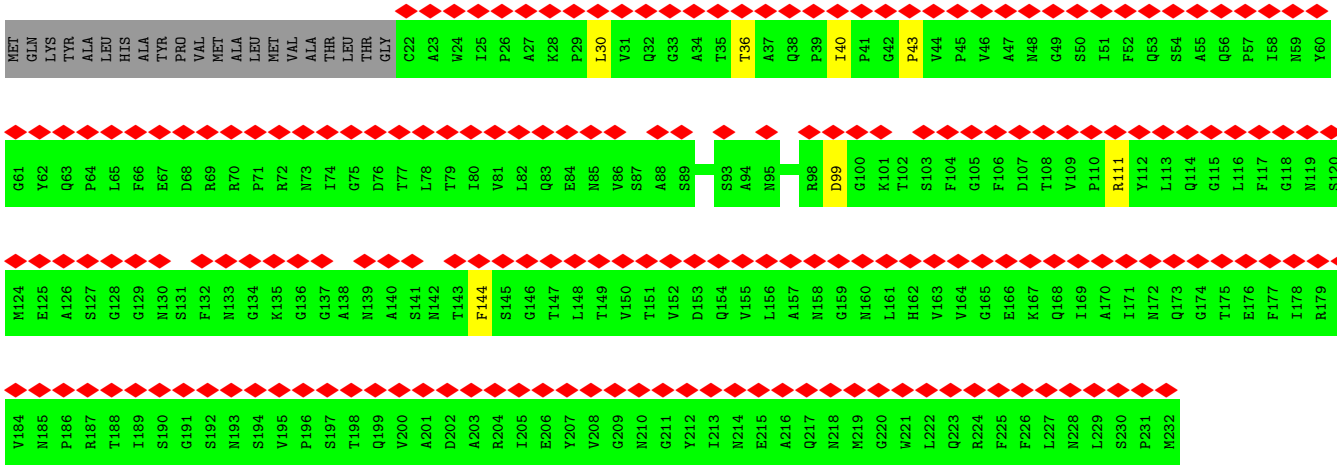




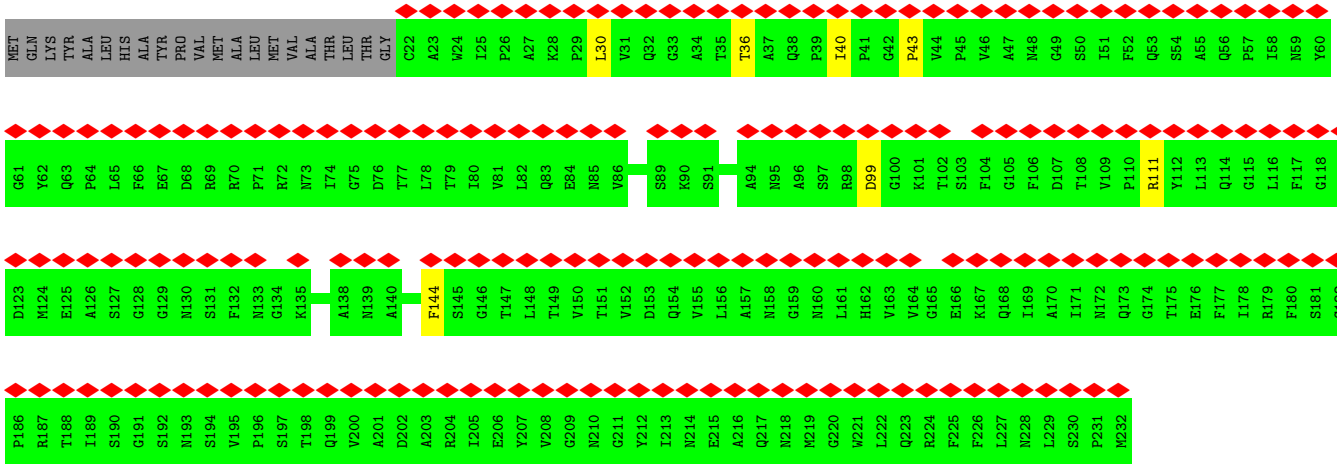

• Molecule 10: Flagellar L-ring protein

Chain G3:



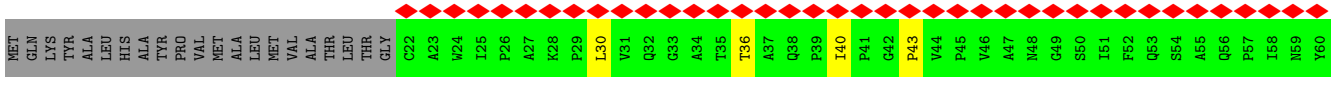

• Molecule 10: Flagellar L-ring protein

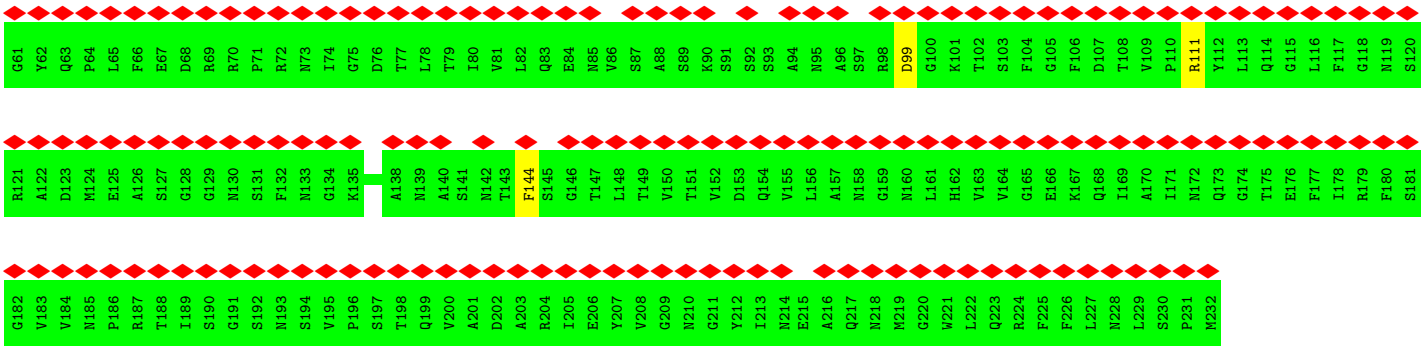
Chain H3:




• Molecule 10: Flagellar L-ring protein

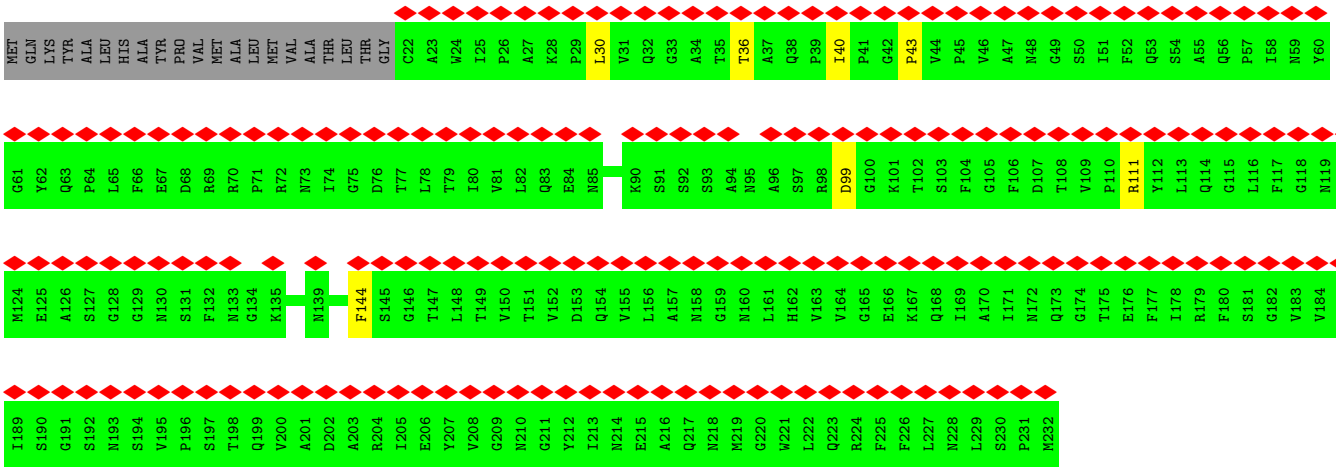
Chain I3:





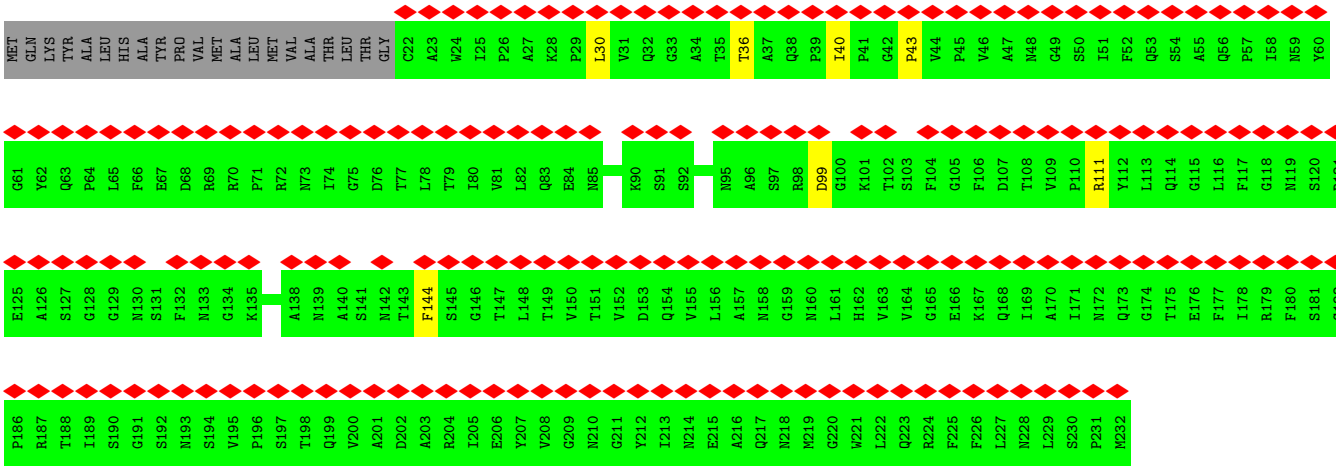

• Molecule 10: Flagellar L-ring protein

Chain J3:



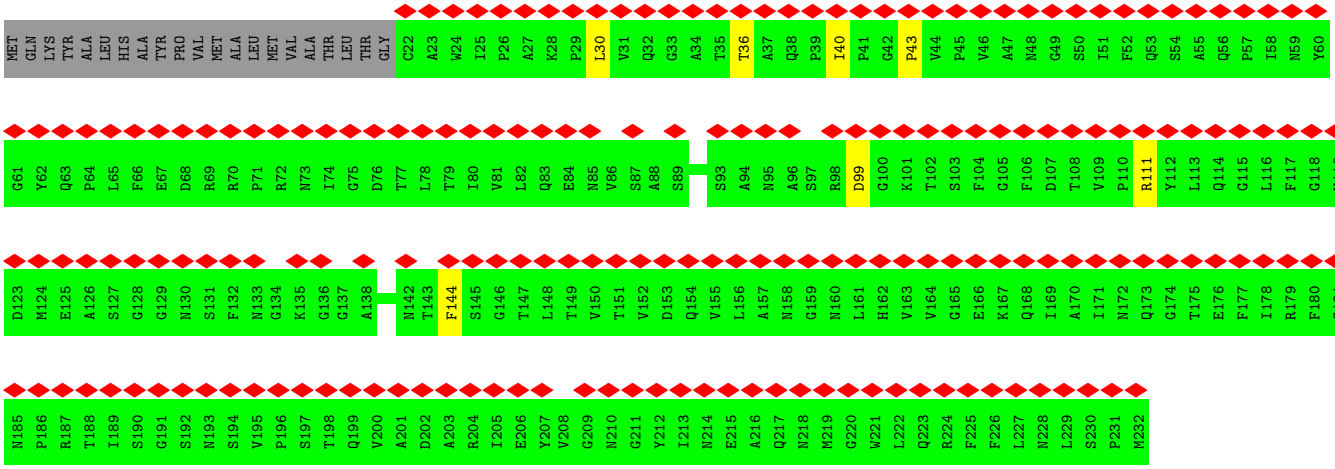

• Molecule 10: Flagellar L-ring protein

Chain K3:



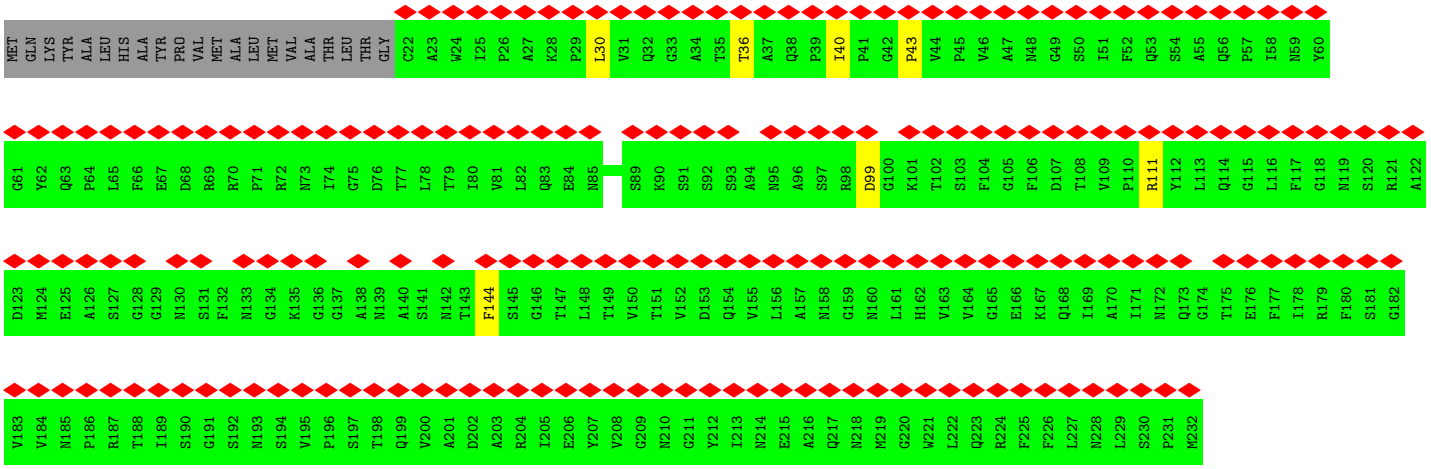

• Molecule 10: Flagellar L-ring protein

Chain L3:



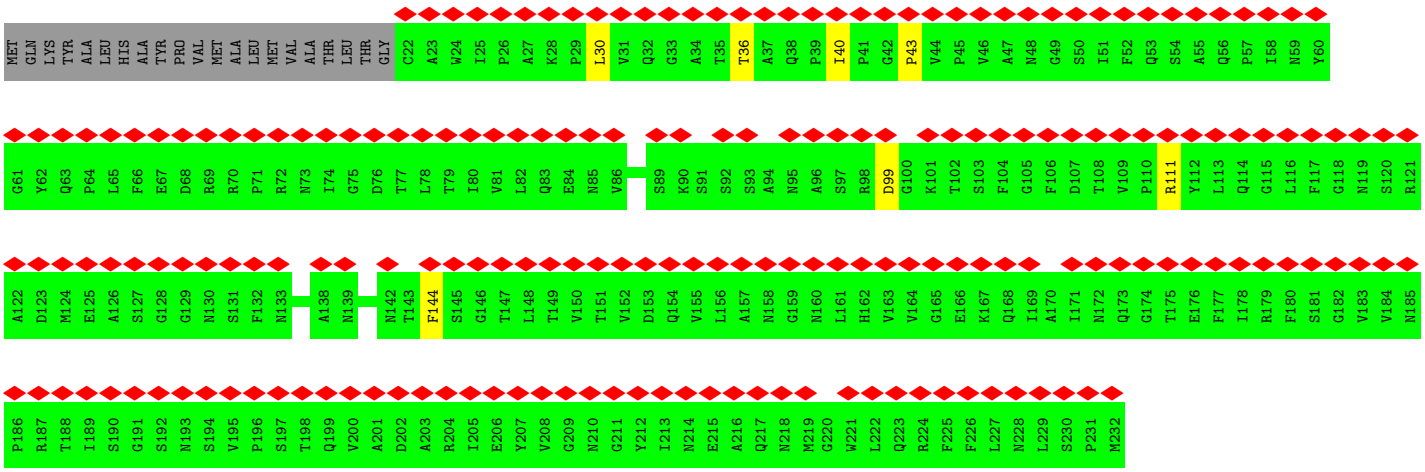

• Molecule 10: Flagellar L-ring protein

Chain M3:



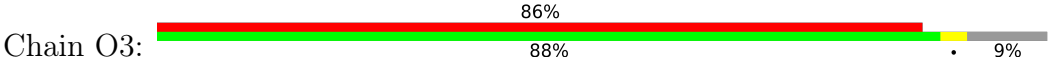

• Molecule 10: Flagellar L-ring protein

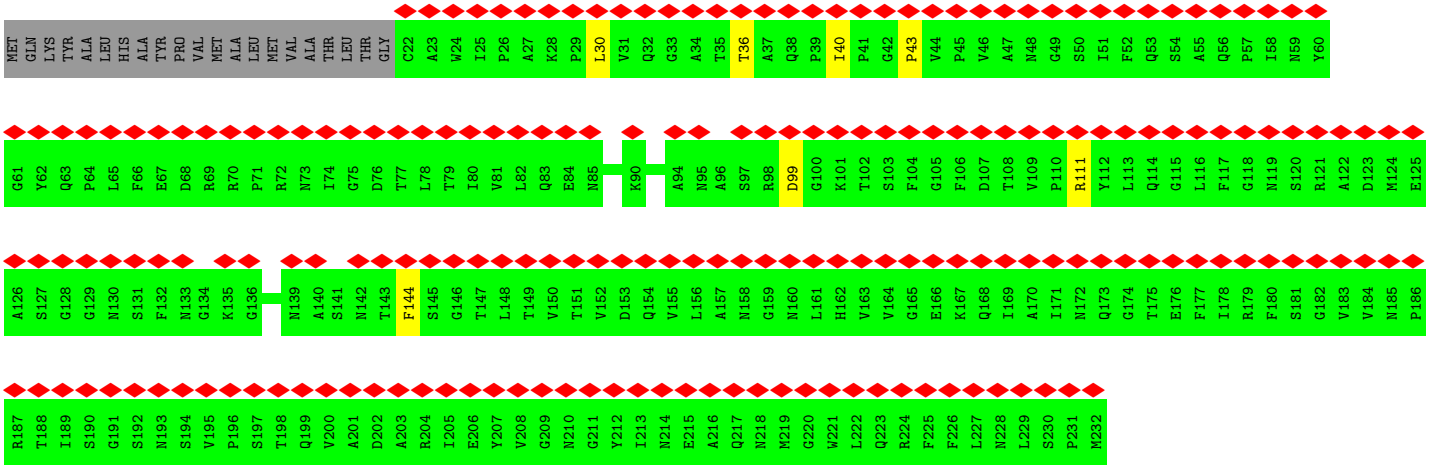
Chain N3:



• Molecule 10: Flagellar L-ring protein

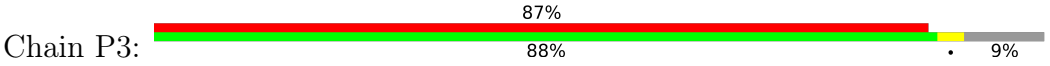
Chain O3:

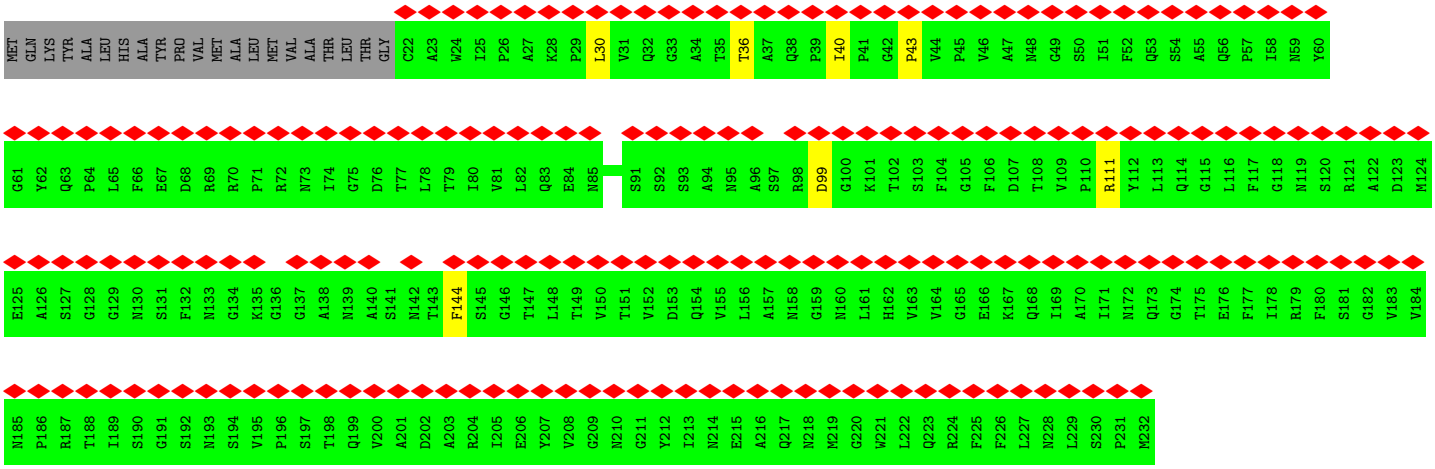



• Molecule 10: Flagellar L-ring protein

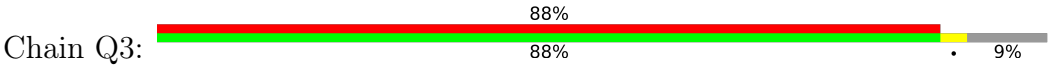
Chain P3:

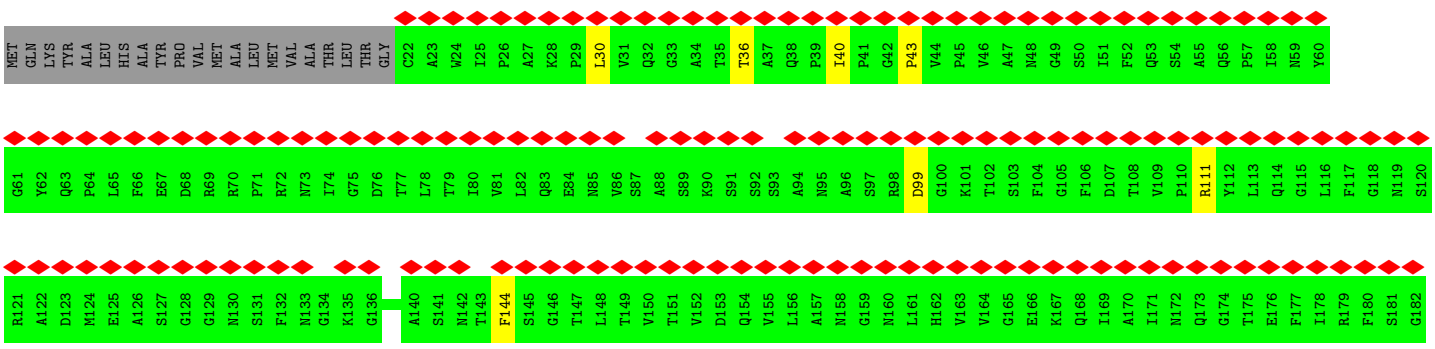


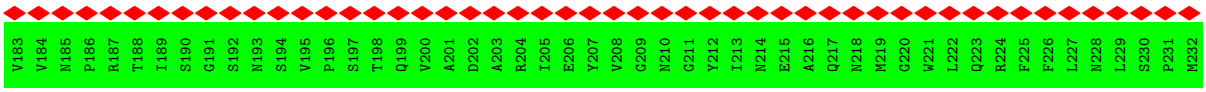




• Molecule 10: Flagellar L-ring protein

Chain Q3:

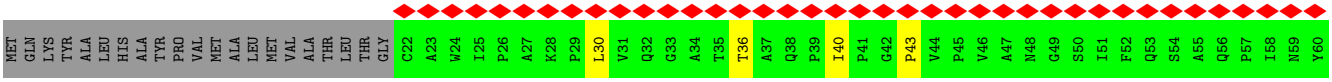


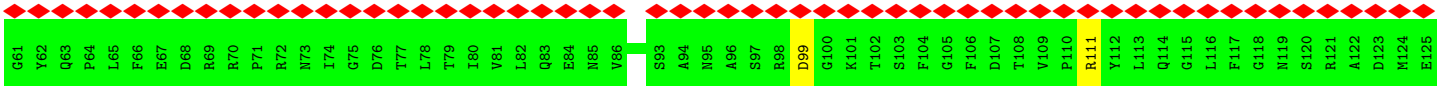



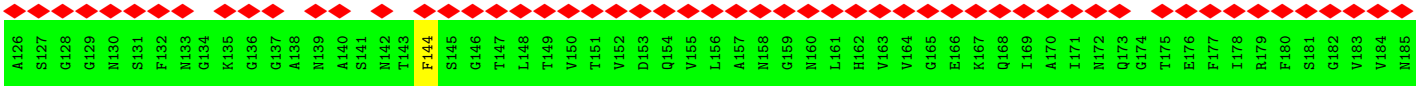


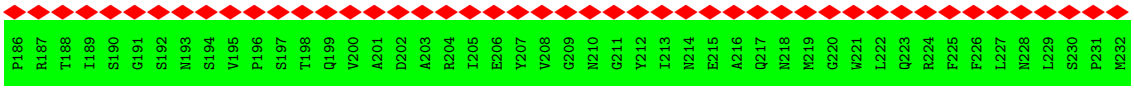

• Molecule 10: Flagellar L-ring protein

Chain R3:



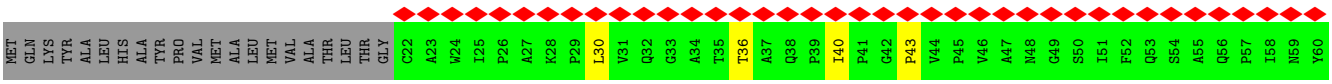



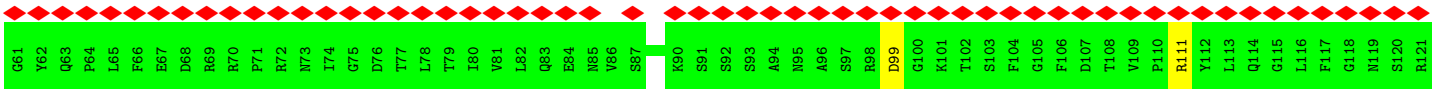



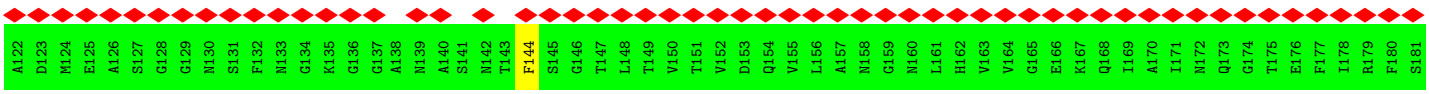



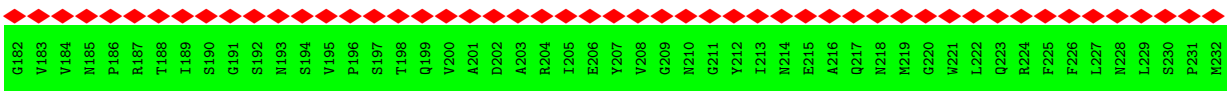

• Molecule 10: Flagellar L-ring protein

Chain S3:



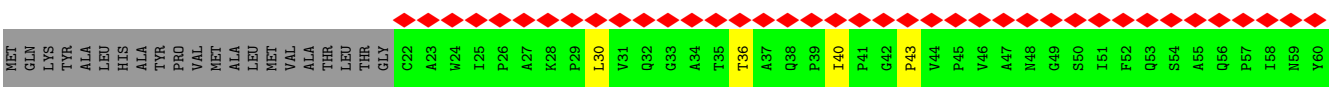



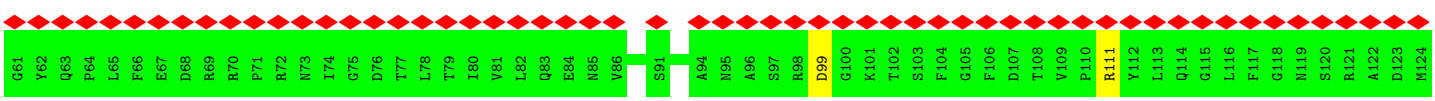



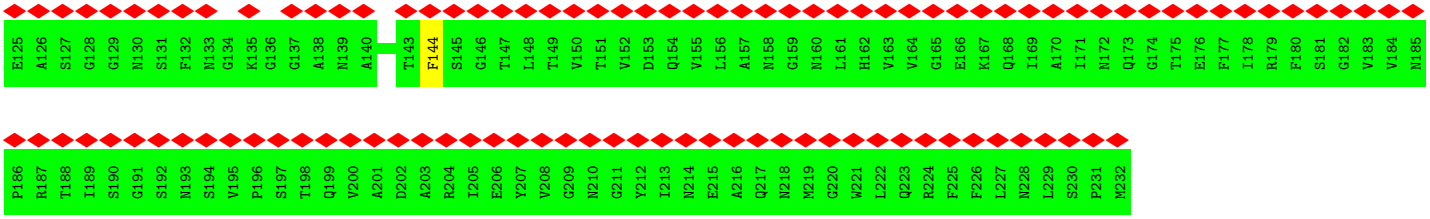




• Molecule 10: Flagellar L-ring protein

Chain T3:

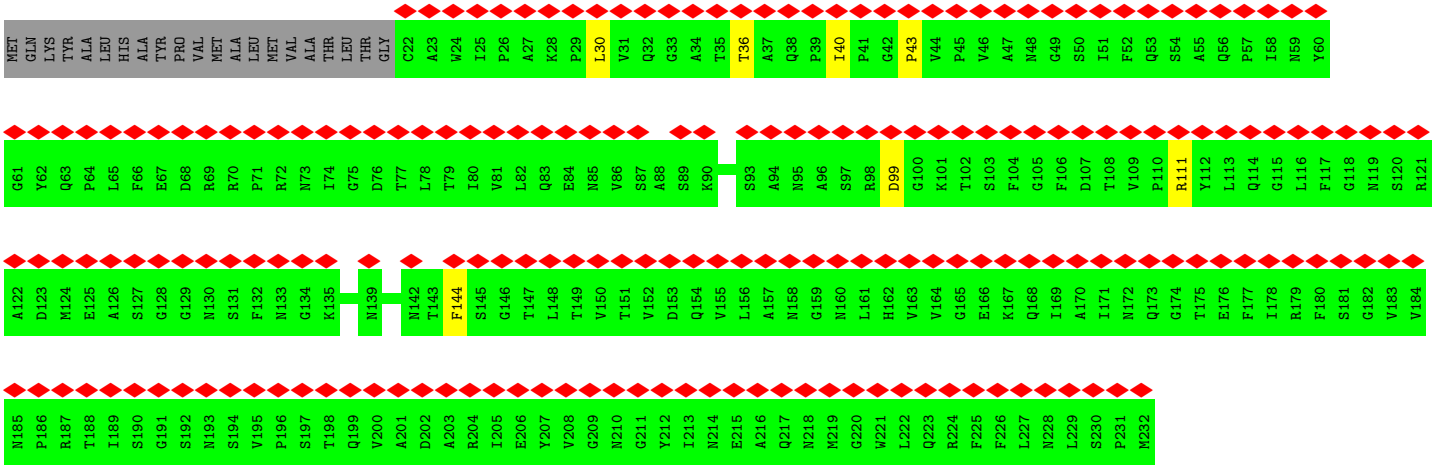




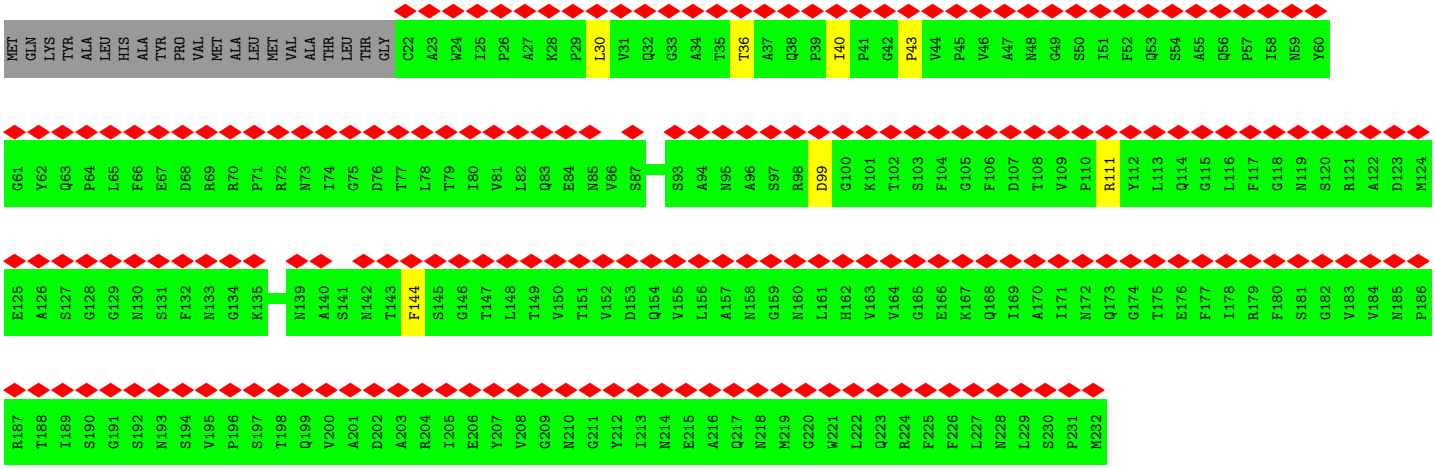

• Molecule 10: Flagellar L-ring protein

Chain U3:



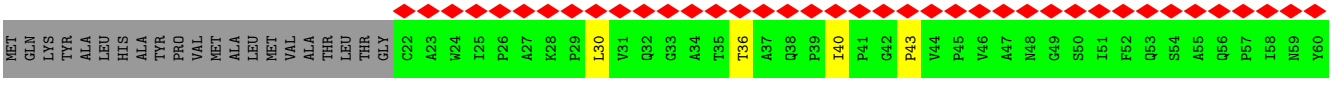

• Molecule 10: Flagellar L-ring protein

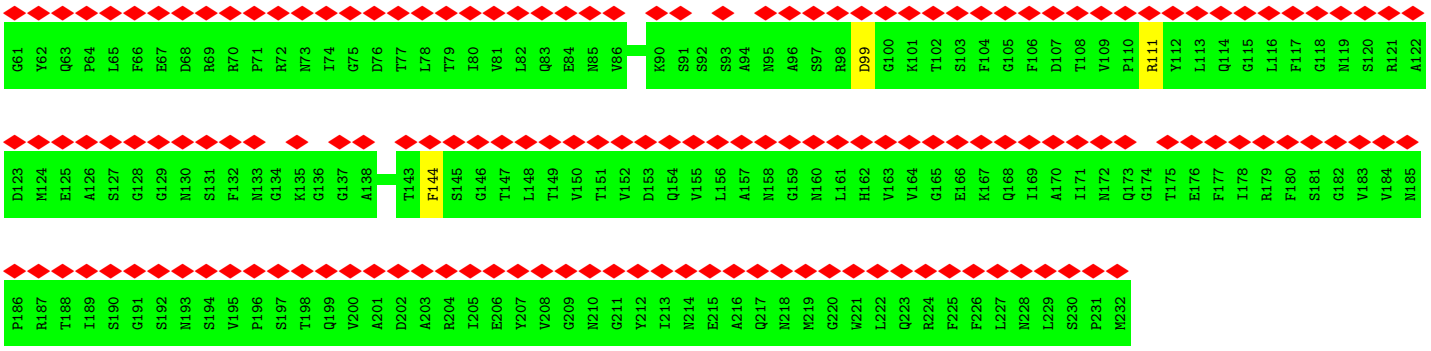
Chain V3:




• Molecule 10: Flagellar L-ring protein

Chain W3:



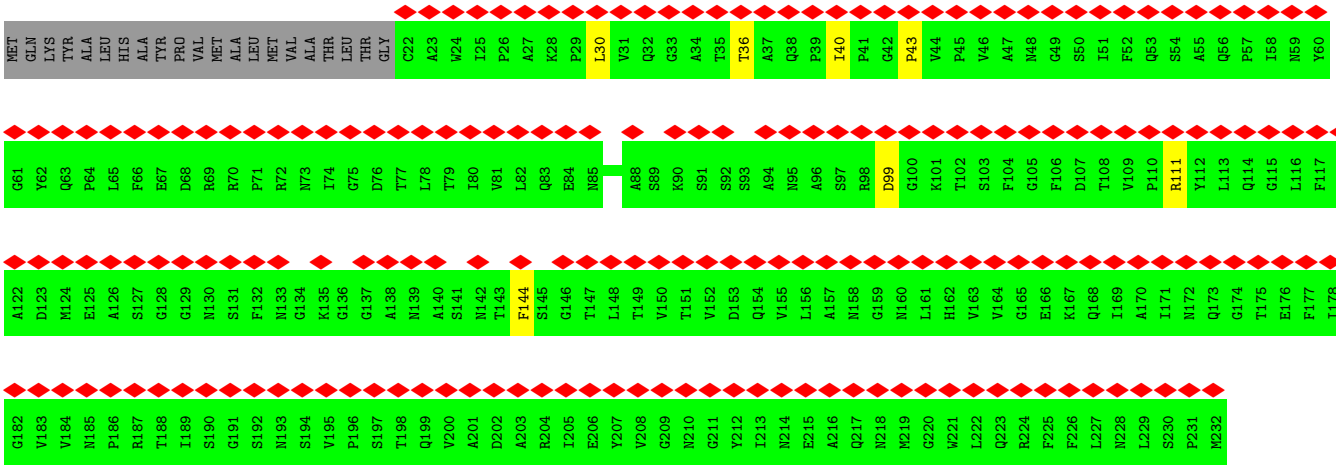



• Molecule 10: Flagellar L-ring protein

Chain X3:

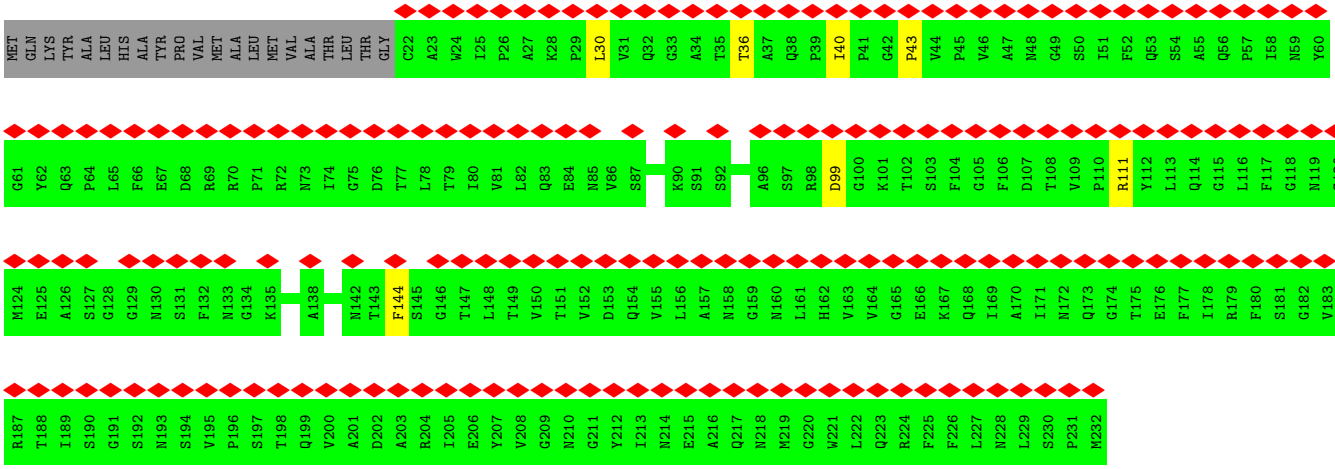
• Molecule 10: Flagellar L-ring protein

Chain Y3:



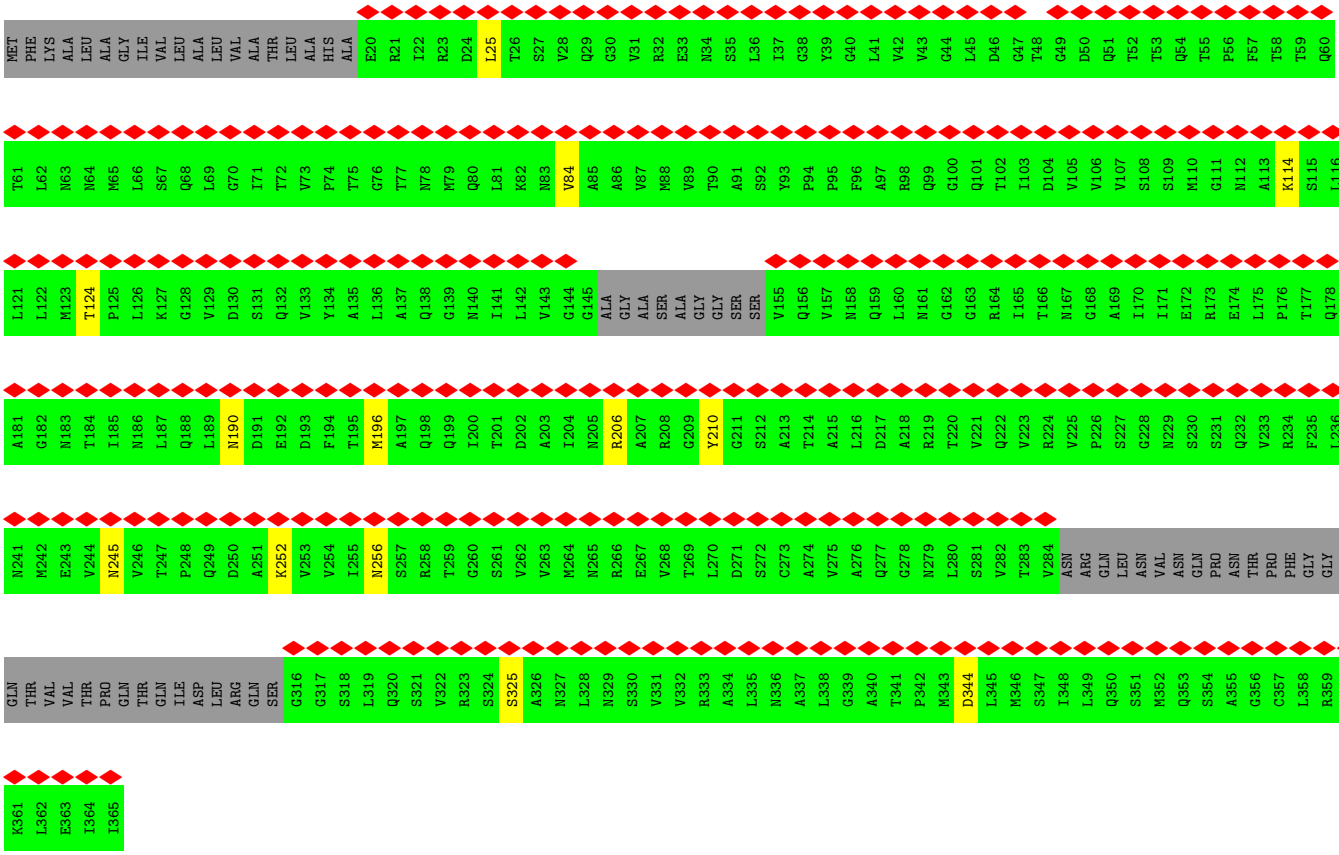

• Molecule 10: Flagellar L-ring protein

Chain Z3:



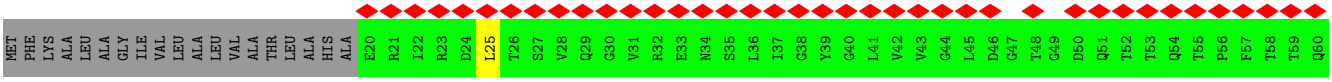

• Molecule 11: Flagellar P-ring protein

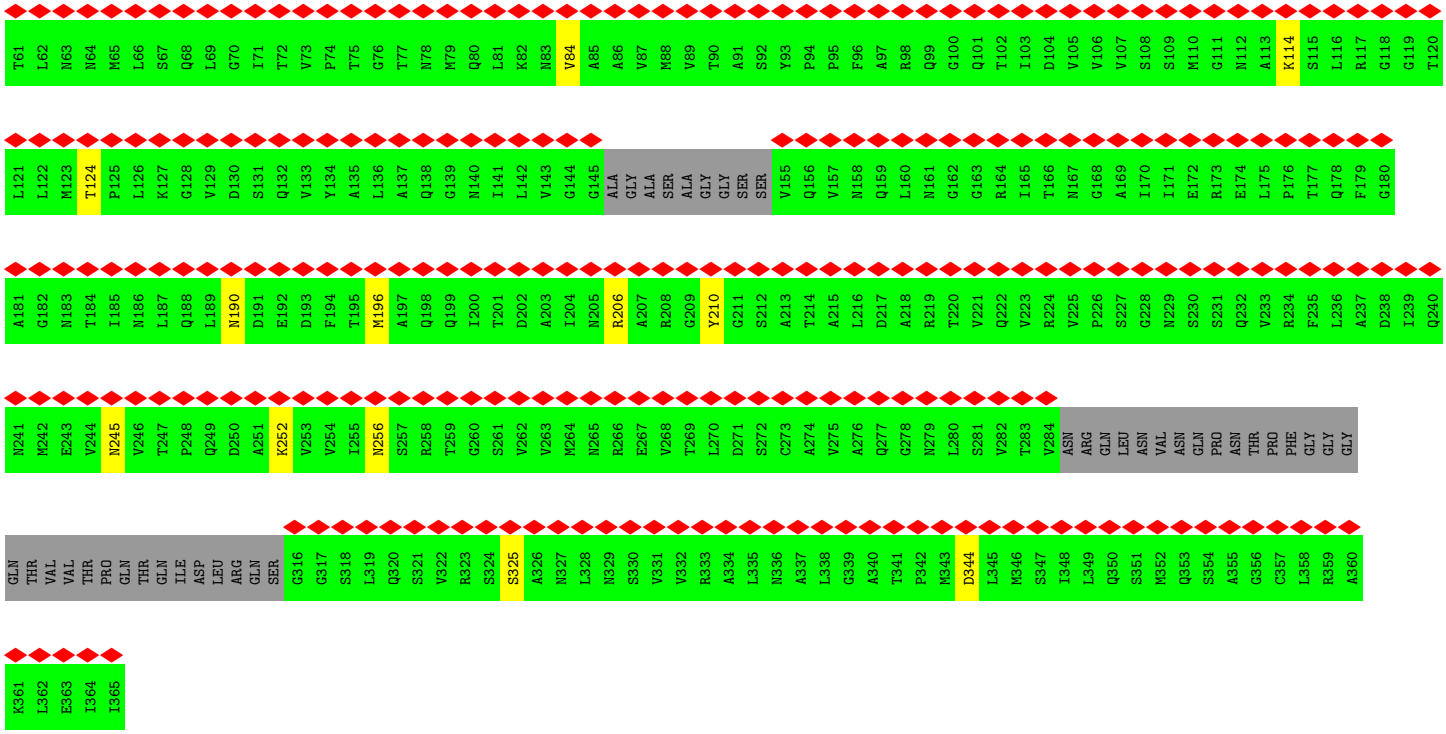
Chain a3:




• Molecule 11: Flagellar P-ring protein

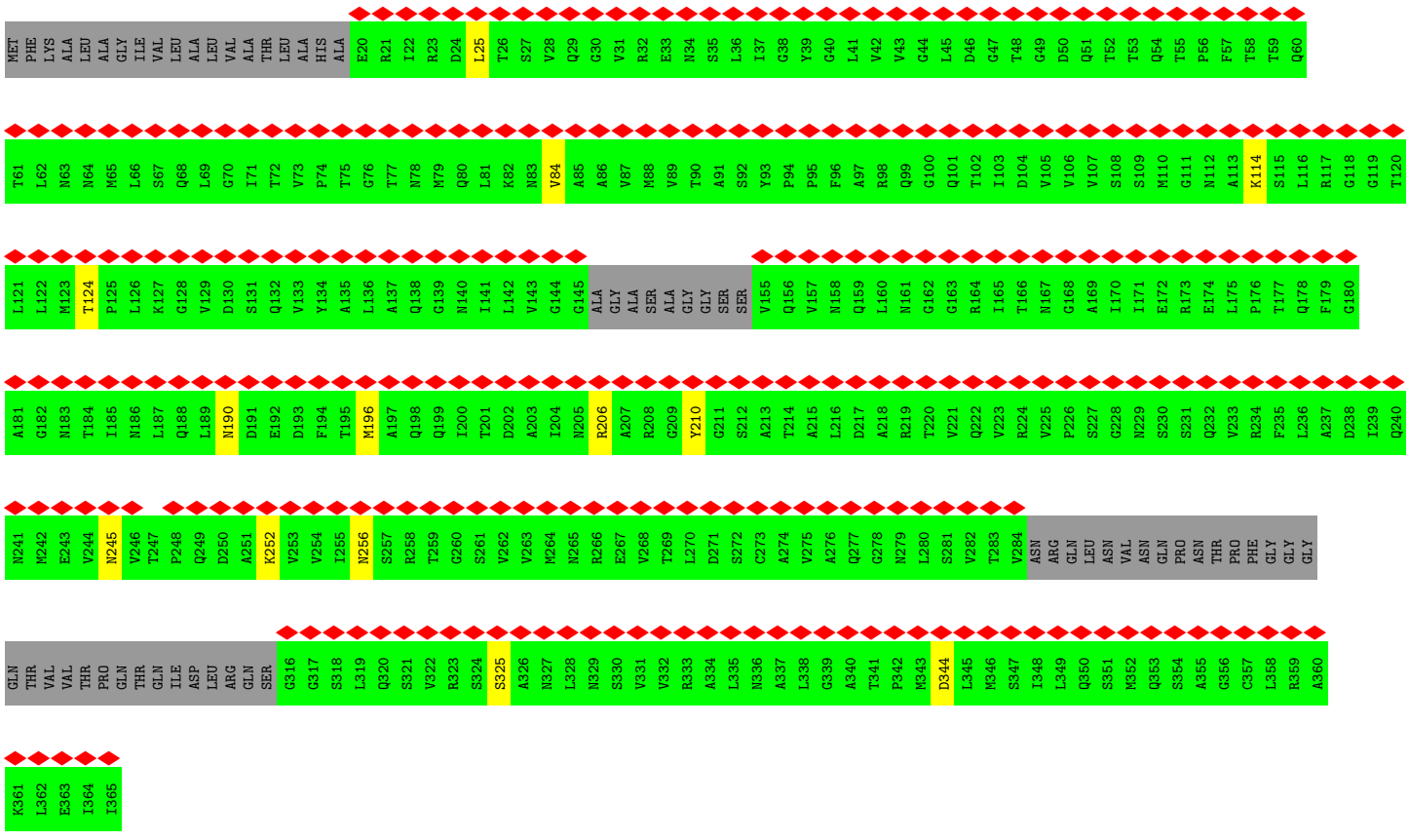
Chain b3:





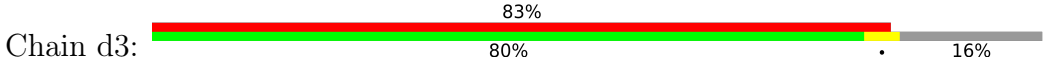

- Molecule 11: Flagellar P-ring protein

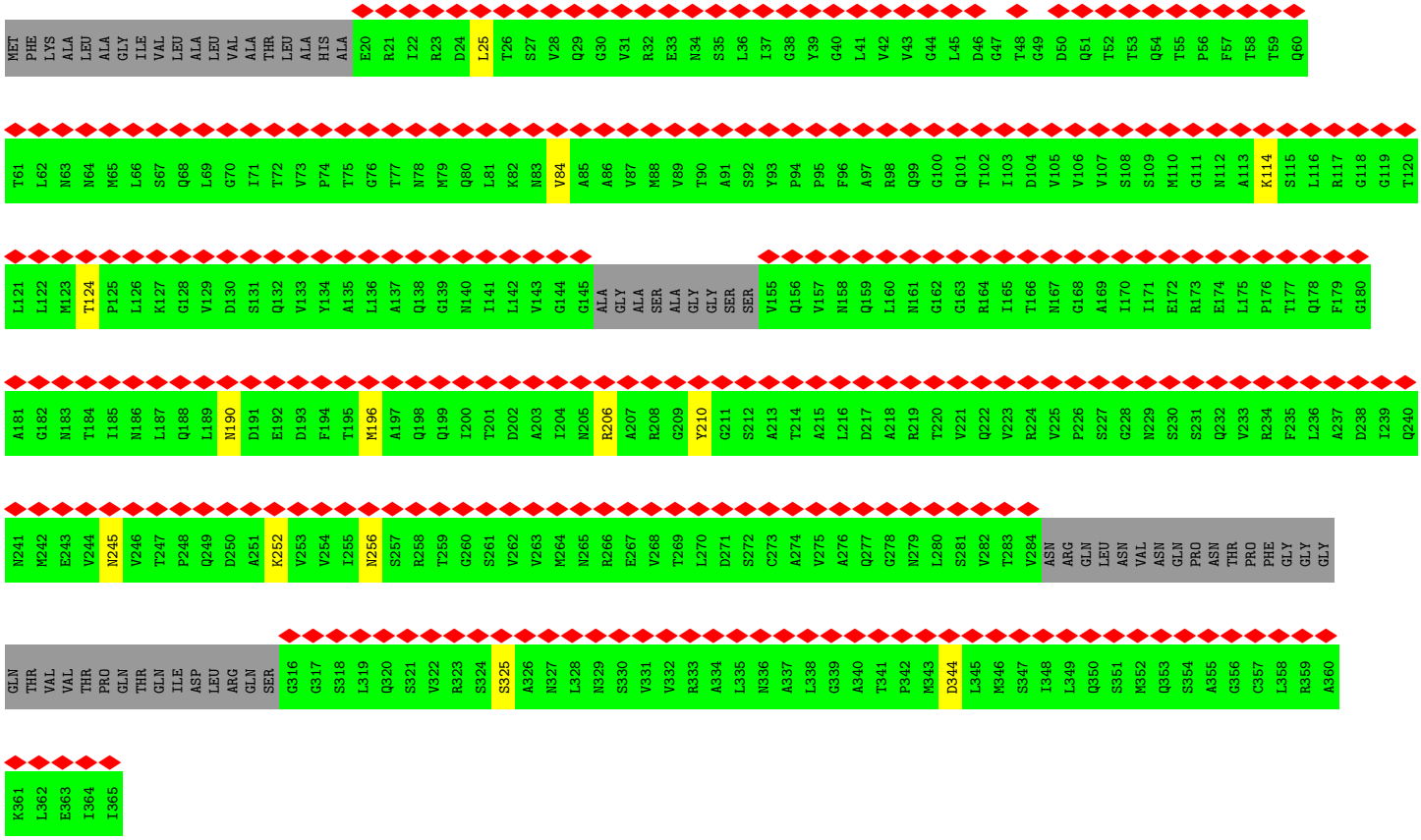
Chain c3:



• Molecule 11: Flagellar P-ring protein

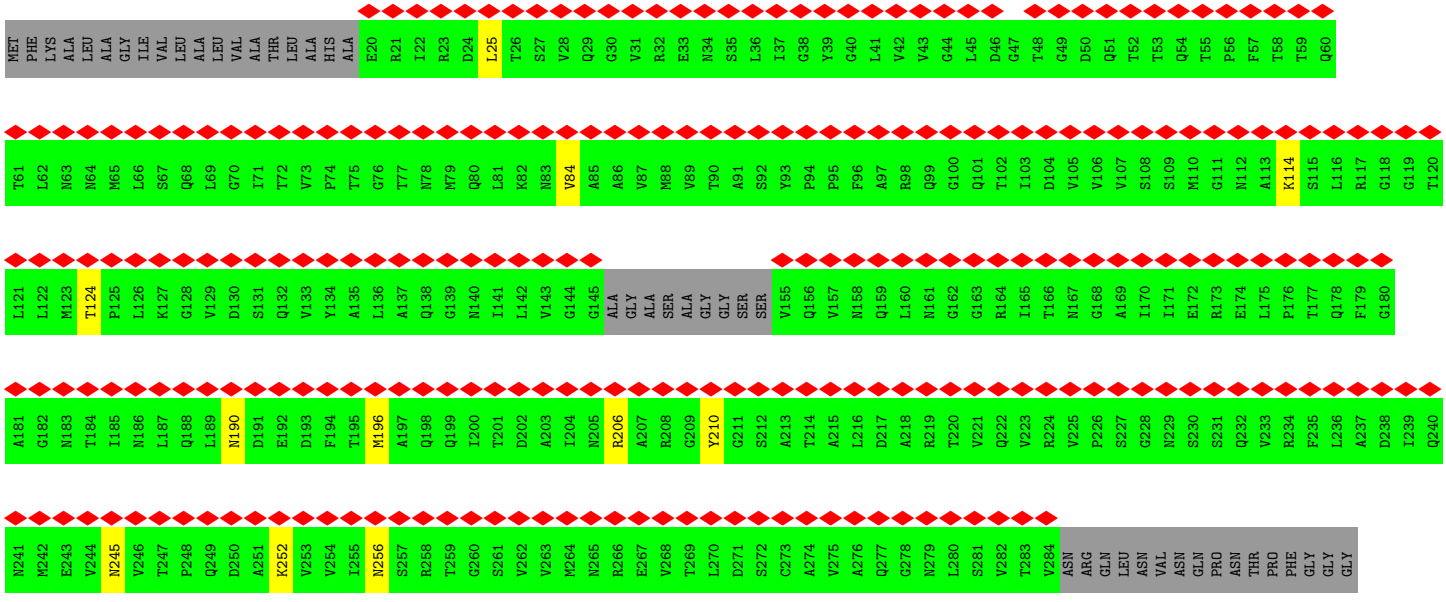
Chain d3:

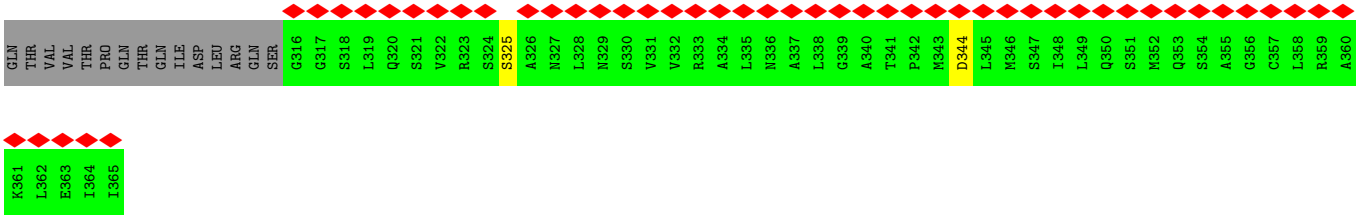



• Molecule 11: Flagellar P-ring protein

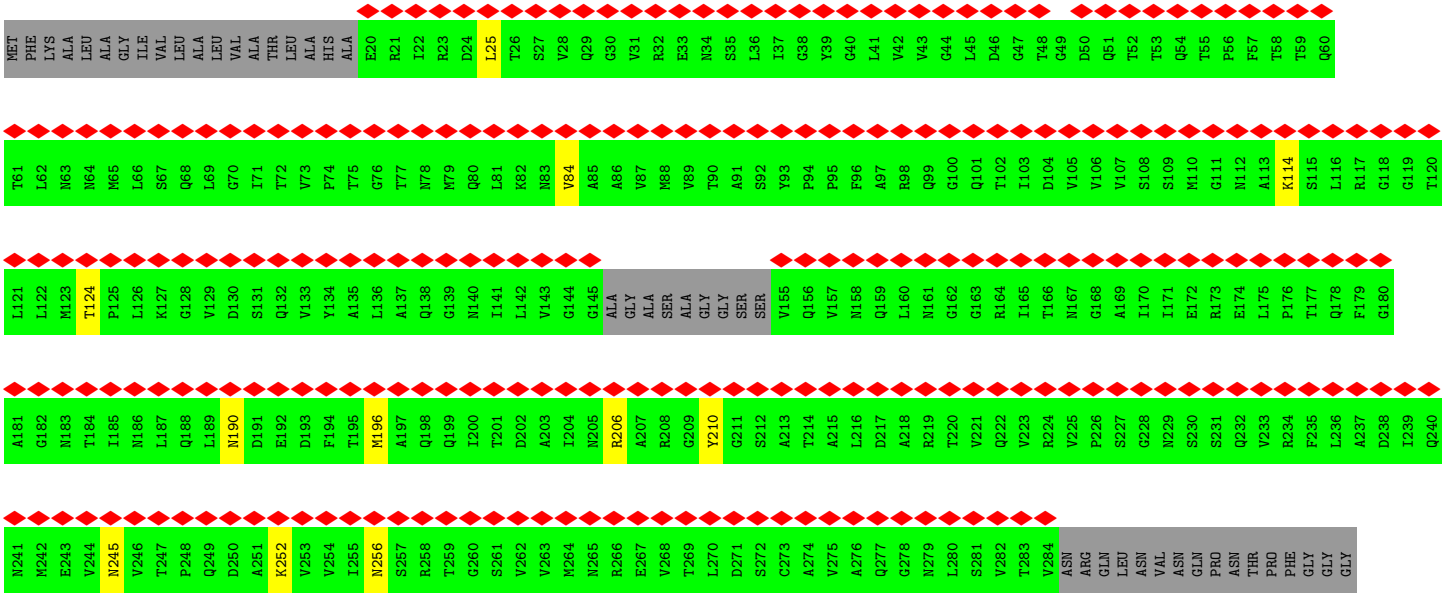
Chain e3:





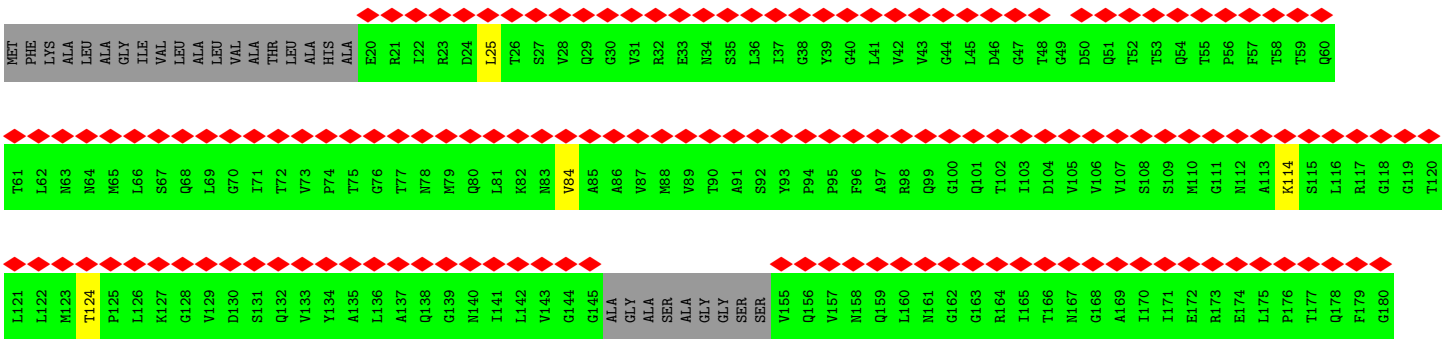

• Molecule 11: Flagellar P-ring protein

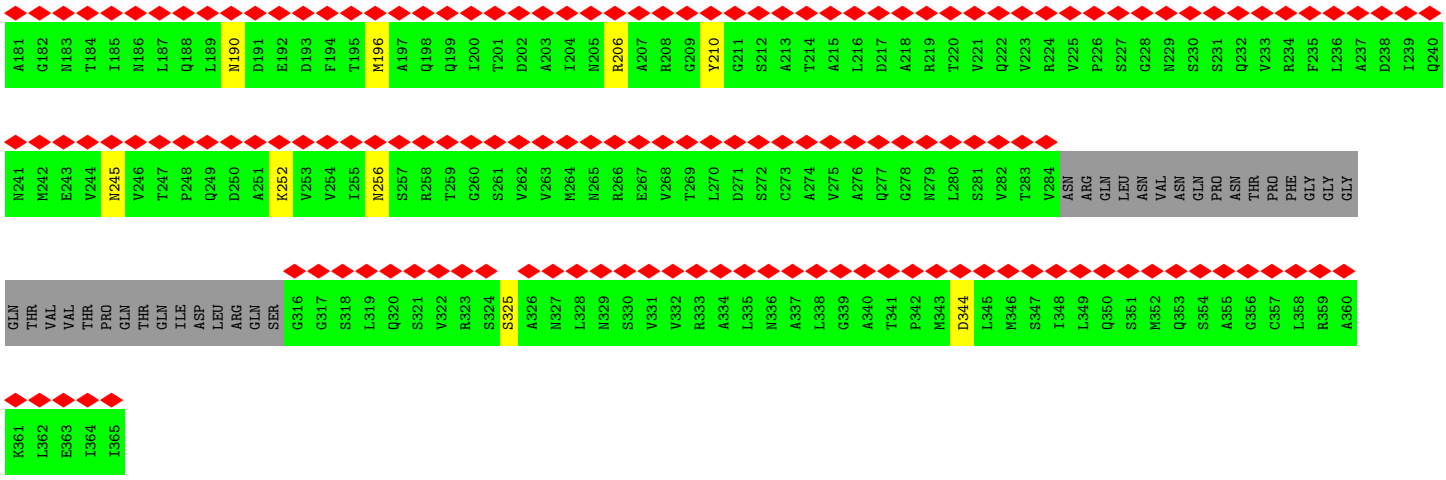
Chain f3:




• Molecule 11: Flagellar P-ring protein

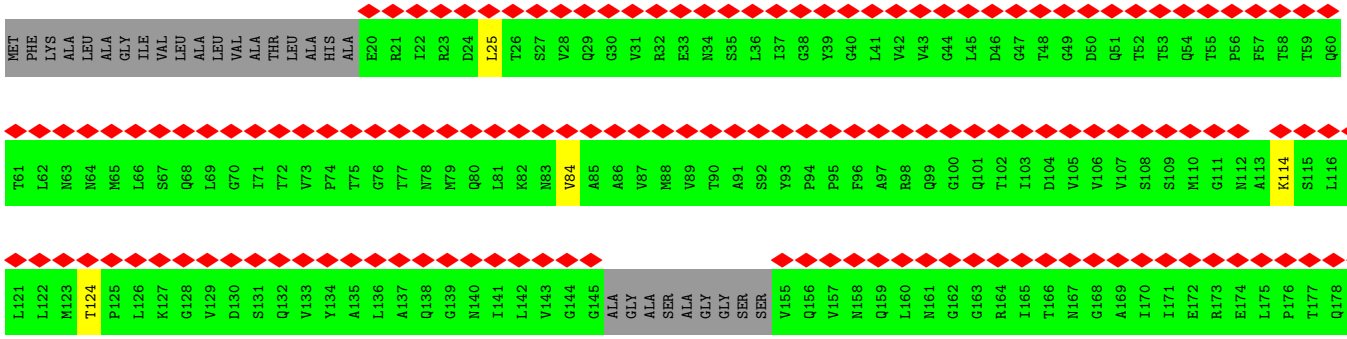
Chain g3:





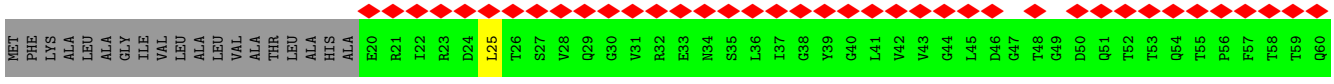

• Molecule 11: Flagellar P-ring protein

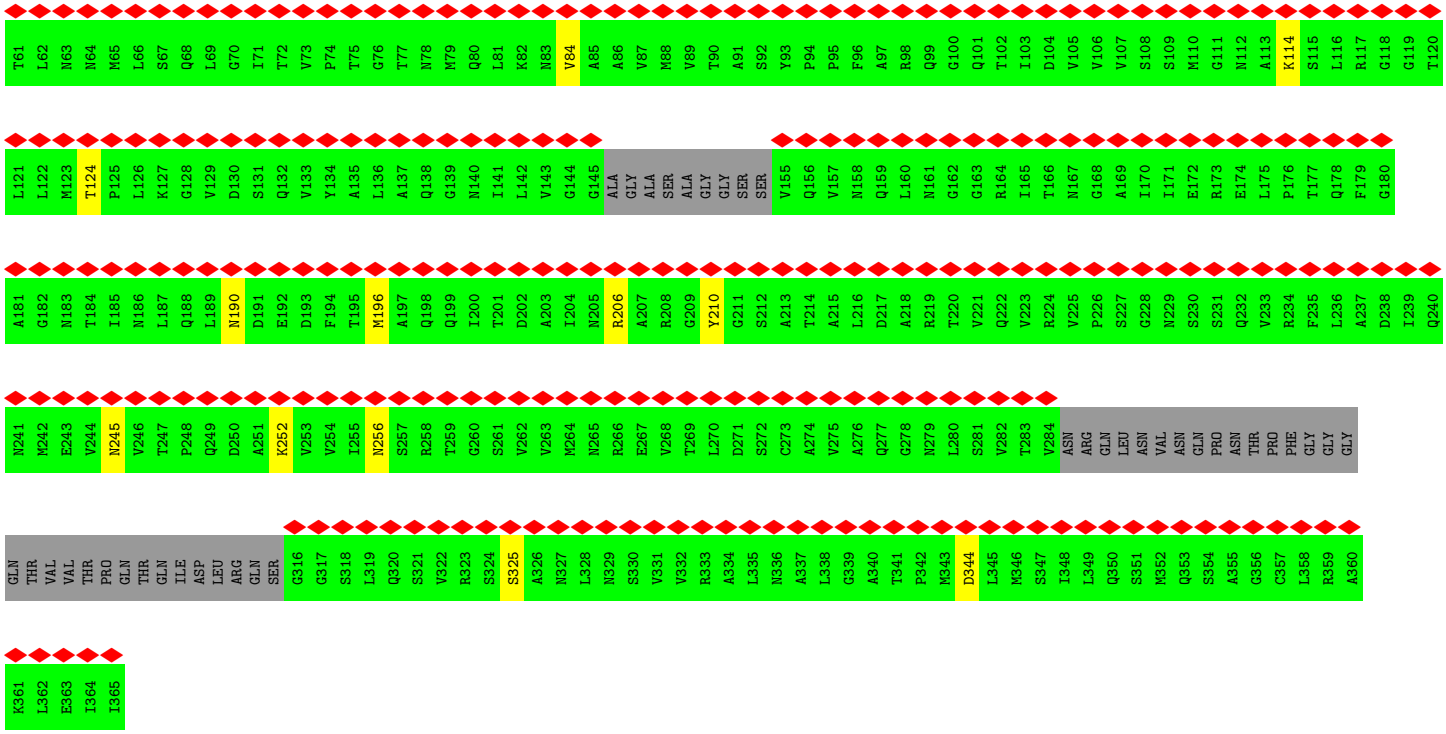
Chain h3:




• Molecule 11: Flagellar P-ring protein

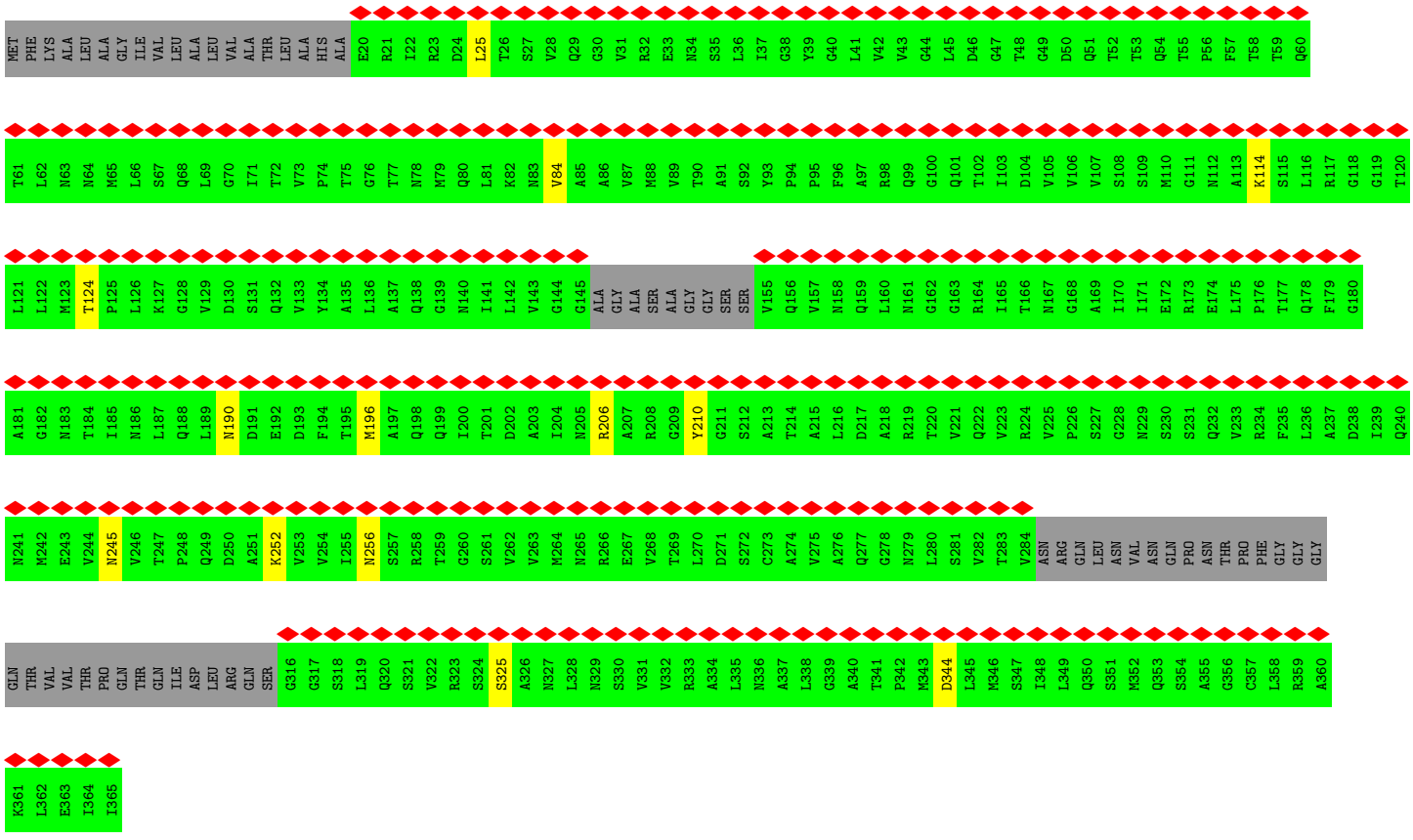
Chain i3:





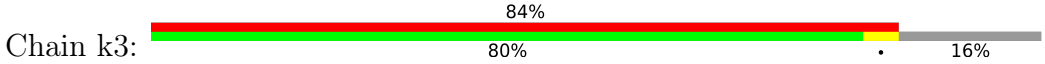

- Molecule 11: Flagellar P-ring protein

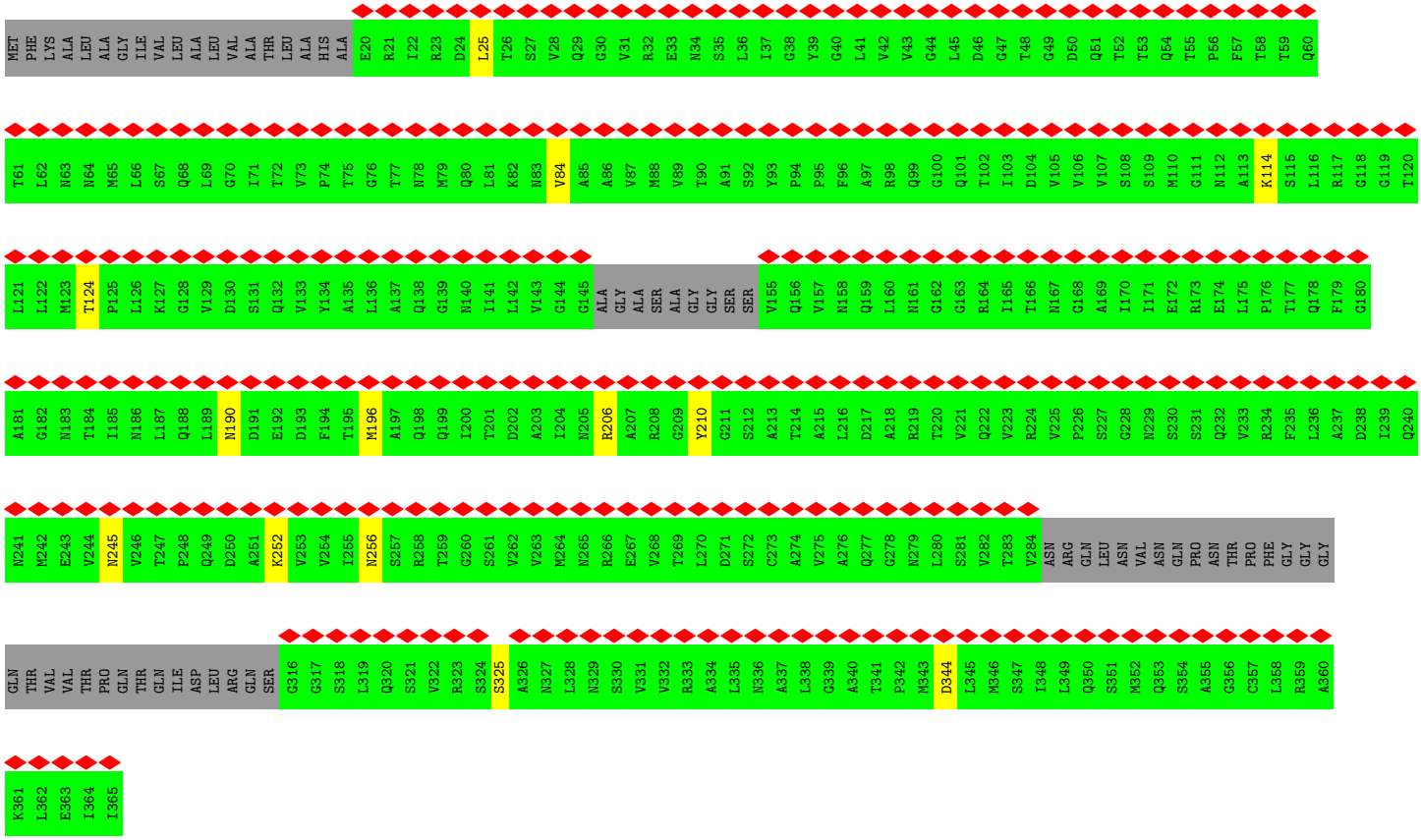
Chain j3:



• Molecule 11: Flagellar P-ring protein

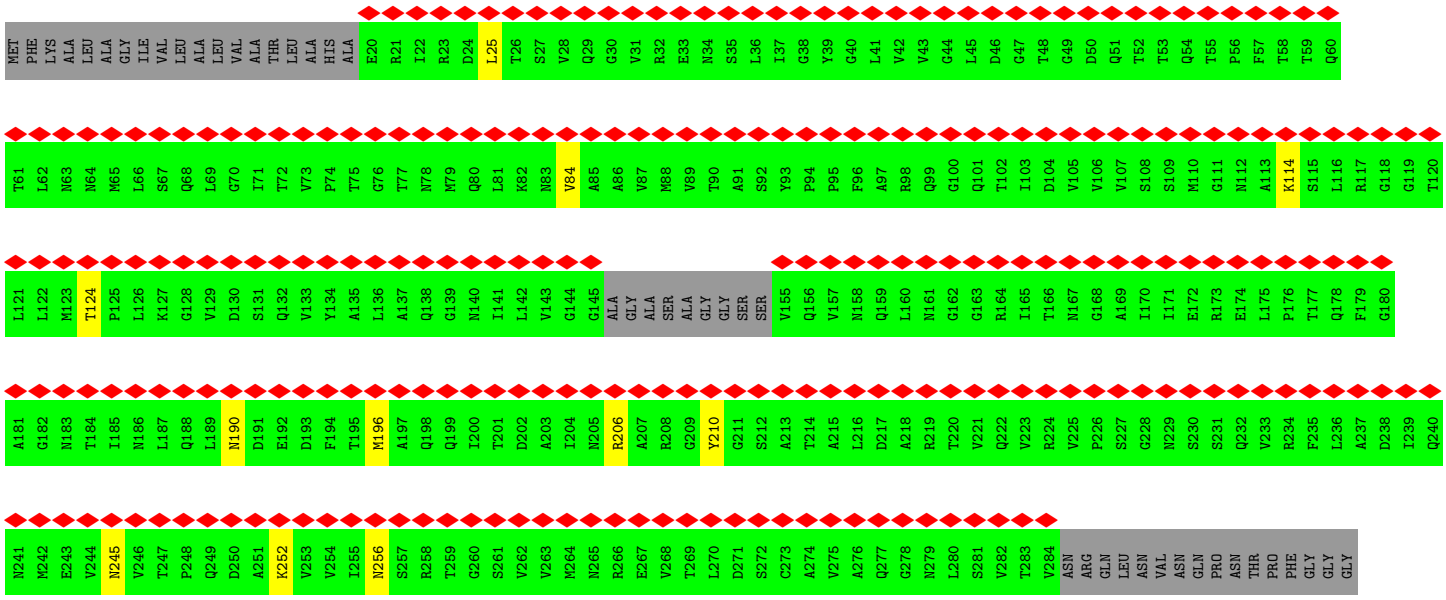
Chain k3:

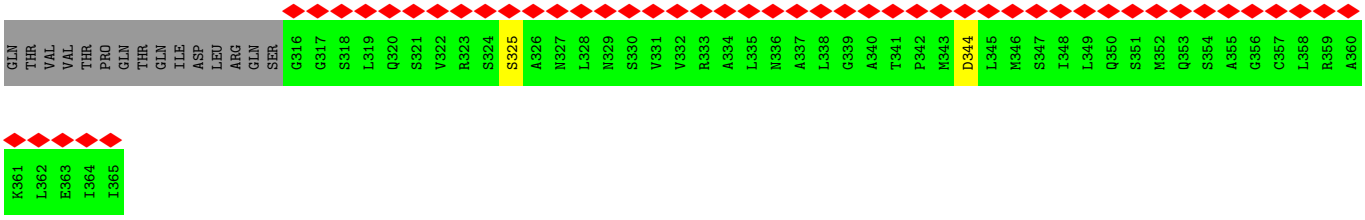



• Molecule 11: Flagellar P-ring protein

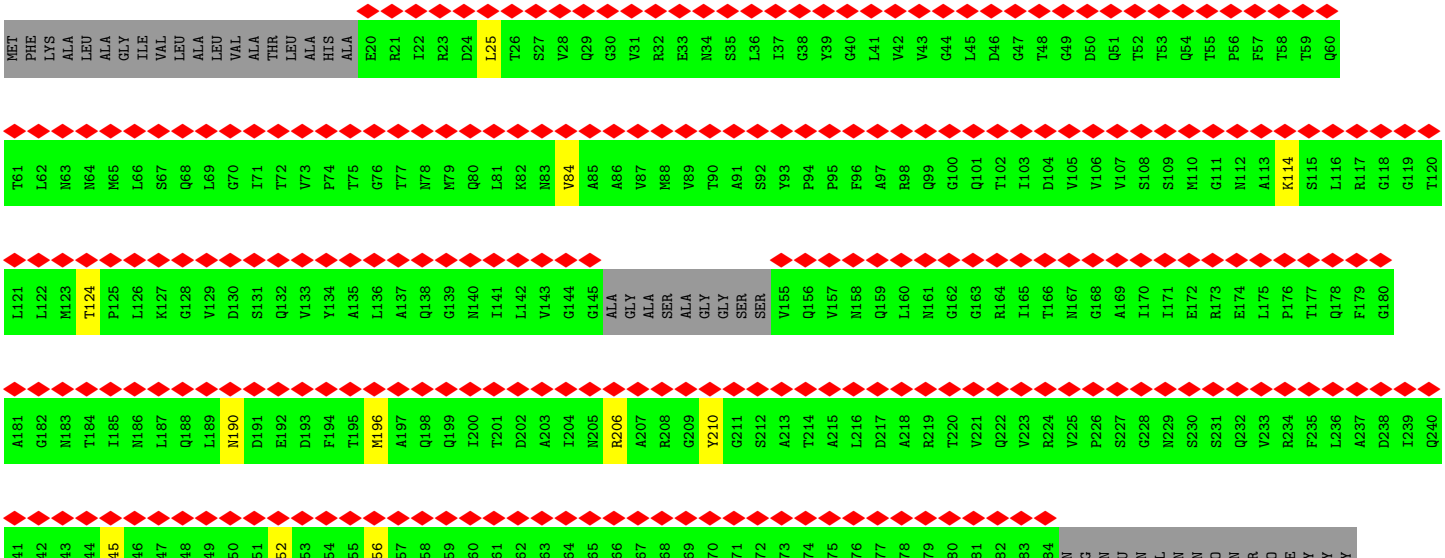
Chain l3:

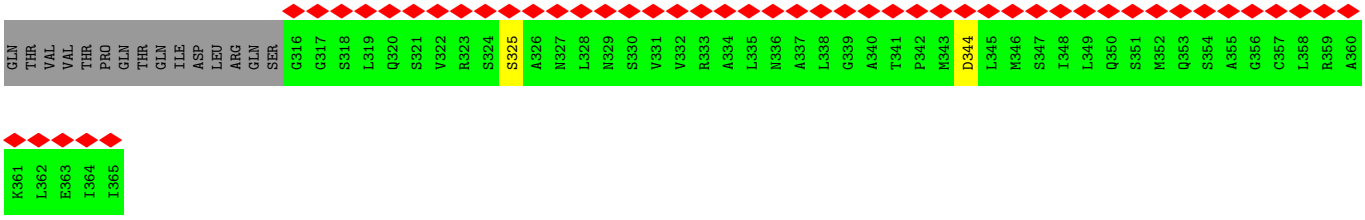





• Molecule 11: Flagellar P-ring protein

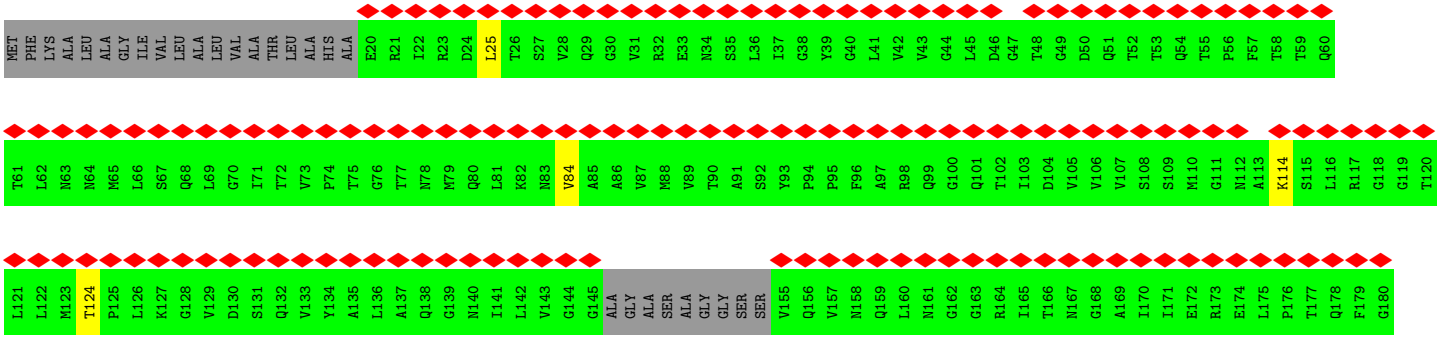
Chain m3:

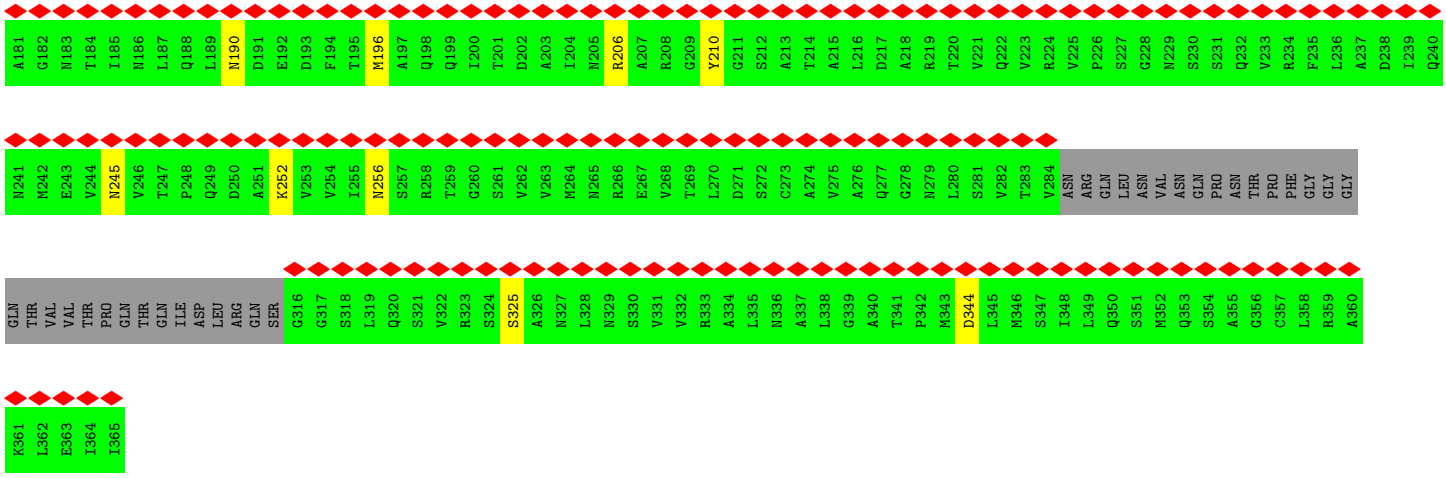



• Molecule 11: Flagellar P-ring protein

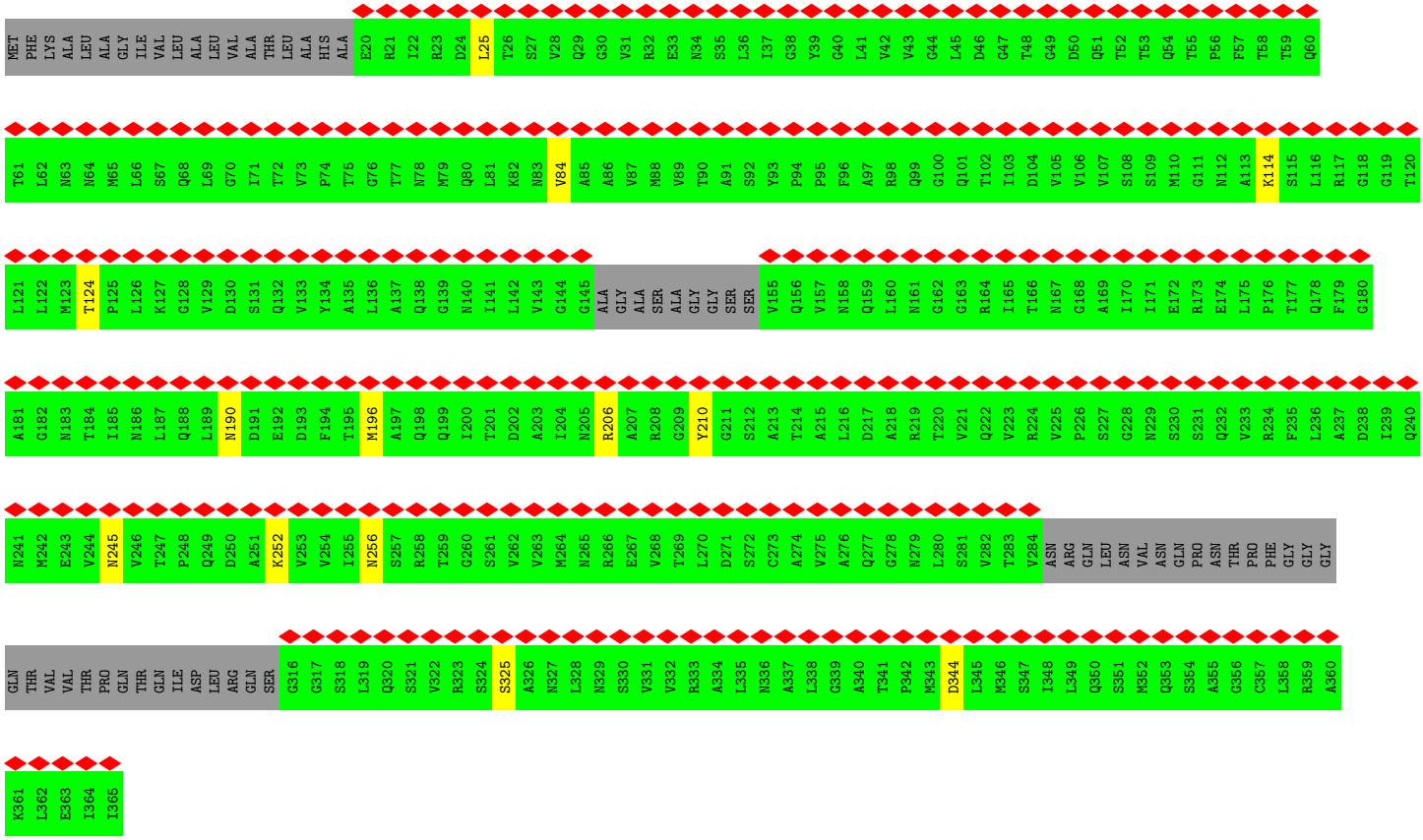
Chain n3:





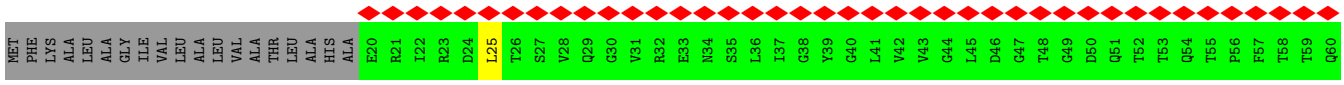

• Molecule 11: Flagellar P-ring protein

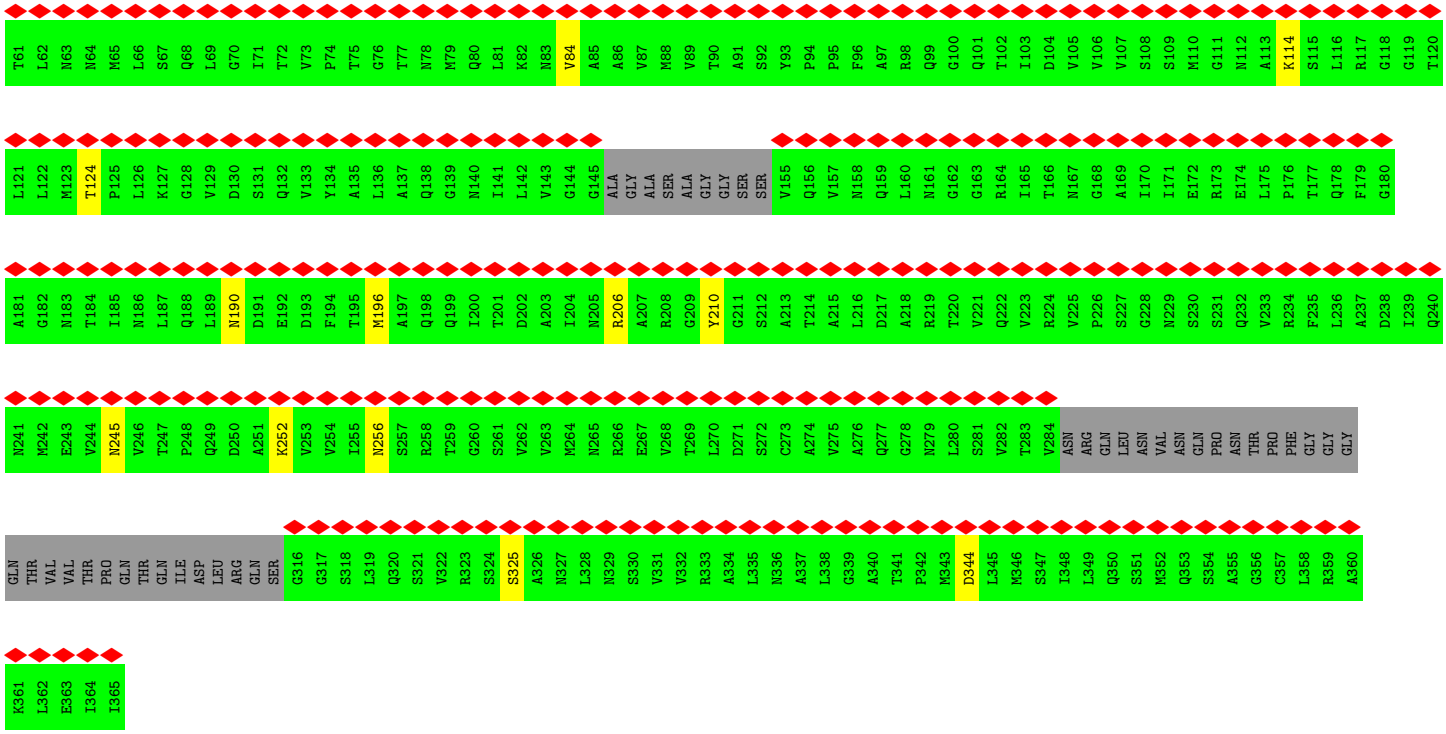
Chain o3:




• Molecule 11: Flagellar P-ring protein

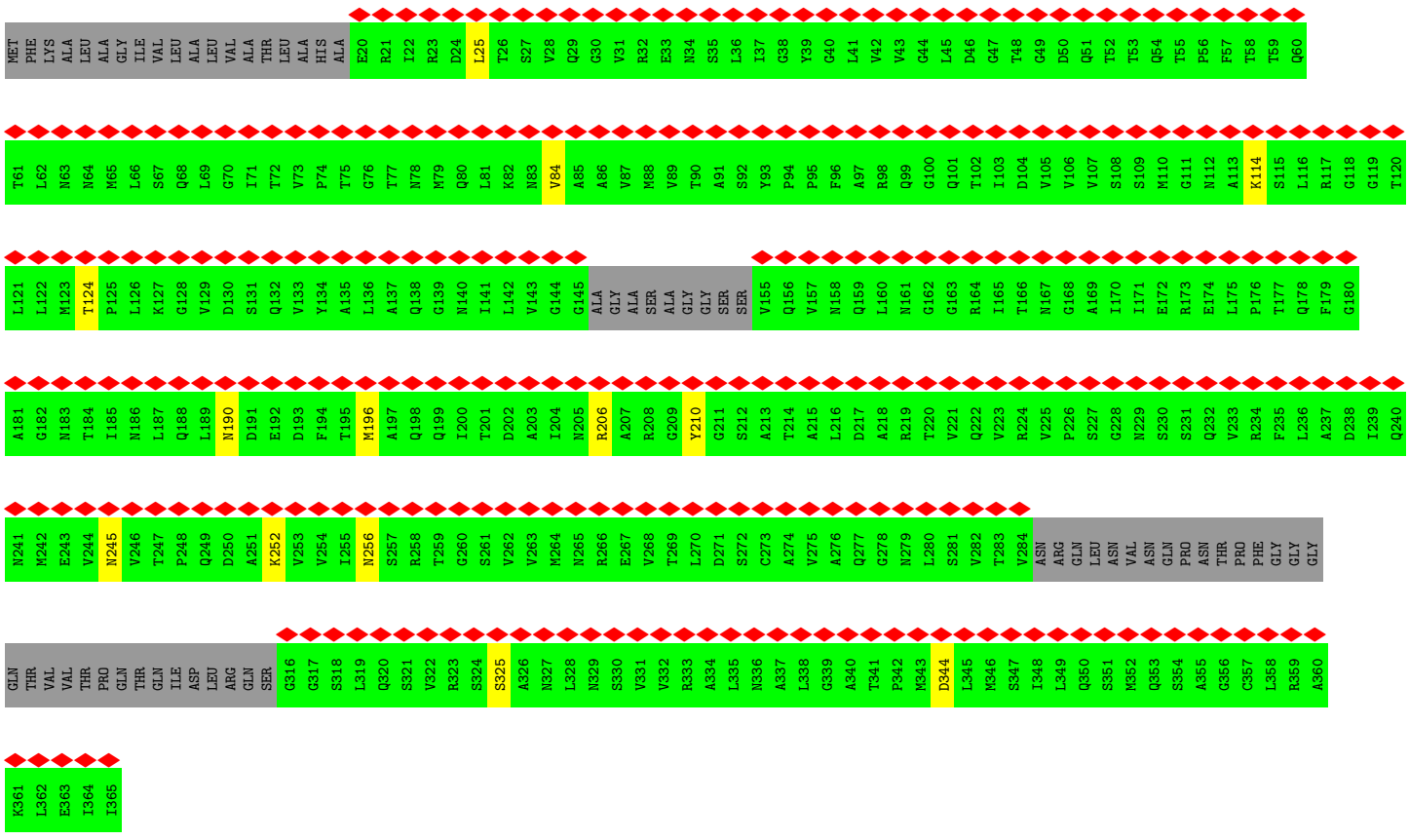
Chain p3:





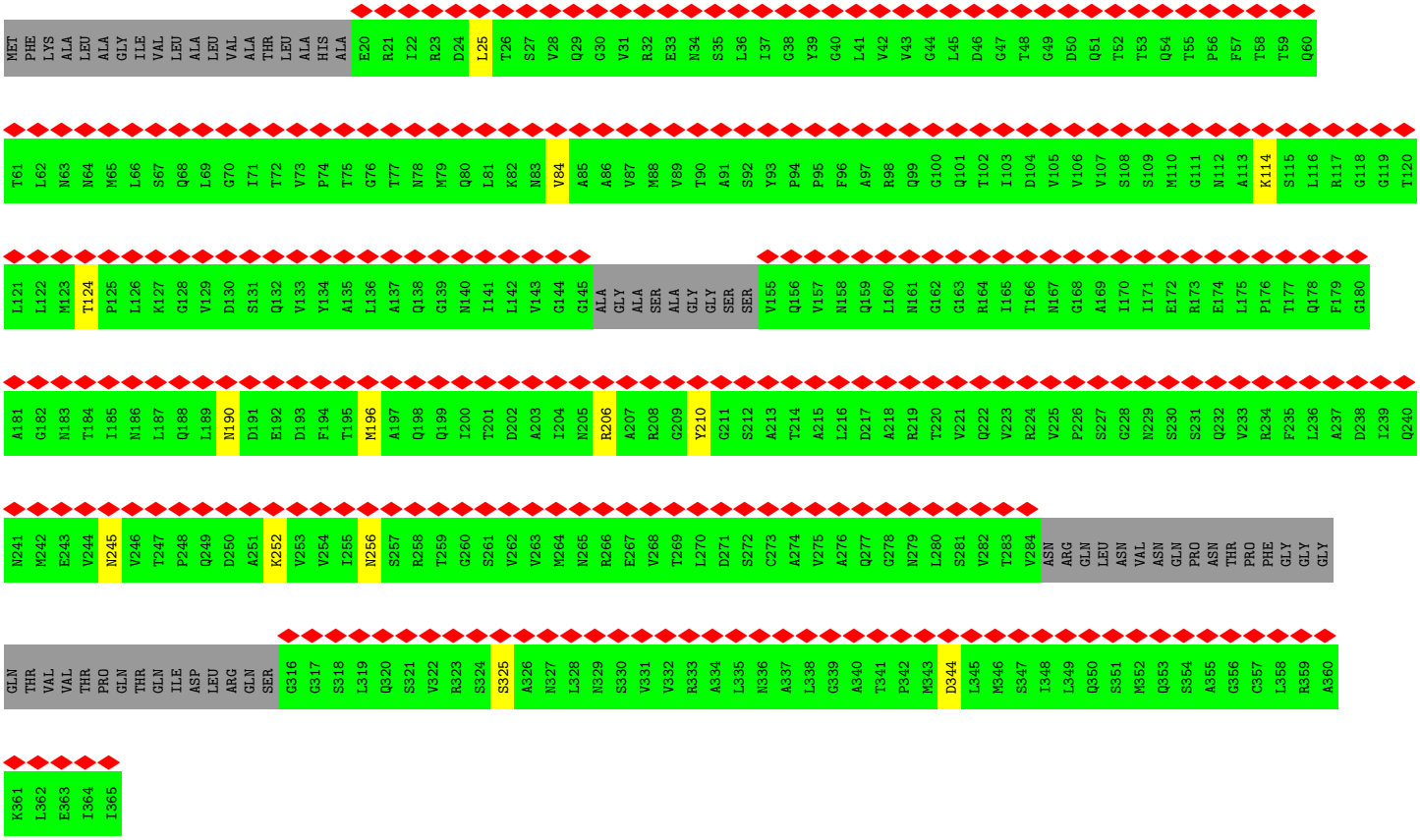

- Molecule 11: Flagellar P-ring protein

Chain q3:



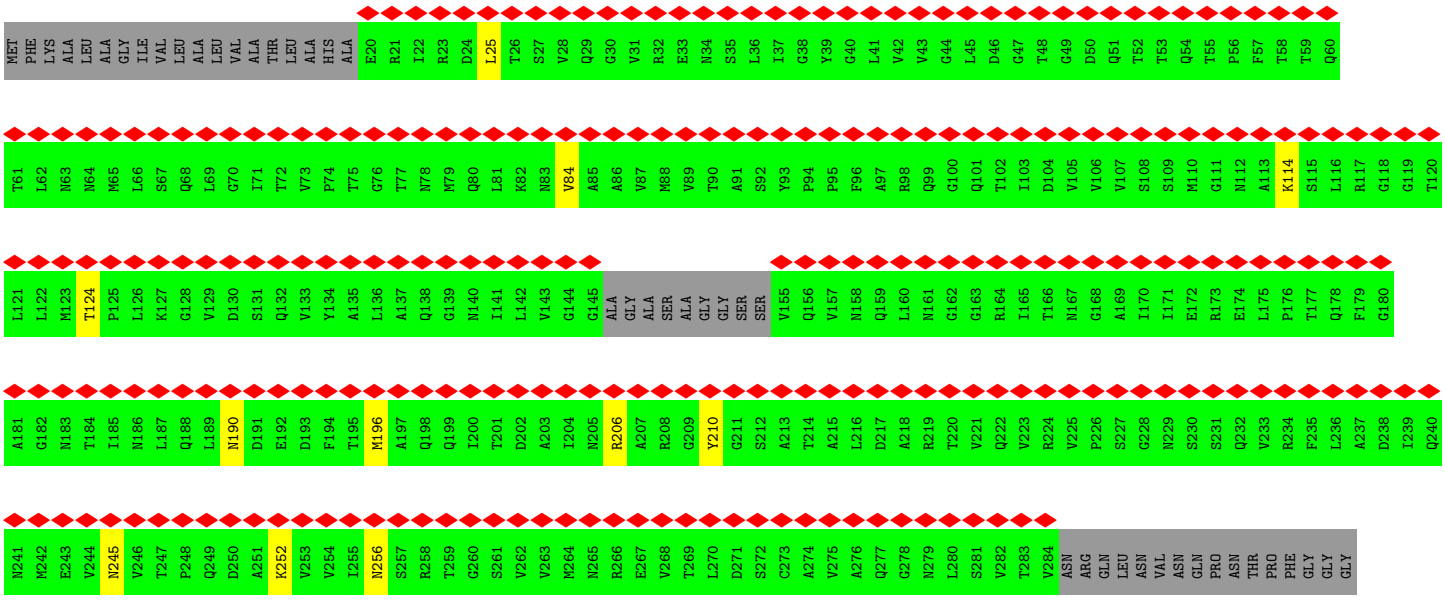
• Molecule 11: Flagellar P-ring protein

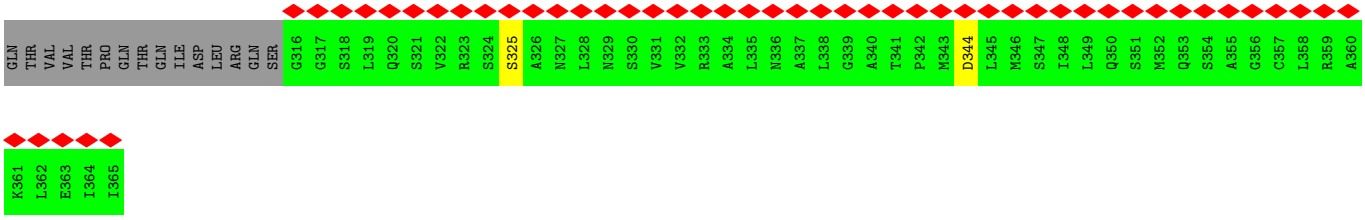
Chain r3:




• Molecule 11: Flagellar P-ring protein

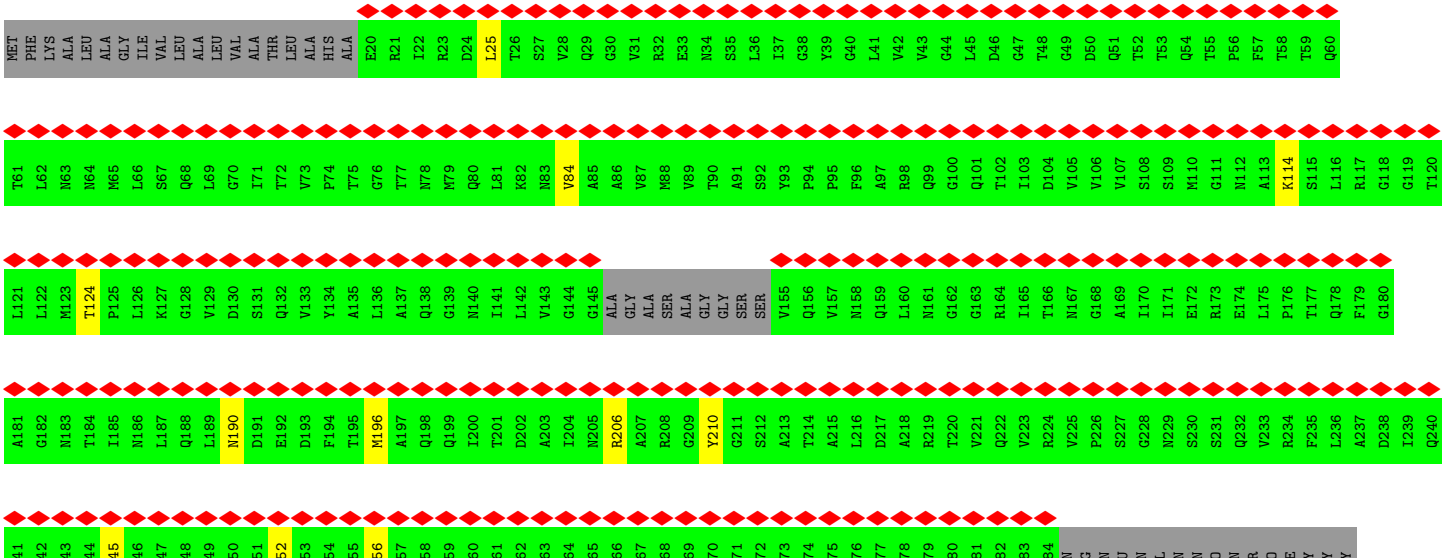
Chain s3:

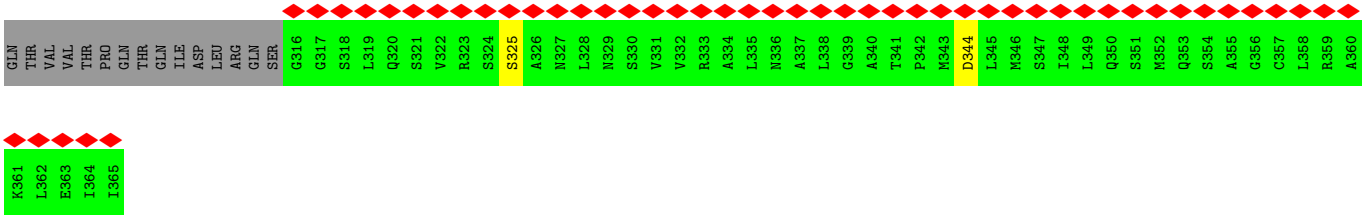





• Molecule 11: Flagellar P-ring protein

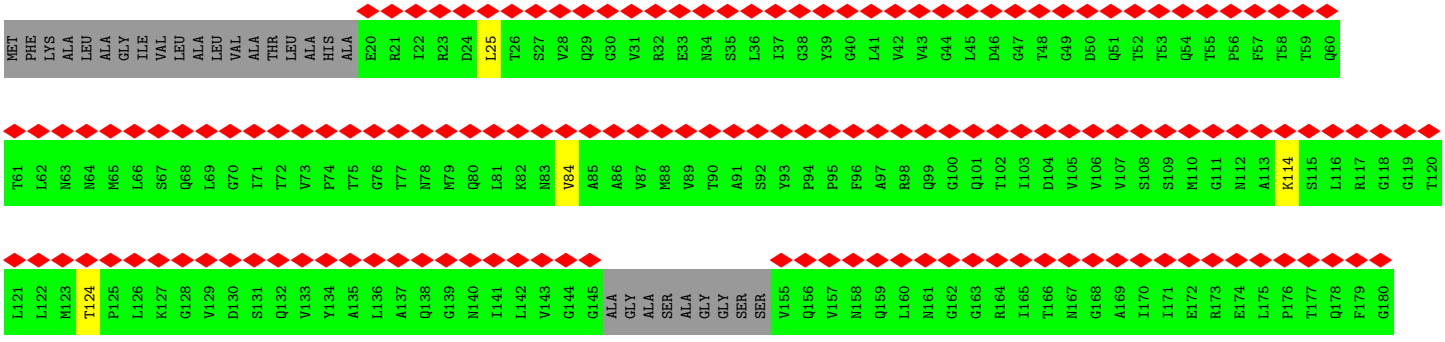
Chain t3:

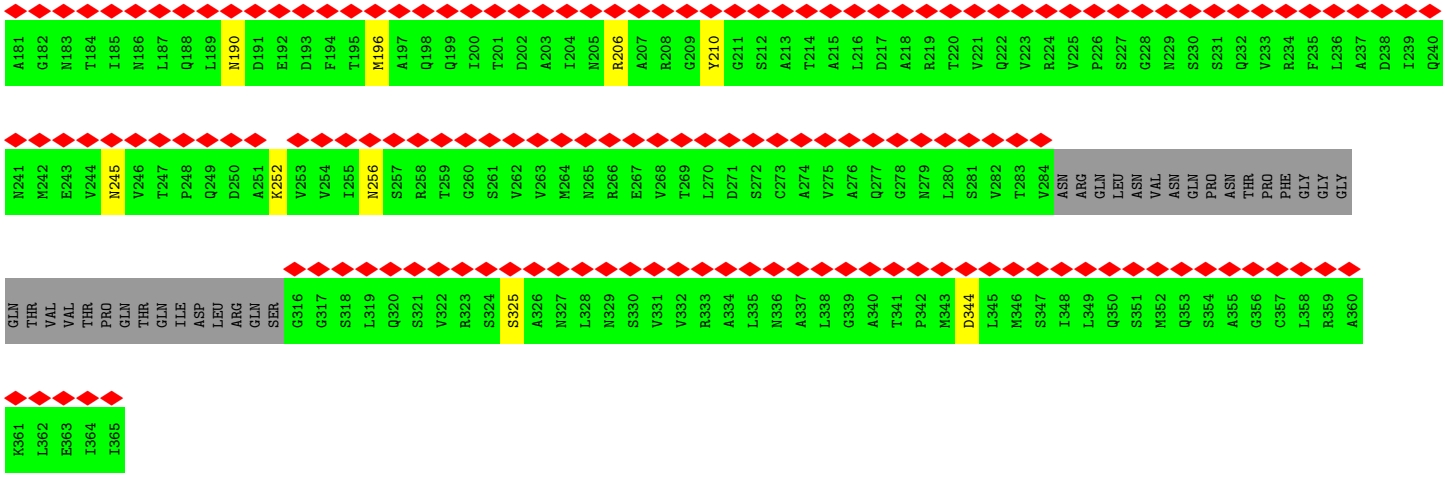



• Molecule 11: Flagellar P-ring protein

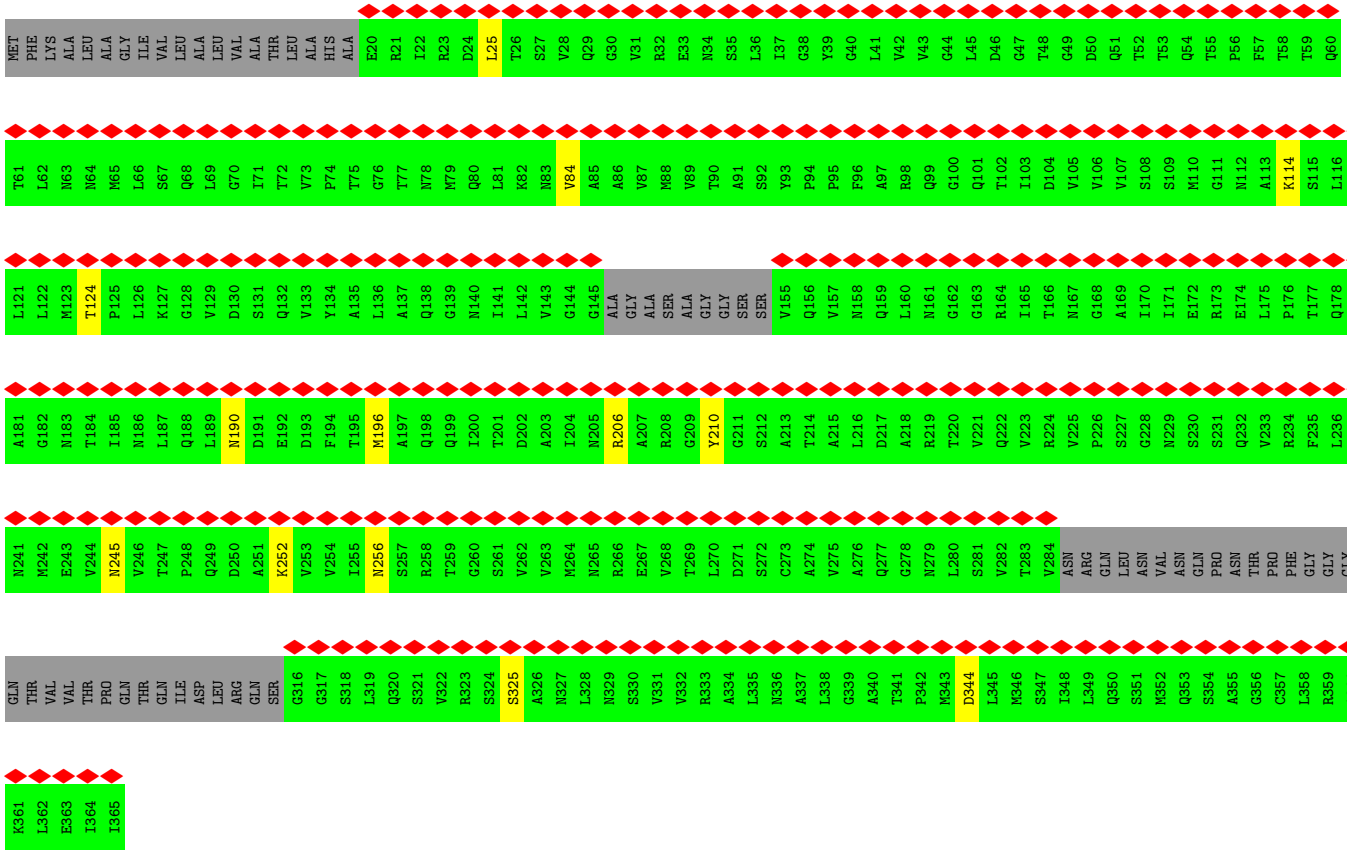
Chain u3:





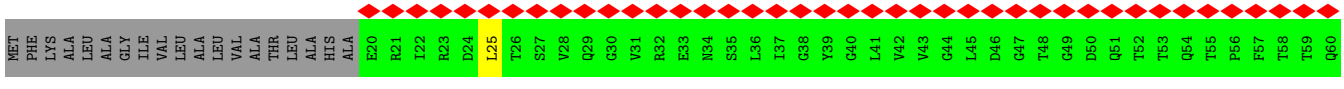

• Molecule 11: Flagellar P-ring protein

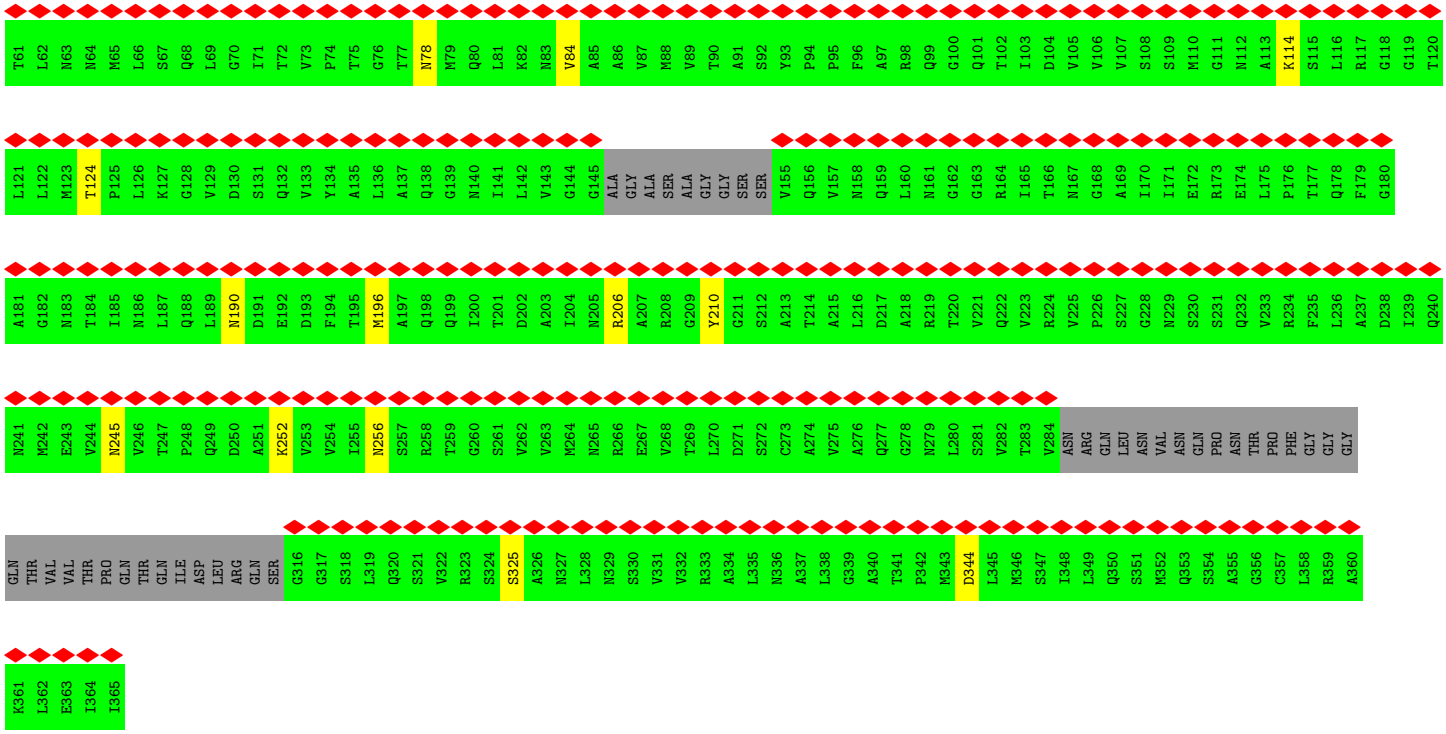
Chain v3:




• Molecule 11: Flagellar P-ring protein

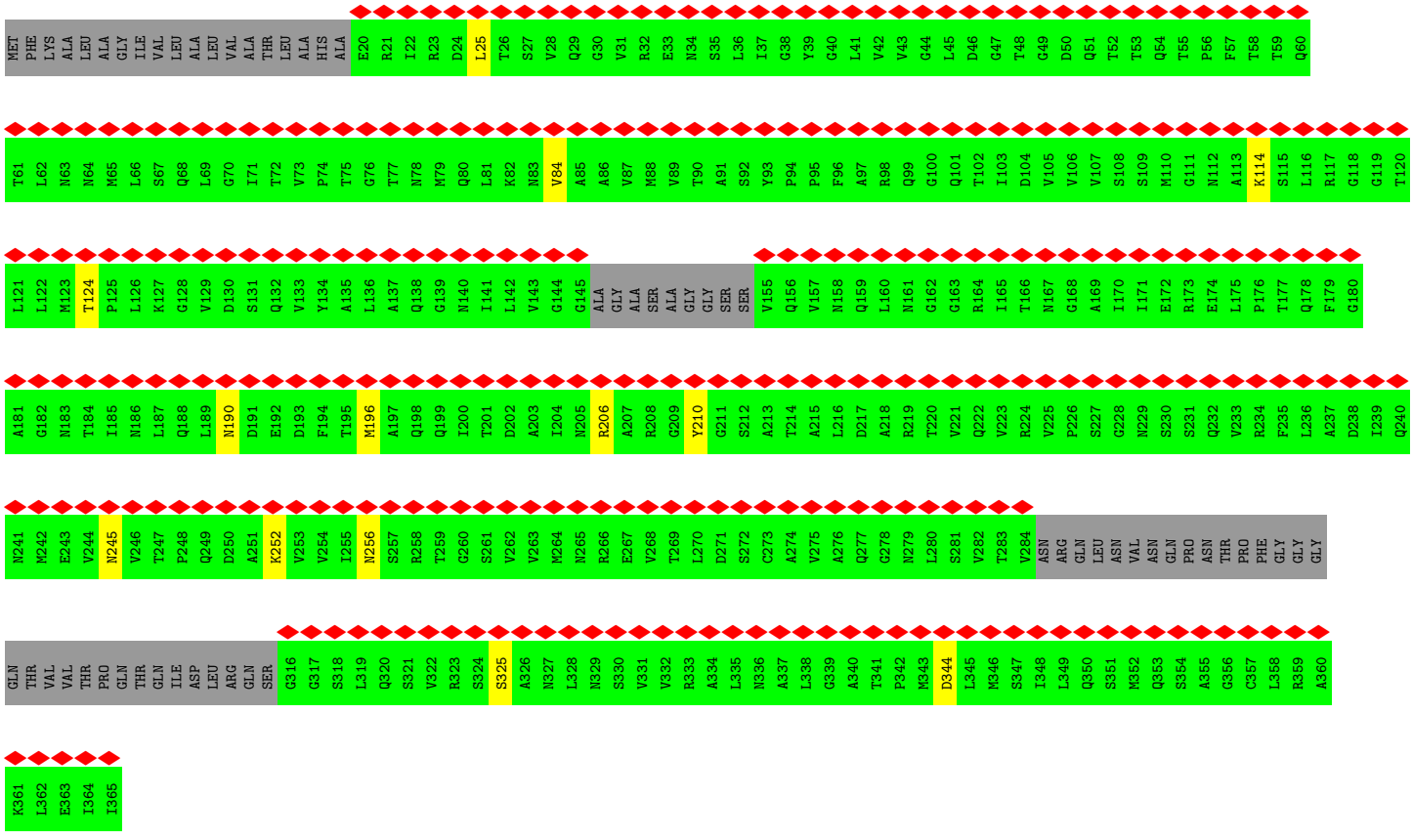
Chain w3:





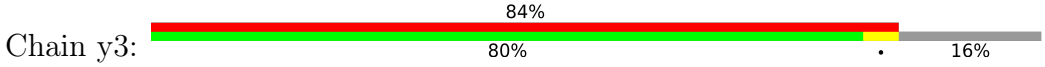

- Molecule 11: Flagellar P-ring protein

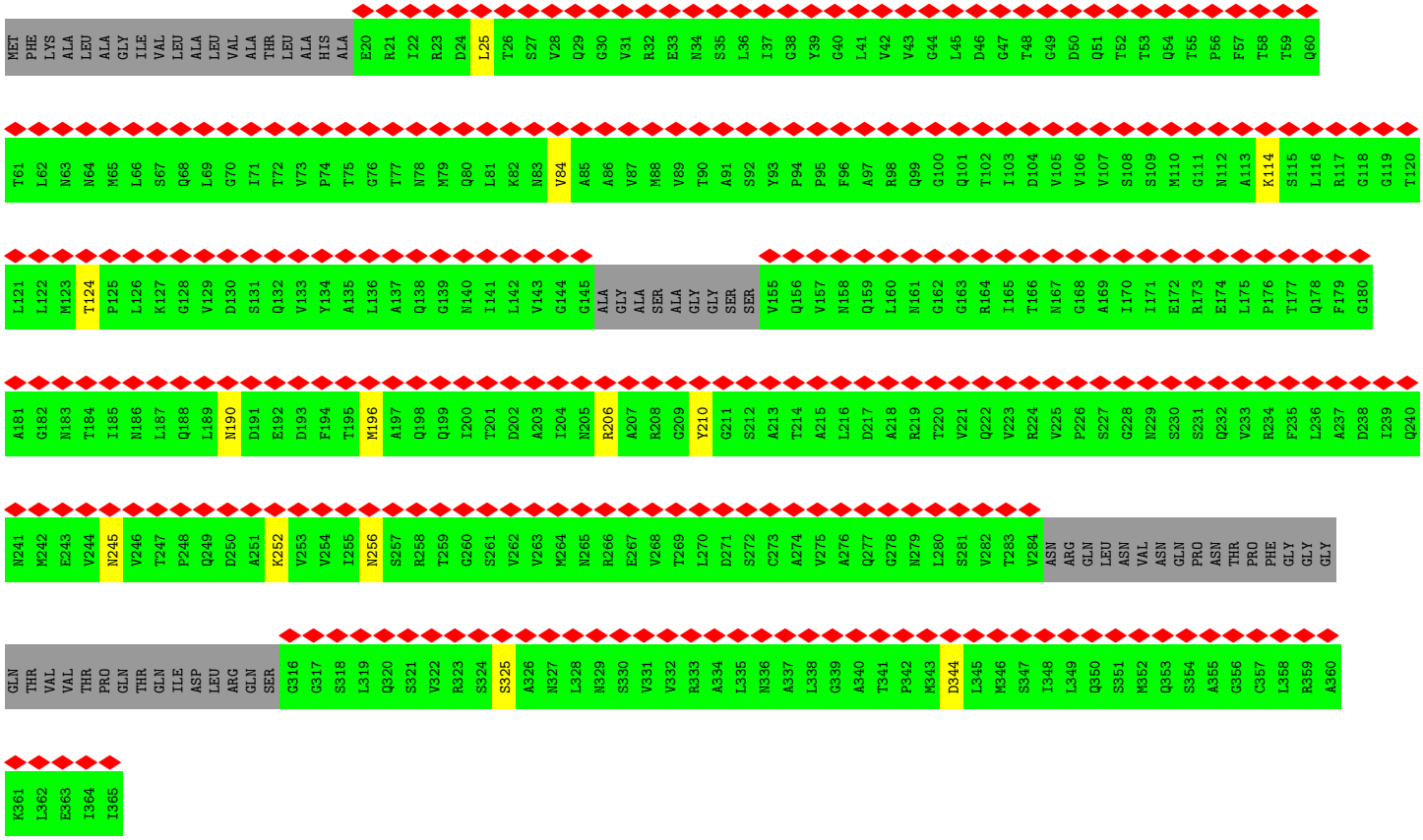
Chain x3:



• Molecule 11: Flagellar P-ring protein

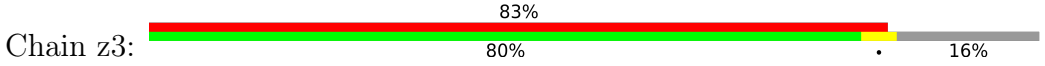
Chain y3:

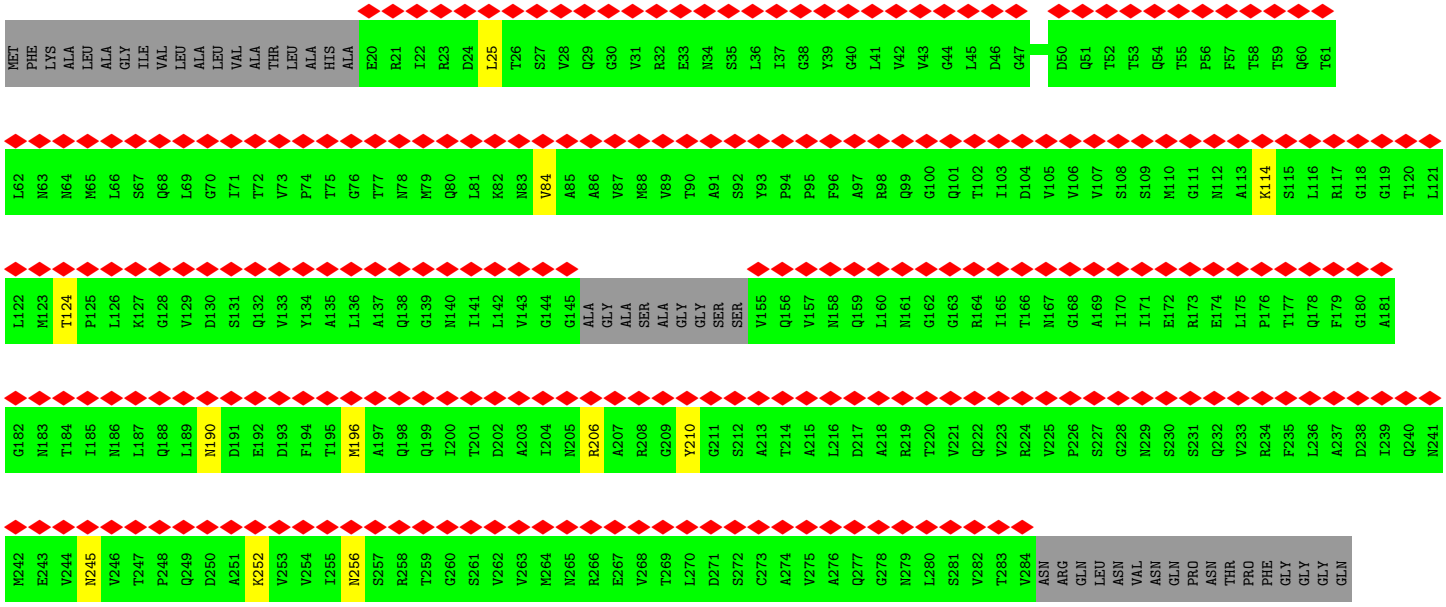


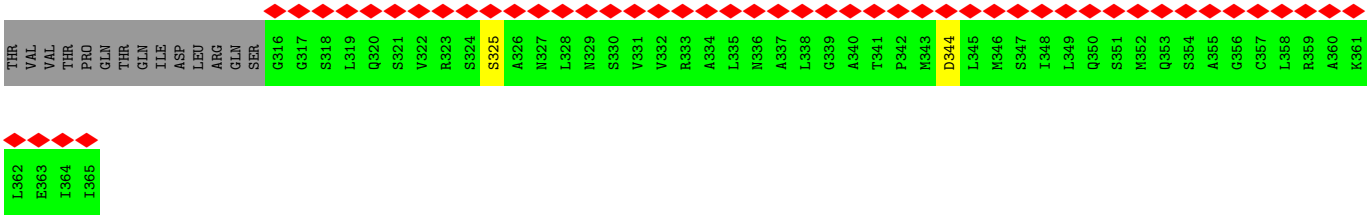




• Molecule 11: Flagellar P-ring protein

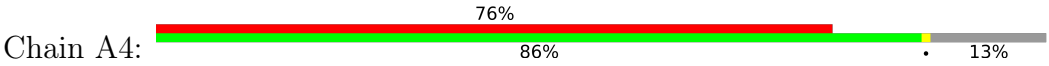
Chain z3:

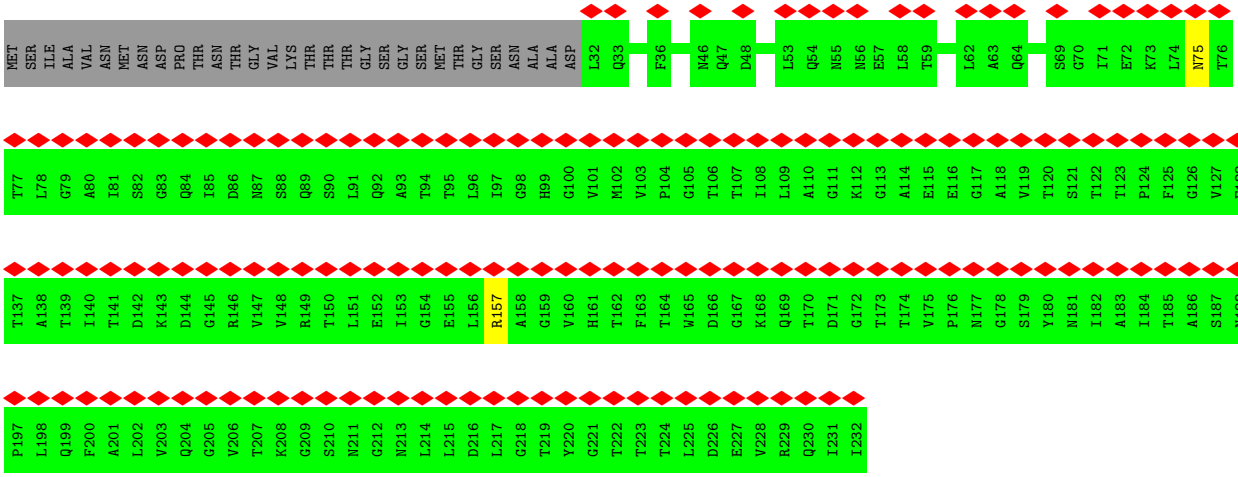


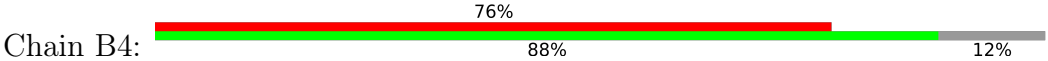


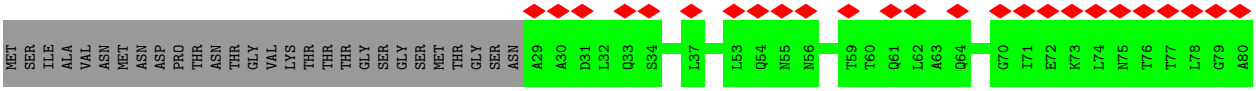

• Molecule 12: Basal-body rod modification protein FlgD

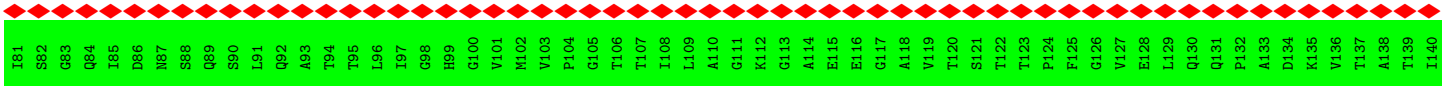


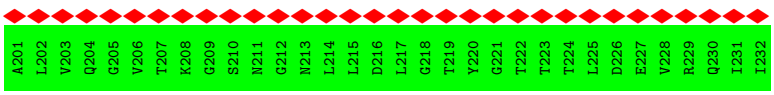




• Molecule 12: Basal-body rod modification protein FlgD

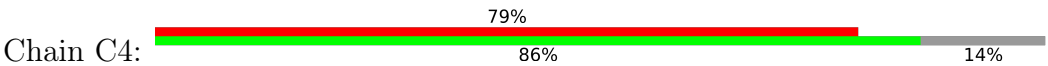


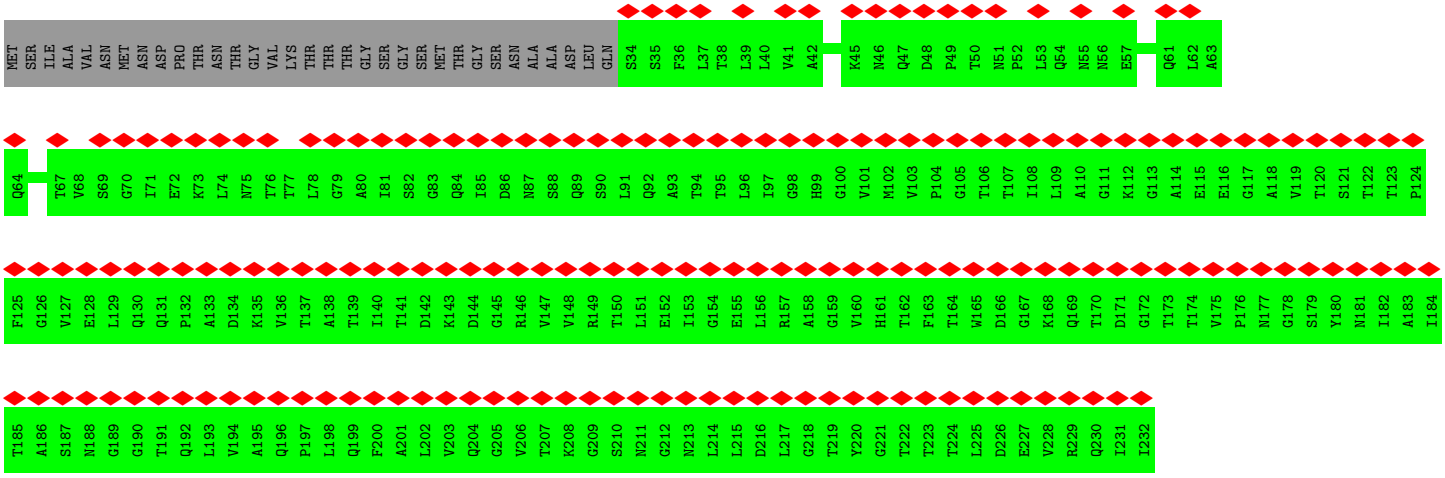



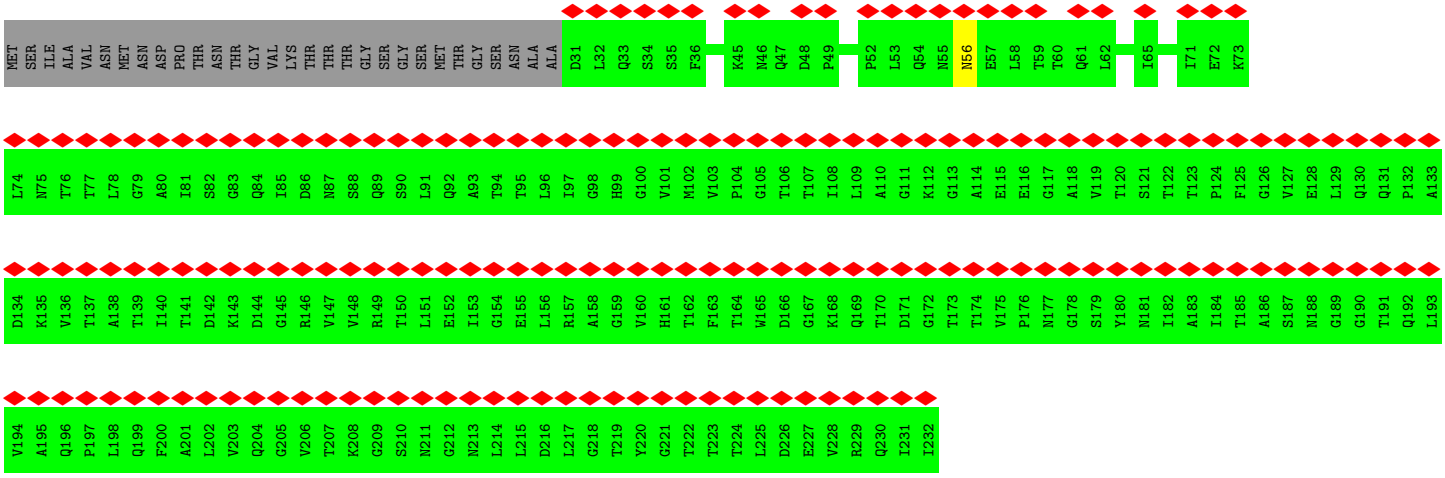

• Molecule 12: Basal-body rod modification protein FlgD





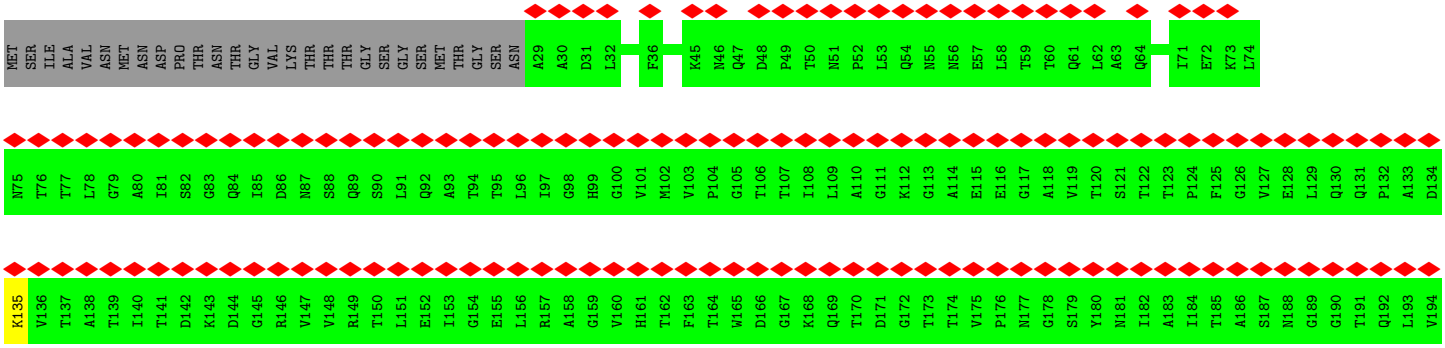

• Molecule 12: Basal-body rod modification protein FlgD

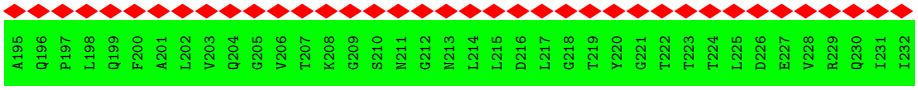
Chain D4:




• Molecule 12: Basal-body rod modification protein FlgD

Chain E4:




A195
Q196
P197
L198
Q199
F200
A201
L202
V203
Q204
G205
V206
T207
K208
G209
S210
N211
G212
N213
L214
L215
D216
L217
G218
T219
Y220
G221
T222
T223
T224
L225
D226
E227
V228
R229
Q230
I231
I232

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 60497 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 59 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.023 | Depositor |
| Minimum map value | -0.010 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.001 | Depositor |
| Recommended contour level | 0.0075 | Depositor |
| Map size (Å) | 638.976, 638.976, 638.976 | wwPDB |
| Map dimensions | 768, 768, 768 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.832, 0.832, 0.832 | 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 | A1 | 0.39 | 0/1205 | 0.52 | 0/1624 |
| 1 | B1 | 0.38 | 0/1955 | 0.55 | 0/2645 |
| 1 | C1 | 0.39 | 0/1955 | 0.54 | 1/2645 (0.0%) |
| 1 | D1 | 0.40 | 0/1205 | 0.53 | 0/1624 |
| 1 | E1 | 0.38 | 0/1955 | 0.55 | 1/2645 (0.0%) |
| 1 | F1 | 0.39 | 0/1205 | 0.57 | 1/1624 (0.1%) |
| 1 | G1 | 0.37 | 0/1955 | 0.54 | 0/2645 |
| 1 | H1 | 0.38 | 0/1955 | 0.56 | 0/2645 |
| 1 | I1 | 0.37 | 0/1955 | 0.53 | 0/2645 |
| 1 | J1 | 0.42 | 0/1205 | 0.53 | 1/1624 (0.1%) |
| 1 | K1 | 0.36 | 0/1955 | 0.52 | 0/2645 |
| 1 | L1 | 0.36 | 0/1955 | 0.54 | 0/2645 |
| 1 | M1 | 0.40 | 0/1205 | 0.55 | 1/1624 (0.1%) |
| 1 | N1 | 0.36 | 0/1955 | 0.55 | 0/2645 |
| 1 | O1 | 0.35 | 0/1955 | 0.53 | 1/2645 (0.0%) |
| 1 | P1 | 0.37 | 0/1205 | 0.52 | 1/1624 (0.1%) |
| 1 | Q1 | 0.35 | 0/1955 | 0.52 | 0/2645 |
| 1 | R1 | 0.35 | 0/1955 | 0.51 | 1/2645 (0.0%) |
| 1 | S1 | 0.38 | 0/1205 | 0.50 | 1/1624 (0.1%) |
| 1 | T1 | 0.35 | 0/1955 | 0.52 | 0/2645 |
| 1 | U1 | 0.36 | 0/1955 | 0.56 | 0/2645 |
| 1 | V1 | 0.38 | 0/1205 | 0.52 | 0/1624 |
| 1 | W1 | 0.35 | 0/1955 | 0.52 | 1/2645 (0.0%) |
| 1 | X1 | 0.35 | 0/1955 | 0.52 | 1/2645 (0.0%) |
| 1 | Y1 | 0.34 | 0/1955 | 0.53 | 0/2645 |
| 1 | Z1 | 0.41 | 0/1205 | 0.54 | 0/1624 |
| 1 | a1 | 0.36 | 0/1955 | 0.53 | 0/2645 |
| 1 | b1 | 0.39 | 0/1205 | 0.51 | 0/1624 |
| 1 | c1 | 0.37 | 0/1955 | 0.53 | 1/2645 (0.0%) |
| 1 | d1 | 0.37 | 0/1955 | 0.54 | 0/2645 |
| 1 | e1 | 0.39 | 0/1205 | 0.52 | 1/1624 (0.1%) |
| 1 | f1 | 0.37 | 0/1955 | 0.53 | 0/2645 |
| 1 | g1 | 0.37 | 0/1955 | 0.54 | 1/2645 (0.0%) |
| 1 | h1 | 0.37 | 0/1955 | 0.51 | 0/2645 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 2 | A2 | 0.39 | 0/1662 | 0.62 | 1/2263 (0.0%) |
| 2 | B2 | 0.41 | 0/1662 | 0.61 | 0/2263 |
| 2 | C2 | 0.40 | 0/1662 | 0.61 | 0/2263 |
| 2 | D2 | 0.43 | 1/1662 (0.1%) | 0.58 | 0/2263 |
| 2 | E2 | 0.61 | 1/1662 (0.1%) | 0.71 | 1/2263 (0.0%) |
| 3 | F2 | 0.35 | 0/2035 | 0.58 | 0/2777 |
| 4 | G2 | 0.34 | 0/681 | 0.61 | 0/930 |
| 4 | H2 | 0.34 | 0/681 | 0.55 | 0/930 |
| 4 | I2 | 0.37 | 0/681 | 0.53 | 0/930 |
| 4 | J2 | 2.82 | 6/681 (0.9%) | 0.65 | 0/930 |
| 5 | K2 | 0.35 | 0/296 | 0.60 | 1/395 (0.3%) |
| 5 | L2 | 0.33 | 0/567 | 0.44 | 0/761 |
| 5 | M2 | 0.36 | 0/567 | 0.45 | 0/761 |
| 5 | N2 | 0.36 | 0/567 | 0.46 | 0/761 |
| 5 | O2 | 0.34 | 0/567 | 0.47 | 0/761 |
| 5 | P2 | 0.36 | 0/567 | 0.47 | 0/761 |
| 6 | Q2 | 0.39 | 0/1035 | 0.52 | 0/1399 |
| 6 | R2 | 0.37 | 0/941 | 0.53 | 0/1269 |
| 6 | S2 | 0.40 | 0/951 | 0.51 | 0/1281 |
| 6 | T2 | 0.40 | 0/842 | 0.53 | 0/1132 |
| 6 | U2 | 0.37 | 0/934 | 0.50 | 0/1259 |
| 7 | V2 | 0.44 | 0/981 | 0.65 | 0/1334 |
| 7 | W2 | 0.44 | 0/976 | 0.57 | 0/1327 |
| 7 | X2 | 0.48 | 0/976 | 0.56 | 0/1327 |
| 7 | Y2 | 0.46 | 0/976 | 0.56 | 0/1327 |
| 7 | Z2 | 0.46 | 0/976 | 0.55 | 0/1327 |
| 7 | a2 | 0.42 | 0/976 | 0.57 | 0/1327 |
| 8 | b2 | 0.39 | 0/1836 | 0.59 | 0/2502 |
| 8 | c2 | 0.42 | 0/1836 | 0.59 | 0/2502 |
| 8 | d2 | 0.44 | 0/1836 | 0.58 | 0/2502 |
| 8 | e2 | 0.43 | 0/1836 | 0.56 | 0/2502 |
| 8 | f2 | 0.40 | 0/1836 | 0.56 | 0/2502 |
| 9 | 12 | 0.38 | 0/1973 | 0.55 | 0/2682 |
| 9 | 22 | 0.37 | 0/1973 | 0.54 | 0/2682 |
| 9 | 32 | 0.36 | 0/1971 | 0.55 | 1/2677 (0.0%) |
| 9 | 42 | 0.31 | 0/1973 | 0.56 | 1/2682 (0.0%) |
| 9 | g2 | 0.41 | 0/1973 | 0.52 | 0/2682 |
| 9 | h2 | 0.43 | 0/1973 | 0.51 | 0/2682 |
| 9 | i2 | 0.43 | 0/1973 | 0.53 | 0/2682 |
| 9 | j2 | 0.44 | 0/1973 | 0.52 | 0/2682 |
| 9 | k2 | 0.43 | 0/1973 | 0.54 | 0/2682 |
| 9 | l2 | 0.43 | 0/1894 | 0.51 | 0/2573 |
| 9 | m2 | 0.46 | 0/1894 | 0.54 | 0/2573 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 9 | n2 | 0.43 | 0/1894 | 0.51 | 0/2573 |
| 9 | o2 | 0.44 | 0/1894 | 0.53 | 0/2573 |
| 9 | p2 | 0.44 | 0/1894 | 0.52 | 0/2573 |
| 9 | q2 | 0.43 | 0/1907 | 0.52 | 0/2590 |
| 9 | r2 | 0.42 | 0/1973 | 0.56 | 0/2682 |
| 9 | s2 | 0.43 | 0/1973 | 0.56 | 0/2682 |
| 9 | t2 | 0.42 | 0/1973 | 0.58 | 2/2682 (0.1%) |
| 9 | u2 | 0.42 | 0/1973 | 0.56 | 0/2682 |
| 9 | v2 | 0.43 | 0/1973 | 0.54 | 0/2682 |
| 9 | w2 | 0.42 | 0/1973 | 0.57 | 1/2682 (0.0%) |
| 9 | x2 | 0.39 | 0/1973 | 0.54 | 0/2682 |
| 9 | y2 | 0.36 | 0/1973 | 0.53 | 0/2682 |
| 9 | z2 | 0.35 | 0/1973 | 0.54 | 2/2682 (0.1%) |
| 10 | A3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | B3 | 0.27 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | C3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | D3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | E3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | F3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | G3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | H3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | I3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | J3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | K3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | L3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | M3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | N3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | O3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | P3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | Q3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | R3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | S3 | 0.27 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | T3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | U3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | V3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | W3 | 0.26 | 0/1611 | 0.52 | 1/2188 (0.0%) |
| 10 | X3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | Y3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 10 | Z3 | 0.26 | 0/1614 | 0.52 | 1/2194 (0.0%) |
| 11 | a3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | b3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | c3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | d3 | 0.24 | 0/2267 | 0.50 | 0/3073 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 11 | e3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | f3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | g3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | h3 | 0.24 | 0/2266 | 0.50 | 0/3071 |
| 11 | i3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | j3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | k3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | l3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | m3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | n3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | o3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | p3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | q3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | r3 | 0.24 | 0/2264 | 0.50 | 0/3066 |
| 11 | s3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | t3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | u3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | v3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | w3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | x3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | y3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 11 | z3 | 0.24 | 0/2267 | 0.50 | 0/3073 |
| 12 | A4 | 0.25 | 0/1491 | 0.47 | 0/2033 |
| 12 | B4 | 0.25 | 0/1509 | 0.48 | 0/2058 |
| 12 | C4 | 0.25 | 0/1474 | 0.48 | 0/2010 |
| 12 | D4 | 0.25 | 0/1496 | 0.49 | 0/2040 |
| 12 | E4 | 0.25 | 0/1509 | 0.48 | 0/2058 |
| All | All | 0.37 | 8/249431 (0.0%) | 0.53 | 50/338382 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | B1 | 0 | 1 |
| 1 | E1 | 0 | 1 |
| 1 | G1 | 0 | 1 |
| 1 | H1 | 0 | 1 |
| 1 | L1 | 0 | 1 |
| 1 | N1 | 0 | 1 |
| 2 | B2 | 0 | 2 |

*Continued on next page...*

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 2 | C2 | 0 | 2 |
| 2 | D2 | 0 | 2 |
| 2 | E2 | 0 | 1 |
| 3 | F2 | 0 | 2 |
| 4 | G2 | 0 | 1 |
| 4 | H2 | 0 | 1 |
| 4 | I2 | 0 | 1 |
| 4 | J2 | 0 | 1 |
| 6 | U2 | 0 | 1 |
| 8 | b2 | 0 | 2 |
| 8 | c2 | 0 | 2 |
| 8 | d2 | 0 | 1 |
| 8 | e2 | 0 | 3 |
| 8 | f2 | 0 | 3 |
| All | All | 0 | 31 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | J2 | 51 | PHE | CE2-CZ | 34.87 | 2.03 | 1.37 |
| 4 | J2 | 51 | PHE | CE1-CZ | 33.72 | 2.01 | 1.37 |
| 4 | J2 | 51 | PHE | CD1-CE1 | 32.60 | 2.04 | 1.39 |
| 4 | J2 | 51 | PHE | CD2-CE2 | 31.33 | 2.02 | 1.39 |
| 4 | J2 | 51 | PHE | CG-CD1 | 21.84 | 1.71 | 1.38 |
| 4 | J2 | 51 | PHE | CG-CD2 | 21.32 | 1.70 | 1.38 |
| 2 | E2 | 205 | MET | SD-CE | 19.73 | 2.88 | 1.77 |
| 2 | D2 | 187 | PHE | CB-CG | -5.18 | 1.42 | 1.51 |

All (50) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | E2 | 205 | MET | CG-SD-CE | 20.16 | 132.46 | 100.20 |
| 9 | t2 | 167 | PRO | CA-N-CD | -8.46 | 99.66 | 111.50 |
| 1 | E1 | 282 | TYR | C-N-CA | -6.66 | 105.04 | 121.70 |
| 1 | g1 | 282 | TYR | C-N-CA | -6.65 | 105.07 | 121.70 |
| 10 | Z3 | 43 | PRO | CA-N-CD | -6.36 | 102.59 | 111.50 |
| 10 | N3 | 43 | PRO | CA-N-CD | -6.36 | 102.59 | 111.50 |
| 1 | M1 | 282 | TYR | C-N-CA | -6.36 | 105.80 | 121.70 |
| 10 | M3 | 43 | PRO | CA-N-CD | -6.36 | 102.60 | 111.50 |
| 10 | A3 | 43 | PRO | CA-N-CD | -6.35 | 102.61 | 111.50 |
| 10 | J3 | 43 | PRO | CA-N-CD | -6.34 | 102.62 | 111.50 |
| 10 | Y3 | 43 | PRO | CA-N-CD | -6.34 | 102.62 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | W3 | 43 | PRO | CA-N-CD | -6.34 | 102.63 | 111.50 |
| 10 | V3 | 43 | PRO | CA-N-CD | -6.34 | 102.63 | 111.50 |
| 10 | B3 | 43 | PRO | CA-N-CD | -6.33 | 102.63 | 111.50 |
| 10 | Q3 | 43 | PRO | CA-N-CD | -6.33 | 102.63 | 111.50 |
| 10 | D3 | 43 | PRO | CA-N-CD | -6.33 | 102.64 | 111.50 |
| 10 | H3 | 43 | PRO | CA-N-CD | -6.33 | 102.64 | 111.50 |
| 10 | I3 | 43 | PRO | CA-N-CD | -6.32 | 102.65 | 111.50 |
| 10 | R3 | 43 | PRO | CA-N-CD | -6.32 | 102.65 | 111.50 |
| 10 | F3 | 43 | PRO | CA-N-CD | -6.32 | 102.65 | 111.50 |
| 10 | S3 | 43 | PRO | CA-N-CD | -6.32 | 102.66 | 111.50 |
| 10 | G3 | 43 | PRO | CA-N-CD | -6.31 | 102.67 | 111.50 |
| 10 | T3 | 43 | PRO | CA-N-CD | -6.31 | 102.67 | 111.50 |
| 10 | C3 | 43 | PRO | CA-N-CD | -6.30 | 102.67 | 111.50 |
| 10 | L3 | 43 | PRO | CA-N-CD | -6.30 | 102.69 | 111.50 |
| 10 | K3 | 43 | PRO | CA-N-CD | -6.29 | 102.69 | 111.50 |
| 10 | U3 | 43 | PRO | CA-N-CD | -6.29 | 102.69 | 111.50 |
| 10 | O3 | 43 | PRO | CA-N-CD | -6.29 | 102.69 | 111.50 |
| 10 | P3 | 43 | PRO | CA-N-CD | -6.29 | 102.70 | 111.50 |
| 10 | X3 | 43 | PRO | CA-N-CD | -6.29 | 102.70 | 111.50 |
| 10 | E3 | 43 | PRO | CA-N-CD | -6.28 | 102.70 | 111.50 |
| 2 | A2 | 224 | MET | CB-CG-SD | -6.22 | 93.75 | 112.40 |
| 9 | t2 | 45 | LEU | CB-CG-CD2 | -6.03 | 100.74 | 111.00 |
| 1 | R1 | 282 | TYR | C-N-CA | -5.98 | 106.75 | 121.70 |
| 1 | F1 | 282 | TYR | C-N-CA | -5.90 | 106.94 | 121.70 |
| 1 | X1 | 282 | TYR | C-N-CA | -5.89 | 106.97 | 121.70 |
| 9 | 32 | 45 | LEU | CA-CB-CG | 5.80 | 128.63 | 115.30 |
| 1 | O1 | 282 | TYR | C-N-CA | -5.76 | 107.30 | 121.70 |
| 1 | e1 | 282 | TYR | C-N-CA | -5.75 | 107.34 | 121.70 |
| 9 | 42 | 253 | MET | CG-SD-CE | -5.73 | 91.03 | 100.20 |
| 5 | K2 | 75 | MET | CA-CB-CG | 5.60 | 122.82 | 113.30 |
| 1 | S1 | 282 | TYR | C-N-CA | -5.39 | 108.21 | 121.70 |
| 1 | J1 | 282 | TYR | C-N-CA | -5.34 | 108.35 | 121.70 |
| 1 | W1 | 282 | TYR | C-N-CA | -5.32 | 108.41 | 121.70 |
| 9 | w2 | 45 | LEU | CB-CG-CD2 | -5.23 | 102.11 | 111.00 |
| 1 | c1 | 282 | TYR | C-N-CA | -5.13 | 108.88 | 121.70 |
| 9 | z2 | 107 | LEU | CA-CB-CG | 5.12 | 127.07 | 115.30 |
| 9 | z2 | 62 | LEU | CA-CB-CG | 5.06 | 126.94 | 115.30 |
| 1 | P1 | 282 | TYR | C-N-CA | -5.04 | 109.10 | 121.70 |
| 1 | C1 | 160 | PRO | C-N-CA | 5.03 | 134.28 | 121.70 |

There are no chirality outliers.

All (31) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | B1 | 163 | SER | Peptide |
| 2 | B2 | 40 | LEU | Peptide |
| 2 | B2 | 41 | SER | Peptide |
| 2 | C2 | 40 | LEU | Peptide |
| 2 | C2 | 41 | SER | Peptide |
| 2 | D2 | 40 | LEU | Peptide |
| 2 | D2 | 41 | SER | Peptide |
| 1 | E1 | 162 | PRO | Peptide |
| 2 | E2 | 38 | TRP | Peptide |
| 3 | F2 | 113 | PHE | Peptide |
| 3 | F2 | 140 | PHE | Peptide |
| 1 | G1 | 165 | PHE | Peptide |
| 4 | G2 | 41 | ALA | Peptide |
| 1 | H1 | 165 | PHE | Peptide |
| 4 | H2 | 41 | ALA | Peptide |
| 4 | I2 | 41 | ALA | Peptide |
| 4 | J2 | 41 | ALA | Peptide |
| 1 | L1 | 125 | GLN | Peptide |
| 1 | N1 | 165 | PHE | Peptide |
| 6 | U2 | 95 | LEU | Peptide |
| 8 | b2 | 116 | GLN | Peptide |
| 8 | b2 | 117 | GLY | Peptide |
| 8 | c2 | 115 | ILE | Peptide |
| 8 | c2 | 117 | GLY | Peptide |
| 8 | d2 | 117 | GLY | Peptide |
| 8 | e2 | 114 | THR | Peptide |
| 8 | e2 | 115 | ILE | Peptide |
| 8 | e2 | 117 | GLY | Peptide |
| 8 | f2 | 114 | THR | Peptide |
| 8 | f2 | 117 | GLY | Peptide |
| 8 | f2 | 70 | GLN | Peptide |

## 5.2 Too-close contacts

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A1 | 145/560 (26%) | 143 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | B1 | 242/560 (43%) | 227 (94%) | 15 (6%) | 0 | 100 | 100 |
| 1 | C1 | 242/560 (43%) | 230 (95%) | 11 (4%) | 1 (0%) | 30 | 62 |
| 1 | D1 | 145/560 (26%) | 142 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | E1 | 242/560 (43%) | 226 (93%) | 16 (7%) | 0 | 100 | 100 |
| 1 | F1 | 145/560 (26%) | 141 (97%) | 4 (3%) | 0 | 100 | 100 |
| 1 | G1 | 242/560 (43%) | 225 (93%) | 16 (7%) | 1 (0%) | 30 | 62 |
| 1 | H1 | 242/560 (43%) | 221 (91%) | 19 (8%) | 2 (1%) | 16 | 49 |
| 1 | I1 | 242/560 (43%) | 229 (95%) | 12 (5%) | 1 (0%) | 30 | 62 |
| 1 | J1 | 145/560 (26%) | 142 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | K1 | 242/560 (43%) | 230 (95%) | 11 (4%) | 1 (0%) | 30 | 62 |
| 1 | L1 | 242/560 (43%) | 224 (93%) | 18 (7%) | 0 | 100 | 100 |
| 1 | M1 | 145/560 (26%) | 141 (97%) | 4 (3%) | 0 | 100 | 100 |
| 1 | N1 | 242/560 (43%) | 223 (92%) | 19 (8%) | 0 | 100 | 100 |
| 1 | O1 | 242/560 (43%) | 231 (96%) | 10 (4%) | 1 (0%) | 30 | 62 |
| 1 | P1 | 145/560 (26%) | 142 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | Q1 | 242/560 (43%) | 224 (93%) | 17 (7%) | 1 (0%) | 30 | 62 |
| 1 | R1 | 242/560 (43%) | 229 (95%) | 13 (5%) | 0 | 100 | 100 |
| 1 | S1 | 145/560 (26%) | 142 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | T1 | 242/560 (43%) | 230 (95%) | 12 (5%) | 0 | 100 | 100 |
| 1 | U1 | 242/560 (43%) | 231 (96%) | 11 (4%) | 0 | 100 | 100 |
| 1 | V1 | 145/560 (26%) | 141 (97%) | 4 (3%) | 0 | 100 | 100 |
| 1 | W1 | 242/560 (43%) | 227 (94%) | 14 (6%) | 1 (0%) | 30 | 62 |
| 1 | X1 | 242/560 (43%) | 225 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | Y1 | 242/560 (43%) | 228 (94%) | 14 (6%) | 0 | 100 | 100 |
| 1 | Z1 | 145/560 (26%) | 142 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | a1 | 242/560 (43%) | 227 (94%) | 14 (6%) | 1 (0%) | 30 | 62 |
| 1 | b1 | 145/560 (26%) | 140 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | c1 | 242/560 (43%) | 225 (93%) | 16 (7%) | 1 (0%) | 30 | 62 |
| 1 | d1 | 242/560 (43%) | 225 (93%) | 16 (7%) | 1 (0%) | 30 | 62 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | e1 | 145/560 (26%) | 144 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | f1 | 242/560 (43%) | 229 (95%) | 12 (5%) | 1 (0%) | 30 | 62 |
| 1 | g1 | 242/560 (43%) | 226 (93%) | 15 (6%) | 1 (0%) | 30 | 62 |
| 1 | h1 | 242/560 (43%) | 232 (96%) | 10 (4%) | 0 | 100 | 100 |
| 2 | A2 | 207/245 (84%) | 182 (88%) | 23 (11%) | 2 (1%) | 13 | 44 |
| 2 | B2 | 207/245 (84%) | 183 (88%) | 22 (11%) | 2 (1%) | 13 | 44 |
| 2 | C2 | 207/245 (84%) | 177 (86%) | 29 (14%) | 1 (0%) | 25 | 57 |
| 2 | D2 | 207/245 (84%) | 181 (87%) | 25 (12%) | 1 (0%) | 25 | 57 |
| 2 | E2 | 207/245 (84%) | 183 (88%) | 22 (11%) | 2 (1%) | 13 | 44 |
| 3 | F2 | 254/264 (96%) | 223 (88%) | 30 (12%) | 1 (0%) | 30 | 62 |
| 4 | G2 | 87/89 (98%) | 75 (86%) | 12 (14%) | 0 | 100 | 100 |
| 4 | H2 | 87/89 (98%) | 77 (88%) | 10 (12%) | 0 | 100 | 100 |
| 4 | I2 | 87/89 (98%) | 78 (90%) | 9 (10%) | 0 | 100 | 100 |
| 4 | J2 | 87/89 (98%) | 77 (88%) | 10 (12%) | 0 | 100 | 100 |
| 5 | K2 | 37/104 (36%) | 37 (100%) | 0 | 0 | 100 | 100 |
| 5 | L2 | 73/104 (70%) | 68 (93%) | 5 (7%) | 0 | 100 | 100 |
| 5 | M2 | 73/104 (70%) | 68 (93%) | 5 (7%) | 0 | 100 | 100 |
| 5 | N2 | 73/104 (70%) | 69 (94%) | 4 (6%) | 0 | 100 | 100 |
| 5 | O2 | 73/104 (70%) | 69 (94%) | 4 (6%) | 0 | 100 | 100 |
| 5 | P2 | 73/104 (70%) | 68 (93%) | 5 (7%) | 0 | 100 | 100 |
| 6 | Q2 | 131/138 (95%) | 115 (88%) | 16 (12%) | 0 | 100 | 100 |
| 6 | R2 | 114/138 (83%) | 98 (86%) | 16 (14%) | 0 | 100 | 100 |
| 6 | S2 | 116/138 (84%) | 104 (90%) | 12 (10%) | 0 | 100 | 100 |
| 6 | T2 | 102/138 (74%) | 95 (93%) | 7 (7%) | 0 | 100 | 100 |
| 6 | U2 | 113/138 (82%) | 102 (90%) | 11 (10%) | 0 | 100 | 100 |
| 7 | V2 | 131/134 (98%) | 112 (86%) | 18 (14%) | 1 (1%) | 16 | 49 |
| 7 | W2 | 130/134 (97%) | 108 (83%) | 22 (17%) | 0 | 100 | 100 |
| 7 | X2 | 130/134 (97%) | 107 (82%) | 22 (17%) | 1 (1%) | 16 | 49 |
| 7 | Y2 | 130/134 (97%) | 109 (84%) | 21 (16%) | 0 | 100 | 100 |
| 7 | Z2 | 130/134 (97%) | 113 (87%) | 17 (13%) | 0 | 100 | 100 |
| 7 | a2 | 130/134 (97%) | 109 (84%) | 21 (16%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 8 | b2 | 247/251 (98%) | 217 (88%) | 29 (12%) | 1 (0%) | 30 | 62 |
| 8 | c2 | 247/251 (98%) | 212 (86%) | 35 (14%) | 0 | 100 | 100 |
| 8 | d2 | 247/251 (98%) | 215 (87%) | 32 (13%) | 0 | 100 | 100 |
| 8 | e2 | 247/251 (98%) | 212 (86%) | 35 (14%) | 0 | 100 | 100 |
| 8 | f2 | 247/251 (98%) | 210 (85%) | 37 (15%) | 0 | 100 | 100 |
| 9 | 12 | 258/260 (99%) | 231 (90%) | 27 (10%) | 0 | 100 | 100 |
| 9 | 22 | 258/260 (99%) | 231 (90%) | 27 (10%) | 0 | 100 | 100 |
| 9 | 32 | 256/260 (98%) | 230 (90%) | 26 (10%) | 0 | 100 | 100 |
| 9 | 42 | 258/260 (99%) | 239 (93%) | 19 (7%) | 0 | 100 | 100 |
| 9 | g2 | 258/260 (99%) | 240 (93%) | 18 (7%) | 0 | 100 | 100 |
| 9 | h2 | 258/260 (99%) | 239 (93%) | 19 (7%) | 0 | 100 | 100 |
| 9 | i2 | 258/260 (99%) | 240 (93%) | 18 (7%) | 0 | 100 | 100 |
| 9 | j2 | 258/260 (99%) | 240 (93%) | 18 (7%) | 0 | 100 | 100 |
| 9 | k2 | 258/260 (99%) | 242 (94%) | 16 (6%) | 0 | 100 | 100 |
| 9 | l2 | 245/260 (94%) | 229 (94%) | 16 (6%) | 0 | 100 | 100 |
| 9 | m2 | 245/260 (94%) | 230 (94%) | 15 (6%) | 0 | 100 | 100 |
| 9 | n2 | 245/260 (94%) | 232 (95%) | 13 (5%) | 0 | 100 | 100 |
| 9 | o2 | 245/260 (94%) | 230 (94%) | 15 (6%) | 0 | 100 | 100 |
| 9 | p2 | 245/260 (94%) | 232 (95%) | 13 (5%) | 0 | 100 | 100 |
| 9 | q2 | 247/260 (95%) | 233 (94%) | 14 (6%) | 0 | 100 | 100 |
| 9 | r2 | 258/260 (99%) | 233 (90%) | 25 (10%) | 0 | 100 | 100 |
| 9 | s2 | 258/260 (99%) | 230 (89%) | 28 (11%) | 0 | 100 | 100 |
| 9 | t2 | 258/260 (99%) | 236 (92%) | 22 (8%) | 0 | 100 | 100 |
| 9 | u2 | 258/260 (99%) | 234 (91%) | 24 (9%) | 0 | 100 | 100 |
| 9 | v2 | 258/260 (99%) | 233 (90%) | 25 (10%) | 0 | 100 | 100 |
| 9 | w2 | 258/260 (99%) | 232 (90%) | 26 (10%) | 0 | 100 | 100 |
| 9 | x2 | 258/260 (99%) | 236 (92%) | 22 (8%) | 0 | 100 | 100 |
| 9 | y2 | 258/260 (99%) | 238 (92%) | 20 (8%) | 0 | 100 | 100 |
| 9 | z2 | 258/260 (99%) | 240 (93%) | 18 (7%) | 0 | 100 | 100 |
| 10 | A3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | B3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 10 | C3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | D3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | E3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | F3 | 209/232 (90%) | 192 (92%) | 17 (8%) | 0 | 100 | 100 |
| 10 | G3 | 209/232 (90%) | 192 (92%) | 17 (8%) | 0 | 100 | 100 |
| 10 | H3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | I3 | 209/232 (90%) | 192 (92%) | 17 (8%) | 0 | 100 | 100 |
| 10 | J3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | K3 | 209/232 (90%) | 192 (92%) | 17 (8%) | 0 | 100 | 100 |
| 10 | L3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | M3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | N3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | O3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | P3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | Q3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | R3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | S3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | T3 | 209/232 (90%) | 192 (92%) | 17 (8%) | 0 | 100 | 100 |
| 10 | U3 | 209/232 (90%) | 192 (92%) | 17 (8%) | 0 | 100 | 100 |
| 10 | V3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | W3 | 208/232 (90%) | 192 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | X3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | Y3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 10 | Z3 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 11 | a3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | b3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | c3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | d3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | e3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | f3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | g3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 11 | h3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | i3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | j3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | k3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | l3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | m3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | n3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | o3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | p3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | q3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | r3 | 299/365 (82%) | 288 (96%) | 11 (4%) | 0 | 100 | 100 |
| 11 | s3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | t3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | u3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | v3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | w3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | x3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | y3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 11 | z3 | 300/365 (82%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 12 | A4 | 199/232 (86%) | 194 (98%) | 5 (2%) | 0 | 100 | 100 |
| 12 | B4 | 202/232 (87%) | 200 (99%) | 2 (1%) | 0 | 100 | 100 |
| 12 | C4 | 197/232 (85%) | 185 (94%) | 12 (6%) | 0 | 100 | 100 |
| 12 | D4 | 200/232 (86%) | 194 (97%) | 6 (3%) | 0 | 100 | 100 |
| 12 | E4 | 202/232 (87%) | 197 (98%) | 5 (2%) | 0 | 100 | 100 |
| All | All | 32138/47180 (68%) | 29936 (93%) | 2176 (7%) | 26 (0%) | 50 | 78 |

All (26) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B2 | 42 | VAL |
| 2 | C2 | 42 | VAL |
| 2 | D2 | 42 | VAL |
| 2 | A2 | 42 | VAL |
| 2 | E2 | 42 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H1 | 160 | PRO |
| 1 | O1 | 160 | PRO |
| 1 | g1 | 160 | PRO |
| 2 | E2 | 41 | SER |
| 1 | K1 | 160 | PRO |
| 1 | a1 | 160 | PRO |
| 2 | A2 | 41 | SER |
| 2 | B2 | 41 | SER |
| 7 | V2 | 58 | ALA |
| 1 | C1 | 160 | PRO |
| 1 | H1 | 166 | VAL |
| 1 | Q1 | 160 | PRO |
| 1 | f1 | 160 | PRO |
| 3 | F2 | 158 | PRO |
| 8 | b2 | 117 | GLY |
| 1 | G1 | 160 | PRO |
| 1 | I1 | 160 | PRO |
| 1 | W1 | 160 | PRO |
| 1 | d1 | 160 | PRO |
| 1 | c1 | 160 | PRO |
| 7 | X2 | 93 | MET |

### 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 | A1 | 134/467 (29%) | 133 (99%) | 1 (1%) | 81 88 |
| 1 | B1 | 217/467 (46%) | 215 (99%) | 2 (1%) | 75 84 |
| 1 | C1 | 217/467 (46%) | 216 (100%) | 1 (0%) | 86 92 |
| 1 | D1 | 134/467 (29%) | 133 (99%) | 1 (1%) | 81 88 |
| 1 | E1 | 217/467 (46%) | 217 (100%) | 0 | 100 100 |
| 1 | F1 | 134/467 (29%) | 133 (99%) | 1 (1%) | 81 88 |
| 1 | G1 | 217/467 (46%) | 216 (100%) | 1 (0%) | 86 92 |
| 1 | H1 | 217/467 (46%) | 216 (100%) | 1 (0%) | 86 92 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | I1 | 217/467 (46%) | 216 (100%) | 1 (0%) | 86 92 |
| 1 | J1 | 134/467 (29%) | 132 (98%) | 2 (2%) | 60 75 |
| 1 | K1 | 217/467 (46%) | 215 (99%) | 2 (1%) | 75 84 |
| 1 | L1 | 217/467 (46%) | 216 (100%) | 1 (0%) | 86 92 |
| 1 | M1 | 134/467 (29%) | 133 (99%) | 1 (1%) | 81 88 |
| 1 | N1 | 217/467 (46%) | 215 (99%) | 2 (1%) | 75 84 |
| 1 | O1 | 217/467 (46%) | 213 (98%) | 4 (2%) | 54 71 |
| 1 | P1 | 134/467 (29%) | 131 (98%) | 3 (2%) | 47 65 |
| 1 | Q1 | 217/467 (46%) | 215 (99%) | 2 (1%) | 75 84 |
| 1 | R1 | 217/467 (46%) | 216 (100%) | 1 (0%) | 86 92 |
| 1 | S1 | 134/467 (29%) | 133 (99%) | 1 (1%) | 81 88 |
| 1 | T1 | 217/467 (46%) | 216 (100%) | 1 (0%) | 86 92 |
| 1 | U1 | 217/467 (46%) | 215 (99%) | 2 (1%) | 75 84 |
| 1 | V1 | 134/467 (29%) | 132 (98%) | 2 (2%) | 60 75 |
| 1 | W1 | 217/467 (46%) | 215 (99%) | 2 (1%) | 75 84 |
| 1 | X1 | 217/467 (46%) | 215 (99%) | 2 (1%) | 75 84 |
| 1 | Y1 | 217/467 (46%) | 215 (99%) | 2 (1%) | 75 84 |
| 1 | Z1 | 134/467 (29%) | 132 (98%) | 2 (2%) | 60 75 |
| 1 | a1 | 217/467 (46%) | 215 (99%) | 2 (1%) | 75 84 |
| 1 | b1 | 134/467 (29%) | 133 (99%) | 1 (1%) | 81 88 |
| 1 | c1 | 217/467 (46%) | 216 (100%) | 1 (0%) | 86 92 |
| 1 | d1 | 217/467 (46%) | 215 (99%) | 2 (1%) | 75 84 |
| 1 | e1 | 134/467 (29%) | 133 (99%) | 1 (1%) | 81 88 |
| 1 | f1 | 217/467 (46%) | 216 (100%) | 1 (0%) | 86 92 |
| 1 | g1 | 217/467 (46%) | 216 (100%) | 1 (0%) | 86 92 |
| 1 | h1 | 217/467 (46%) | 216 (100%) | 1 (0%) | 86 92 |
| 2 | A2 | 179/204 (88%) | 179 (100%) | 0 | 100 100 |
| 2 | B2 | 179/204 (88%) | 179 (100%) | 0 | 100 100 |
| 2 | C2 | 179/204 (88%) | 178 (99%) | 1 (1%) | 84 90 |
| 2 | D2 | 179/204 (88%) | 179 (100%) | 0 | 100 100 |
| 2 | E2 | 179/204 (88%) | 179 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 3 | F2 | 215/221 (97%) | 215 (100%) | 0 | 100 100 |
| 4 | G2 | 74/74 (100%) | 74 (100%) | 0 | 100 100 |
| 4 | H2 | 74/74 (100%) | 74 (100%) | 0 | 100 100 |
| 4 | I2 | 74/74 (100%) | 74 (100%) | 0 | 100 100 |
| 4 | J2 | 74/74 (100%) | 74 (100%) | 0 | 100 100 |
| 5 | K2 | 33/79 (42%) | 33 (100%) | 0 | 100 100 |
| 5 | L2 | 59/79 (75%) | 59 (100%) | 0 | 100 100 |
| 5 | M2 | 59/79 (75%) | 59 (100%) | 0 | 100 100 |
| 5 | N2 | 59/79 (75%) | 59 (100%) | 0 | 100 100 |
| 5 | O2 | 59/79 (75%) | 59 (100%) | 0 | 100 100 |
| 5 | P2 | 59/79 (75%) | 59 (100%) | 0 | 100 100 |
| 6 | Q2 | 109/113 (96%) | 109 (100%) | 0 | 100 100 |
| 6 | R2 | 100/113 (88%) | 100 (100%) | 0 | 100 100 |
| 6 | S2 | 100/113 (88%) | 99 (99%) | 1 (1%) | 73 82 |
| 6 | T2 | 89/113 (79%) | 88 (99%) | 1 (1%) | 70 80 |
| 6 | U2 | 99/113 (88%) | 97 (98%) | 2 (2%) | 50 68 |
| 7 | V2 | 104/105 (99%) | 103 (99%) | 1 (1%) | 73 82 |
| 7 | W2 | 104/105 (99%) | 104 (100%) | 0 | 100 100 |
| 7 | X2 | 104/105 (99%) | 104 (100%) | 0 | 100 100 |
| 7 | Y2 | 104/105 (99%) | 104 (100%) | 0 | 100 100 |
| 7 | Z2 | 104/105 (99%) | 103 (99%) | 1 (1%) | 73 82 |
| 7 | a2 | 104/105 (99%) | 104 (100%) | 0 | 100 100 |
| 8 | b2 | 191/193 (99%) | 191 (100%) | 0 | 100 100 |
| 8 | c2 | 191/193 (99%) | 191 (100%) | 0 | 100 100 |
| 8 | d2 | 191/193 (99%) | 191 (100%) | 0 | 100 100 |
| 8 | e2 | 191/193 (99%) | 191 (100%) | 0 | 100 100 |
| 8 | f2 | 191/193 (99%) | 191 (100%) | 0 | 100 100 |
| 9 | 12 | 215/215 (100%) | 215 (100%) | 0 | 100 100 |
| 9 | 22 | 215/215 (100%) | 215 (100%) | 0 | 100 100 |
| 9 | 32 | 214/215 (100%) | 214 (100%) | 0 | 100 100 |
| 9 | 42 | 215/215 (100%) | 214 (100%) | 1 (0%) | 86 92 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 9 | g2 | 215/215 (100%) | 215 (100%) | 0 | 100 | 100 |
| 9 | h2 | 215/215 (100%) | 215 (100%) | 0 | 100 | 100 |
| 9 | i2 | 215/215 (100%) | 215 (100%) | 0 | 100 | 100 |
| 9 | j2 | 215/215 (100%) | 215 (100%) | 0 | 100 | 100 |
| 9 | k2 | 215/215 (100%) | 215 (100%) | 0 | 100 | 100 |
| 9 | l2 | 206/215 (96%) | 206 (100%) | 0 | 100 | 100 |
| 9 | m2 | 206/215 (96%) | 206 (100%) | 0 | 100 | 100 |
| 9 | n2 | 206/215 (96%) | 205 (100%) | 1 (0%) | 86 | 92 |
| 9 | o2 | 206/215 (96%) | 206 (100%) | 0 | 100 | 100 |
| 9 | p2 | 206/215 (96%) | 206 (100%) | 0 | 100 | 100 |
| 9 | q2 | 207/215 (96%) | 206 (100%) | 1 (0%) | 86 | 92 |
| 9 | r2 | 215/215 (100%) | 214 (100%) | 1 (0%) | 86 | 92 |
| 9 | s2 | 215/215 (100%) | 215 (100%) | 0 | 100 | 100 |
| 9 | t2 | 215/215 (100%) | 215 (100%) | 0 | 100 | 100 |
| 9 | u2 | 215/215 (100%) | 215 (100%) | 0 | 100 | 100 |
| 9 | v2 | 215/215 (100%) | 215 (100%) | 0 | 100 | 100 |
| 9 | w2 | 215/215 (100%) | 215 (100%) | 0 | 100 | 100 |
| 9 | x2 | 215/215 (100%) | 215 (100%) | 0 | 100 | 100 |
| 9 | y2 | 215/215 (100%) | 214 (100%) | 1 (0%) | 86 | 92 |
| 9 | z2 | 215/215 (100%) | 215 (100%) | 0 | 100 | 100 |
| 10 | A3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | B3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | C3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | D3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | E3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | F3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | G3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | H3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | I3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | J3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | K3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 10 | L3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | M3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | N3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | O3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | P3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | Q3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | R3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | S3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | T3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | U3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | V3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | W3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | X3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | Y3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 10 | Z3 | 170/186 (91%) | 164 (96%) | 6 (4%) | 31 | 56 |
| 11 | a3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | b3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | c3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | d3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | e3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | f3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | g3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | h3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | i3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | j3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | k3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | l3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | m3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | n3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | o3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | p3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 11 | q3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | r3 | 250/294 (85%) | 237 (95%) | 13 (5%) | 19 | 46 |
| 11 | s3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | t3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | u3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | v3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | w3 | 251/294 (85%) | 237 (94%) | 14 (6%) | 17 | 45 |
| 11 | x3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | y3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 11 | z3 | 251/294 (85%) | 238 (95%) | 13 (5%) | 19 | 46 |
| 12 | A4 | 164/188 (87%) | 162 (99%) | 2 (1%) | 67 | 79 |
| 12 | B4 | 165/188 (88%) | 165 (100%) | 0 | 100 | 100 |
| 12 | C4 | 162/188 (86%) | 162 (100%) | 0 | 100 | 100 |
| 12 | D4 | 164/188 (87%) | 163 (99%) | 1 (1%) | 84 | 90 |
| 12 | E4 | 165/188 (88%) | 164 (99%) | 1 (1%) | 84 | 90 |
| All | All | 27146/38629 (70%) | 26584 (98%) | 562 (2%) | 49 | 67 |

All (562) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 410 | LYS |
| 1 | B1 | 394 | LYS |
| 1 | B1 | 410 | LYS |
| 1 | C1 | 394 | LYS |
| 1 | D1 | 394 | LYS |
| 1 | F1 | 394 | LYS |
| 1 | G1 | 394 | LYS |
| 1 | H1 | 394 | LYS |
| 1 | I1 | 410 | LYS |
| 1 | J1 | 394 | LYS |
| 1 | J1 | 410 | LYS |
| 1 | K1 | 394 | LYS |
| 1 | K1 | 410 | LYS |
| 1 | L1 | 394 | LYS |
| 1 | M1 | 394 | LYS |
| 1 | N1 | 394 | LYS |
| 1 | N1 | 410 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O1 | 161 | LYS |
| 1 | O1 | 170 | LYS |
| 1 | O1 | 394 | LYS |
| 1 | O1 | 410 | LYS |
| 1 | P1 | 394 | LYS |
| 1 | P1 | 410 | LYS |
| 1 | P1 | 431 | ASN |
| 1 | Q1 | 394 | LYS |
| 1 | Q1 | 410 | LYS |
| 1 | R1 | 394 | LYS |
| 1 | S1 | 394 | LYS |
| 1 | T1 | 394 | LYS |
| 1 | U1 | 394 | LYS |
| 1 | U1 | 410 | LYS |
| 1 | V1 | 281 | HIS |
| 1 | V1 | 394 | LYS |
| 1 | W1 | 394 | LYS |
| 1 | W1 | 410 | LYS |
| 1 | X1 | 394 | LYS |
| 1 | X1 | 410 | LYS |
| 1 | Y1 | 394 | LYS |
| 1 | Y1 | 410 | LYS |
| 1 | Z1 | 394 | LYS |
| 1 | Z1 | 410 | LYS |
| 1 | a1 | 394 | LYS |
| 1 | a1 | 410 | LYS |
| 1 | b1 | 394 | LYS |
| 1 | c1 | 394 | LYS |
| 1 | d1 | 394 | LYS |
| 1 | d1 | 410 | LYS |
| 1 | e1 | 394 | LYS |
| 1 | f1 | 394 | LYS |
| 1 | g1 | 394 | LYS |
| 1 | h1 | 394 | LYS |
| 2 | C2 | 236 | MET |
| 6 | S2 | 17 | ASN |
| 6 | T2 | 17 | ASN |
| 6 | U2 | 112 | ASN |
| 6 | U2 | 117 | GLN |
| 7 | V2 | 59 | THR |
| 7 | Z2 | 75 | LYS |
| 9 | n2 | 172 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | q2 | 169 | GLN |
| 9 | r2 | 135 | GLN |
| 9 | y2 | 196 | GLN |
| 9 | 42 | 243 | ASN |
| 10 | A3 | 30 | LEU |
| 10 | A3 | 36 | THR |
| 10 | A3 | 40 | ILE |
| 10 | A3 | 99 | ASP |
| 10 | A3 | 111 | ARG |
| 10 | A3 | 144 | PHE |
| 10 | B3 | 30 | LEU |
| 10 | B3 | 36 | THR |
| 10 | B3 | 40 | ILE |
| 10 | B3 | 99 | ASP |
| 10 | B3 | 111 | ARG |
| 10 | B3 | 144 | PHE |
| 10 | C3 | 30 | LEU |
| 10 | C3 | 36 | THR |
| 10 | C3 | 40 | ILE |
| 10 | C3 | 99 | ASP |
| 10 | C3 | 111 | ARG |
| 10 | C3 | 144 | PHE |
| 10 | D3 | 30 | LEU |
| 10 | D3 | 36 | THR |
| 10 | D3 | 40 | ILE |
| 10 | D3 | 99 | ASP |
| 10 | D3 | 111 | ARG |
| 10 | D3 | 144 | PHE |
| 10 | E3 | 30 | LEU |
| 10 | E3 | 36 | THR |
| 10 | E3 | 40 | ILE |
| 10 | E3 | 99 | ASP |
| 10 | E3 | 111 | ARG |
| 10 | E3 | 144 | PHE |
| 10 | F3 | 30 | LEU |
| 10 | F3 | 36 | THR |
| 10 | F3 | 40 | ILE |
| 10 | F3 | 99 | ASP |
| 10 | F3 | 111 | ARG |
| 10 | F3 | 144 | PHE |
| 10 | G3 | 30 | LEU |
| 10 | G3 | 36 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | G3 | 40 | ILE |
| 10 | G3 | 99 | ASP |
| 10 | G3 | 111 | ARG |
| 10 | G3 | 144 | PHE |
| 10 | H3 | 30 | LEU |
| 10 | H3 | 36 | THR |
| 10 | H3 | 40 | ILE |
| 10 | H3 | 99 | ASP |
| 10 | H3 | 111 | ARG |
| 10 | H3 | 144 | PHE |
| 10 | I3 | 30 | LEU |
| 10 | I3 | 36 | THR |
| 10 | I3 | 40 | ILE |
| 10 | I3 | 99 | ASP |
| 10 | I3 | 111 | ARG |
| 10 | I3 | 144 | PHE |
| 10 | J3 | 30 | LEU |
| 10 | J3 | 36 | THR |
| 10 | J3 | 40 | ILE |
| 10 | J3 | 99 | ASP |
| 10 | J3 | 111 | ARG |
| 10 | J3 | 144 | PHE |
| 10 | K3 | 30 | LEU |
| 10 | K3 | 36 | THR |
| 10 | K3 | 40 | ILE |
| 10 | K3 | 99 | ASP |
| 10 | K3 | 111 | ARG |
| 10 | K3 | 144 | PHE |
| 10 | L3 | 30 | LEU |
| 10 | L3 | 36 | THR |
| 10 | L3 | 40 | ILE |
| 10 | L3 | 99 | ASP |
| 10 | L3 | 111 | ARG |
| 10 | L3 | 144 | PHE |
| 10 | M3 | 30 | LEU |
| 10 | M3 | 36 | THR |
| 10 | M3 | 40 | ILE |
| 10 | M3 | 99 | ASP |
| 10 | M3 | 111 | ARG |
| 10 | M3 | 144 | PHE |
| 10 | N3 | 30 | LEU |
| 10 | N3 | 36 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | N3 | 40 | ILE |
| 10 | N3 | 99 | ASP |
| 10 | N3 | 111 | ARG |
| 10 | N3 | 144 | PHE |
| 10 | O3 | 30 | LEU |
| 10 | O3 | 36 | THR |
| 10 | O3 | 40 | ILE |
| 10 | O3 | 99 | ASP |
| 10 | O3 | 111 | ARG |
| 10 | O3 | 144 | PHE |
| 10 | P3 | 30 | LEU |
| 10 | P3 | 36 | THR |
| 10 | P3 | 40 | ILE |
| 10 | P3 | 99 | ASP |
| 10 | P3 | 111 | ARG |
| 10 | P3 | 144 | PHE |
| 10 | Q3 | 30 | LEU |
| 10 | Q3 | 36 | THR |
| 10 | Q3 | 40 | ILE |
| 10 | Q3 | 99 | ASP |
| 10 | Q3 | 111 | ARG |
| 10 | Q3 | 144 | PHE |
| 10 | R3 | 30 | LEU |
| 10 | R3 | 36 | THR |
| 10 | R3 | 40 | ILE |
| 10 | R3 | 99 | ASP |
| 10 | R3 | 111 | ARG |
| 10 | R3 | 144 | PHE |
| 10 | S3 | 30 | LEU |
| 10 | S3 | 36 | THR |
| 10 | S3 | 40 | ILE |
| 10 | S3 | 99 | ASP |
| 10 | S3 | 111 | ARG |
| 10 | S3 | 144 | PHE |
| 10 | T3 | 30 | LEU |
| 10 | T3 | 36 | THR |
| 10 | T3 | 40 | ILE |
| 10 | T3 | 99 | ASP |
| 10 | T3 | 111 | ARG |
| 10 | T3 | 144 | PHE |
| 10 | U3 | 30 | LEU |
| 10 | U3 | 36 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | U3 | 40 | ILE |
| 10 | U3 | 99 | ASP |
| 10 | U3 | 111 | ARG |
| 10 | U3 | 144 | PHE |
| 10 | V3 | 30 | LEU |
| 10 | V3 | 36 | THR |
| 10 | V3 | 40 | ILE |
| 10 | V3 | 99 | ASP |
| 10 | V3 | 111 | ARG |
| 10 | V3 | 144 | PHE |
| 10 | W3 | 30 | LEU |
| 10 | W3 | 36 | THR |
| 10 | W3 | 40 | ILE |
| 10 | W3 | 99 | ASP |
| 10 | W3 | 111 | ARG |
| 10 | W3 | 144 | PHE |
| 10 | X3 | 30 | LEU |
| 10 | X3 | 36 | THR |
| 10 | X3 | 40 | ILE |
| 10 | X3 | 99 | ASP |
| 10 | X3 | 111 | ARG |
| 10 | X3 | 144 | PHE |
| 10 | Y3 | 30 | LEU |
| 10 | Y3 | 36 | THR |
| 10 | Y3 | 40 | ILE |
| 10 | Y3 | 99 | ASP |
| 10 | Y3 | 111 | ARG |
| 10 | Y3 | 144 | PHE |
| 10 | Z3 | 30 | LEU |
| 10 | Z3 | 36 | THR |
| 10 | Z3 | 40 | ILE |
| 10 | Z3 | 99 | ASP |
| 10 | Z3 | 111 | ARG |
| 10 | Z3 | 144 | PHE |
| 11 | a3 | 25 | LEU |
| 11 | a3 | 84 | VAL |
| 11 | a3 | 114 | LYS |
| 11 | a3 | 124 | THR |
| 11 | a3 | 190 | ASN |
| 11 | a3 | 196 | MET |
| 11 | a3 | 206 | ARG |
| 11 | a3 | 210 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | a3 | 245 | ASN |
| 11 | a3 | 252 | LYS |
| 11 | a3 | 256 | ASN |
| 11 | a3 | 325 | SER |
| 11 | a3 | 344 | ASP |
| 11 | b3 | 25 | LEU |
| 11 | b3 | 84 | VAL |
| 11 | b3 | 114 | LYS |
| 11 | b3 | 124 | THR |
| 11 | b3 | 190 | ASN |
| 11 | b3 | 196 | MET |
| 11 | b3 | 206 | ARG |
| 11 | b3 | 210 | TYR |
| 11 | b3 | 245 | ASN |
| 11 | b3 | 252 | LYS |
| 11 | b3 | 256 | ASN |
| 11 | b3 | 325 | SER |
| 11 | b3 | 344 | ASP |
| 11 | c3 | 25 | LEU |
| 11 | c3 | 84 | VAL |
| 11 | c3 | 114 | LYS |
| 11 | c3 | 124 | THR |
| 11 | c3 | 190 | ASN |
| 11 | c3 | 196 | MET |
| 11 | c3 | 206 | ARG |
| 11 | c3 | 210 | TYR |
| 11 | c3 | 245 | ASN |
| 11 | c3 | 252 | LYS |
| 11 | c3 | 256 | ASN |
| 11 | c3 | 325 | SER |
| 11 | c3 | 344 | ASP |
| 11 | d3 | 25 | LEU |
| 11 | d3 | 84 | VAL |
| 11 | d3 | 114 | LYS |
| 11 | d3 | 124 | THR |
| 11 | d3 | 190 | ASN |
| 11 | d3 | 196 | MET |
| 11 | d3 | 206 | ARG |
| 11 | d3 | 210 | TYR |
| 11 | d3 | 245 | ASN |
| 11 | d3 | 252 | LYS |
| 11 | d3 | 256 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | d3 | 325 | SER |
| 11 | d3 | 344 | ASP |
| 11 | e3 | 25 | LEU |
| 11 | e3 | 84 | VAL |
| 11 | e3 | 114 | LYS |
| 11 | e3 | 124 | THR |
| 11 | e3 | 190 | ASN |
| 11 | e3 | 196 | MET |
| 11 | e3 | 206 | ARG |
| 11 | e3 | 210 | TYR |
| 11 | e3 | 245 | ASN |
| 11 | e3 | 252 | LYS |
| 11 | e3 | 256 | ASN |
| 11 | e3 | 325 | SER |
| 11 | e3 | 344 | ASP |
| 11 | f3 | 25 | LEU |
| 11 | f3 | 84 | VAL |
| 11 | f3 | 114 | LYS |
| 11 | f3 | 124 | THR |
| 11 | f3 | 190 | ASN |
| 11 | f3 | 196 | MET |
| 11 | f3 | 206 | ARG |
| 11 | f3 | 210 | TYR |
| 11 | f3 | 245 | ASN |
| 11 | f3 | 252 | LYS |
| 11 | f3 | 256 | ASN |
| 11 | f3 | 325 | SER |
| 11 | f3 | 344 | ASP |
| 11 | g3 | 25 | LEU |
| 11 | g3 | 84 | VAL |
| 11 | g3 | 114 | LYS |
| 11 | g3 | 124 | THR |
| 11 | g3 | 190 | ASN |
| 11 | g3 | 196 | MET |
| 11 | g3 | 206 | ARG |
| 11 | g3 | 210 | TYR |
| 11 | g3 | 245 | ASN |
| 11 | g3 | 252 | LYS |
| 11 | g3 | 256 | ASN |
| 11 | g3 | 325 | SER |
| 11 | g3 | 344 | ASP |
| 11 | h3 | 25 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | h3 | 84 | VAL |
| 11 | h3 | 114 | LYS |
| 11 | h3 | 124 | THR |
| 11 | h3 | 190 | ASN |
| 11 | h3 | 196 | MET |
| 11 | h3 | 206 | ARG |
| 11 | h3 | 210 | TYR |
| 11 | h3 | 245 | ASN |
| 11 | h3 | 252 | LYS |
| 11 | h3 | 256 | ASN |
| 11 | h3 | 325 | SER |
| 11 | h3 | 344 | ASP |
| 11 | i3 | 25 | LEU |
| 11 | i3 | 84 | VAL |
| 11 | i3 | 114 | LYS |
| 11 | i3 | 124 | THR |
| 11 | i3 | 190 | ASN |
| 11 | i3 | 196 | MET |
| 11 | i3 | 206 | ARG |
| 11 | i3 | 210 | TYR |
| 11 | i3 | 245 | ASN |
| 11 | i3 | 252 | LYS |
| 11 | i3 | 256 | ASN |
| 11 | i3 | 325 | SER |
| 11 | i3 | 344 | ASP |
| 11 | j3 | 25 | LEU |
| 11 | j3 | 84 | VAL |
| 11 | j3 | 114 | LYS |
| 11 | j3 | 124 | THR |
| 11 | j3 | 190 | ASN |
| 11 | j3 | 196 | MET |
| 11 | j3 | 206 | ARG |
| 11 | j3 | 210 | TYR |
| 11 | j3 | 245 | ASN |
| 11 | j3 | 252 | LYS |
| 11 | j3 | 256 | ASN |
| 11 | j3 | 325 | SER |
| 11 | j3 | 344 | ASP |
| 11 | k3 | 25 | LEU |
| 11 | k3 | 84 | VAL |
| 11 | k3 | 114 | LYS |
| 11 | k3 | 124 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | k3 | 190 | ASN |
| 11 | k3 | 196 | MET |
| 11 | k3 | 206 | ARG |
| 11 | k3 | 210 | TYR |
| 11 | k3 | 245 | ASN |
| 11 | k3 | 252 | LYS |
| 11 | k3 | 256 | ASN |
| 11 | k3 | 325 | SER |
| 11 | k3 | 344 | ASP |
| 11 | l3 | 25 | LEU |
| 11 | l3 | 84 | VAL |
| 11 | l3 | 114 | LYS |
| 11 | l3 | 124 | THR |
| 11 | l3 | 190 | ASN |
| 11 | l3 | 196 | MET |
| 11 | l3 | 206 | ARG |
| 11 | l3 | 210 | TYR |
| 11 | l3 | 245 | ASN |
| 11 | l3 | 252 | LYS |
| 11 | l3 | 256 | ASN |
| 11 | l3 | 325 | SER |
| 11 | l3 | 344 | ASP |
| 11 | m3 | 25 | LEU |
| 11 | m3 | 84 | VAL |
| 11 | m3 | 114 | LYS |
| 11 | m3 | 124 | THR |
| 11 | m3 | 190 | ASN |
| 11 | m3 | 196 | MET |
| 11 | m3 | 206 | ARG |
| 11 | m3 | 210 | TYR |
| 11 | m3 | 245 | ASN |
| 11 | m3 | 252 | LYS |
| 11 | m3 | 256 | ASN |
| 11 | m3 | 325 | SER |
| 11 | m3 | 344 | ASP |
| 11 | n3 | 25 | LEU |
| 11 | n3 | 84 | VAL |
| 11 | n3 | 114 | LYS |
| 11 | n3 | 124 | THR |
| 11 | n3 | 190 | ASN |
| 11 | n3 | 196 | MET |
| 11 | n3 | 206 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | n3 | 210 | TYR |
| 11 | n3 | 245 | ASN |
| 11 | n3 | 252 | LYS |
| 11 | n3 | 256 | ASN |
| 11 | n3 | 325 | SER |
| 11 | n3 | 344 | ASP |
| 11 | o3 | 25 | LEU |
| 11 | o3 | 84 | VAL |
| 11 | o3 | 114 | LYS |
| 11 | o3 | 124 | THR |
| 11 | o3 | 190 | ASN |
| 11 | o3 | 196 | MET |
| 11 | o3 | 206 | ARG |
| 11 | o3 | 210 | TYR |
| 11 | o3 | 245 | ASN |
| 11 | o3 | 252 | LYS |
| 11 | o3 | 256 | ASN |
| 11 | o3 | 325 | SER |
| 11 | o3 | 344 | ASP |
| 11 | p3 | 25 | LEU |
| 11 | p3 | 84 | VAL |
| 11 | p3 | 114 | LYS |
| 11 | p3 | 124 | THR |
| 11 | p3 | 190 | ASN |
| 11 | p3 | 196 | MET |
| 11 | p3 | 206 | ARG |
| 11 | p3 | 210 | TYR |
| 11 | p3 | 245 | ASN |
| 11 | p3 | 252 | LYS |
| 11 | p3 | 256 | ASN |
| 11 | p3 | 325 | SER |
| 11 | p3 | 344 | ASP |
| 11 | q3 | 25 | LEU |
| 11 | q3 | 84 | VAL |
| 11 | q3 | 114 | LYS |
| 11 | q3 | 124 | THR |
| 11 | q3 | 190 | ASN |
| 11 | q3 | 196 | MET |
| 11 | q3 | 206 | ARG |
| 11 | q3 | 210 | TYR |
| 11 | q3 | 245 | ASN |
| 11 | q3 | 252 | LYS |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | q3 | 256 | ASN |
| 11 | q3 | 325 | SER |
| 11 | q3 | 344 | ASP |
| 11 | r3 | 25 | LEU |
| 11 | r3 | 84 | VAL |
| 11 | r3 | 114 | LYS |
| 11 | r3 | 124 | THR |
| 11 | r3 | 190 | ASN |
| 11 | r3 | 196 | MET |
| 11 | r3 | 206 | ARG |
| 11 | r3 | 210 | TYR |
| 11 | r3 | 245 | ASN |
| 11 | r3 | 252 | LYS |
| 11 | r3 | 256 | ASN |
| 11 | r3 | 325 | SER |
| 11 | r3 | 344 | ASP |
| 11 | s3 | 25 | LEU |
| 11 | s3 | 84 | VAL |
| 11 | s3 | 114 | LYS |
| 11 | s3 | 124 | THR |
| 11 | s3 | 190 | ASN |
| 11 | s3 | 196 | MET |
| 11 | s3 | 206 | ARG |
| 11 | s3 | 210 | TYR |
| 11 | s3 | 245 | ASN |
| 11 | s3 | 252 | LYS |
| 11 | s3 | 256 | ASN |
| 11 | s3 | 325 | SER |
| 11 | s3 | 344 | ASP |
| 11 | t3 | 25 | LEU |
| 11 | t3 | 84 | VAL |
| 11 | t3 | 114 | LYS |
| 11 | t3 | 124 | THR |
| 11 | t3 | 190 | ASN |
| 11 | t3 | 196 | MET |
| 11 | t3 | 206 | ARG |
| 11 | t3 | 210 | TYR |
| 11 | t3 | 245 | ASN |
| 11 | t3 | 252 | LYS |
| 11 | t3 | 256 | ASN |
| 11 | t3 | 325 | SER |
| 11 | t3 | 344 | ASP |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | u3 | 25 | LEU |
| 11 | u3 | 84 | VAL |
| 11 | u3 | 114 | LYS |
| 11 | u3 | 124 | THR |
| 11 | u3 | 190 | ASN |
| 11 | u3 | 196 | MET |
| 11 | u3 | 206 | ARG |
| 11 | u3 | 210 | TYR |
| 11 | u3 | 245 | ASN |
| 11 | u3 | 252 | LYS |
| 11 | u3 | 256 | ASN |
| 11 | u3 | 325 | SER |
| 11 | u3 | 344 | ASP |
| 11 | v3 | 25 | LEU |
| 11 | v3 | 84 | VAL |
| 11 | v3 | 114 | LYS |
| 11 | v3 | 124 | THR |
| 11 | v3 | 190 | ASN |
| 11 | v3 | 196 | MET |
| 11 | v3 | 206 | ARG |
| 11 | v3 | 210 | TYR |
| 11 | v3 | 245 | ASN |
| 11 | v3 | 252 | LYS |
| 11 | v3 | 256 | ASN |
| 11 | v3 | 325 | SER |
| 11 | v3 | 344 | ASP |
| 11 | w3 | 25 | LEU |
| 11 | w3 | 78 | ASN |
| 11 | w3 | 84 | VAL |
| 11 | w3 | 114 | LYS |
| 11 | w3 | 124 | THR |
| 11 | w3 | 190 | ASN |
| 11 | w3 | 196 | MET |
| 11 | w3 | 206 | ARG |
| 11 | w3 | 210 | TYR |
| 11 | w3 | 245 | ASN |
| 11 | w3 | 252 | LYS |
| 11 | w3 | 256 | ASN |
| 11 | w3 | 325 | SER |
| 11 | w3 | 344 | ASP |
| 11 | x3 | 25 | LEU |
| 11 | x3 | 84 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | x3 | 114 | LYS |
| 11 | x3 | 124 | THR |
| 11 | x3 | 190 | ASN |
| 11 | x3 | 196 | MET |
| 11 | x3 | 206 | ARG |
| 11 | x3 | 210 | TYR |
| 11 | x3 | 245 | ASN |
| 11 | x3 | 252 | LYS |
| 11 | x3 | 256 | ASN |
| 11 | x3 | 325 | SER |
| 11 | x3 | 344 | ASP |
| 11 | y3 | 25 | LEU |
| 11 | y3 | 84 | VAL |
| 11 | y3 | 114 | LYS |
| 11 | y3 | 124 | THR |
| 11 | y3 | 190 | ASN |
| 11 | y3 | 196 | MET |
| 11 | y3 | 206 | ARG |
| 11 | y3 | 210 | TYR |
| 11 | y3 | 245 | ASN |
| 11 | y3 | 252 | LYS |
| 11 | y3 | 256 | ASN |
| 11 | y3 | 325 | SER |
| 11 | y3 | 344 | ASP |
| 11 | z3 | 25 | LEU |
| 11 | z3 | 84 | VAL |
| 11 | z3 | 114 | LYS |
| 11 | z3 | 124 | THR |
| 11 | z3 | 190 | ASN |
| 11 | z3 | 196 | MET |
| 11 | z3 | 206 | ARG |
| 11 | z3 | 210 | TYR |
| 11 | z3 | 245 | ASN |
| 11 | z3 | 252 | LYS |
| 11 | z3 | 256 | ASN |
| 11 | z3 | 325 | SER |
| 11 | z3 | 344 | ASP |
| 12 | A4 | 75 | ASN |
| 12 | A4 | 157 | ARG |
| 12 | D4 | 56 | ASN |
| 12 | E4 | 135 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (200)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A1 | 434 | ASN |
| 1 | B1 | 156 | HIS |
| 1 | B1 | 434 | ASN |
| 1 | C1 | 246 | GLN |
| 1 | D1 | 434 | ASN |
| 1 | E1 | 169 | GLN |
| 1 | E1 | 297 | GLN |
| 1 | E1 | 365 | ASN |
| 1 | E1 | 434 | ASN |
| 1 | G1 | 156 | HIS |
| 1 | G1 | 169 | GLN |
| 1 | H1 | 434 | ASN |
| 1 | I1 | 169 | GLN |
| 1 | J1 | 434 | ASN |
| 1 | K1 | 133 | GLN |
| 1 | K1 | 261 | ASN |
| 1 | M1 | 277 | GLN |
| 1 | M1 | 431 | ASN |
| 1 | M1 | 434 | ASN |
| 1 | N1 | 297 | GLN |
| 1 | O1 | 361 | ASN |
| 1 | P1 | 299 | ASN |
| 1 | P1 | 359 | GLN |
| 1 | P1 | 434 | ASN |
| 1 | S1 | 411 | GLN |
| 1 | S1 | 434 | ASN |
| 1 | T1 | 156 | HIS |
| 1 | W1 | 156 | HIS |
| 1 | W1 | 431 | ASN |
| 1 | W1 | 434 | ASN |
| 1 | X1 | 434 | ASN |
| 1 | Y1 | 359 | GLN |
| 1 | Z1 | 297 | GLN |
| 1 | Z1 | 299 | ASN |
| 1 | Z1 | 434 | ASN |
| 1 | a1 | 434 | ASN |
| 1 | b1 | 265 | GLN |
| 1 | d1 | 133 | GLN |
| 1 | d1 | 218 | HIS |
| 1 | e1 | 277 | GLN |
| 1 | e1 | 434 | ASN |
| 1 | f1 | 434 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A2 | 119 | GLN |
| 2 | C2 | 119 | GLN |
| 3 | F2 | 105 | GLN |
| 3 | F2 | 141 | ASN |
| 6 | Q2 | 13 | GLN |
| 6 | Q2 | 92 | GLN |
| 6 | Q2 | 112 | ASN |
| 6 | S2 | 92 | GLN |
| 6 | T2 | 92 | GLN |
| 7 | V2 | 134 | GLN |
| 7 | W2 | 22 | ASN |
| 7 | X2 | 22 | ASN |
| 8 | b2 | 37 | GLN |
| 8 | c2 | 230 | GLN |
| 8 | e2 | 83 | GLN |
| 8 | e2 | 106 | GLN |
| 9 | g2 | 67 | GLN |
| 9 | h2 | 24 | ASN |
| 9 | h2 | 47 | GLN |
| 9 | h2 | 67 | GLN |
| 9 | i2 | 121 | GLN |
| 9 | j2 | 169 | GLN |
| 9 | k2 | 135 | GLN |
| 9 | m2 | 67 | GLN |
| 9 | m2 | 135 | GLN |
| 9 | m2 | 164 | GLN |
| 9 | n2 | 169 | GLN |
| 9 | n2 | 209 | ASN |
| 9 | o2 | 67 | GLN |
| 9 | o2 | 127 | GLN |
| 9 | o2 | 161 | GLN |
| 9 | o2 | 164 | GLN |
| 9 | o2 | 169 | GLN |
| 9 | o2 | 235 | GLN |
| 9 | p2 | 85 | ASN |
| 9 | p2 | 88 | GLN |
| 9 | p2 | 145 | ASN |
| 9 | p2 | 172 | GLN |
| 9 | r2 | 180 | ASN |
| 9 | s2 | 127 | GLN |
| 9 | t2 | 67 | GLN |
| 9 | t2 | 127 | GLN |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | t2 | 137 | GLN |
| 9 | u2 | 55 | GLN |
| 9 | u2 | 202 | ASN |
| 9 | v2 | 88 | GLN |
| 9 | w2 | 83 | GLN |
| 9 | y2 | 16 | GLN |
| 9 | y2 | 91 | ASN |
| 9 | z2 | 164 | GLN |
| 9 | z2 | 237 | GLN |
| 9 | 12 | 237 | GLN |
| 9 | 22 | 237 | GLN |
| 9 | 32 | 255 | GLN |
| 9 | 42 | 47 | GLN |
| 9 | 42 | 55 | GLN |
| 11 | a3 | 99 | GLN |
| 11 | a3 | 161 | ASN |
| 11 | a3 | 350 | GLN |
| 11 | b3 | 78 | ASN |
| 11 | b3 | 99 | GLN |
| 11 | b3 | 161 | ASN |
| 11 | b3 | 350 | GLN |
| 11 | c3 | 51 | GLN |
| 11 | c3 | 54 | GLN |
| 11 | c3 | 80 | GLN |
| 11 | c3 | 99 | GLN |
| 11 | c3 | 161 | ASN |
| 11 | c3 | 350 | GLN |
| 11 | d3 | 99 | GLN |
| 11 | d3 | 161 | ASN |
| 11 | d3 | 350 | GLN |
| 11 | e3 | 99 | GLN |
| 11 | e3 | 161 | ASN |
| 11 | e3 | 350 | GLN |
| 11 | f3 | 99 | GLN |
| 11 | f3 | 161 | ASN |
| 11 | f3 | 350 | GLN |
| 11 | g3 | 99 | GLN |
| 11 | g3 | 161 | ASN |
| 11 | g3 | 350 | GLN |
| 11 | h3 | 99 | GLN |
| 11 | h3 | 161 | ASN |
| 11 | h3 | 350 | GLN |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | i3 | 99 | GLN |
| 11 | i3 | 161 | ASN |
| 11 | i3 | 350 | GLN |
| 11 | j3 | 99 | GLN |
| 11 | j3 | 161 | ASN |
| 11 | j3 | 350 | GLN |
| 11 | k3 | 78 | ASN |
| 11 | k3 | 99 | GLN |
| 11 | k3 | 161 | ASN |
| 11 | k3 | 350 | GLN |
| 11 | l3 | 54 | GLN |
| 11 | l3 | 78 | ASN |
| 11 | l3 | 99 | GLN |
| 11 | l3 | 161 | ASN |
| 11 | l3 | 350 | GLN |
| 11 | m3 | 54 | GLN |
| 11 | m3 | 99 | GLN |
| 11 | m3 | 161 | ASN |
| 11 | m3 | 350 | GLN |
| 11 | n3 | 99 | GLN |
| 11 | n3 | 161 | ASN |
| 11 | n3 | 350 | GLN |
| 11 | o3 | 80 | GLN |
| 11 | o3 | 99 | GLN |
| 11 | o3 | 161 | ASN |
| 11 | o3 | 350 | GLN |
| 11 | p3 | 78 | ASN |
| 11 | p3 | 99 | GLN |
| 11 | p3 | 161 | ASN |
| 11 | p3 | 350 | GLN |
| 11 | q3 | 54 | GLN |
| 11 | q3 | 99 | GLN |
| 11 | q3 | 161 | ASN |
| 11 | q3 | 350 | GLN |
| 11 | r3 | 78 | ASN |
| 11 | r3 | 99 | GLN |
| 11 | r3 | 161 | ASN |
| 11 | r3 | 350 | GLN |
| 11 | s3 | 78 | ASN |
| 11 | s3 | 80 | GLN |
| 11 | s3 | 99 | GLN |
| 11 | s3 | 161 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | s3 | 350 | GLN |
| 11 | t3 | 99 | GLN |
| 11 | t3 | 161 | ASN |
| 11 | t3 | 350 | GLN |
| 11 | u3 | 80 | GLN |
| 11 | u3 | 99 | GLN |
| 11 | u3 | 161 | ASN |
| 11 | u3 | 350 | GLN |
| 11 | v3 | 78 | ASN |
| 11 | v3 | 99 | GLN |
| 11 | v3 | 161 | ASN |
| 11 | v3 | 350 | GLN |
| 11 | w3 | 99 | GLN |
| 11 | w3 | 161 | ASN |
| 11 | w3 | 350 | GLN |
| 11 | x3 | 78 | ASN |
| 11 | x3 | 99 | GLN |
| 11 | x3 | 161 | ASN |
| 11 | x3 | 350 | GLN |
| 11 | y3 | 99 | GLN |
| 11 | y3 | 161 | ASN |
| 11 | y3 | 350 | GLN |
| 11 | z3 | 80 | GLN |
| 11 | z3 | 99 | GLN |
| 11 | z3 | 161 | ASN |
| 11 | z3 | 350 | GLN |
| 12 | A4 | 55 | ASN |
| 12 | A4 | 230 | GLN |
| 12 | B4 | 46 | ASN |
| 12 | B4 | 55 | ASN |
| 12 | C4 | 84 | GLN |
| 12 | E4 | 54 | 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)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 3 | F2 | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | F2 | 115:ASP | C | 116:PRO | N | 5.09 |

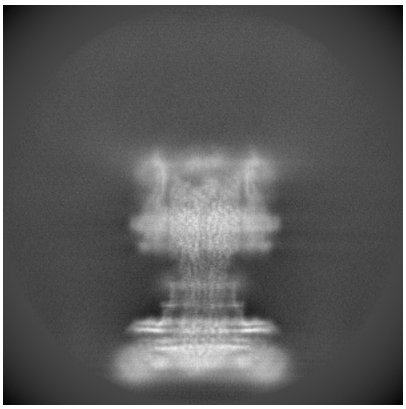
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12603. These allow visual inspection of the internal detail of the map and identification of artifacts.

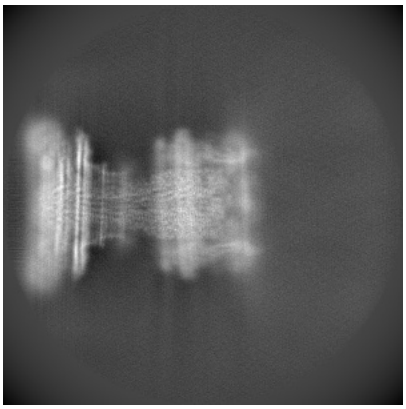
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

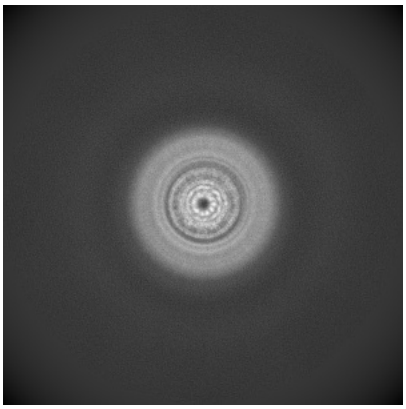
### 6.1.1 Primary map



X

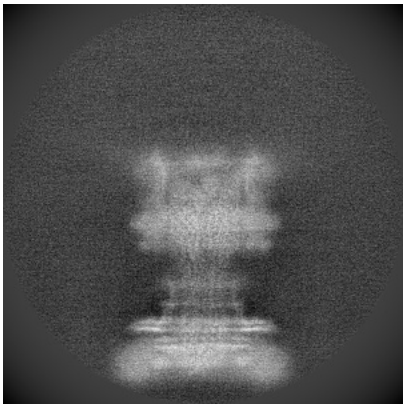


Y

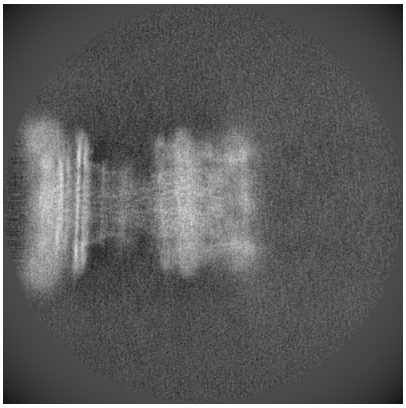


Z

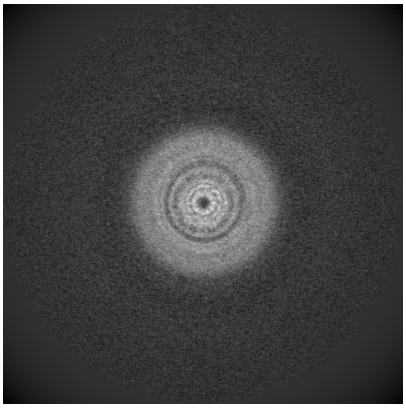
### 6.1.2 Raw map



X



Y

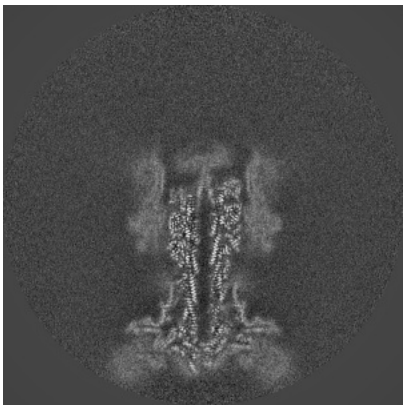


Z

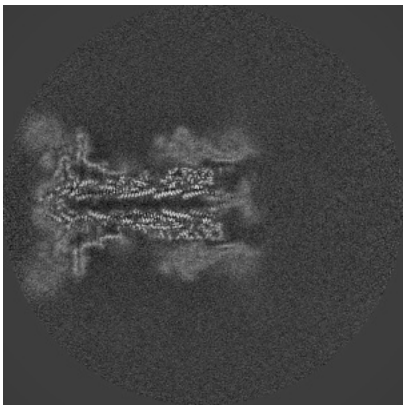
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

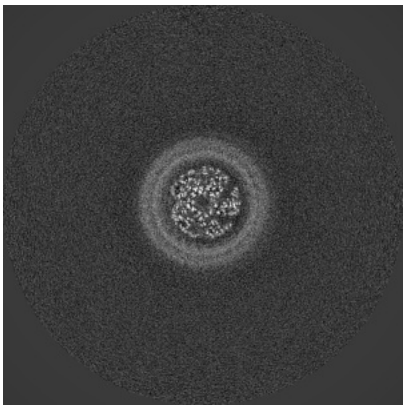
### 6.2.1 Primary map



X Index: 384

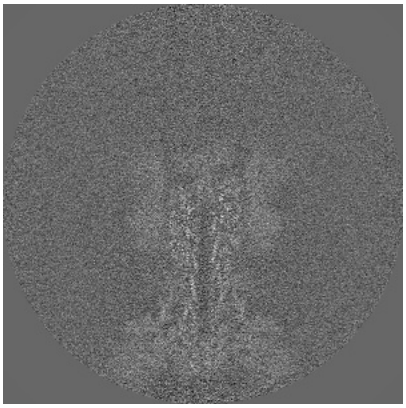


Y Index: 384

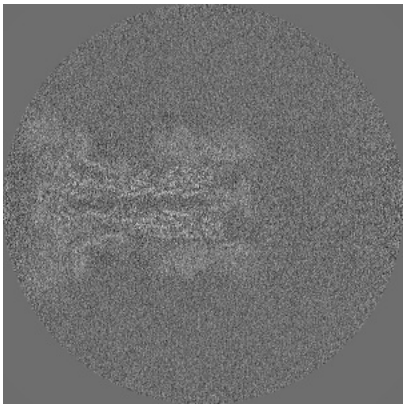


Z Index: 384

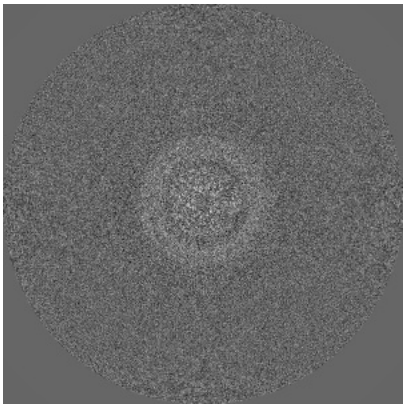
### 6.2.2 Raw map



X Index: 384



Y Index: 384

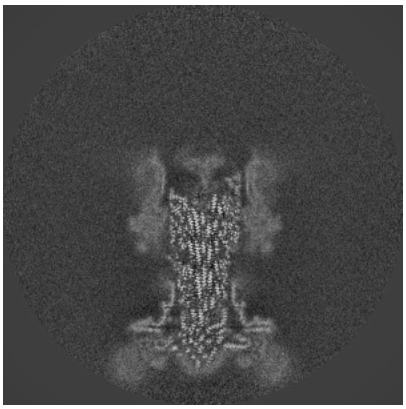


Z Index: 384

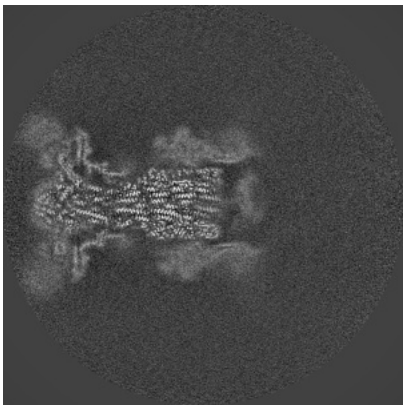
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

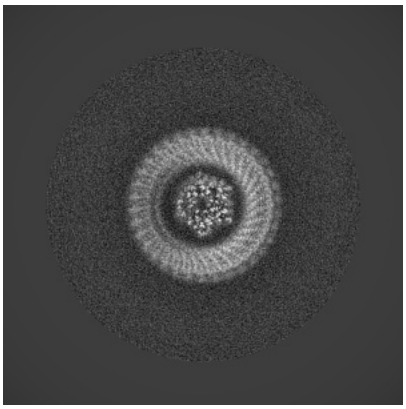
### 6.3.1 Primary map



X Index: 402

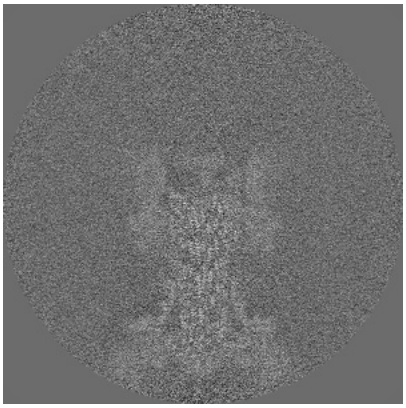


Y Index: 371

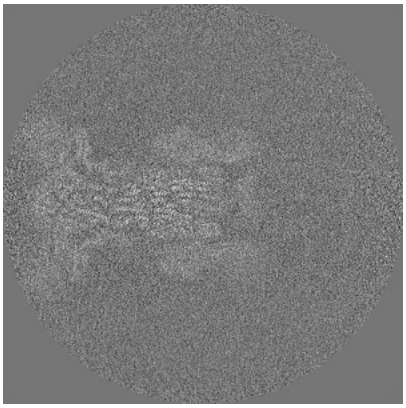


Z Index: 144

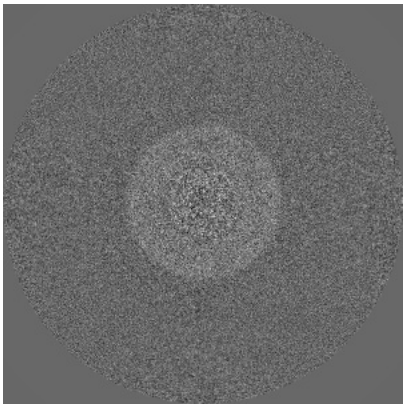
### 6.3.2 Raw map



X Index: 402



Y Index: 371

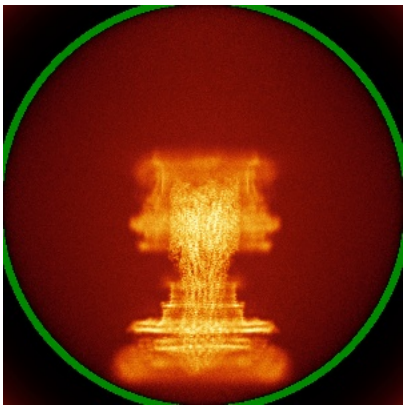


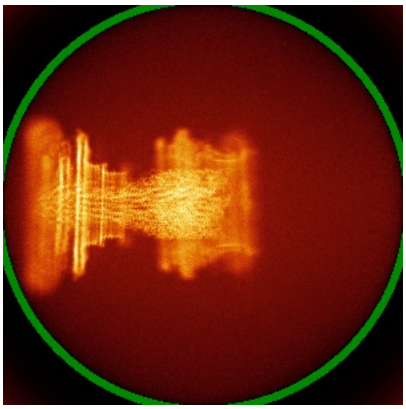
Z Index: 350

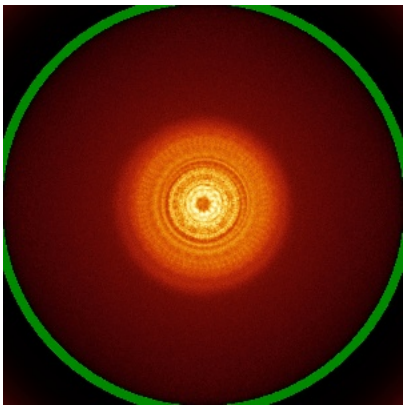
The images above show the largest variance slices of the map in three orthogonal directions.

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

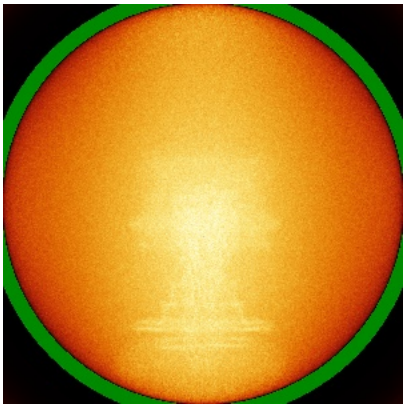
### 6.4.1 Primary map

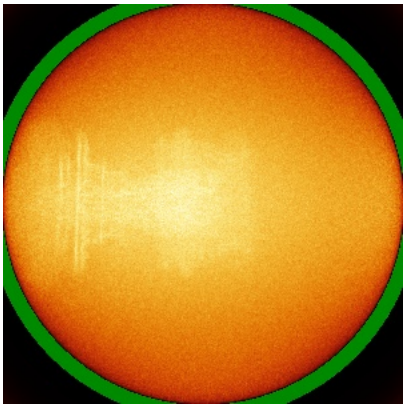

X

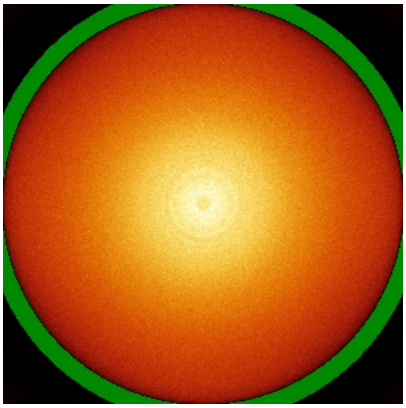

Y


Z

### 6.4.2 Raw map


X

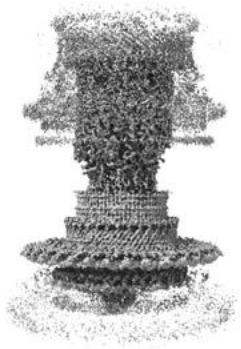

Y


Z

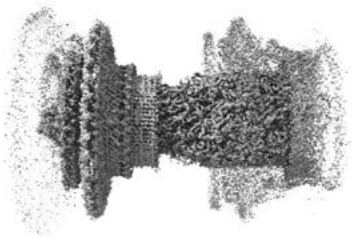
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

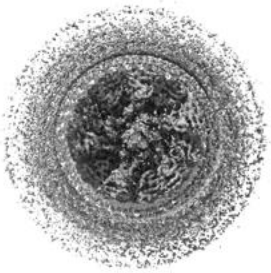
### 6.5.1 Primary map



X



Y

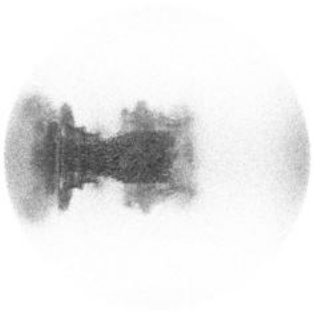


Z

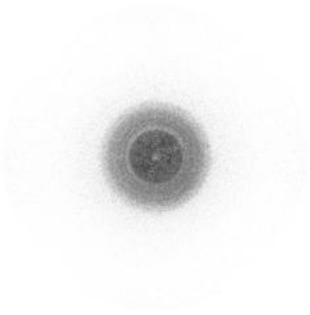
The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map

X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

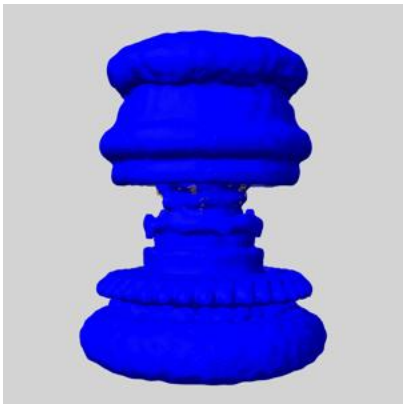
## 6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

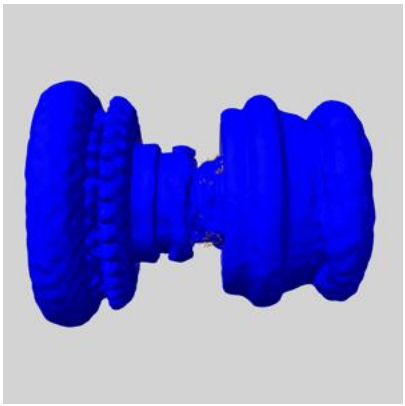
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

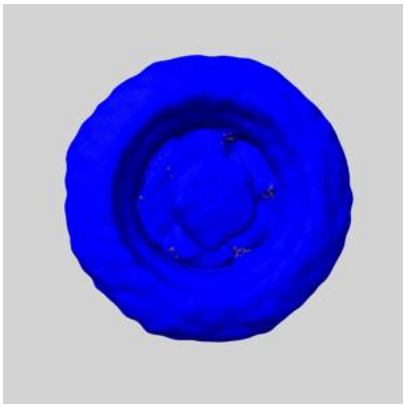
### 6.6.1 emd_12603_msk_1.map (i)



X



Y

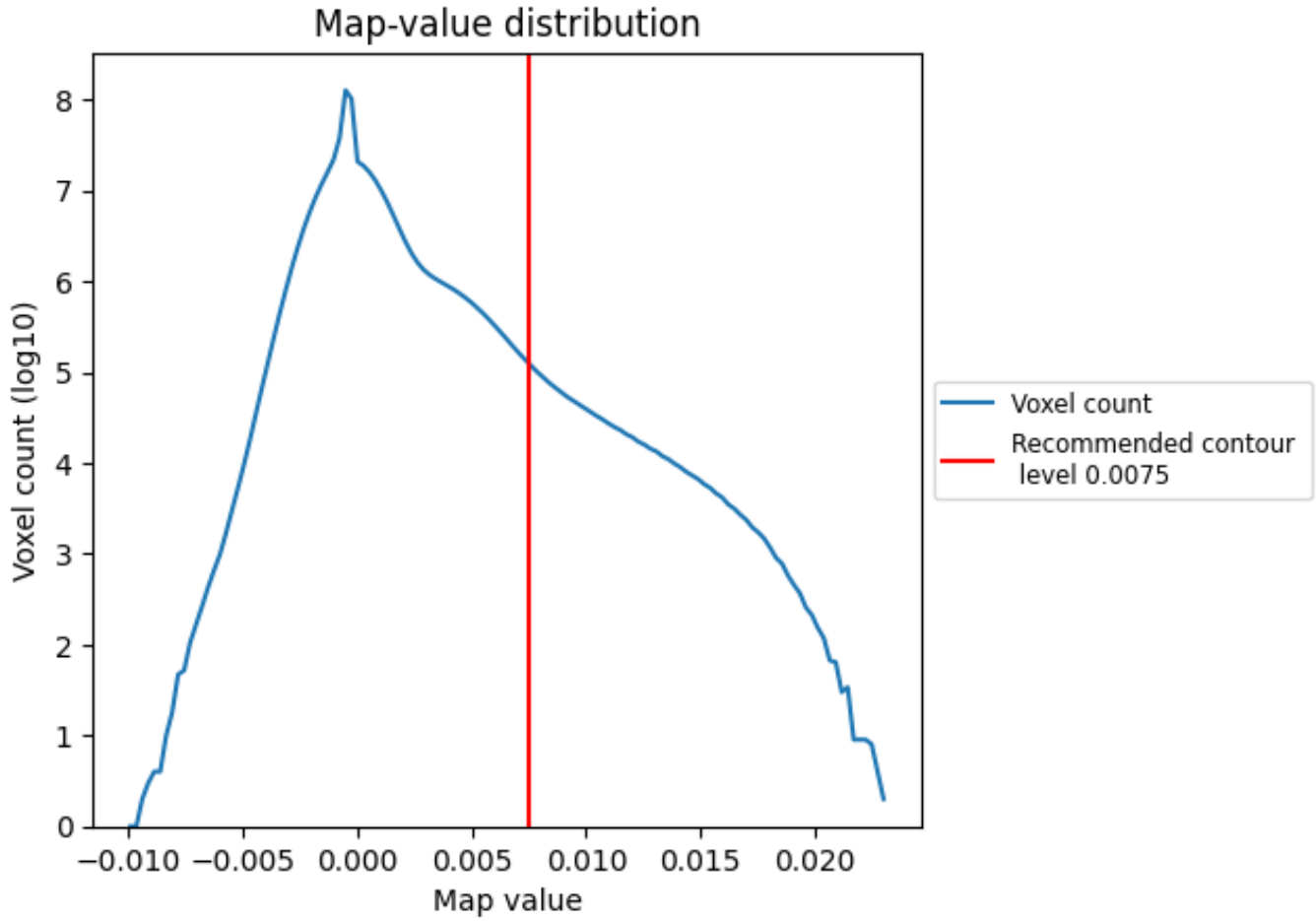


Z

# 7 Map analysis

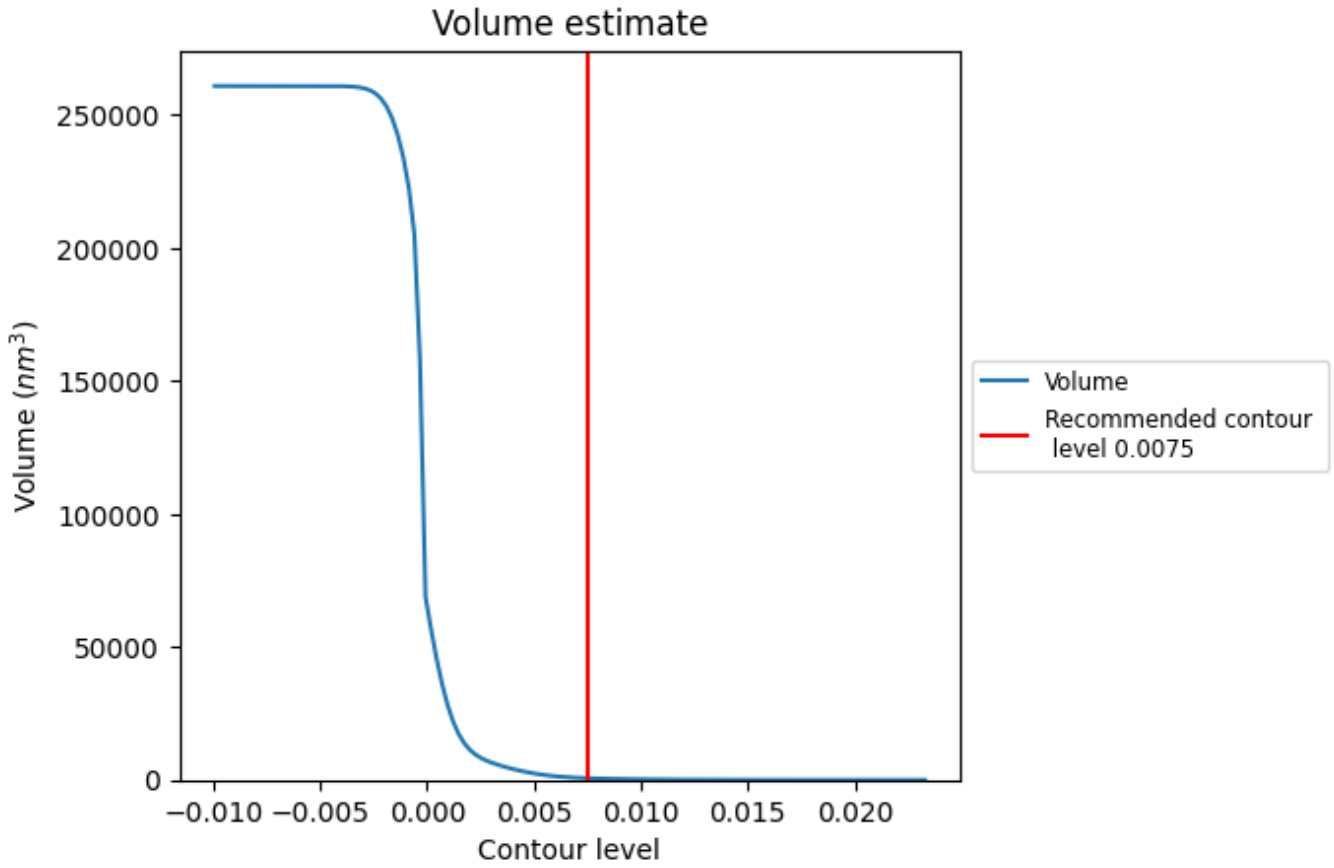
This section contains the results of statistical analysis of the map.

## 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.

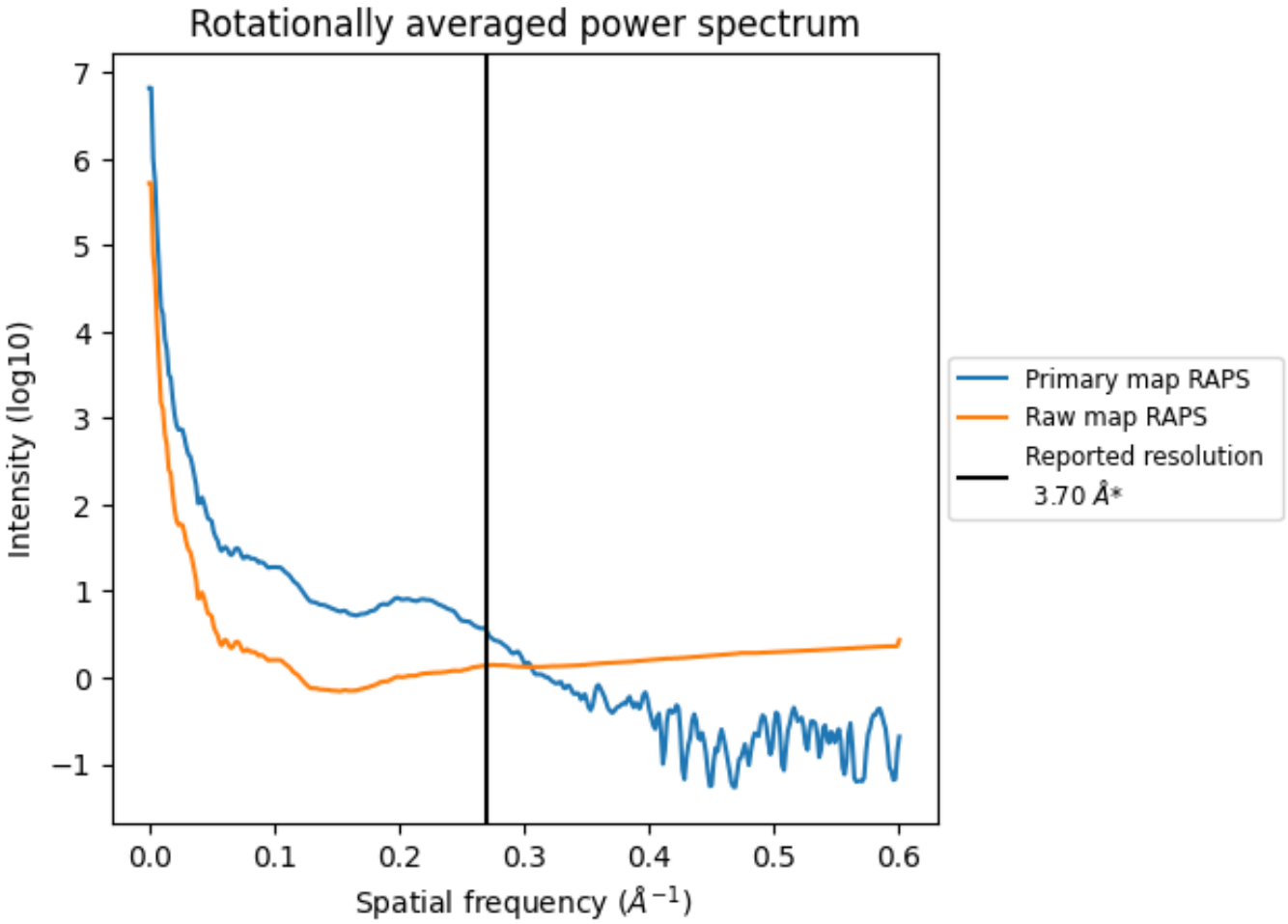
## 7.2 Volume estimate




The volume at the recommended contour level is 648 $nm^3$; this corresponds to an approximate mass of 586 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)

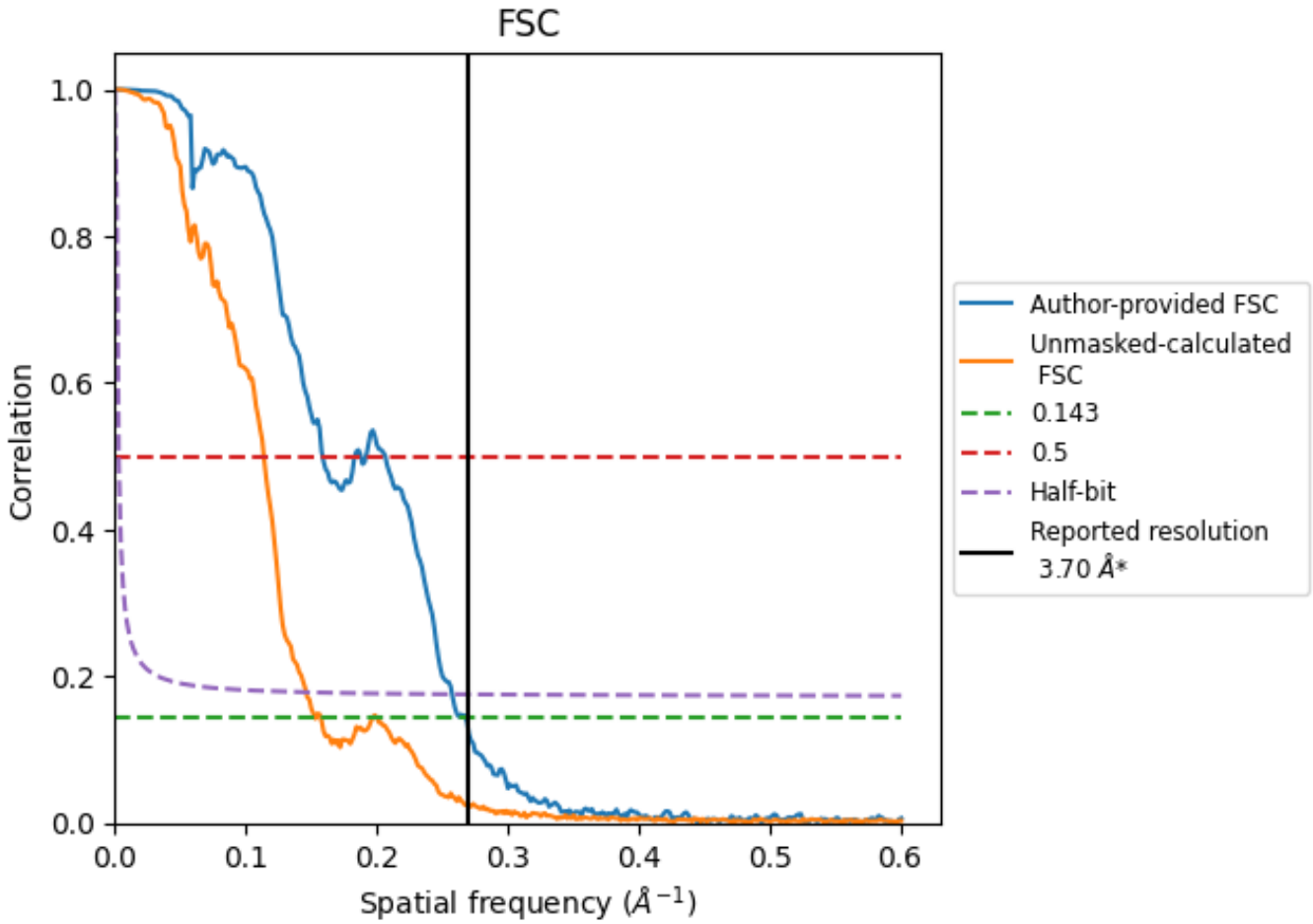



*Reported resolution corresponds to spatial frequency of 0.270 Å$^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.270 Å$^{-1}$

## 8.2 Resolution estimates (i)

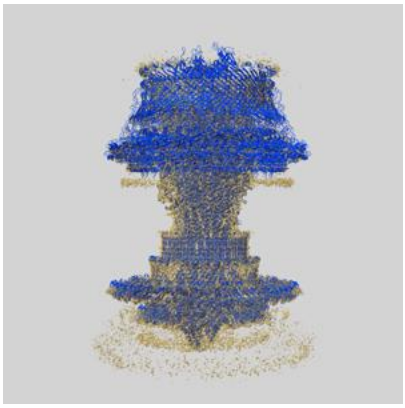
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.70 | - | - |
| Author-provided FSC curve | 3.73 | 6.30 | 3.88 |
| Unmasked-calculated* | 6.53 | 8.78 | 6.84 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.53 differs from the reported value 3.7 by more than 10 %

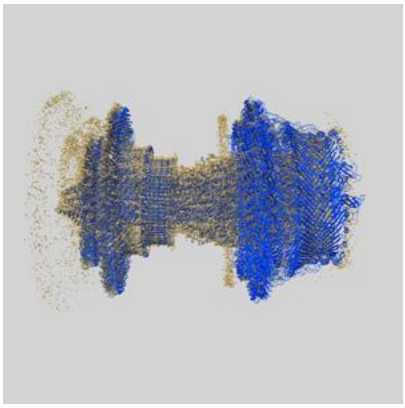
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12603 and PDB model 7NVG. Per-residue inclusion information can be found in section 3 on page 18.

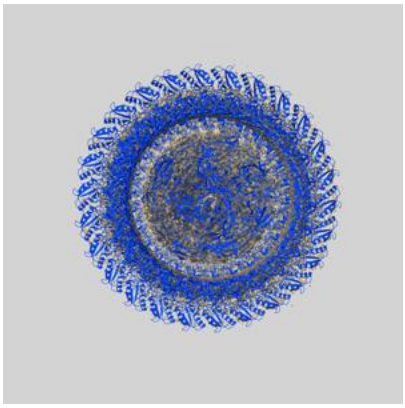
## 9.1 Map-model overlay



X



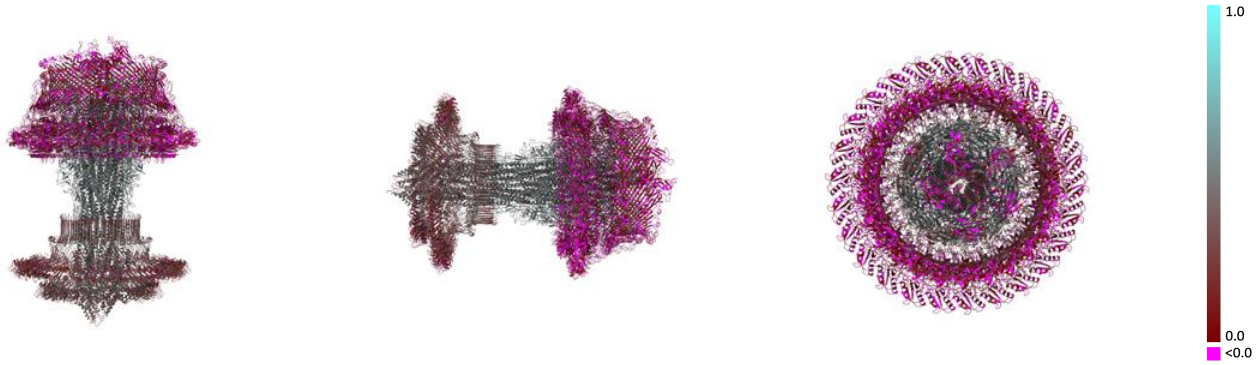
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0075 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.

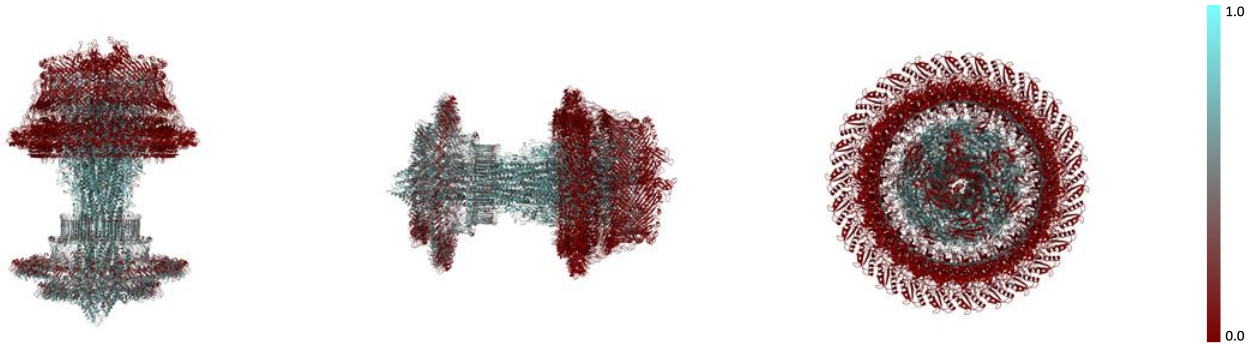
## 9.2 Q-score mapped to coordinate model (i)




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.

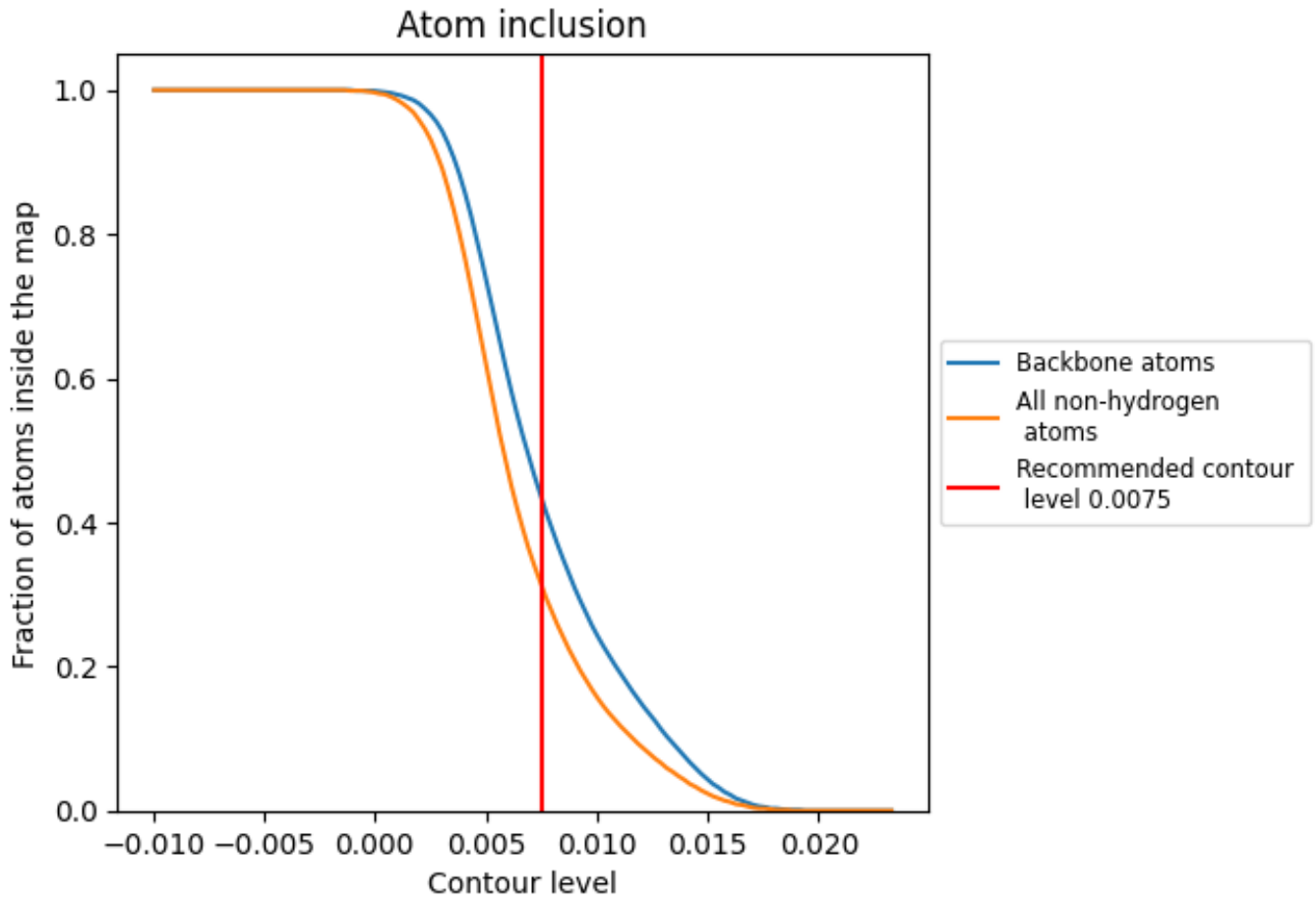
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.0075).

## 9.4 Atom inclusion (i)




At the recommended contour level, 44% of all backbone atoms, 31% 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 (0.0075) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.3140 | 0.2600 |
| 12 | 0.5820 | 0.4540 |
| 22 | 0.5740 | 0.4590 |
| 32 | 0.5370 | 0.4490 |
| 42 | 0.2200 | 0.3100 |
| A1 | 0.4300 | 0.2750 |
| A2 | 0.5380 | 0.4390 |
| A3 | 0.0690 | 0.0910 |
| A4 | 0.0850 | 0.1010 |
| B1 | 0.4340 | 0.3030 |
| B2 | 0.5800 | 0.4430 |
| B3 | 0.0710 | 0.1080 |
| B4 | 0.1010 | 0.0920 |
| C1 | 0.4640 | 0.3060 |
| C2 | 0.6100 | 0.4410 |
| C3 | 0.0720 | 0.1010 |
| C4 | 0.0760 | 0.1210 |
| D1 | 0.4240 | 0.2850 |
| D2 | 0.5880 | 0.4330 |
| D3 | 0.0710 | 0.0870 |
| D4 | 0.0690 | 0.0820 |
| E1 | 0.4420 | 0.3140 |
| E2 | 0.5410 | 0.4190 |
| E3 | 0.0840 | 0.1060 |
| E4 | 0.0870 | 0.1120 |
| F1 | 0.4230 | 0.3020 |
| F2 | 0.4960 | 0.4070 |
| F3 | 0.0740 | 0.1080 |
| G1 | 0.4420 | 0.3180 |
| G2 | 0.5370 | 0.3880 |
| G3 | 0.0820 | 0.1110 |
| H1 | 0.4500 | 0.3230 |
| H2 | 0.6050 | 0.4120 |
| H3 | 0.0790 | 0.1110 |
| I1 | 0.4290 | 0.3090 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| I2 | 0.5700 | 0.4000 |
| I3 | 0.0710 | 0.1020 |
| J1 | 0.4160 | 0.2950 |
| J2 | 0.4990 | 0.3730 |
| J3 | 0.0770 | 0.1060 |
| K1 | 0.4060 | 0.2910 |
| K2 | 0.5490 | 0.4530 |
| K3 | 0.0600 | 0.0850 |
| L1 | 0.3980 | 0.3000 |
| L2 | 0.5450 | 0.4600 |
| L3 | 0.0660 | 0.0880 |
| M1 | 0.4170 | 0.2860 |
| M2 | 0.5960 | 0.4700 |
| M3 | 0.0580 | 0.0840 |
| N1 | 0.3840 | 0.2760 |
| N2 | 0.6070 | 0.4750 |
| N3 | 0.0690 | 0.0920 |
| O1 | 0.3940 | 0.2840 |
| O2 | 0.5720 | 0.4610 |
| O3 | 0.0650 | 0.0800 |
| P1 | 0.4130 | 0.2780 |
| P2 | 0.5520 | 0.4700 |
| P3 | 0.0530 | 0.0860 |
| Q1 | 0.3510 | 0.2740 |
| Q2 | 0.5120 | 0.4850 |
| Q3 | 0.0510 | 0.1000 |
| R1 | 0.3270 | 0.2640 |
| R2 | 0.6080 | 0.4760 |
| R3 | 0.0490 | 0.0760 |
| S1 | 0.3950 | 0.2700 |
| S2 | 0.6050 | 0.4750 |
| S3 | 0.0430 | 0.0760 |
| T1 | 0.2860 | 0.2480 |
| T2 | 0.6450 | 0.4990 |
| T3 | 0.0480 | 0.0960 |
| U1 | 0.2810 | 0.2090 |
| U2 | 0.5750 | 0.4800 |
| U3 | 0.0520 | 0.0880 |
| V1 | 0.3510 | 0.2380 |
| V2 | 0.5560 | 0.4590 |
| V3 | 0.0550 | 0.0850 |
| W1 | 0.2980 | 0.2380 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| W2 | 0.6130 | 0.4770 |
| W3 | 0.0580 | 0.0740 |
| X1 | 0.3350 | 0.2480 |
| X2 | 0.6340 | 0.4930 |
| X3 | 0.0430 | 0.0870 |
| Y1 | 0.3600 | 0.2720 |
| Y2 | 0.6360 | 0.4890 |
| Y3 | 0.0570 | 0.0980 |
| Z1 | 0.3890 | 0.2530 |
| Z2 | 0.6360 | 0.4810 |
| Z3 | 0.0700 | 0.1080 |
| a1 | 0.4160 | 0.2790 |
| a2 | 0.6140 | 0.4580 |
| a3 | 0.0180 | 0.0990 |
| b1 | 0.4100 | 0.2630 |
| b2 | 0.6010 | 0.5010 |
| b3 | 0.0240 | 0.0990 |
| c1 | 0.4270 | 0.2960 |
| c2 | 0.6670 | 0.5000 |
| c3 | 0.0260 | 0.0820 |
| d1 | 0.4540 | 0.2960 |
| d2 | 0.6980 | 0.5070 |
| d3 | 0.0270 | 0.1050 |
| e1 | 0.4590 | 0.2880 |
| e2 | 0.6820 | 0.5060 |
| e3 | 0.0210 | 0.0810 |
| f1 | 0.4580 | 0.3080 |
| f2 | 0.6650 | 0.5050 |
| f3 | 0.0300 | 0.1040 |
| g1 | 0.4720 | 0.3040 |
| g2 | 0.6390 | 0.4990 |
| g3 | 0.0280 | 0.0810 |
| h1 | 0.4570 | 0.3010 |
| h2 | 0.6560 | 0.5060 |
| h3 | 0.0230 | 0.0980 |
| i2 | 0.6690 | 0.5130 |
| i3 | 0.0300 | 0.0890 |
| j2 | 0.6560 | 0.5050 |
| j3 | 0.0150 | 0.0810 |
| k2 | 0.6640 | 0.5070 |
| k3 | 0.0160 | 0.0840 |
| l2 | 0.6570 | 0.5090 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| l3 | 0.0110 | 0.0710 |
| m2 | 0.6610 | 0.5130 |
| m3 | 0.0060 | 0.0480 |
| n2 | 0.6630 | 0.5160 |
| n3 | 0.0120 | 0.0500 |
| o2 | 0.6640 | 0.5040 |
| o3 | 0.0140 | 0.0610 |
| p2 | 0.6600 | 0.5020 |
| p3 | 0.0070 | 0.0430 |
| q2 | 0.6710 | 0.5110 |
| q3 | 0.0050 | 0.0530 |
| r2 | 0.6620 | 0.5030 |
| r3 | 0.0060 | 0.0570 |
| s2 | 0.6590 | 0.5030 |
| s3 | 0.0060 | 0.0580 |
| t2 | 0.6570 | 0.4970 |
| t3 | 0.0110 | 0.0570 |
| u2 | 0.6580 | 0.4910 |
| u3 | 0.0080 | 0.0530 |
| v2 | 0.6700 | 0.4960 |
| v3 | 0.0060 | 0.0640 |
| w2 | 0.6740 | 0.4930 |
| w3 | 0.0110 | 0.0690 |
| x2 | 0.6430 | 0.4870 |
| x3 | 0.0160 | 0.0790 |
| y2 | 0.5760 | 0.4470 |
| y3 | 0.0170 | 0.0750 |
| z2 | 0.5250 | 0.4040 |
| z3 | 0.0170 | 0.0910 |