# wwPDB EM Validation Summary Report

Mar 18, 2025 – 11:10 PM JST

| | | |
|---|---|---|
| PDB ID | : | 8YJT |
| EMDB ID | : | EMD-39349 |
| Title | : | Cryo-EM structure of the flagellar C ring in the CCW state |
| Authors | : | Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q. |
| Deposited on | : | 2024-03-02 |
| Resolution | : | 5.90 Å(reported) |
| Based on initial models | : | ., ? |

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

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

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

---

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

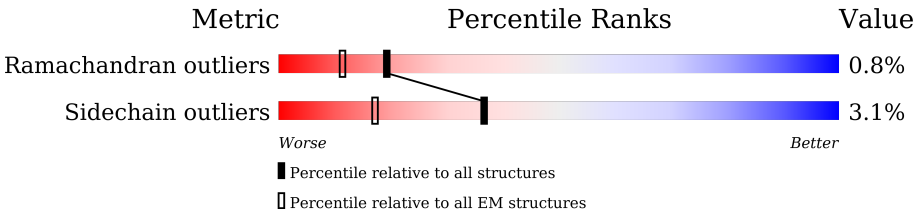
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev117 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.41.4 |

# 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 5.90 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Ramachandran outliers | 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 | 3 | 331 | 7% 93% · 5% |
| 1 | 9 | 331 | 7% 93% · 5% |
| 1 | A1 | 331 | 7% 93% · 5% |
| 1 | A7 | 331 | 6% 93% · 5% |
| 1 | AE | 331 | 7% 93% · 5% |
| 1 | AK | 331 | 6% 93% · 5% |
| 1 | AQ | 331 | 7% 93% · 5% |
| 1 | AW | 331 | 7% 93% · 5% |
| 1 | Ac | 331 | 7% 93% · 5% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | Ai | 331 | 6% 93% 5% |
| 1 | Ao | 331 | 8% 93% 5% |
| 1 | Au | 331 | 7% 93% 5% |
| 1 | B5 | 331 | 7% 93% 5% |
| 1 | BC | 331 | 7% 93% 5% |
| 1 | BI | 331 | 8% 93% 5% |
| 1 | BO | 331 | 7% 93% 5% |
| 1 | BU | 331 | 7% 93% 5% |
| 1 | Ba | 331 | 7% 93% 5% |
| 1 | Bg | 331 | 7% 93% 5% |
| 1 | Bm | 331 | 7% 93% 5% |
| 1 | Bs | 331 | 7% 93% 5% |
| 1 | By | 331 | 6% 93% 5% |
| 1 | CA | 331 | 7% 93% 5% |
| 1 | CG | 331 | 7% 93% 5% |
| 1 | CM | 331 | 6% 93% 5% |
| 1 | CS | 331 | 8% 93% 5% |
| 1 | CY | 331 | 7% 93% 5% |
| 1 | Ce | 331 | 7% 93% 5% |
| 1 | Ck | 331 | 6% 93% 5% |
| 1 | Cq | 331 | 7% 93% 5% |
| 1 | Cw | 331 | 8% 93% 5% |
| 1 | k | 331 | 7% 93% 5% |
| 1 | q | 331 | 7% 93% 5% |
| 1 | w | 331 | 7% 93% 5% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | 0 | 560 | 5% 95% |
| 2 | 4 | 560 | 5% 95% |
| 2 | A2 | 560 | 5% 95% |
| 2 | A8 | 560 | 5% 95% |
| 2 | AF | 560 | 5% 95% |
| 2 | AL | 560 | 5% 95% |
| 2 | AR | 560 | 5% 95% |
| 2 | AX | 560 | 5% 95% |
| 2 | Ad | 560 | 5% 95% |
| 2 | Aj | 560 | 5% 95% |
| 2 | Ap | 560 | 5% 95% |
| 2 | Av | 560 | 5% 95% |
| 2 | B6 | 560 | 5% 95% |
| 2 | BD | 560 | 5% 95% |
| 2 | BJ | 560 | 5% 95% |
| 2 | BP | 560 | 5% 95% |
| 2 | BV | 560 | 5% 95% |
| 2 | Bb | 560 | 5% 95% |
| 2 | Bh | 560 | 5% 95% |
| 2 | Bn | 560 | 5% 95% |
| 2 | Bt | 560 | 5% 95% |
| 2 | Bz | 560 | 5% 95% |
| 2 | CB | 560 | 5% 95% |
| 2 | CH | 560 | 5% 95% |
| 2 | CN | 560 | 5% 95% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | CT | 560 | 5% 95% |
| 2 | CZ | 560 | 5% 95% |
| 2 | Cf | 560 | 5% 95% |
| 2 | Cl | 560 | 5% 95% |
| 2 | Cr | 560 | 5% 95% |
| 2 | Cx | 560 | 5% 95% |
| 2 | l | 560 | 5% 95% |
| 2 | r | 560 | 5% 95% |
| 2 | x | 560 | 5% 95% |
| 3 | 5 | 334 | 82% 13% |
| 3 | A3 | 334 | 82% 13% |
| 3 | A9 | 334 | 82% 13% |
| 3 | AA | 334 | 82% 13% |
| 3 | AG | 334 | 82% 13% |
| 3 | AM | 334 | 82% 13% |
| 3 | AS | 334 | 82% 13% |
| 3 | AY | 334 | 82% 13% |
| 3 | Ae | 334 | 82% 13% |
| 3 | Ak | 334 | 82% 13% |
| 3 | Aq | 334 | 82% 13% |
| 3 | Aw | 334 | 82% 13% |
| 3 | B1 | 334 | 82% 13% |
| 3 | B7 | 334 | 82% 13% |
| 3 | BE | 334 | 82% 13% |
| 3 | BK | 334 | 82% 13% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | BQ | 334 | 82% 13% |
| 3 | BW | 334 | 82% 13% |
| 3 | Bc | 334 | 82% 13% |
| 3 | Bi | 334 | 82% 13% |
| 3 | Bo | 334 | 82% 13% |
| 3 | Bu | 334 | 82% 13% |
| 3 | CC | 334 | 82% 13% |
| 3 | CI | 334 | 82% 13% |
| 3 | CO | 334 | 82% 13% |
| 3 | CU | 334 | 82% 13% |
| 3 | Ca | 334 | 82% 13% |
| 3 | Cg | 334 | 82% 13% |
| 3 | Cm | 334 | 82% 13% |
| 3 | Cs | 334 | 82% 13% |
| 3 | Cy | 334 | 82% 13% |
| 3 | m | 334 | 82% 13% |
| 3 | s | 334 | 82% 13% |
| 3 | y | 334 | 82% 13% |
| 4 | 1 | 137 | 61% 36% |
| 4 | 2 | 137 | 61% 36% |
| 4 | 6 | 137 | 61% 36% |
| 4 | 7 | 137 | 61% 36% |
| 4 | 8 | 137 | 61% 36% |
| 4 | A0 | 137 | 61% 36% |
| 4 | A4 | 137 | 61% 36% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | A5 | 137 | 61% 36% |
| 4 | A6 | 137 | 61% 36% |
| 4 | AB | 137 | 61% 36% |
| 4 | AC | 137 | 61% 36% |
| 4 | AD | 137 | 61% 36% |
| 4 | AH | 137 | 61% 36% |
| 4 | AI | 137 | 61% 36% |
| 4 | AJ | 137 | 61% 36% |
| 4 | AN | 137 | 61% 36% |
| 4 | AO | 137 | 61% 36% |
| 4 | AP | 137 | 61% 36% |
| 4 | AT | 137 | 61% 36% |
| 4 | AU | 137 | 61% 36% |
| 4 | AV | 137 | 61% 36% |
| 4 | AZ | 137 | 61% 36% |
| 4 | Aa | 137 | 61% 36% |
| 4 | Ab | 137 | 61% 36% |
| 4 | Af | 137 | 61% 36% |
| 4 | Ag | 137 | 61% 36% |
| 4 | Ah | 137 | 61% 36% |
| 4 | Al | 137 | 61% 36% |
| 4 | Am | 137 | 61% 36% |
| 4 | An | 137 | 61% 36% |
| 4 | Ar | 137 | 61% 36% |
| 4 | As | 137 | 61% 36% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | At | 137 | 61% 36% |
| 4 | Ax | 137 | 61% 36% |
| 4 | Ay | 137 | 61% 36% |
| 4 | Az | 137 | 61% 36% |
| 4 | B0 | 137 | 61% 36% |
| 4 | B2 | 137 | 61% 36% |
| 4 | B3 | 137 | 61% 36% |
| 4 | B4 | 137 | 61% 36% |
| 4 | B8 | 137 | 61% 36% |
| 4 | B9 | 137 | 61% 36% |
| 4 | BA | 137 | 61% 36% |
| 4 | BB | 137 | 61% 36% |
| 4 | BF | 137 | 61% 36% |
| 4 | BG | 137 | 61% 36% |
| 4 | BH | 137 | 61% 36% |
| 4 | BL | 137 | 61% 36% |
| 4 | BM | 137 | 61% 36% |
| 4 | BN | 137 | 61% 36% |
| 4 | BR | 137 | 61% 36% |
| 4 | BS | 137 | 61% 36% |
| 4 | BT | 137 | 61% 36% |
| 4 | BX | 137 | 61% 36% |
| 4 | BY | 137 | 61% 36% |
| 4 | BZ | 137 | 61% 36% |
| 4 | Bd | 137 | 61% 36% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | Be | 137 | 61% 36% |
| 4 | Bf | 137 | 61% 36% |
| 4 | Bj | 137 | 61% 36% |
| 4 | Bk | 137 | 61% 36% |
| 4 | Bl | 137 | 61% 36% |
| 4 | Bp | 137 | 61% 36% |
| 4 | Bq | 137 | 61% 36% |
| 4 | Br | 137 | 61% 36% |
| 4 | Bv | 137 | 61% 36% |
| 4 | Bw | 137 | 61% 36% |
| 4 | Bx | 137 | 61% 36% |
| 4 | C1 | 137 | 61% 36% |
| 4 | C2 | 137 | 61% 36% |
| 4 | CD | 137 | 61% 36% |
| 4 | CE | 137 | 61% 36% |
| 4 | CF | 137 | 61% 36% |
| 4 | CJ | 137 | 61% 36% |
| 4 | CK | 137 | 61% 36% |
| 4 | CL | 137 | 61% 36% |
| 4 | CP | 137 | 61% 36% |
| 4 | CQ | 137 | 61% 36% |
| 4 | CR | 137 | 61% 36% |
| 4 | CV | 137 | 61% 36% |
| 4 | CW | 137 | 61% 36% |
| 4 | CX | 137 | 61% 36% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | Cb | 137 | 61% 36% |
| 4 | Cc | 137 | 61% 36% |
| 4 | Cd | 137 | 61% 36% |
| 4 | Ch | 137 | 61% 36% |
| 4 | Ci | 137 | 61% 36% |
| 4 | Cj | 137 | 61% 36% |
| 4 | Cn | 137 | 61% 36% |
| 4 | Co | 137 | 61% 36% |
| 4 | Cp | 137 | 61% 36% |
| 4 | Ct | 137 | 61% 36% |
| 4 | Cu | 137 | 61% 36% |
| 4 | Cv | 137 | 61% 36% |
| 4 | Cz | 137 | 61% 36% |
| 4 | n | 137 | 61% 36% |
| 4 | o | 137 | 61% 36% |
| 4 | p | 137 | 61% 36% |
| 4 | t | 137 | 61% 36% |
| 4 | u | 137 | 61% 36% |
| 4 | v | 137 | 61% 36% |
| 4 | z | 137 | 61% 36% |

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 239768 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 motor switch protein FliG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | k | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | q | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | w | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | 3 | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | 9 | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | AE | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | AK | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | AQ | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | AW | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | Ac | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | Ai | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | Ao | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | Au | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | A1 | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | A7 | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | BC | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | BI | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | BO | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | BU | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | Ba | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | Bg | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | Bm | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | Bs | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | By | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | B5 | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | CA | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | CG | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | CM | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | CS | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | CY | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | Ce | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | Ck | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | Cq | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |
| 1 | Cw | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2462 | 1535 | 435 | 483 | 9 | | |

- Molecule 2 is a protein called Flagellar M-ring protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | l | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | r | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | x | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | 4 | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | 0 | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | AF | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | AL | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | AR | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | AX | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | Ad | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | Aj | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | Ap | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | Av | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | A2 | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | A8 | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | BD | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | BJ | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | BP | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | BV | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | Bb | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | Bh | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | Bn | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | Bt | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | Bz | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | B6 | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | CB | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | CH | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | CN | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | CT | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | CZ | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | Cf | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | Cl | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | Cr | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |
| 2 | Cx | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 224 | 135 | 44 | 42 | 3 | | |

- Molecule 3 is a protein called Flagellar motor switch protein FliM.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | m | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | s | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | y | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | 5 | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | AA | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | AG | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | AM | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | AS | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | AY | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | Ae | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | Ak | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | Aq | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | Aw | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | A3 | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | A9 | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | BE | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | BK | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | BQ | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | BW | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | Bc | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | Bi | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | Bo | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | Bu | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | B1 | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | B7 | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | CC | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | CI | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | CO | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | CU | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | Ca | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | Cg | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | Cm | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | Cs | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |
| 3 | Cy | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2341 | 1492 | 423 | 421 | 5 | | |

- Molecule 4 is a protein called Flagellar motor switch protein FliN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | n | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | o | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | p | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | t | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | u | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | v | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | z | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | 1 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | 2 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | 6 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | 7 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | 8 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | AB | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | AC | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | AD | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | AH | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | AI | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | AJ | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | AN | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | AO | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | AP | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | AT | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | AU | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | AV | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | AZ | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Aa | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Ab | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Af | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Ag | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Ah | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Al | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Am | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | An | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Ar | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | As | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | At | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Ax | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Ay | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Az | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | A4 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | A5 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | A6 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | A0 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | BA | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | BB | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | BF | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | BG | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | BH | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | BL | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | BM | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | BN | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | BR | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | BS | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | BT | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | BX | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | BY | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | BZ | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Bd | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Be | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Bf | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Bj | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Bk | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Bl | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Bp | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Bq | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Br | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Bv | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Bw | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Bx | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | B2 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | B3 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | B4 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | B8 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | B9 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | B0 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | CD | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | CE | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | CF | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | CJ | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | CK | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | CL | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | CP | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | CQ | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | CR | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | CV | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | CW | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | CX | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Cb | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Cc | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Cd | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Ch | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Ci | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Cj | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Cn | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Co | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Cp | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Ct | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Cu | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |

*Continued on next page...*

*Continued from previous page...*

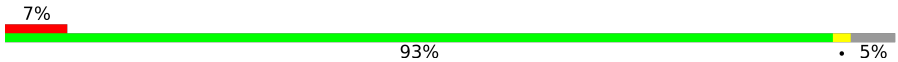
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | Cv | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | Cz | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | C1 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |
| 4 | C2 | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 427 | 118 | 126 | 4 | | |

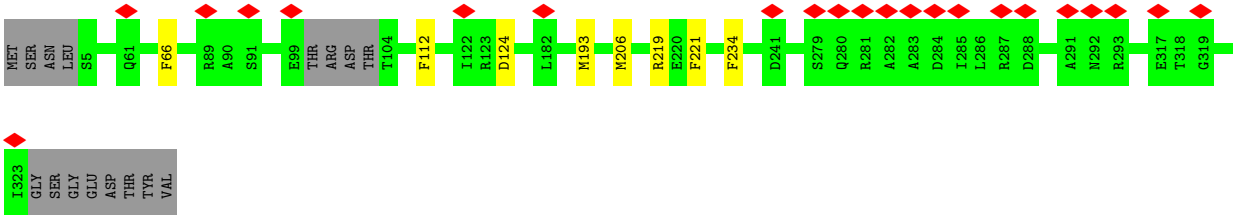
# 3 Residue-property plots (i)

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 motor switch protein FliG

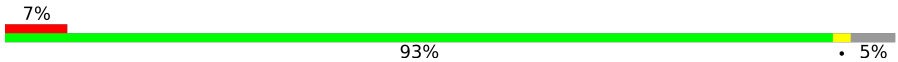
Chain k:

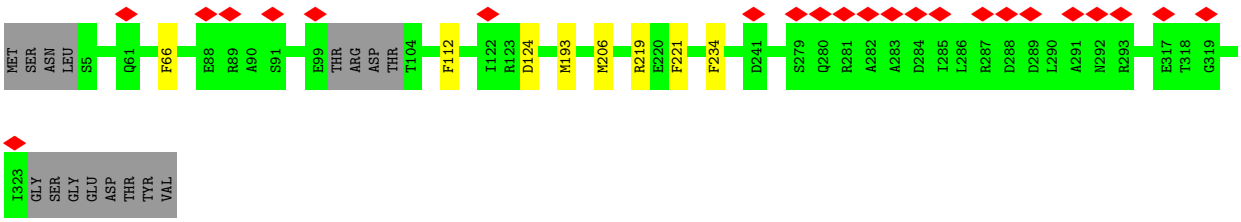



• Molecule 1: Flagellar motor switch protein FliG

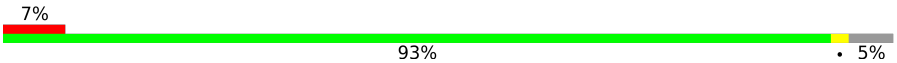
Chain q:

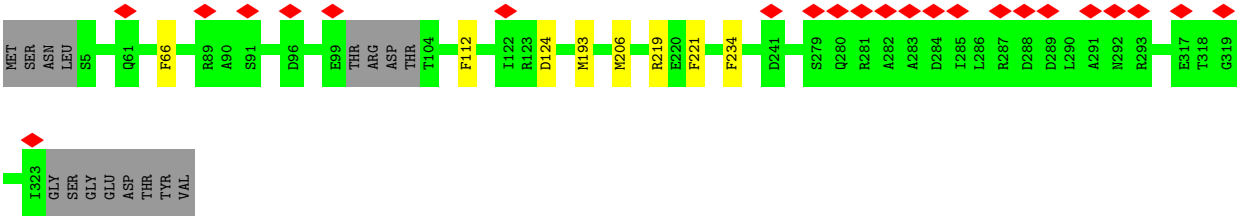



• Molecule 1: Flagellar motor switch protein FliG

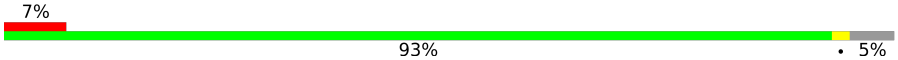
Chain w:

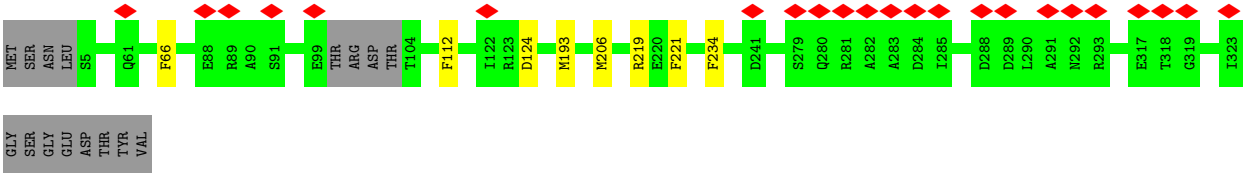



• Molecule 1: Flagellar motor switch protein FliG

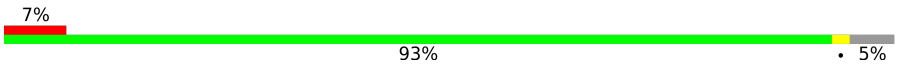
Chain 3:

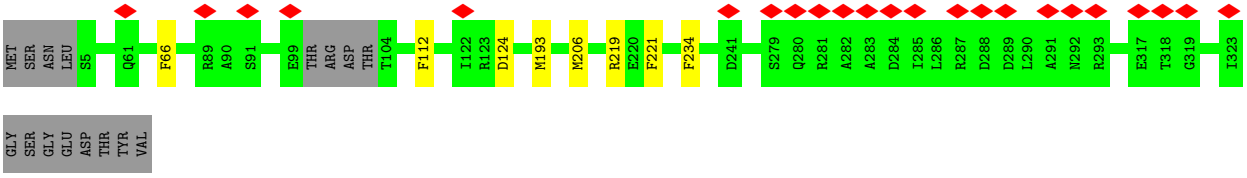





• Molecule 1: Flagellar motor switch protein FliG

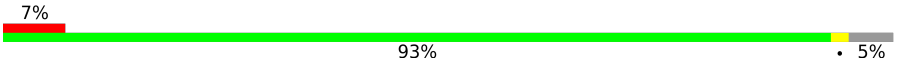
Chain 9:

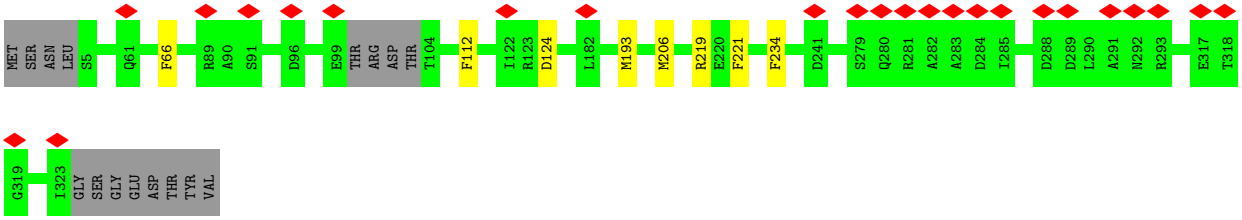



• Molecule 1: Flagellar motor switch protein FliG

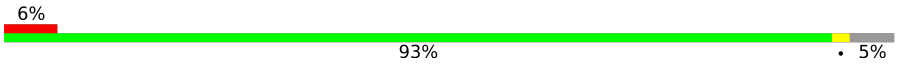
Chain AE:

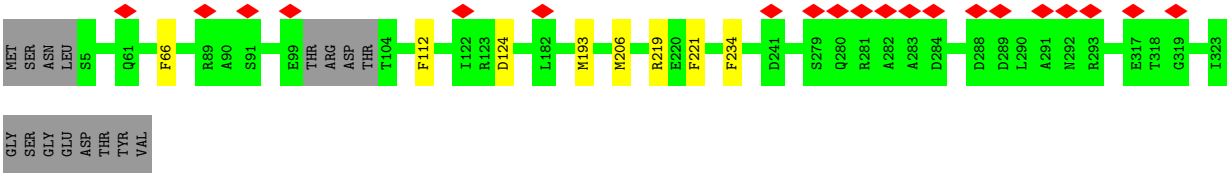



• Molecule 1: Flagellar motor switch protein FliG

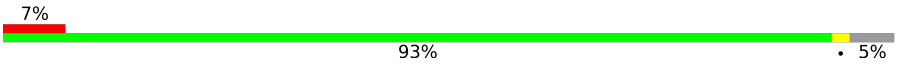
Chain AK:

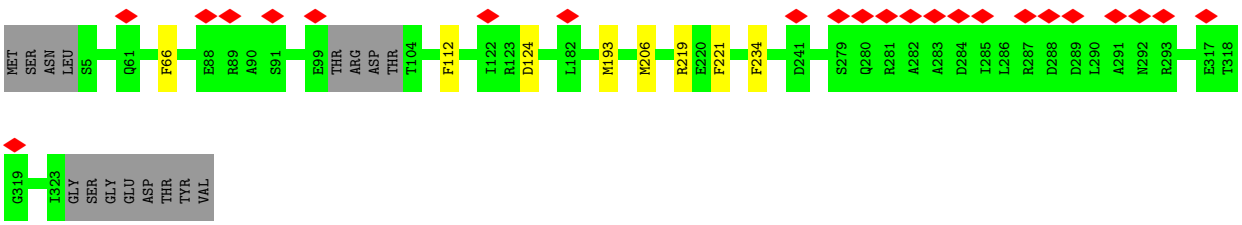



• Molecule 1: Flagellar motor switch protein FliG

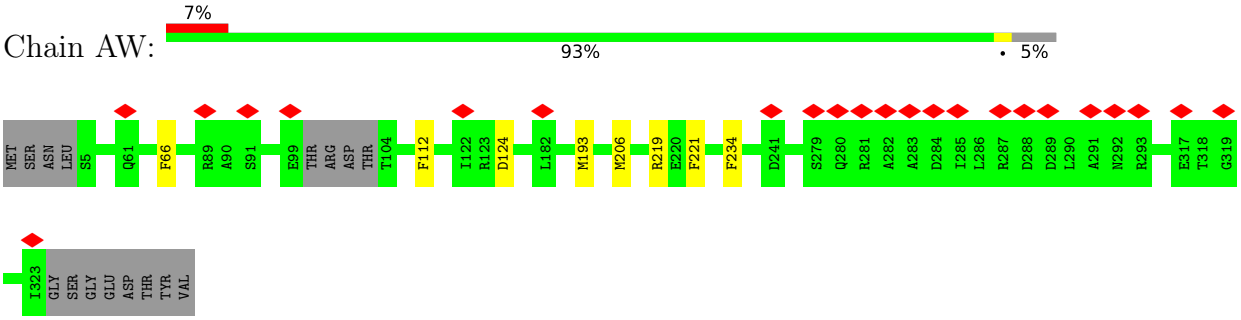
Chain AQ:



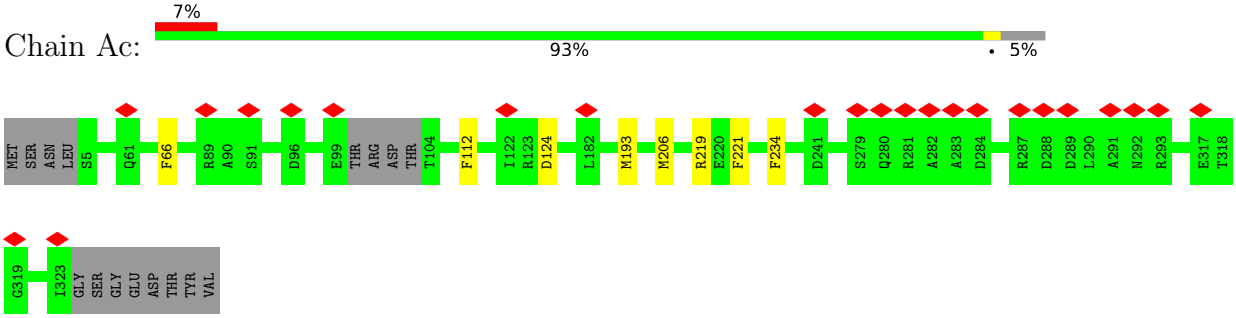

• Molecule 1: Flagellar motor switch protein FliG

Chain AW:



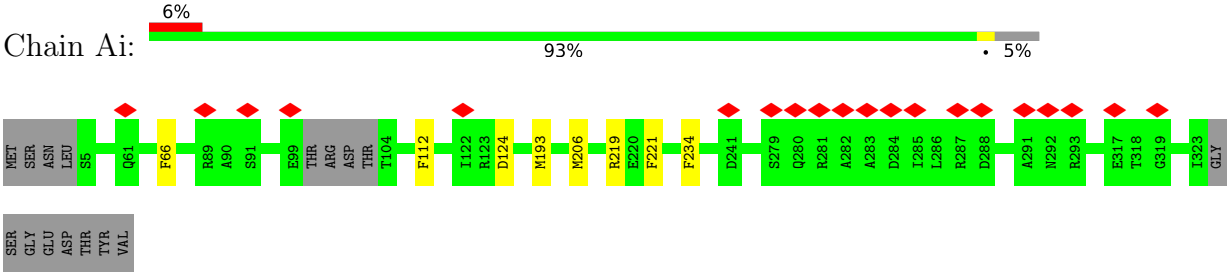

• Molecule 1: Flagellar motor switch protein FliG

Chain Ac:



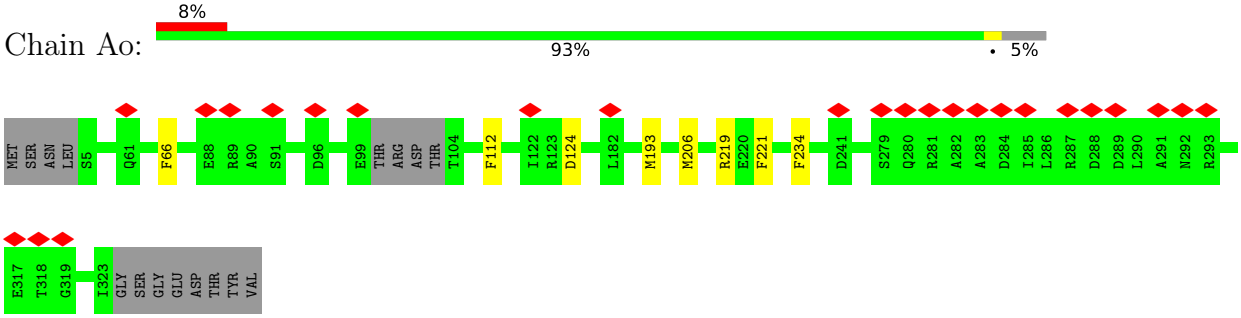

• Molecule 1: Flagellar motor switch protein FliG

Chain Ai:



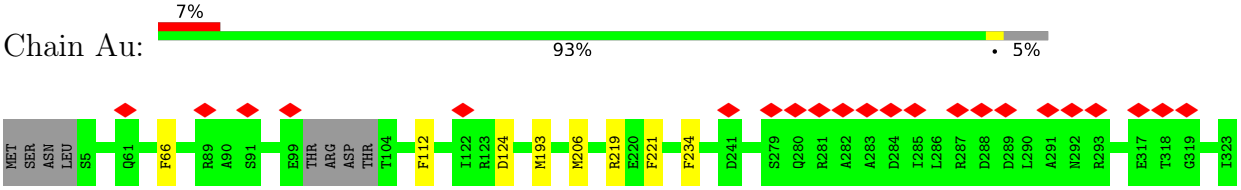

• Molecule 1: Flagellar motor switch protein FliG

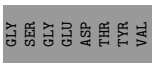
Chain Ao:




• Molecule 1: Flagellar motor switch protein FliG

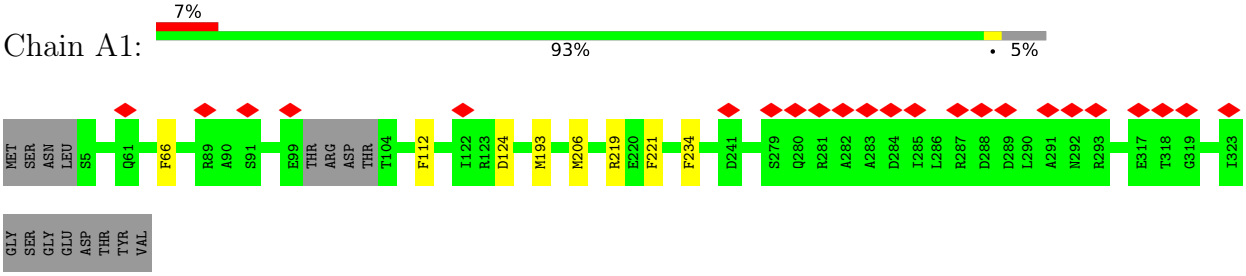
Chain Au:





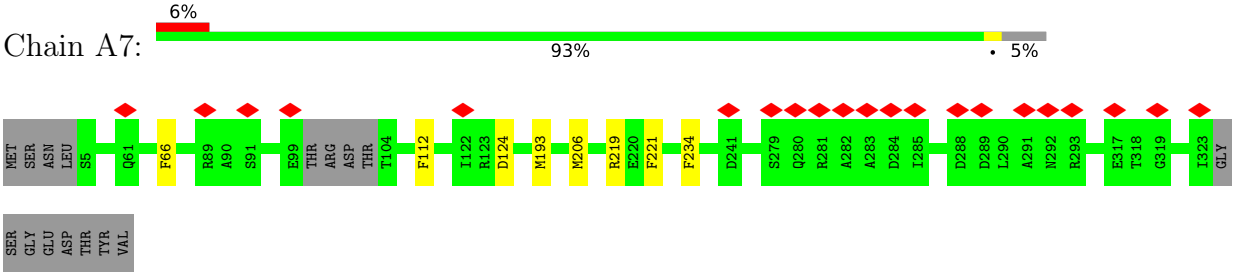

• Molecule 1: Flagellar motor switch protein FliG

Chain A1:



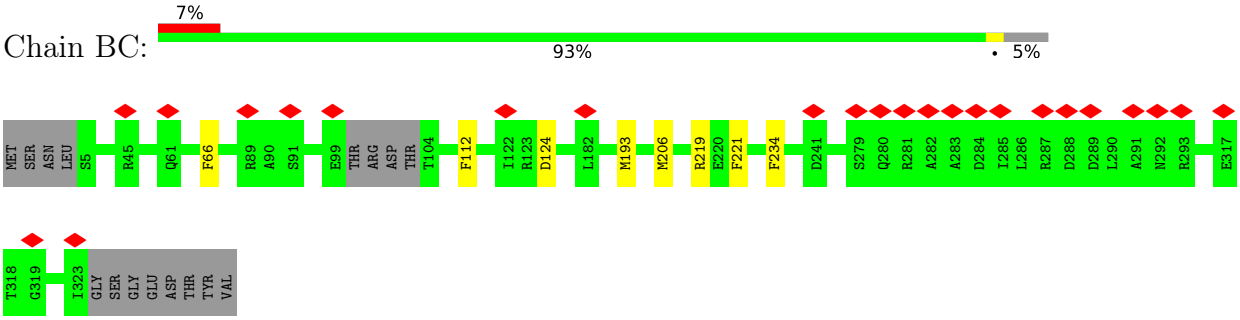

• Molecule 1: Flagellar motor switch protein FliG

Chain A7:



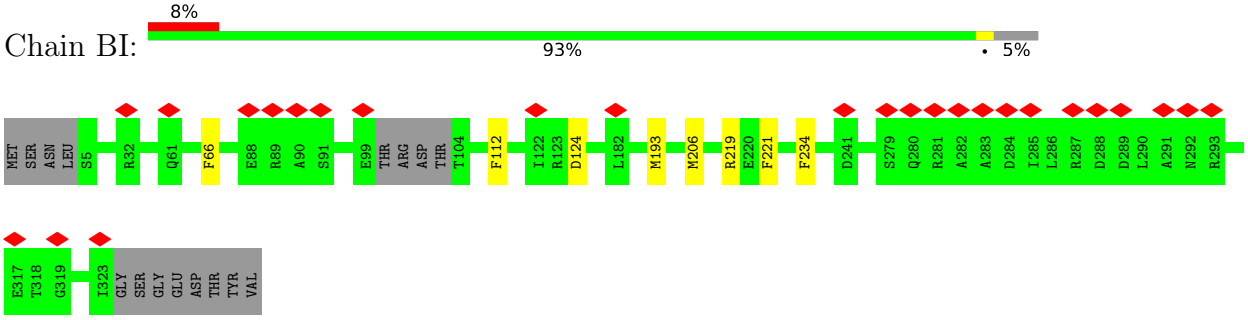

• Molecule 1: Flagellar motor switch protein FliG

Chain BC:



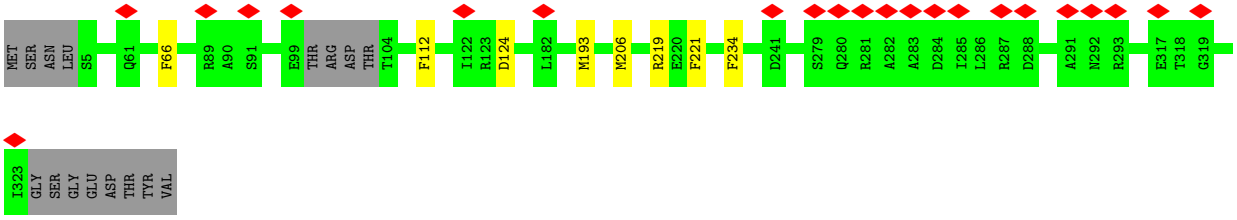

• Molecule 1: Flagellar motor switch protein FliG

Chain BI:

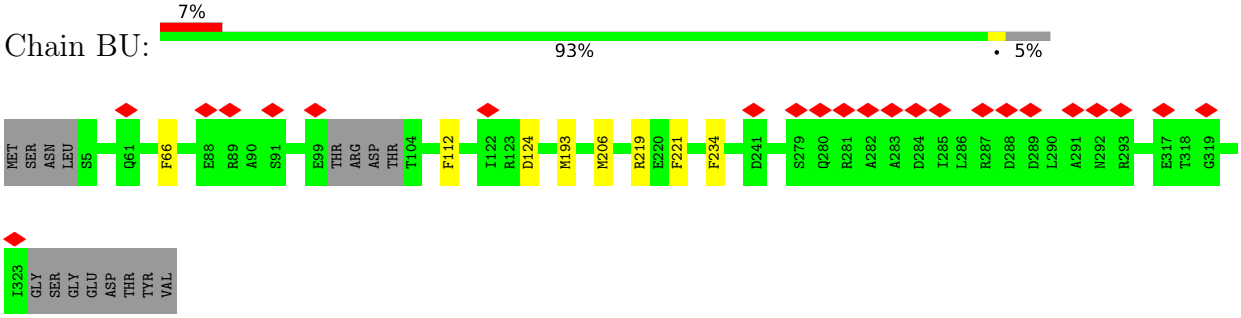



• Molecule 1: Flagellar motor switch protein FliG

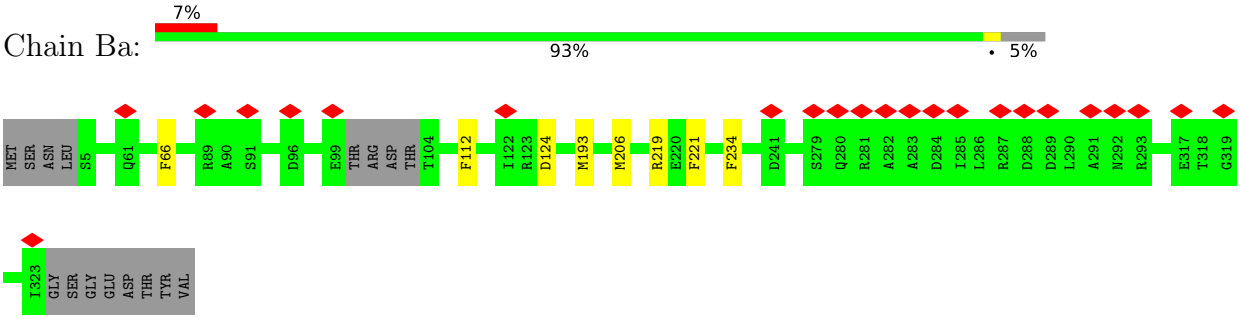
Chain BO:



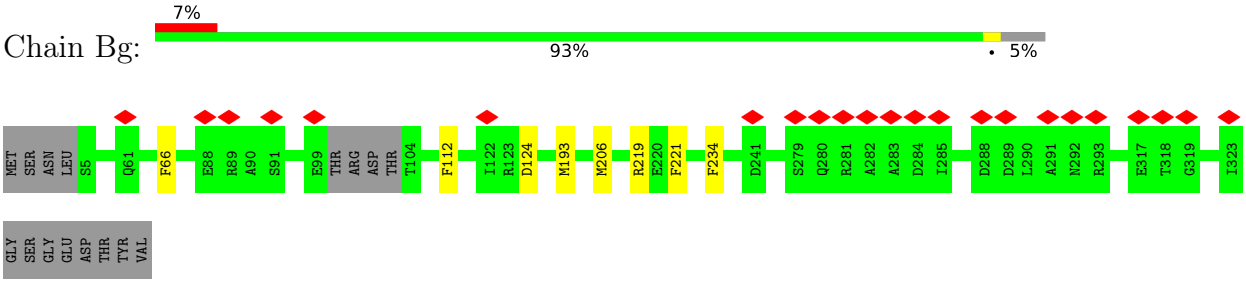

• Molecule 1: Flagellar motor switch protein FliG



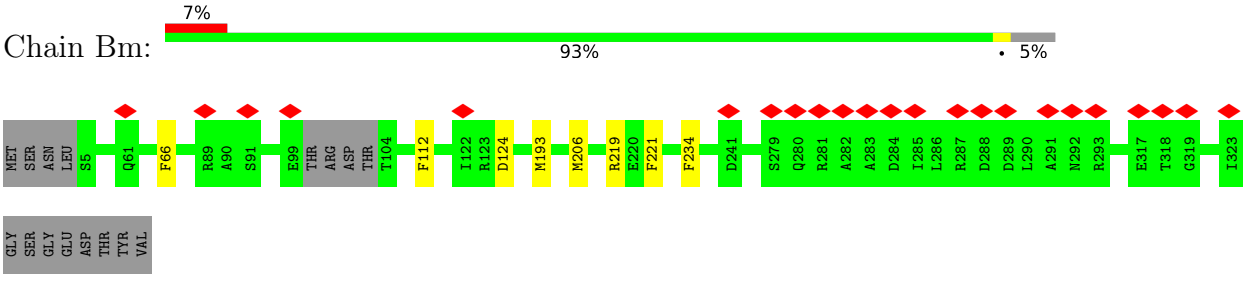

• Molecule 1: Flagellar motor switch protein FliG




• Molecule 1: Flagellar motor switch protein FliG

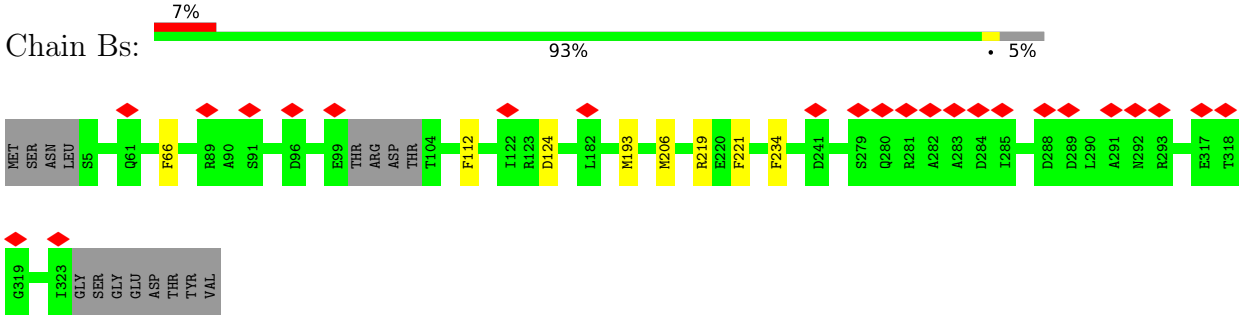



• Molecule 1: Flagellar motor switch protein FliG



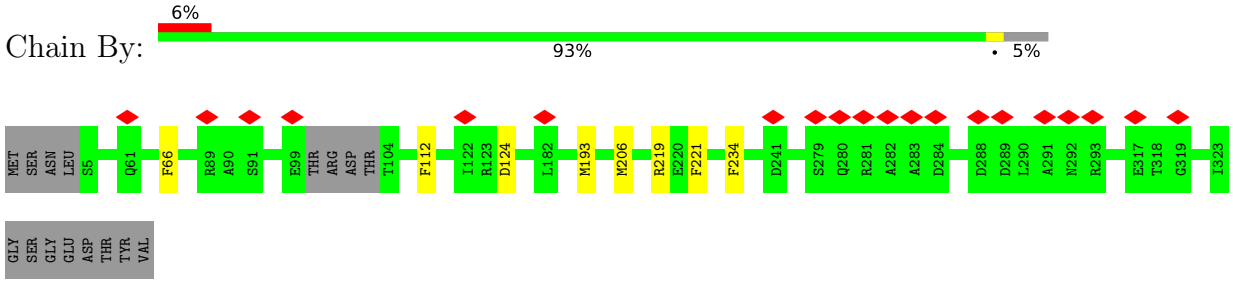
• Molecule 1: Flagellar motor switch protein FliG

Chain Bs:



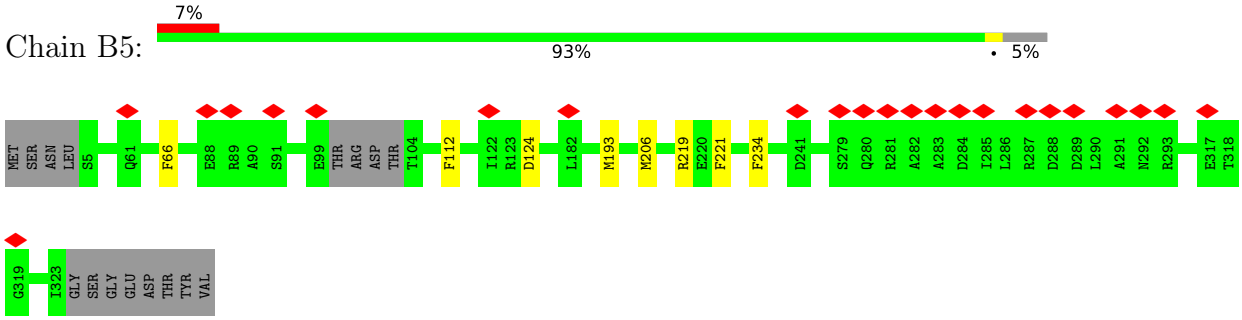

• Molecule 1: Flagellar motor switch protein FliG

Chain By:



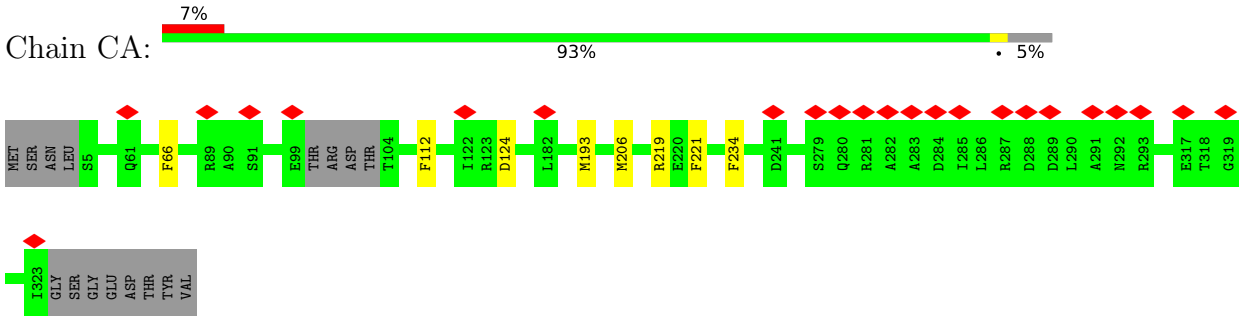

• Molecule 1: Flagellar motor switch protein FliG

Chain B5:



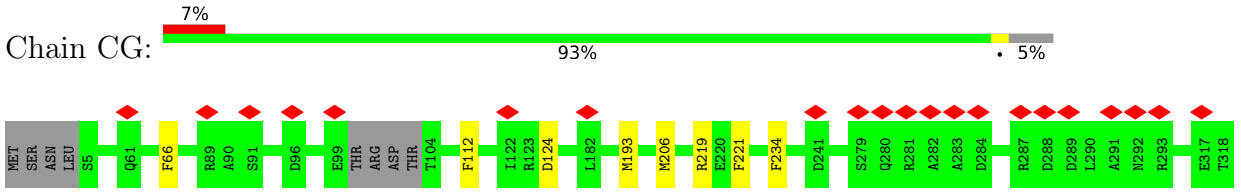

• Molecule 1: Flagellar motor switch protein FliG

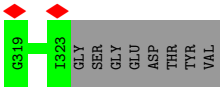
Chain CA:




• Molecule 1: Flagellar motor switch protein FliG

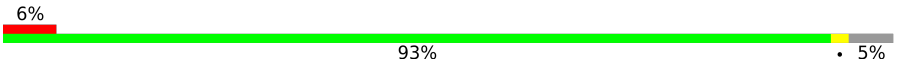
Chain CG:





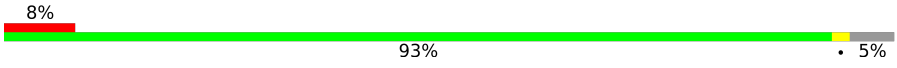

• Molecule 1: Flagellar motor switch protein FliG

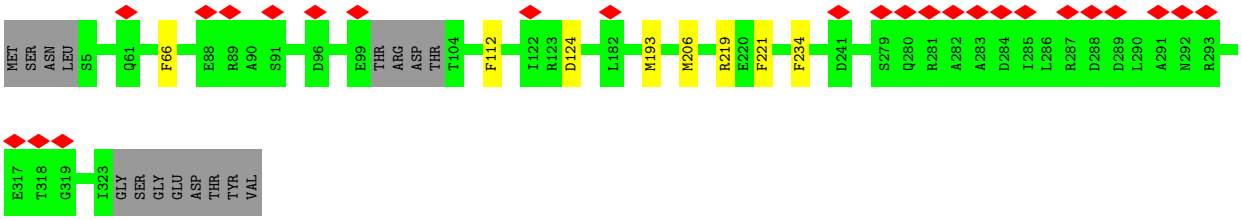
Chain CM:



• Molecule 1: Flagellar motor switch protein FliG

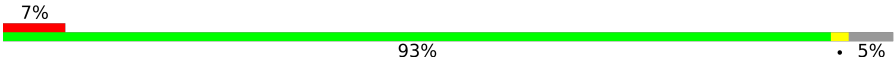
Chain CS:

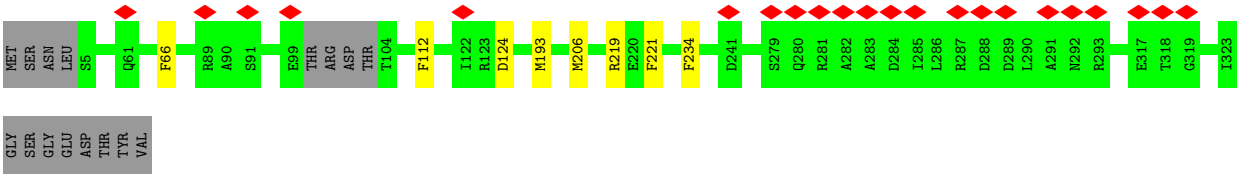



• Molecule 1: Flagellar motor switch protein FliG

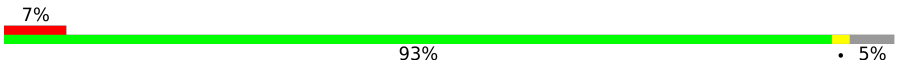
Chain CY:



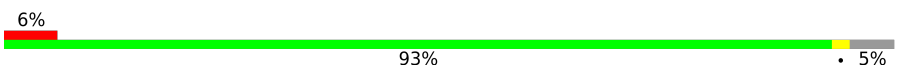

• Molecule 1: Flagellar motor switch protein FliG

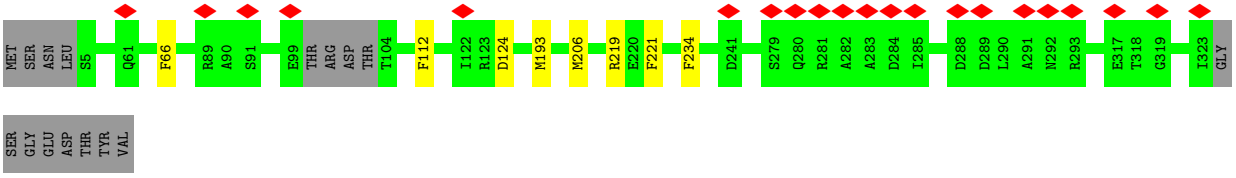
Chain Ce:



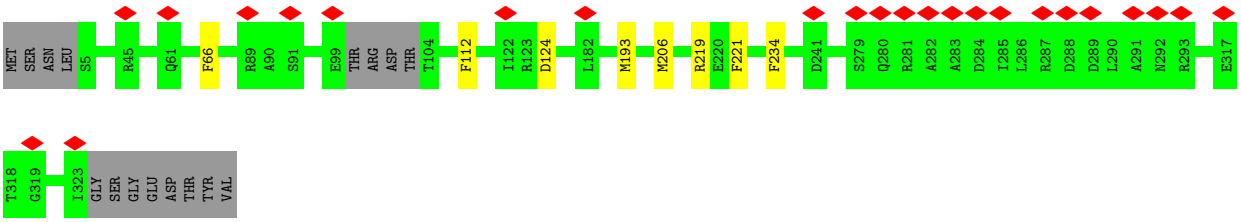
• Molecule 1: Flagellar motor switch protein FliG

Chain Ck:

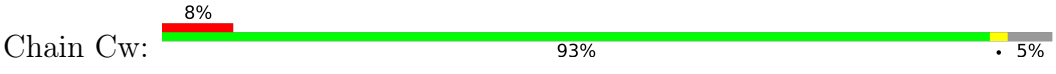


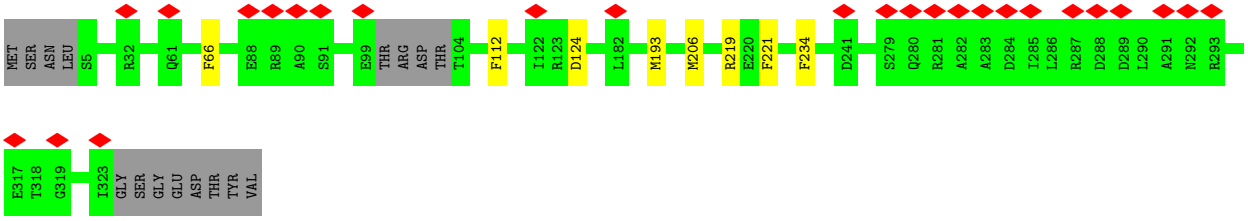



• Molecule 1: Flagellar motor switch protein FliG

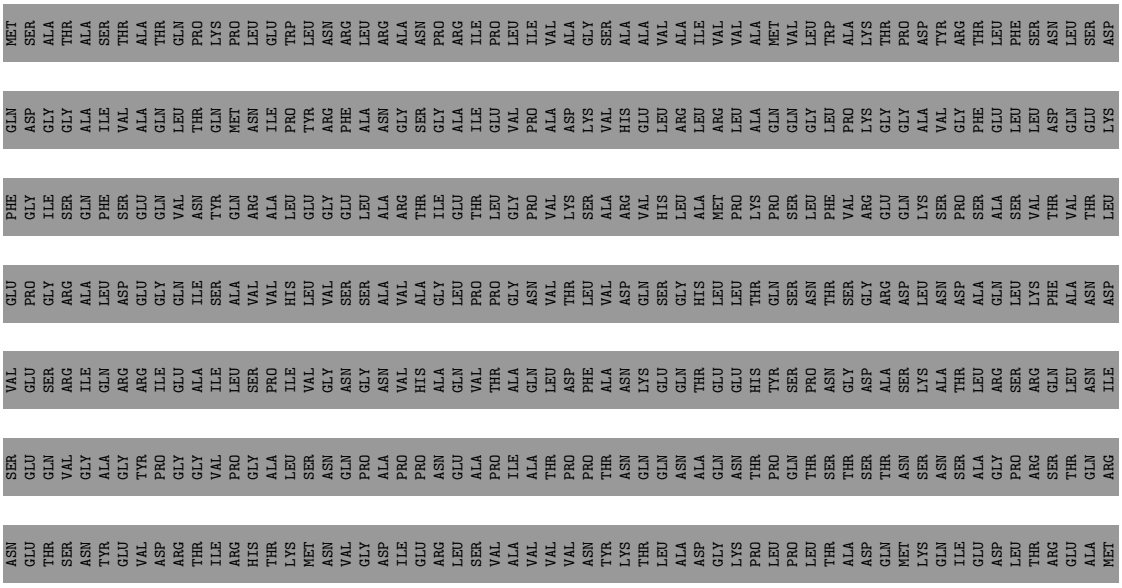


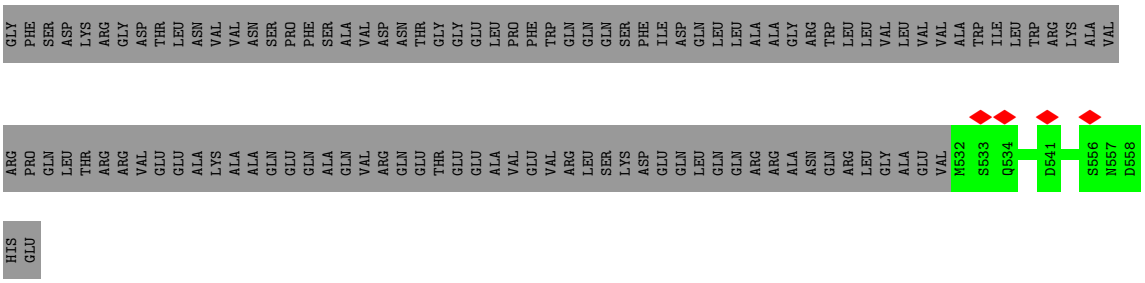

• Molecule 1: Flagellar motor switch protein FliG



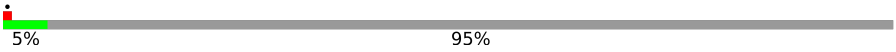

• Molecule 2: Flagellar M-ring protein

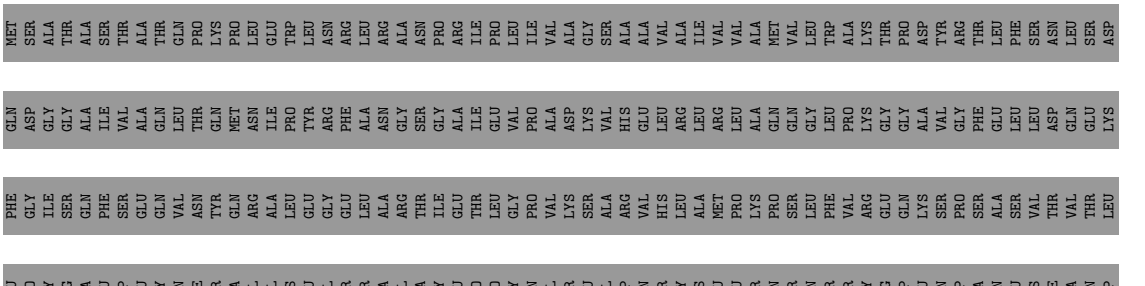





• Molecule 2: Flagellar M-ring protein

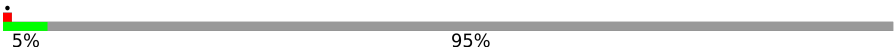
Chain r:

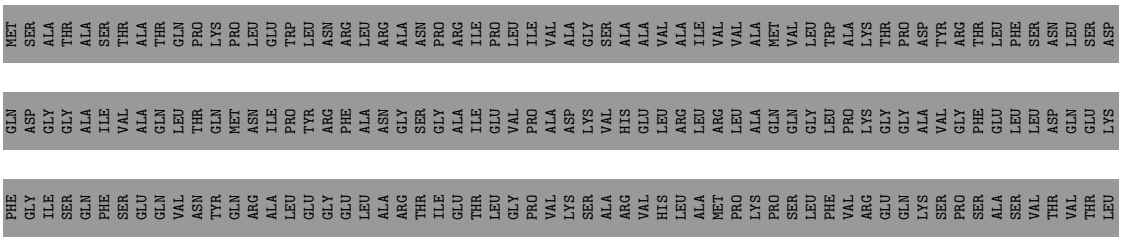


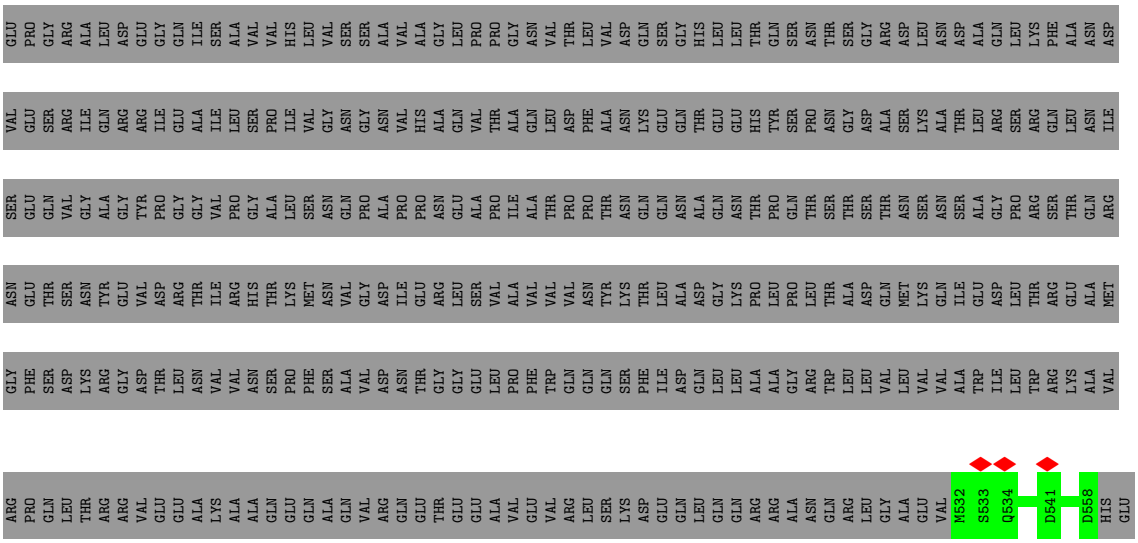




• Molecule 2: Flagellar M-ring protein

Chain x:

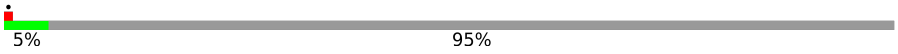


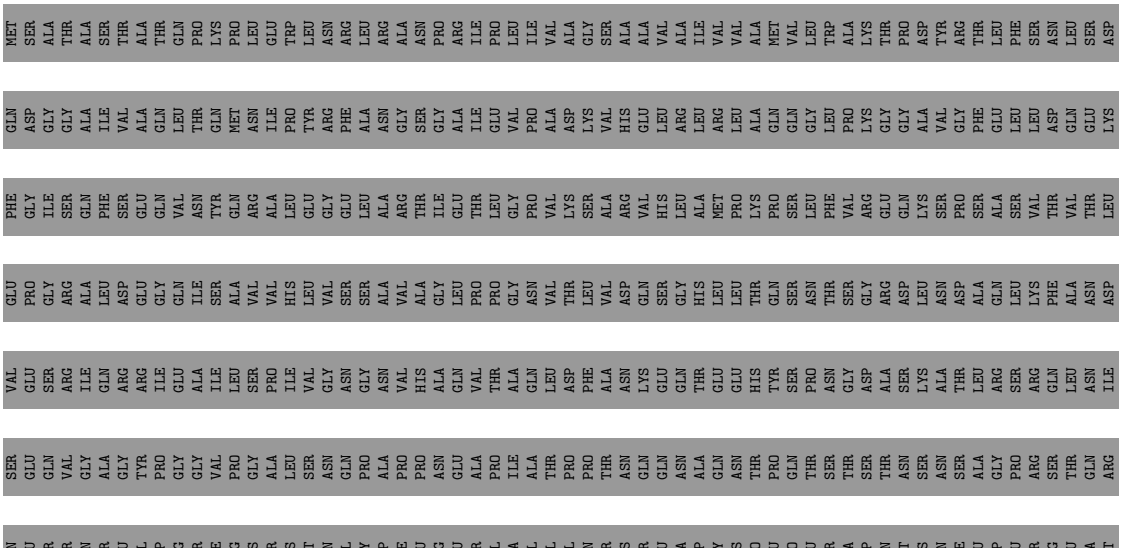






• Molecule 2: Flagellar M-ring protein

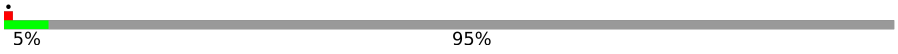
Chain 4:

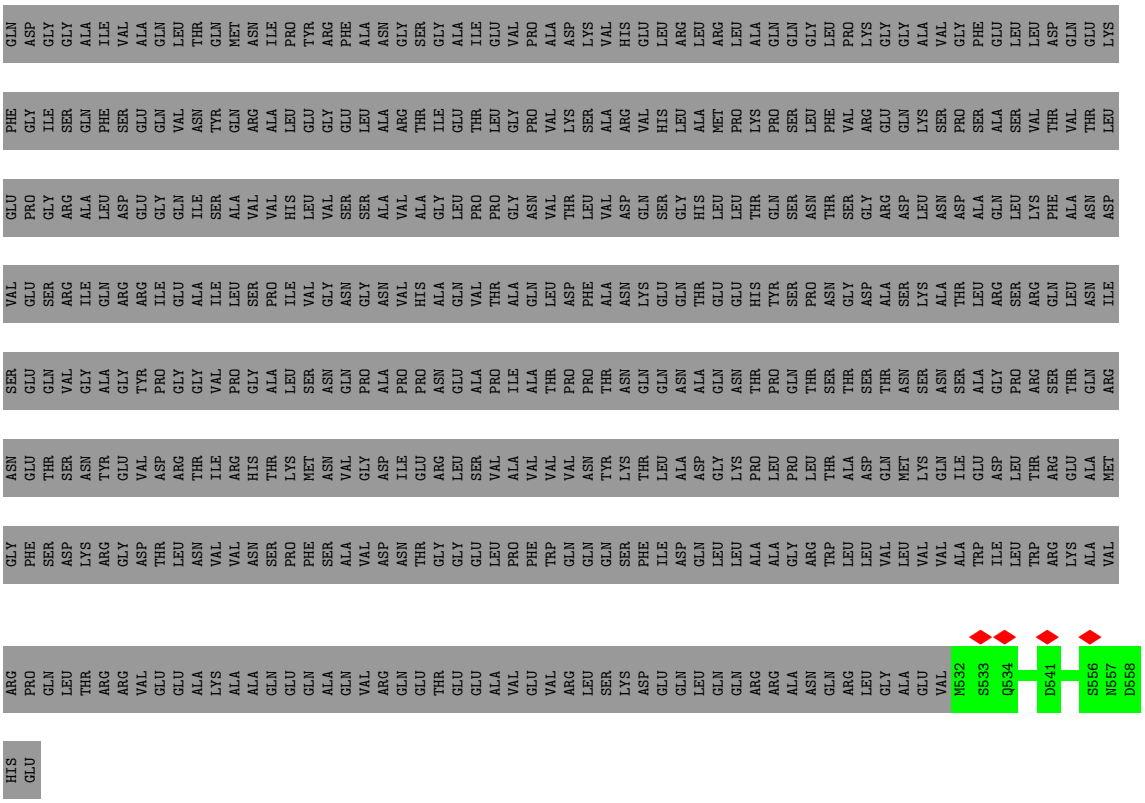



• Molecule 2: Flagellar M-ring protein

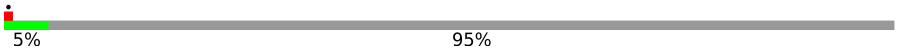
Chain 0:

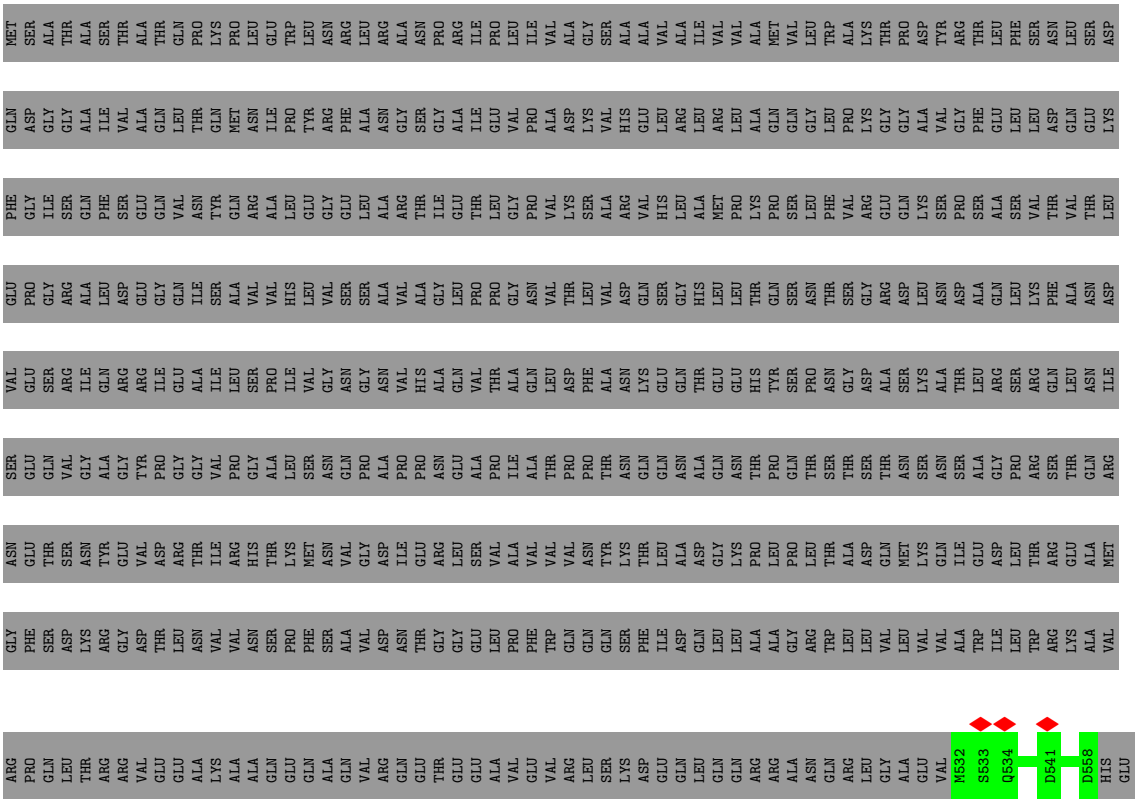





• Molecule 2: Flagellar M-ring protein

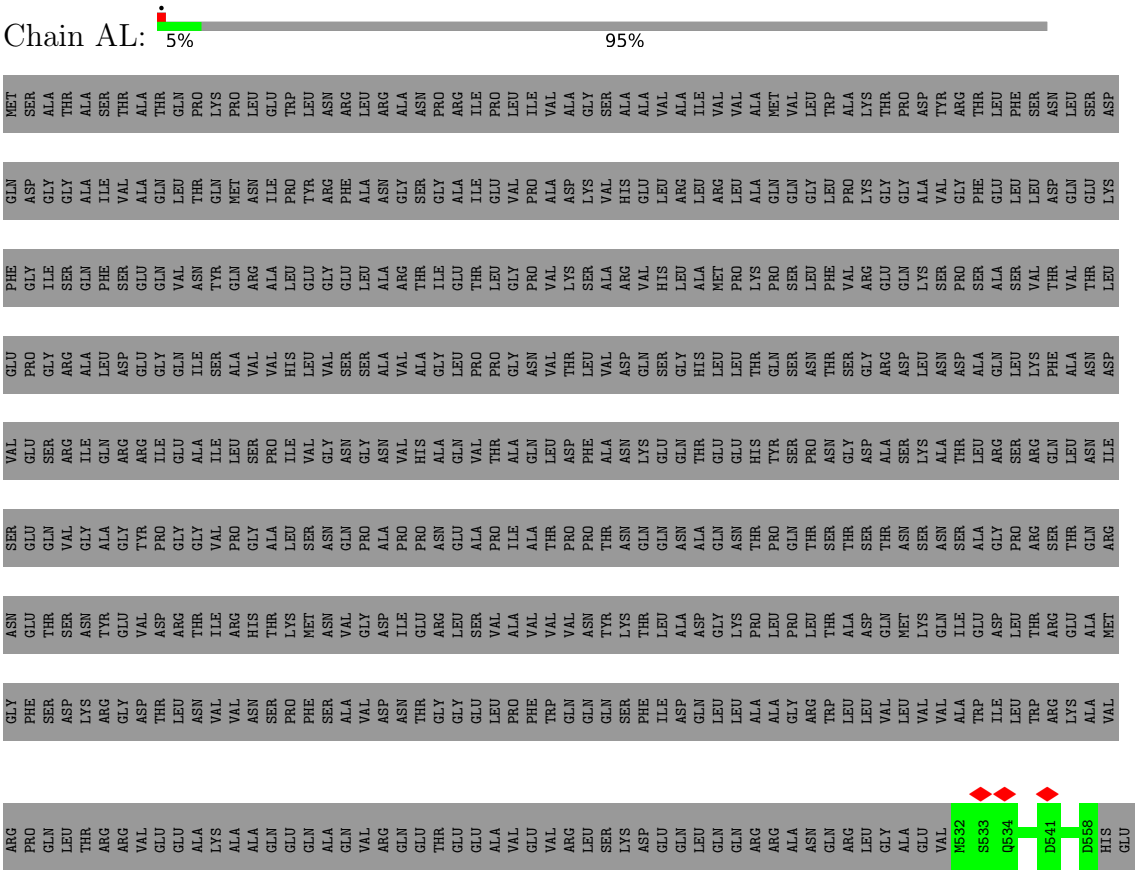
Chain AF:



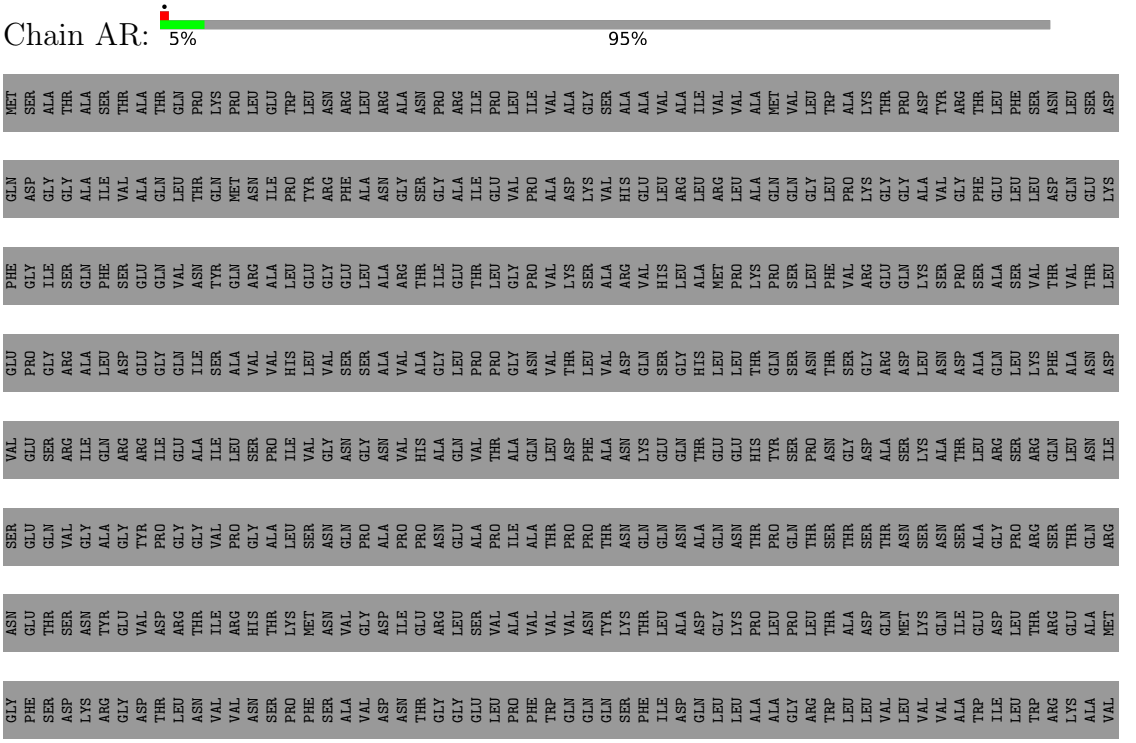
• Molecule 2: Flagellar M-ring protein

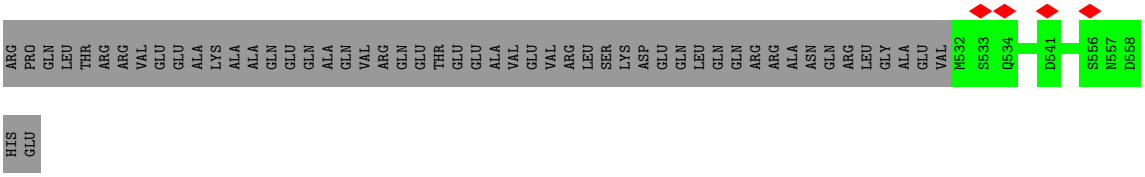
Chain AL:




• Molecule 2: Flagellar M-ring protein

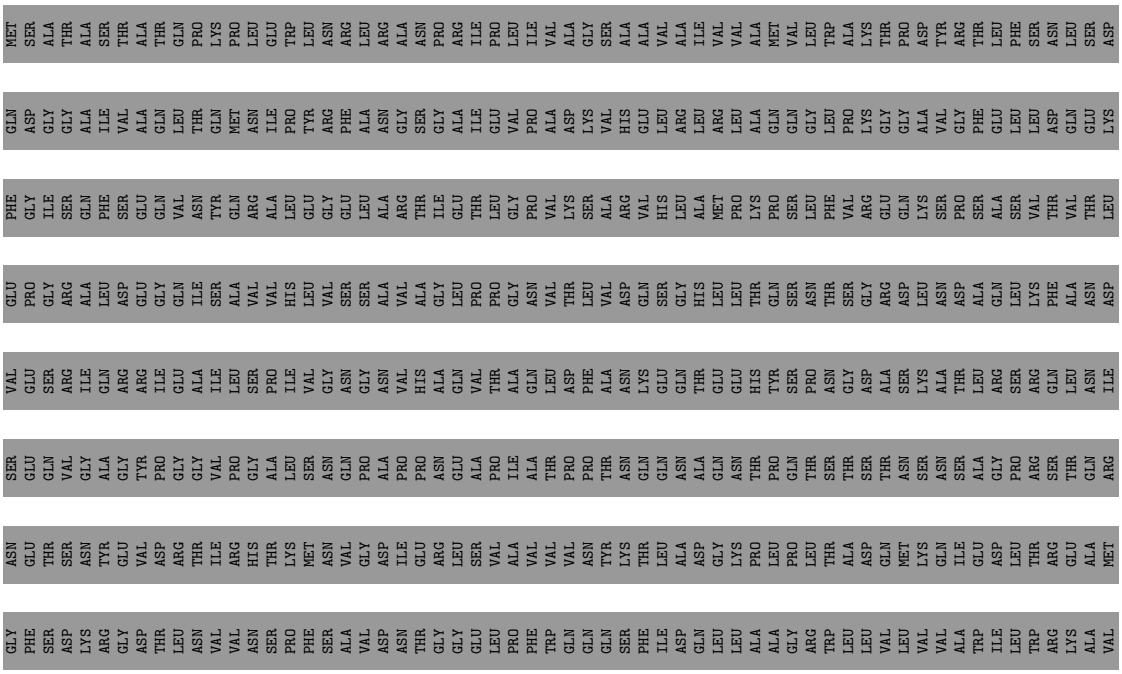
Chain AR:





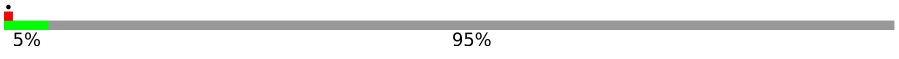

• Molecule 2: Flagellar M-ring protein

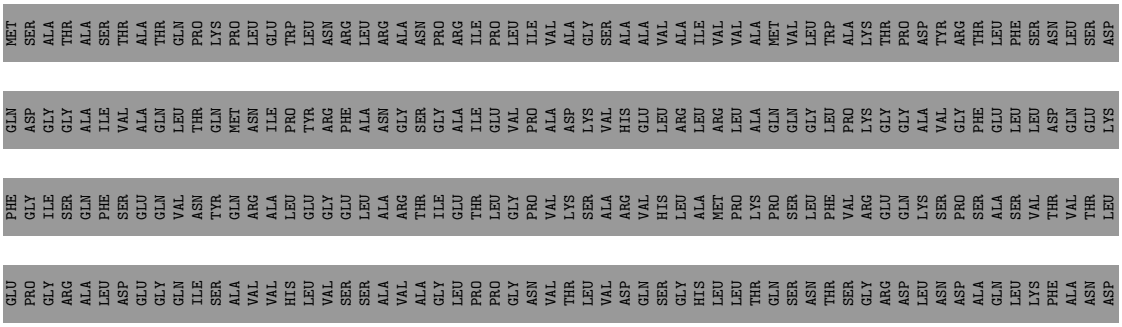
Chain AX:



• Molecule 2: Flagellar M-ring protein

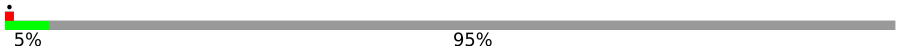
Chain Ad:

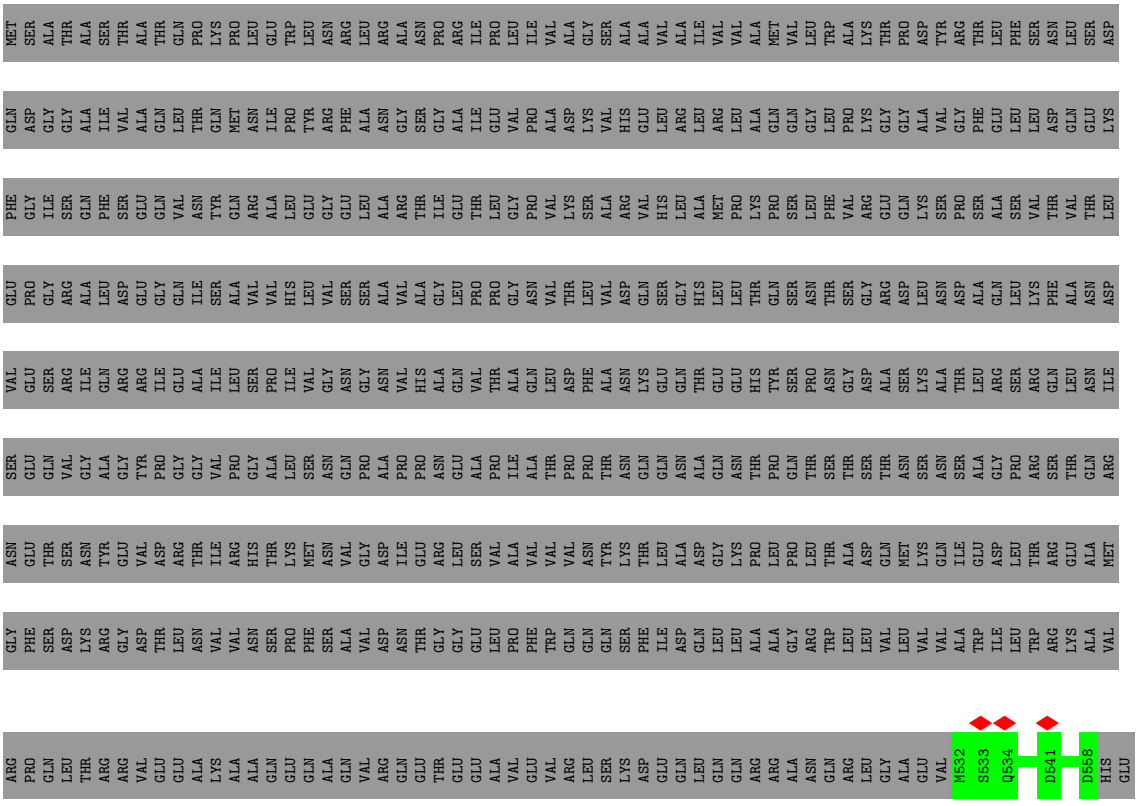


• Molecule 2: Flagellar M-ring protein

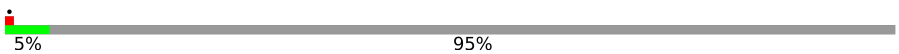
Chain Aj:

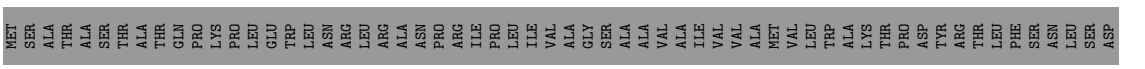


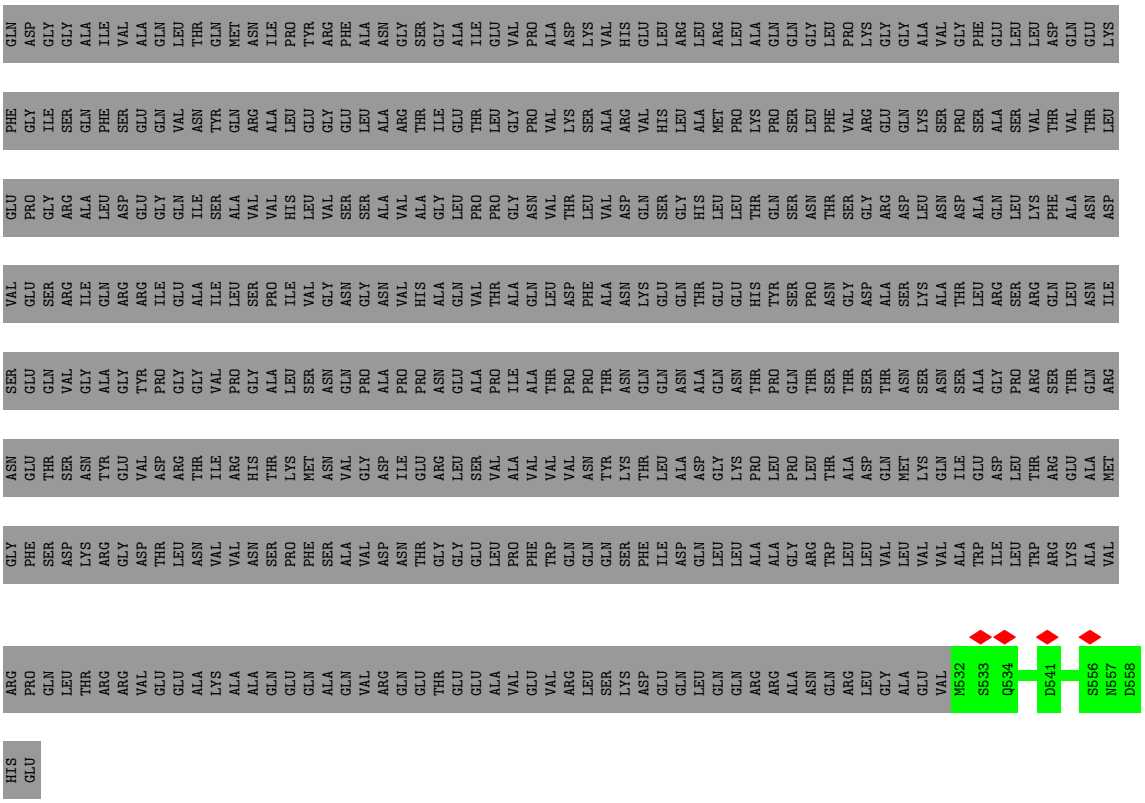




• Molecule 2: Flagellar M-ring protein

Chain Ap:

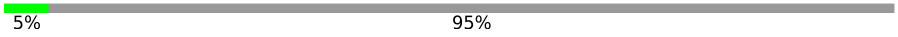


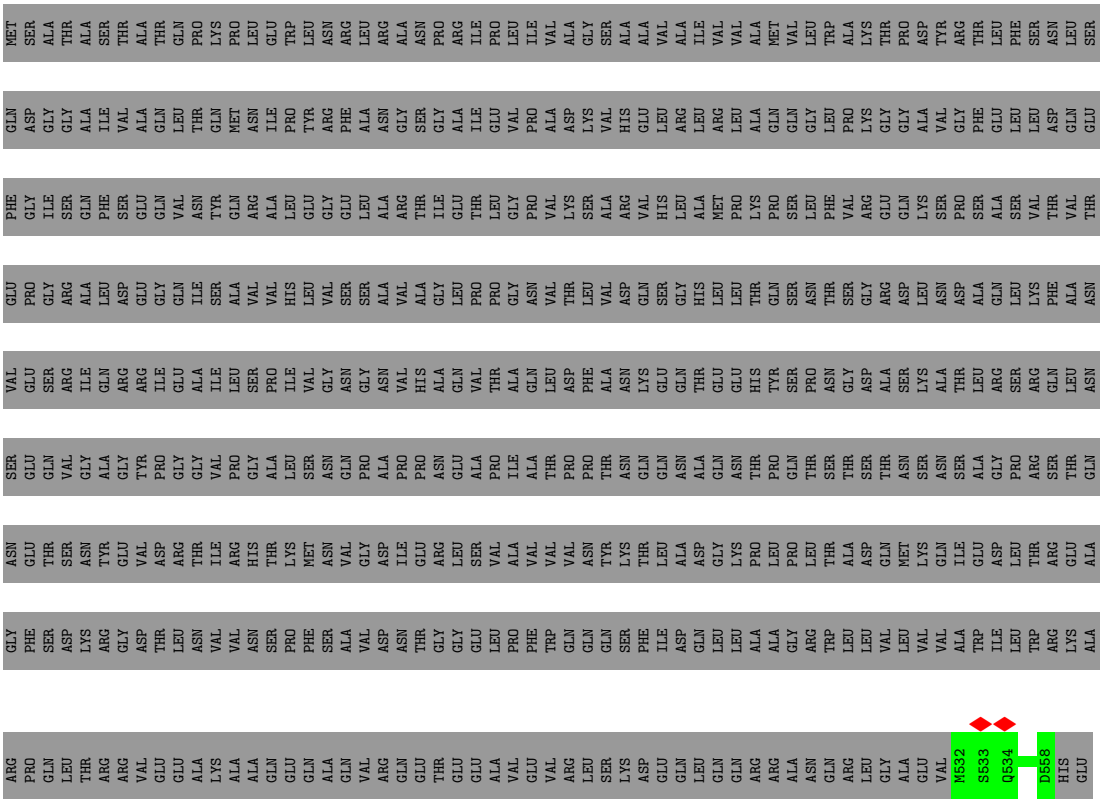






• Molecule 2: Flagellar M-ring protein

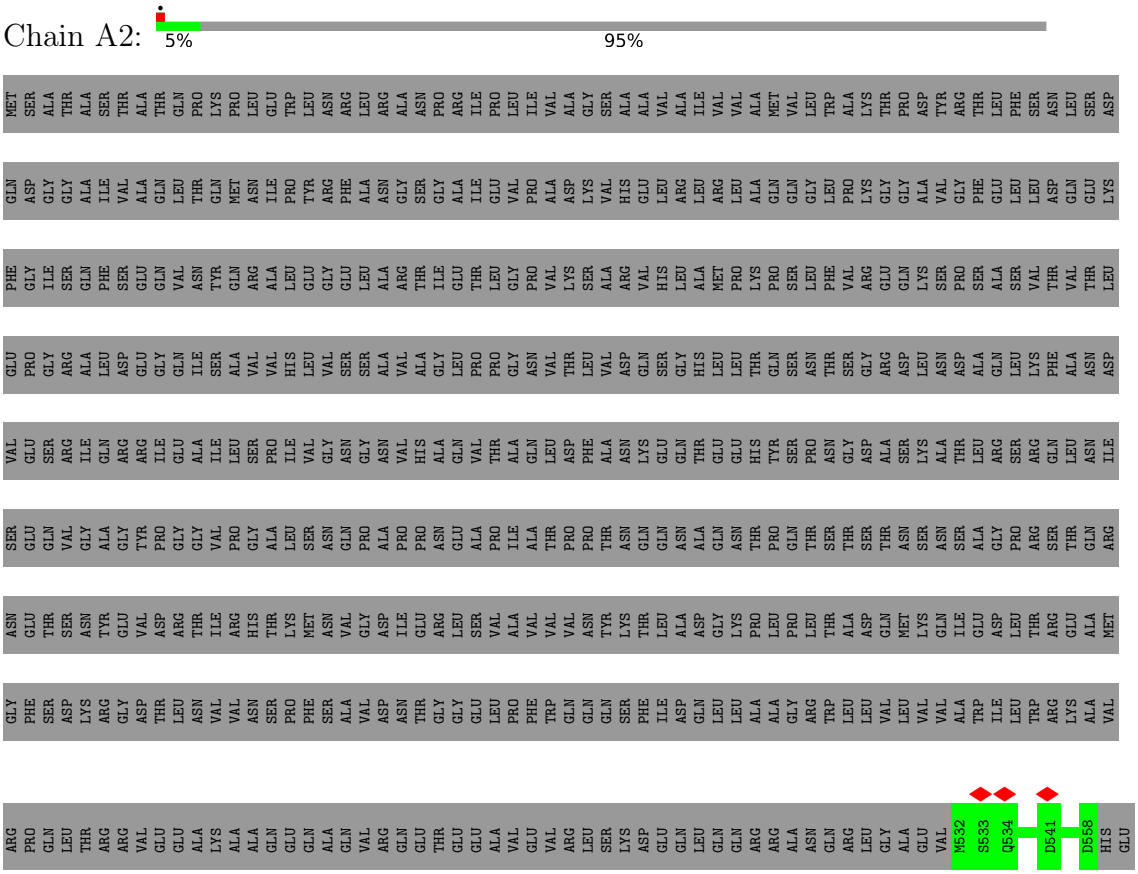
Chain Av:



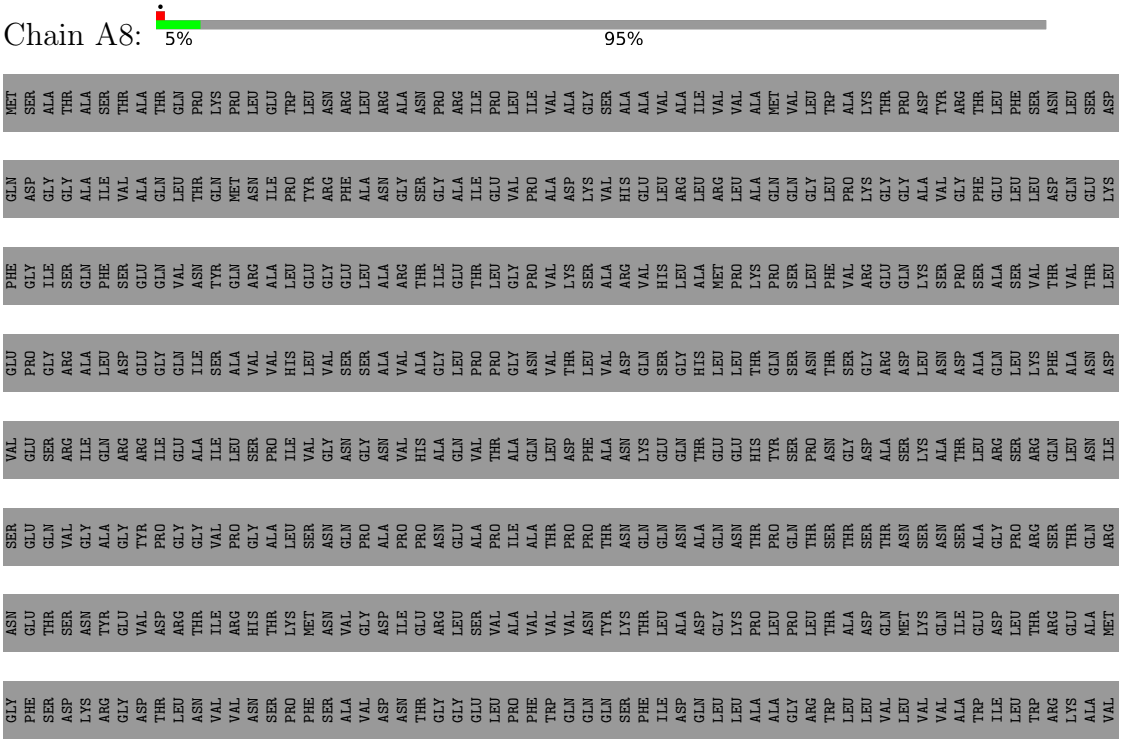
• Molecule 2: Flagellar M-ring protein

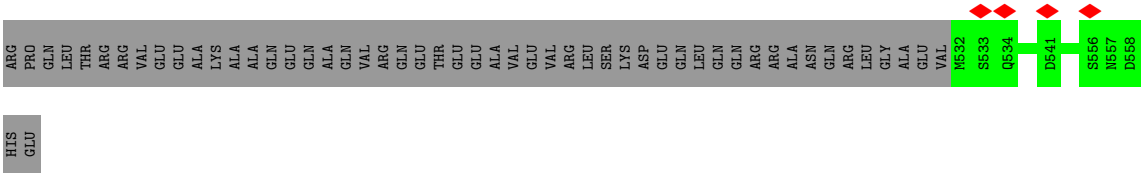
Chain A2:




• Molecule 2: Flagellar M-ring protein

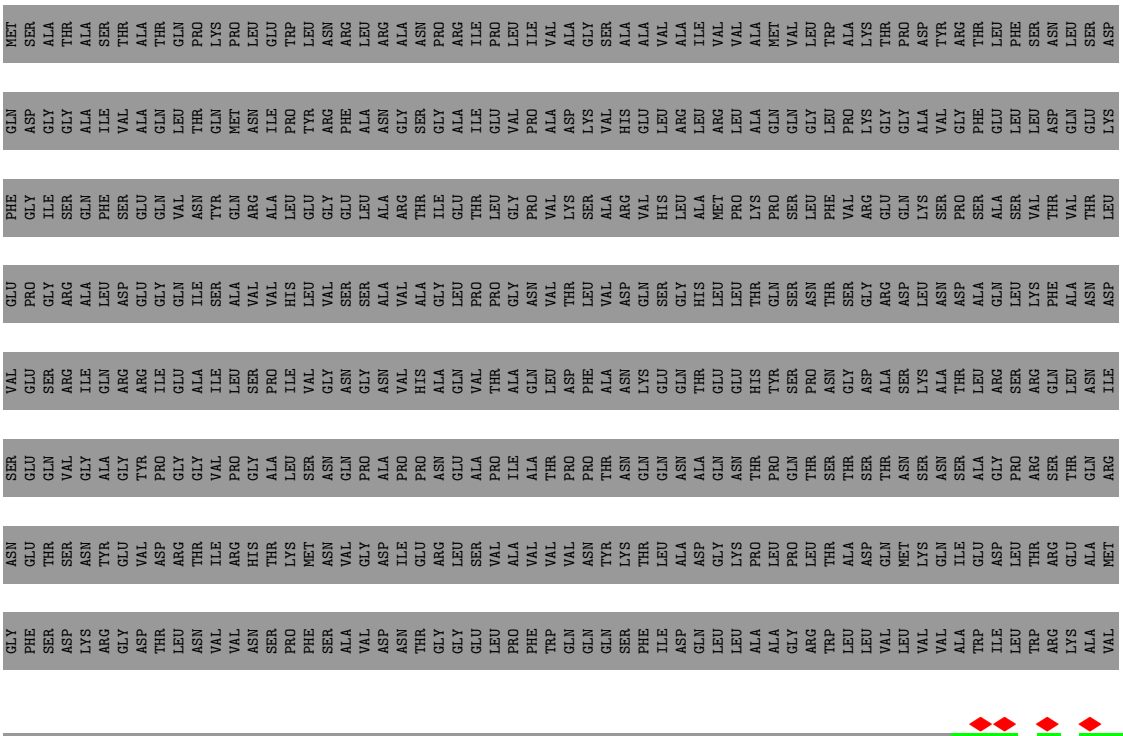
Chain A8:





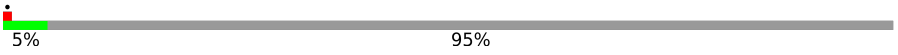

• Molecule 2: Flagellar M-ring protein

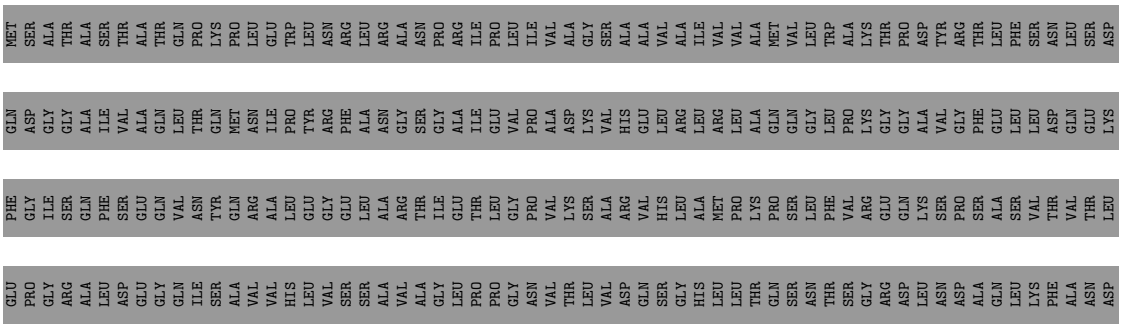
Chain BD:

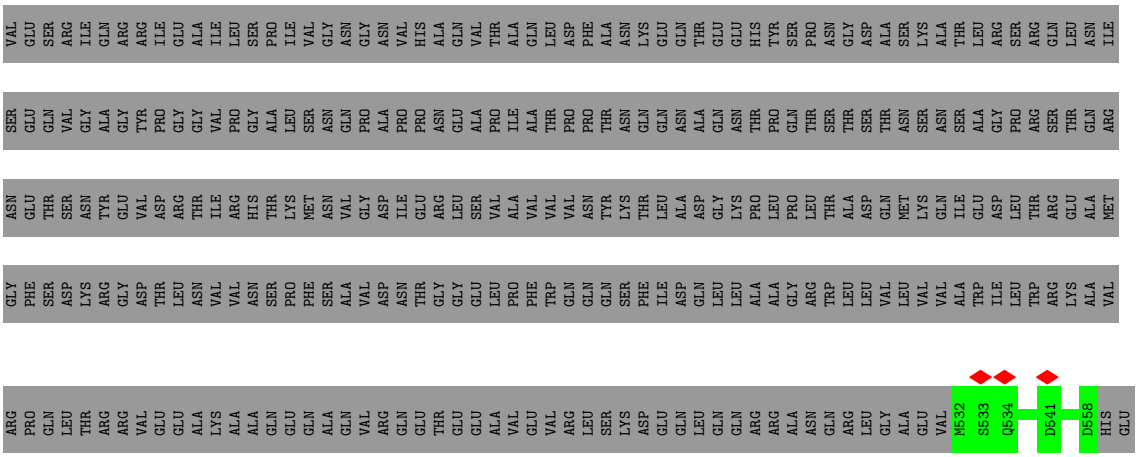


• Molecule 2: Flagellar M-ring protein

Chain BJ:

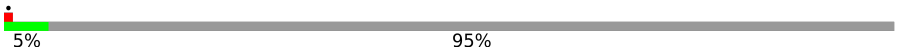


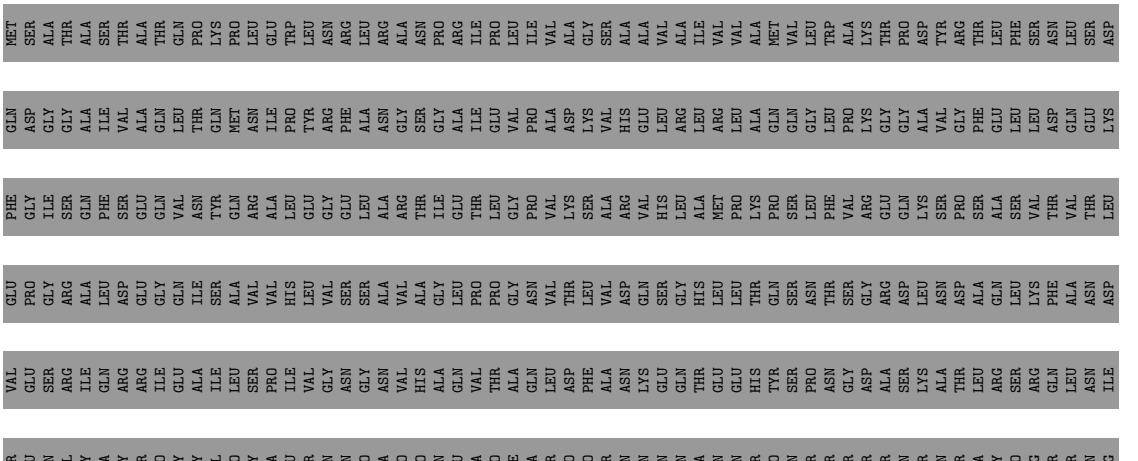






• Molecule 2: Flagellar M-ring protein

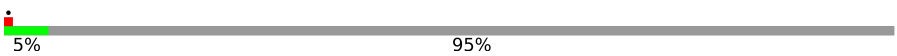
Chain BP:

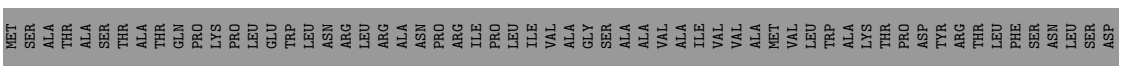


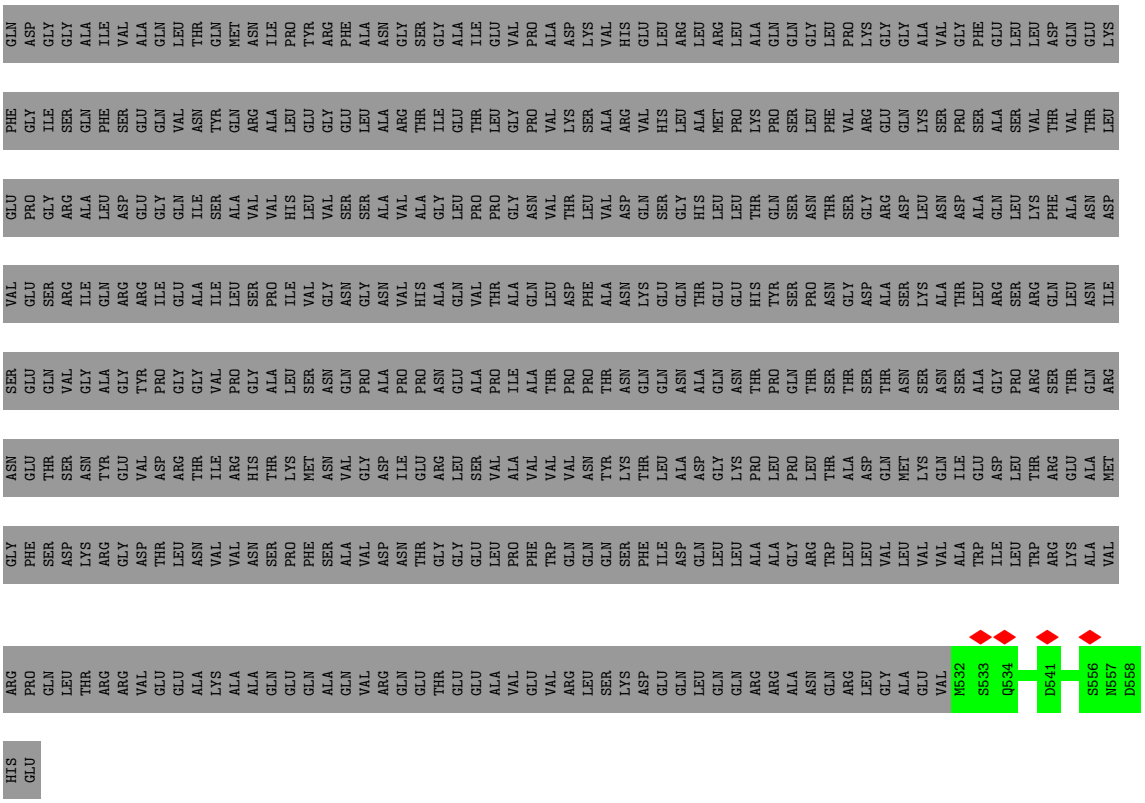




• Molecule 2: Flagellar M-ring protein

Chain BV:

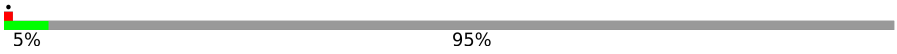


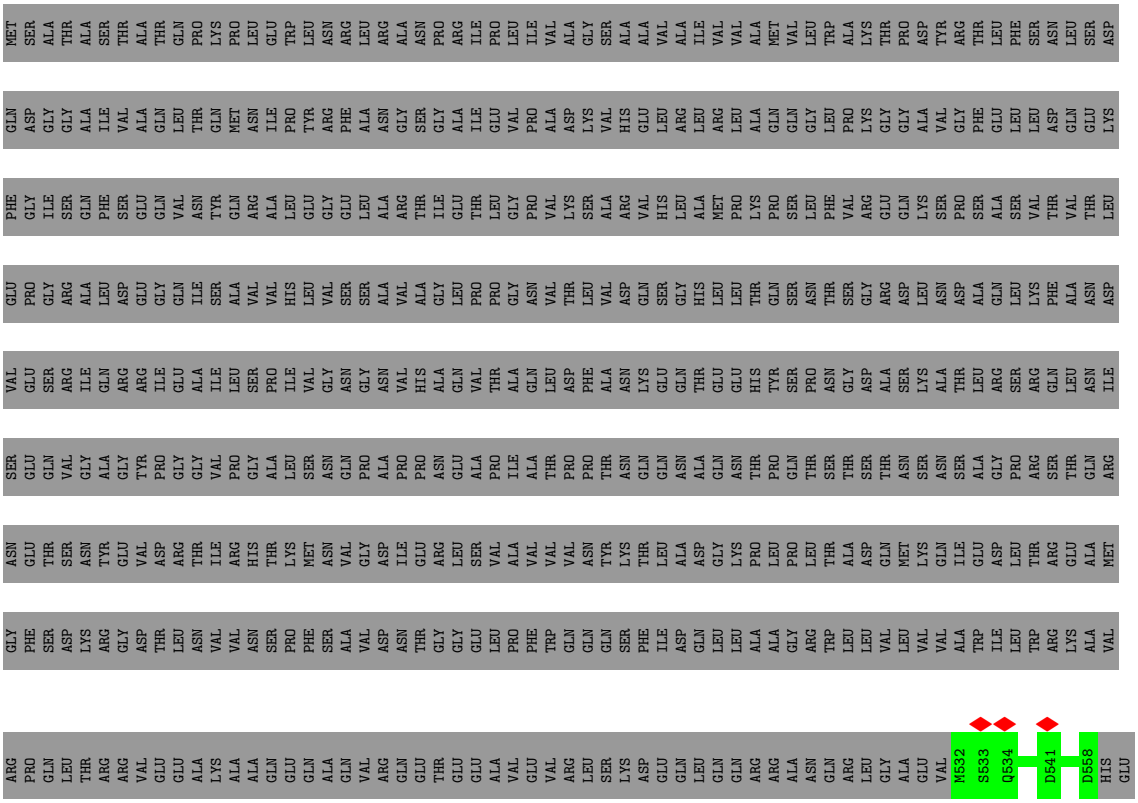






• Molecule 2: Flagellar M-ring protein

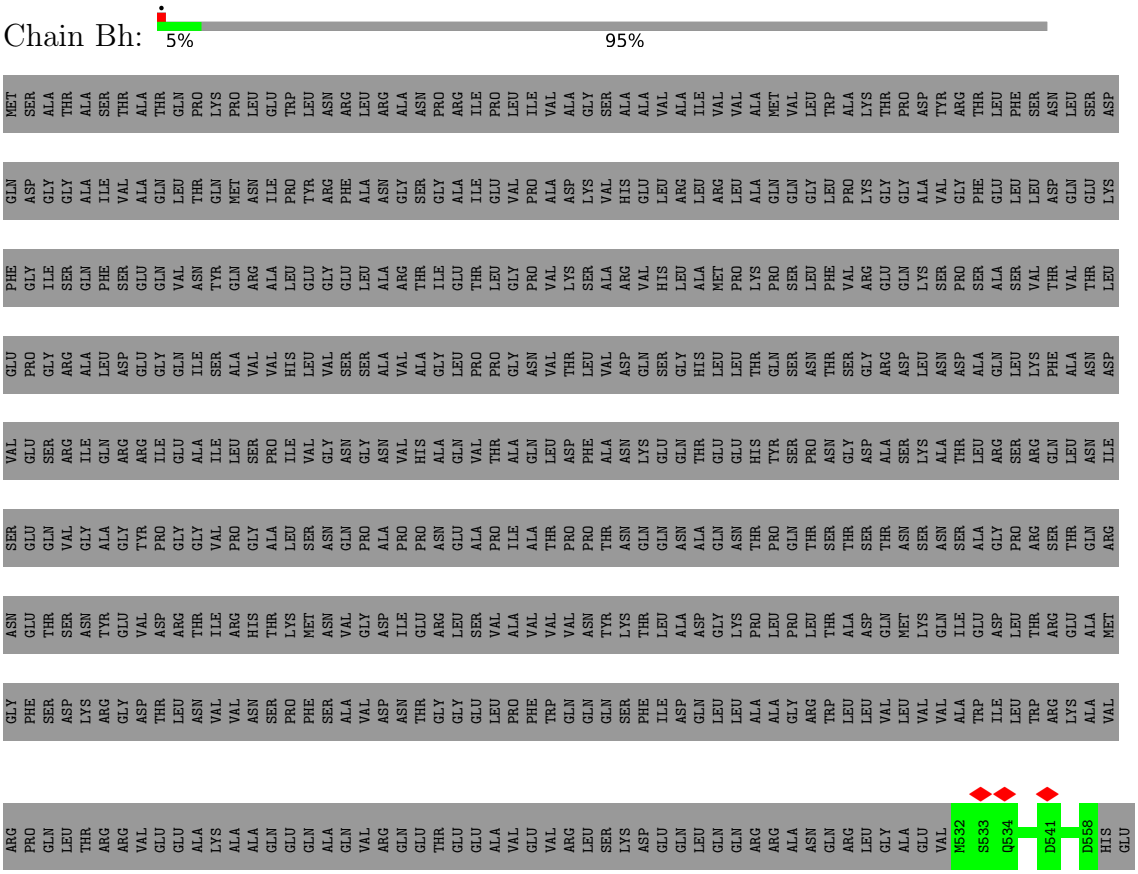
Chain Bb:



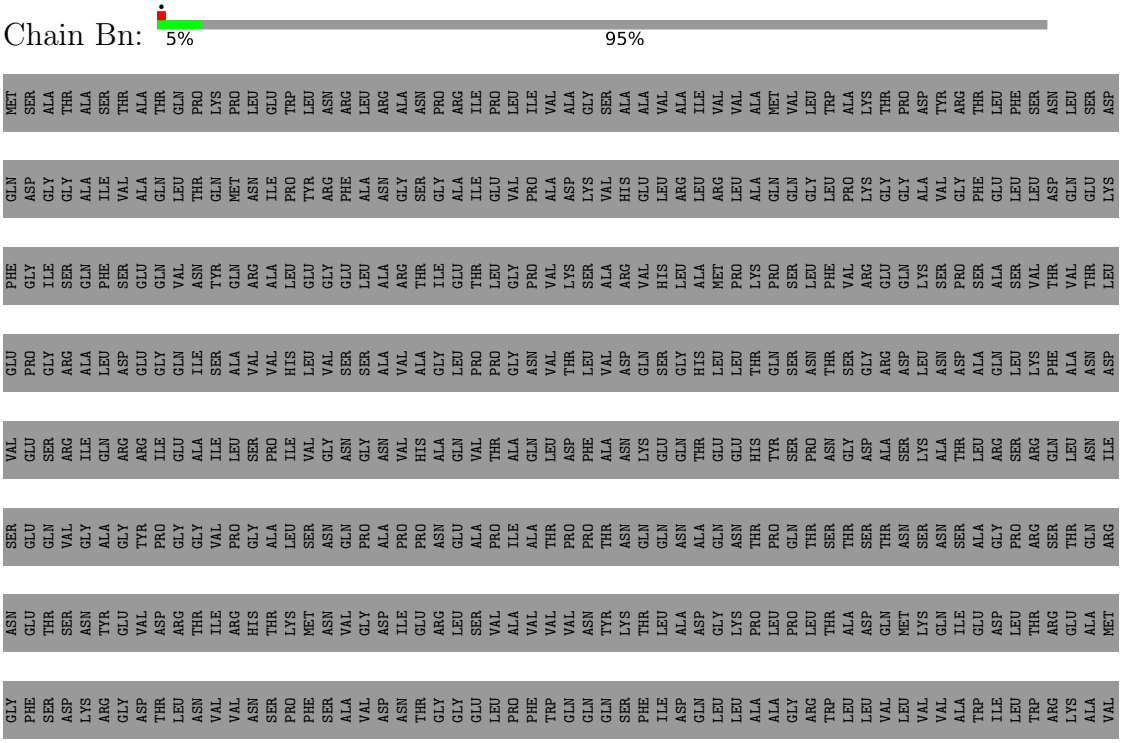
• Molecule 2: Flagellar M-ring protein

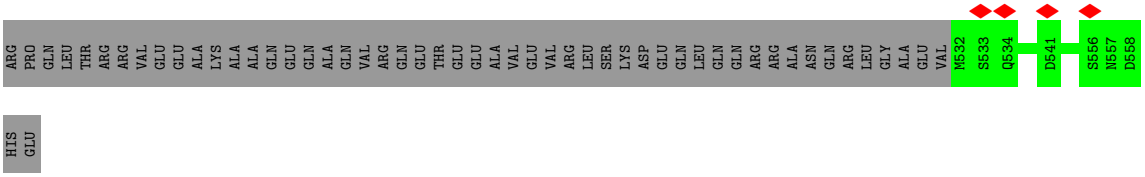
Chain Bh:




• Molecule 2: Flagellar M-ring protein

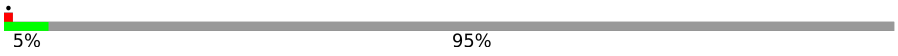
Chain Bn:

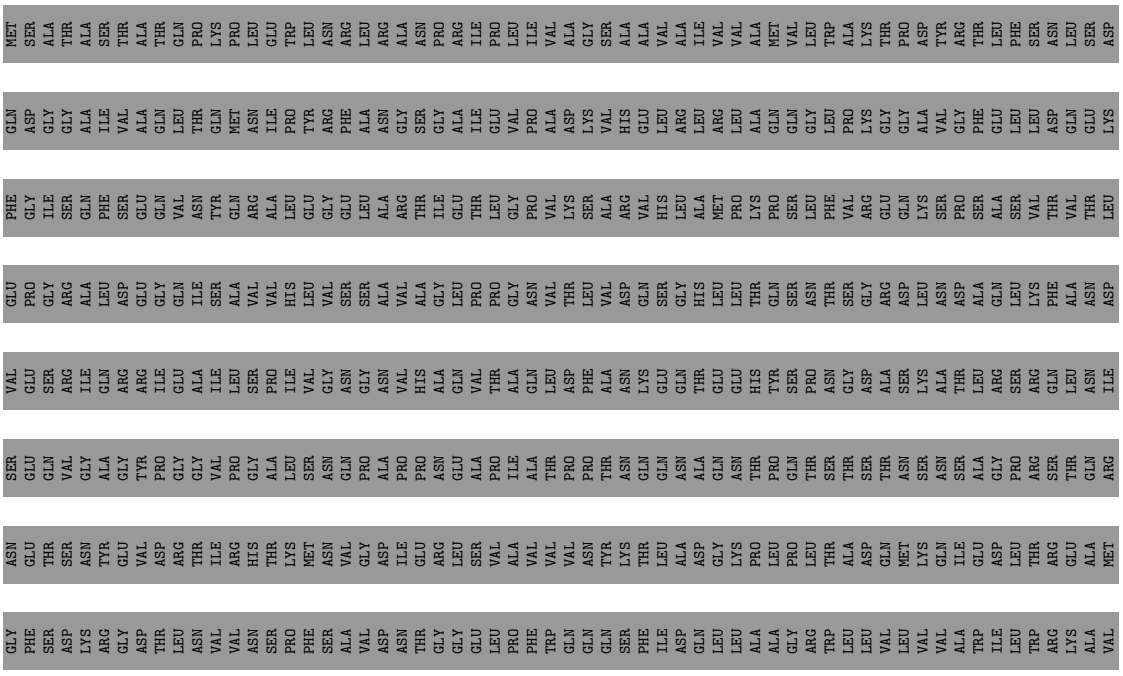


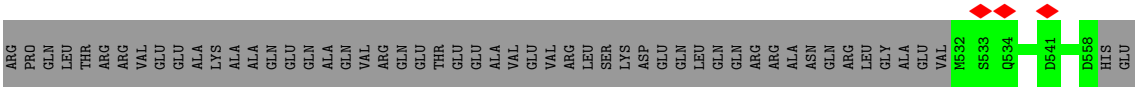



• Molecule 2: Flagellar M-ring protein

Chain Bt:

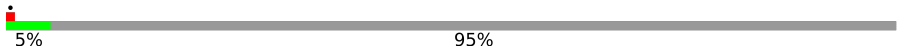


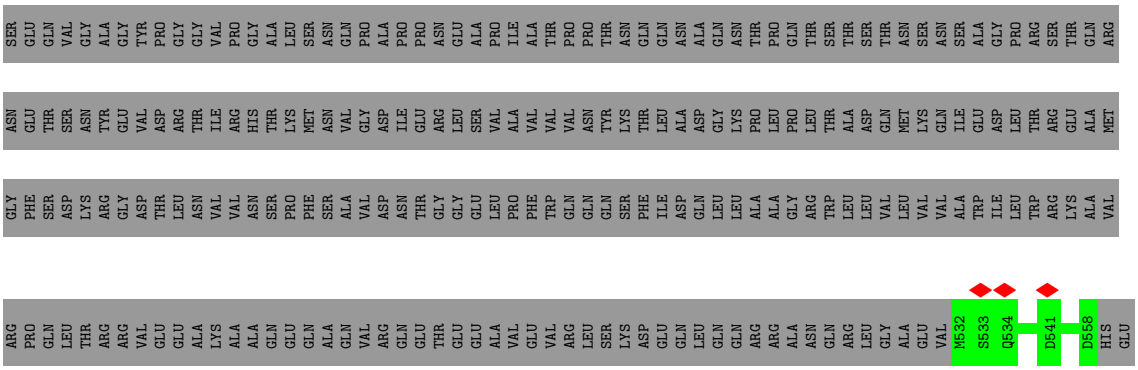




• Molecule 2: Flagellar M-ring protein

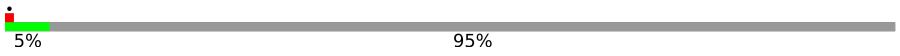
Chain Bz:

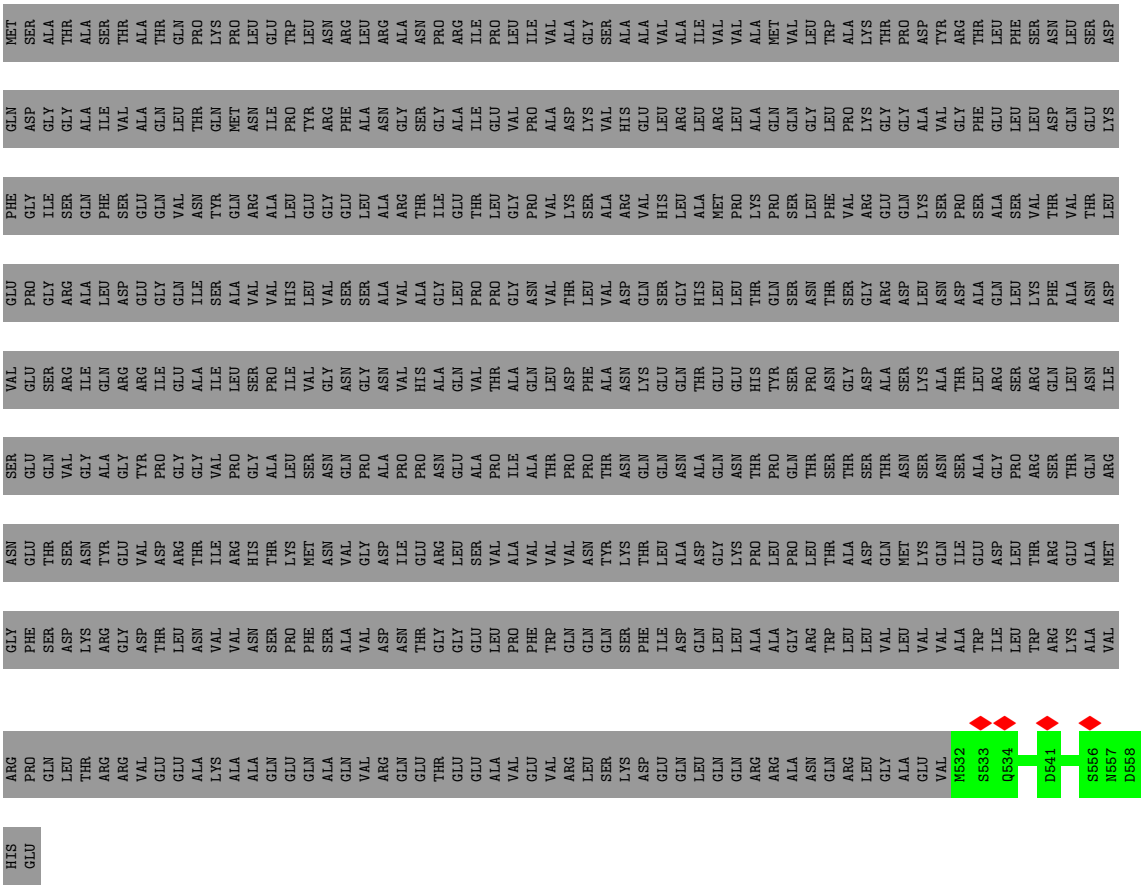





• Molecule 2: Flagellar M-ring protein

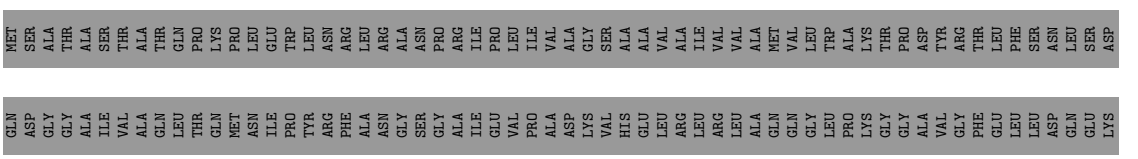
Chain B6:



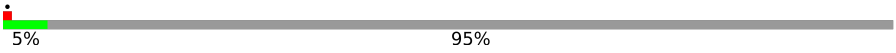

• Molecule 2: Flagellar M-ring protein

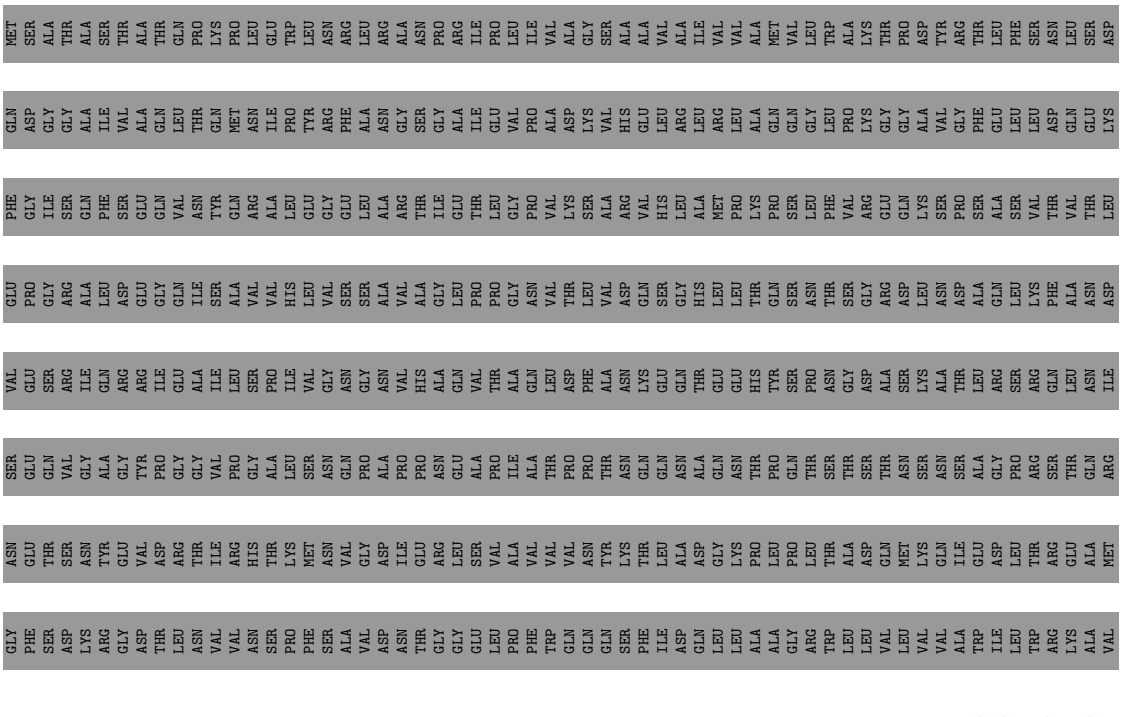
Chain CB:



- Molecule 2: Flagellar M-ring protein

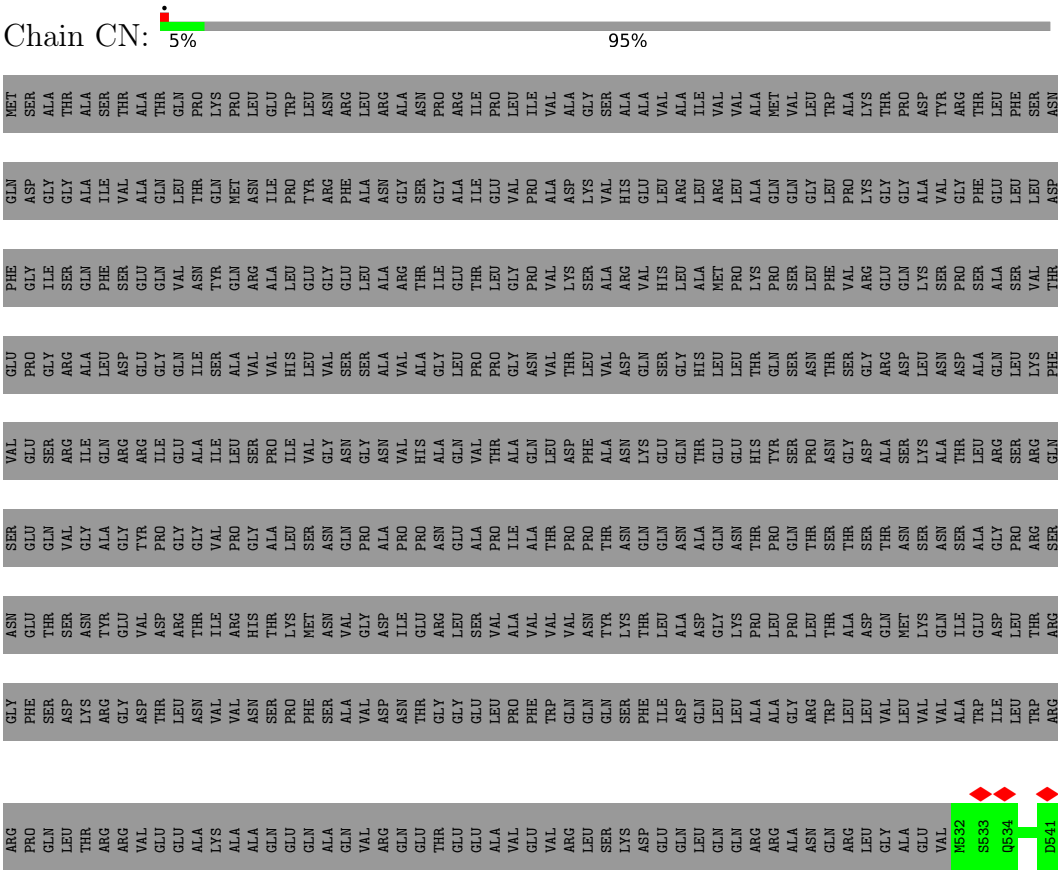
Chain CH:



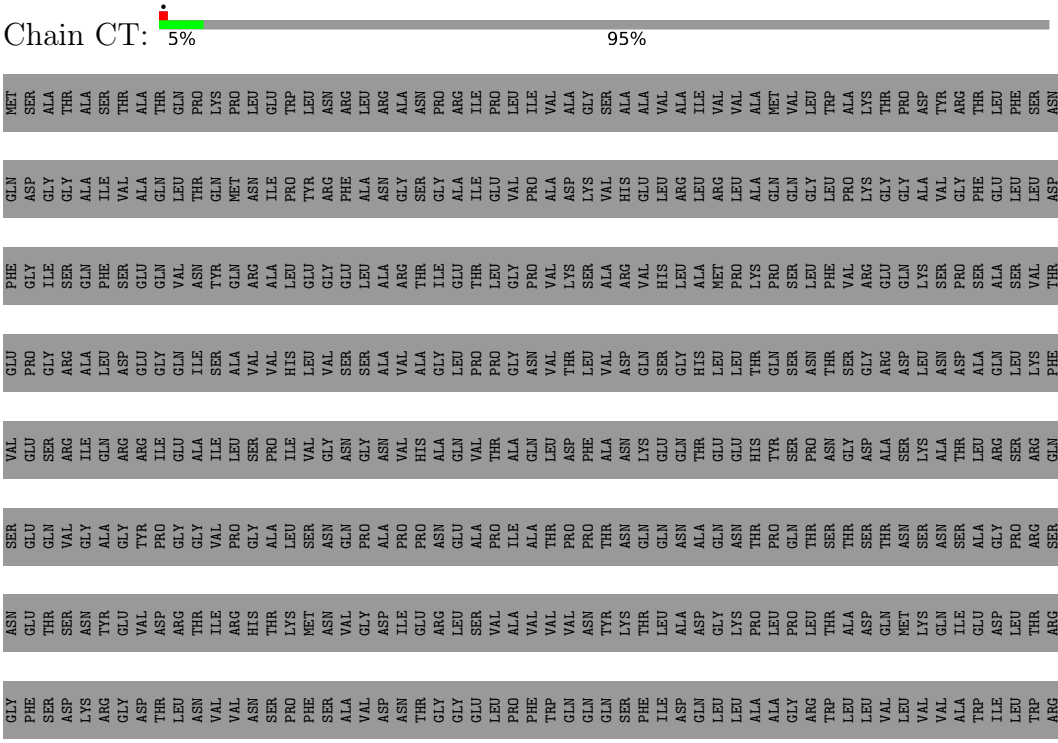
• Molecule 2: Flagellar M-ring protein

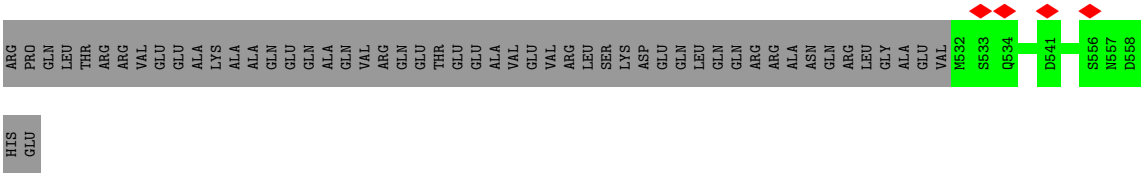
Chain CN:




• Molecule 2: Flagellar M-ring protein

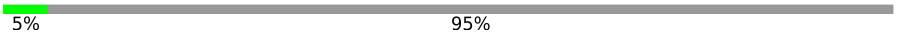
Chain CT:

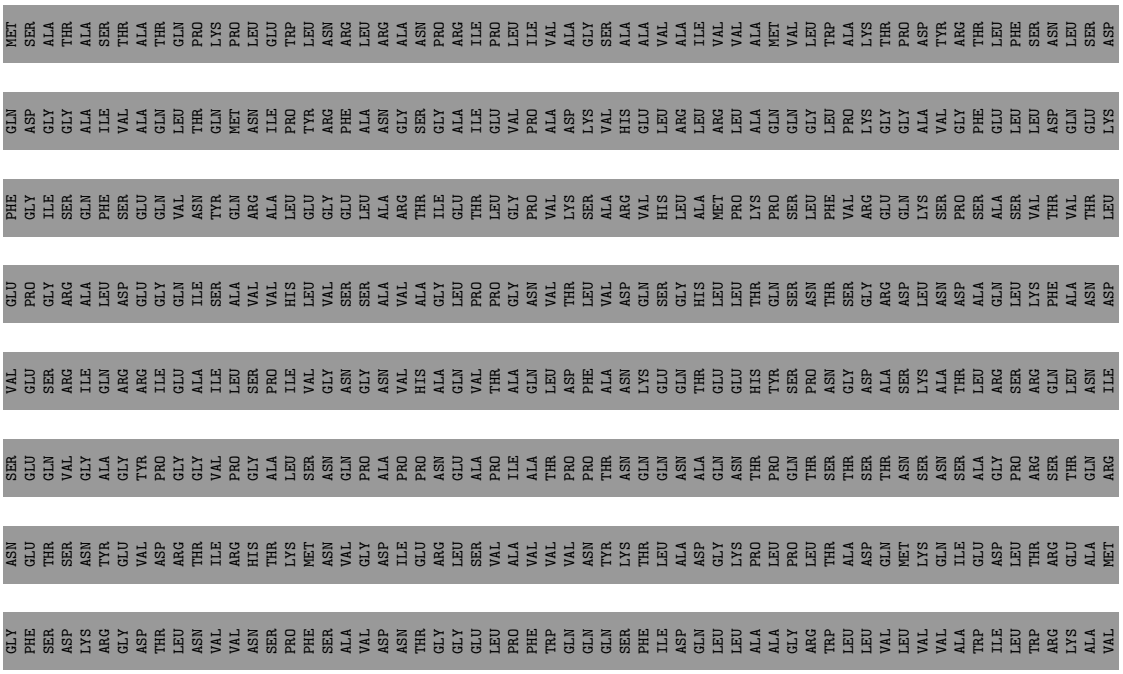


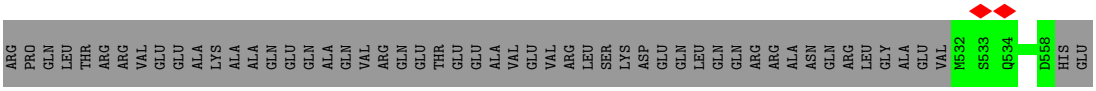



• Molecule 2: Flagellar M-ring protein

Chain CZ:

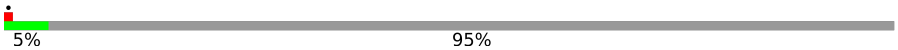


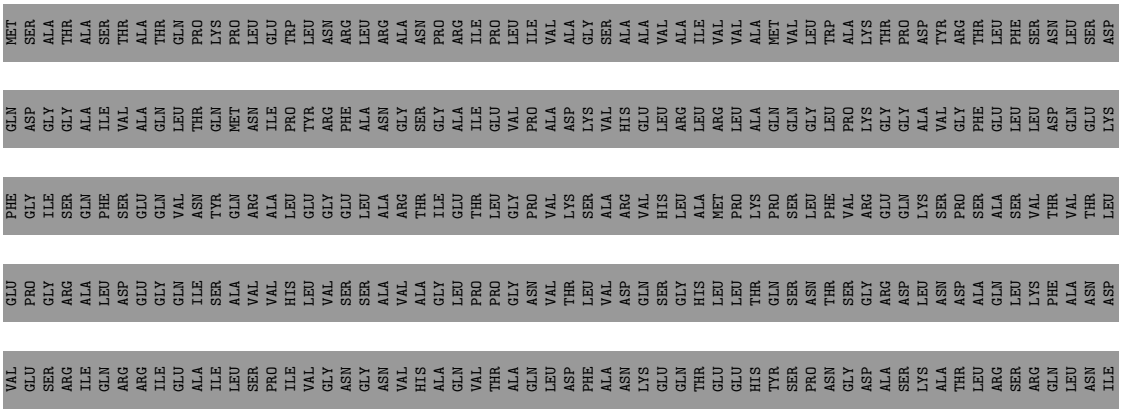



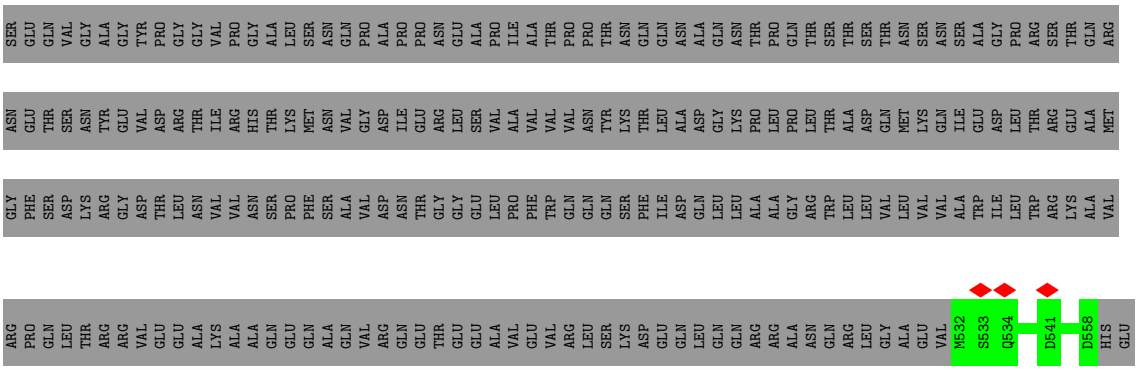




• Molecule 2: Flagellar M-ring protein

Chain Cf:

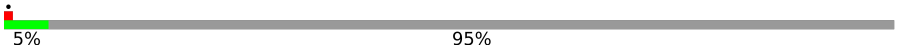


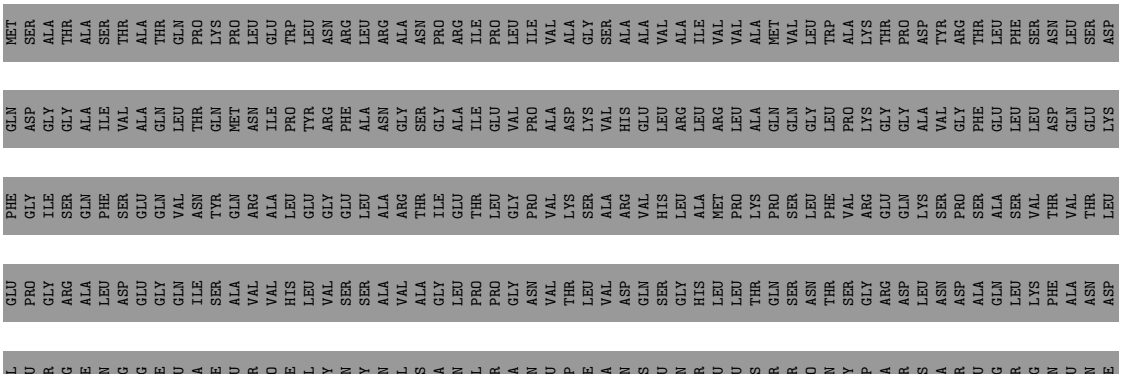






• Molecule 2: Flagellar M-ring protein

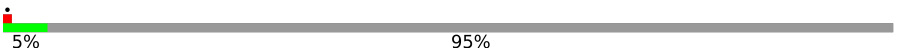
Chain Cl:

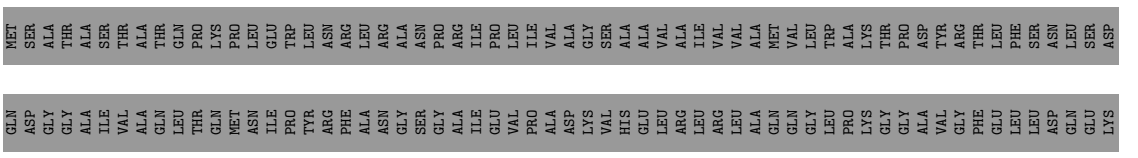



• Molecule 2: Flagellar M-ring protein

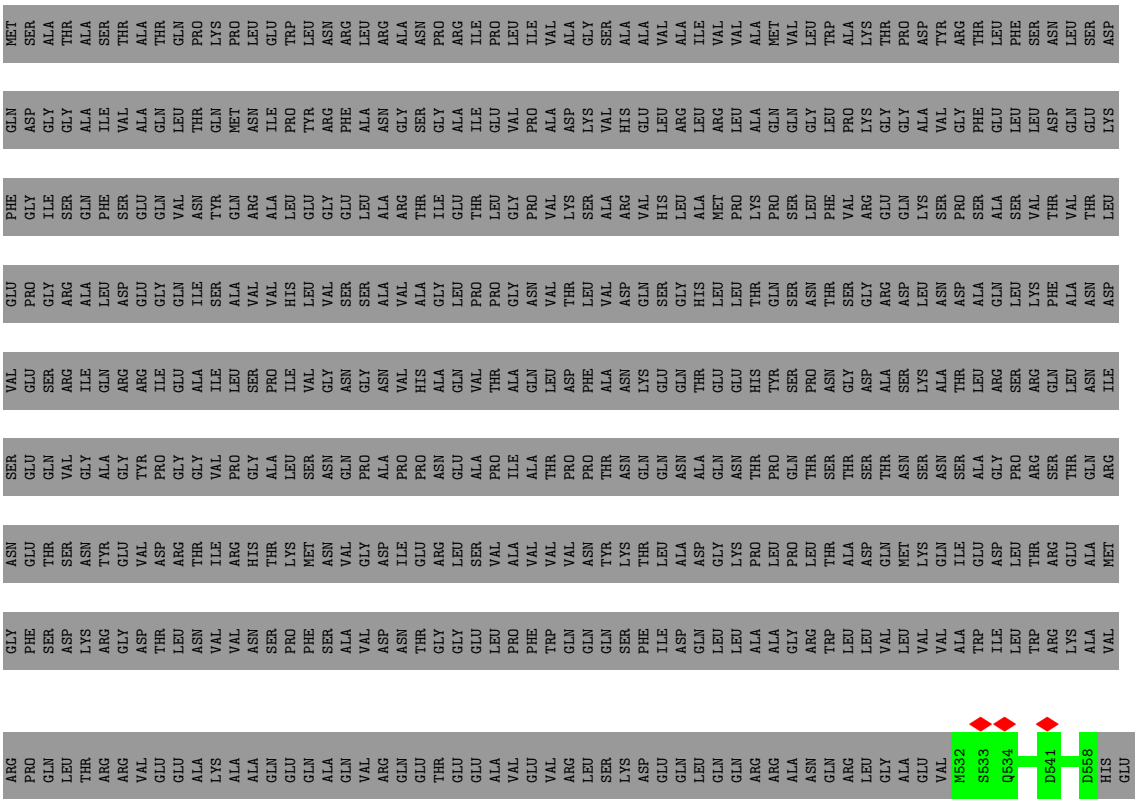
Chain Cr:



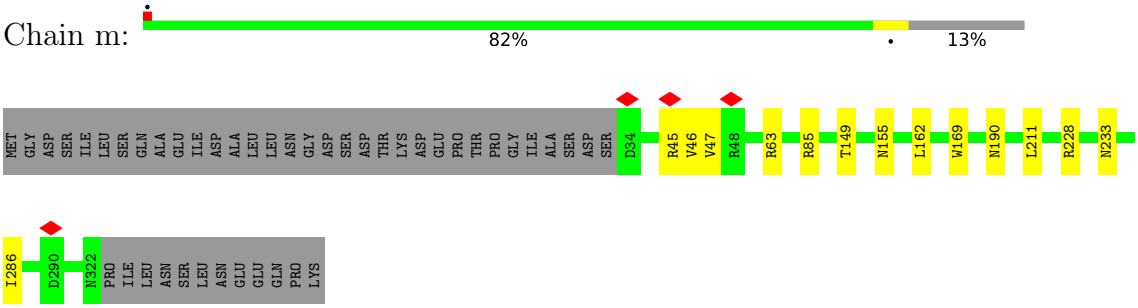
• Molecule 2: Flagellar M-ring protein

Chain Cx: 5% 95%



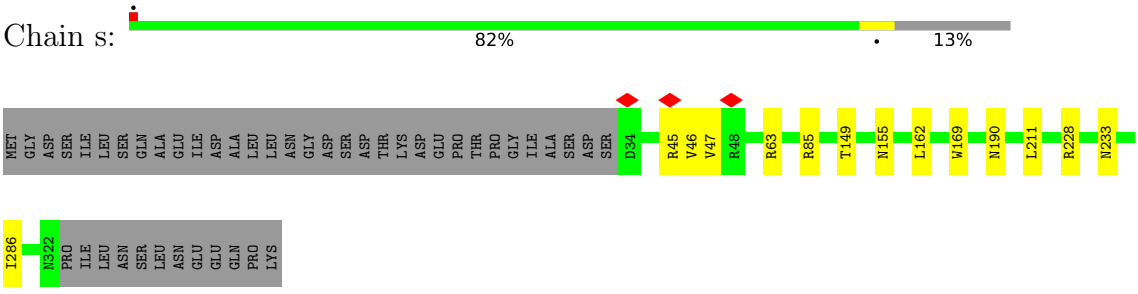

• Molecule 3: Flagellar motor switch protein FliM

Chain m:



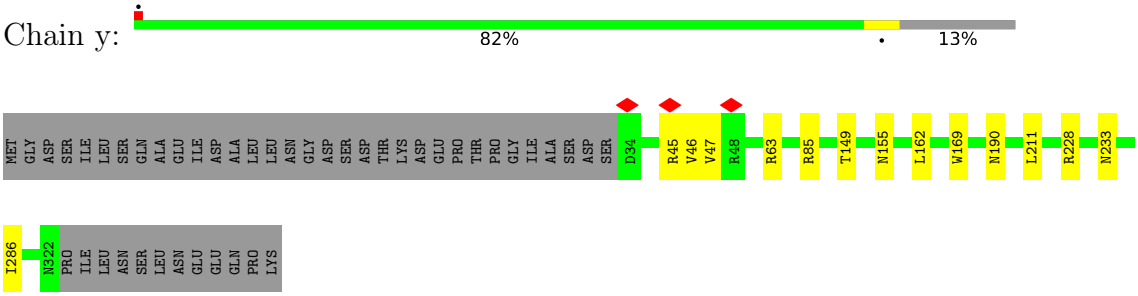

• Molecule 3: Flagellar motor switch protein FliM

Chain s:



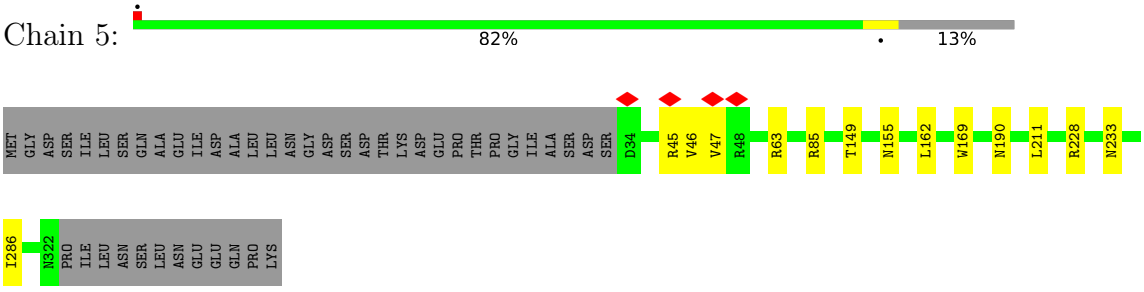

• Molecule 3: Flagellar motor switch protein FliM

Chain y:



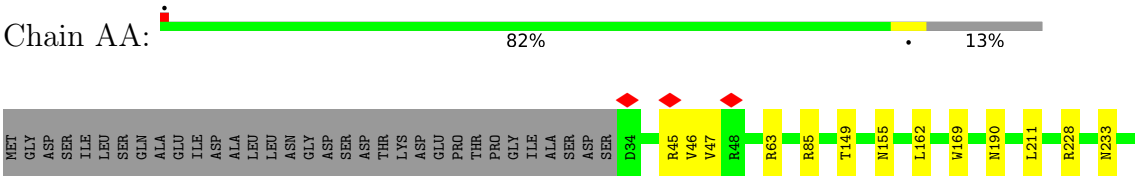

• Molecule 3: Flagellar motor switch protein FliM

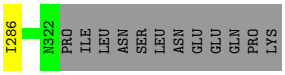
Chain 5:




• Molecule 3: Flagellar motor switch protein FliM

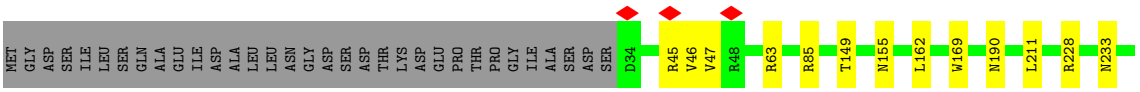
Chain AA:

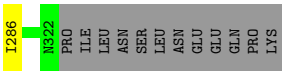





• Molecule 3: Flagellar motor switch protein FliM

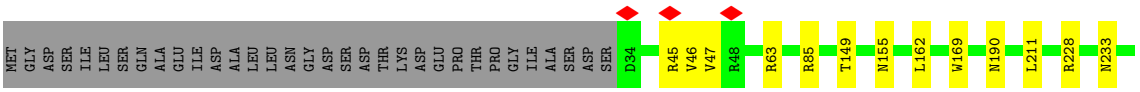
Chain AG:

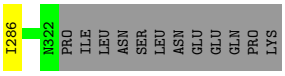



• Molecule 3: Flagellar motor switch protein FliM

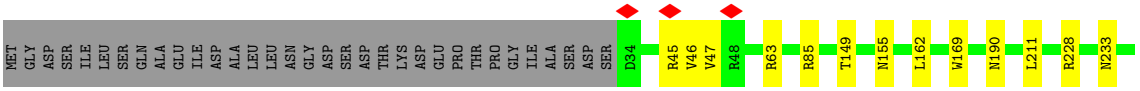
Chain AM:

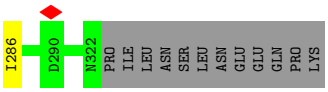



• Molecule 3: Flagellar motor switch protein FliM

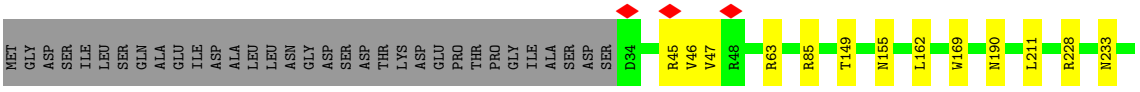
Chain AS:

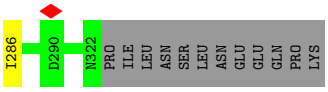



• Molecule 3: Flagellar motor switch protein FliM

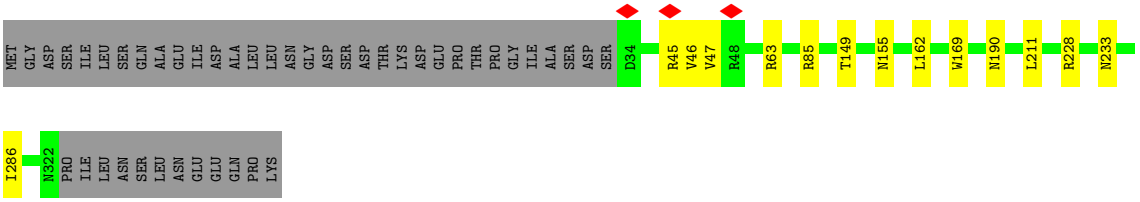
Chain AY:



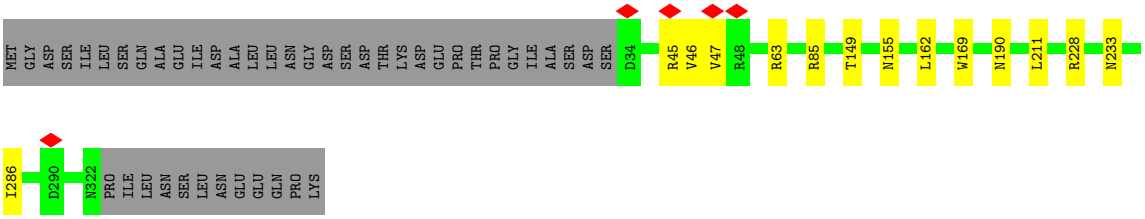

• Molecule 3: Flagellar motor switch protein FliM

Chain Ae:



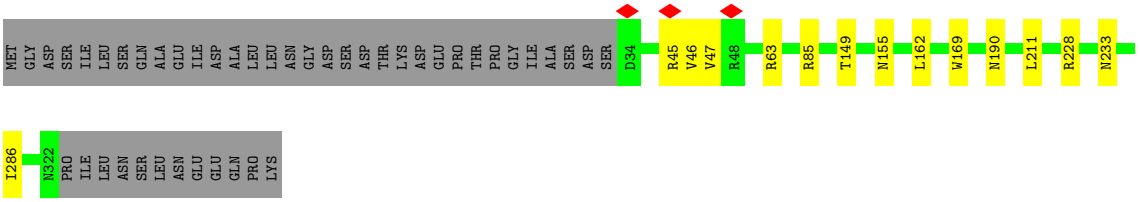

• Molecule 3: Flagellar motor switch protein FliM

Chain Ak:



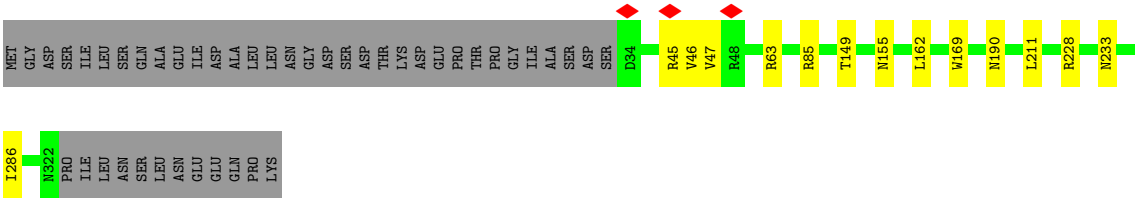

• Molecule 3: Flagellar motor switch protein FliM

Chain Aq:



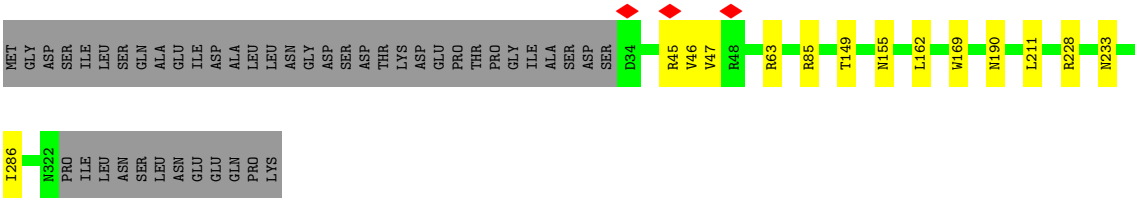

• Molecule 3: Flagellar motor switch protein FliM

Chain Aw:



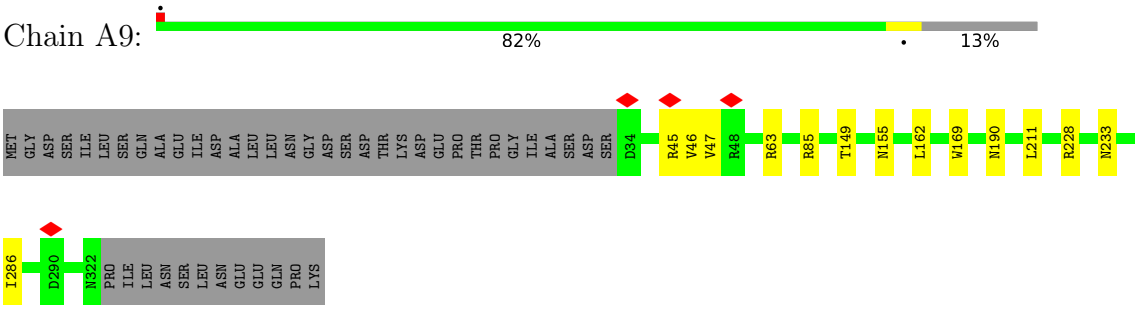

• Molecule 3: Flagellar motor switch protein FliM

Chain A3:



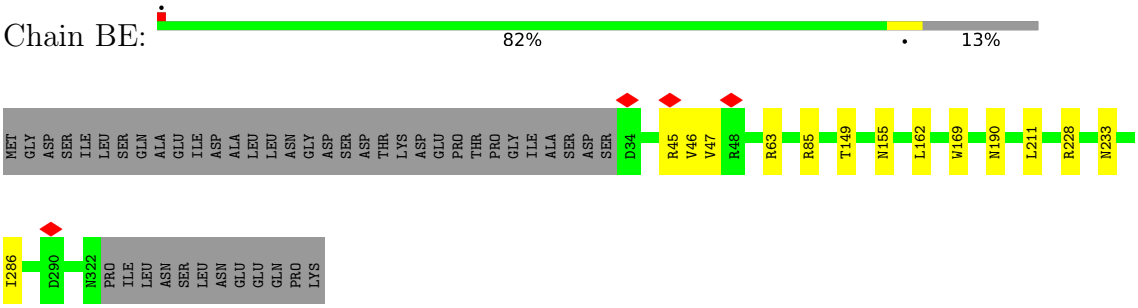
• Molecule 3: Flagellar motor switch protein FliM

Chain A9:



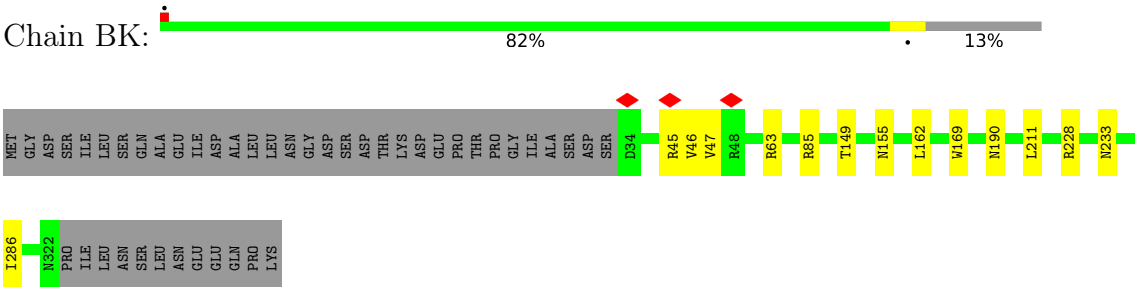

• Molecule 3: Flagellar motor switch protein FliM

Chain BE:



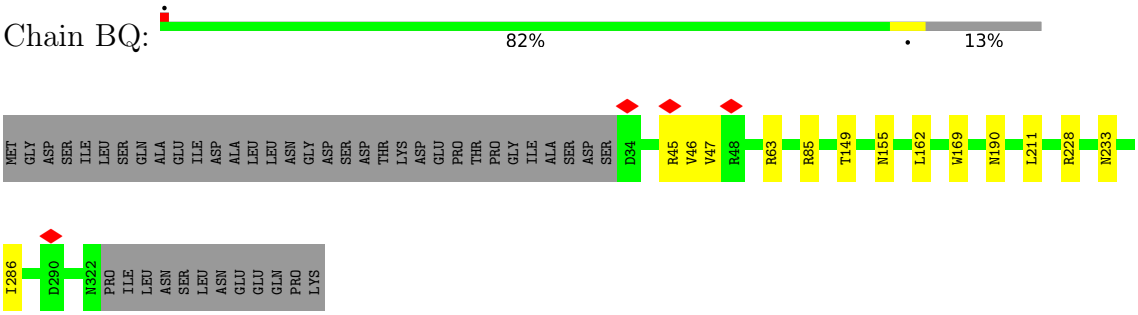

• Molecule 3: Flagellar motor switch protein FliM

Chain BK:



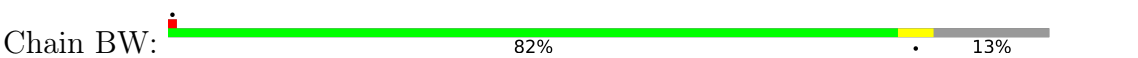

• Molecule 3: Flagellar motor switch protein FliM

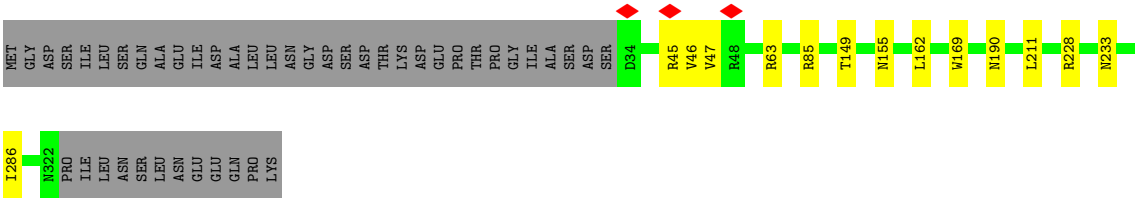
Chain BQ:




• Molecule 3: Flagellar motor switch protein FliM

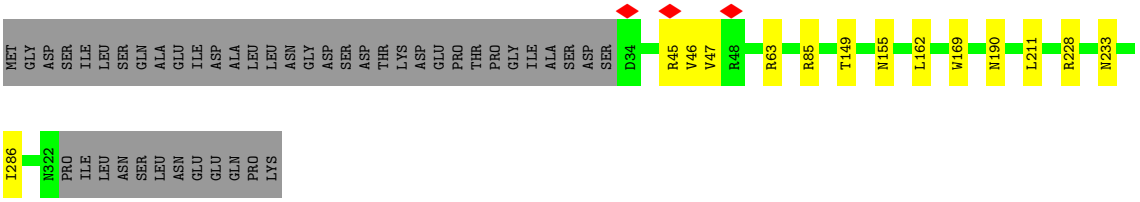
Chain BW:






• Molecule 3: Flagellar motor switch protein FliM

Chain Bc:

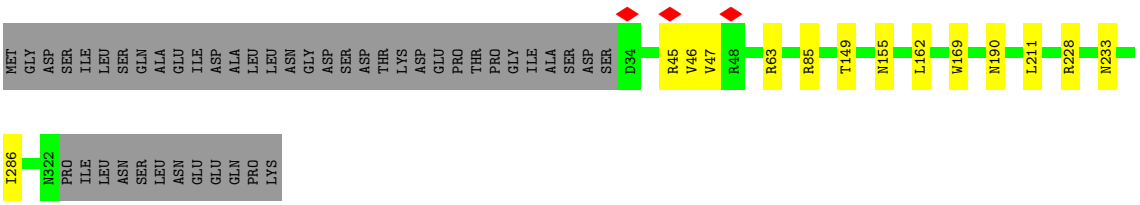



• Molecule 3: Flagellar motor switch protein FliM

Chain Bi:

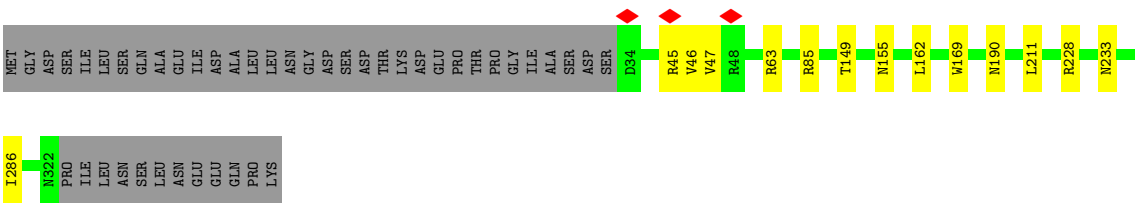
• Molecule 3: Flagellar motor switch protein FliM

Chain Bo:



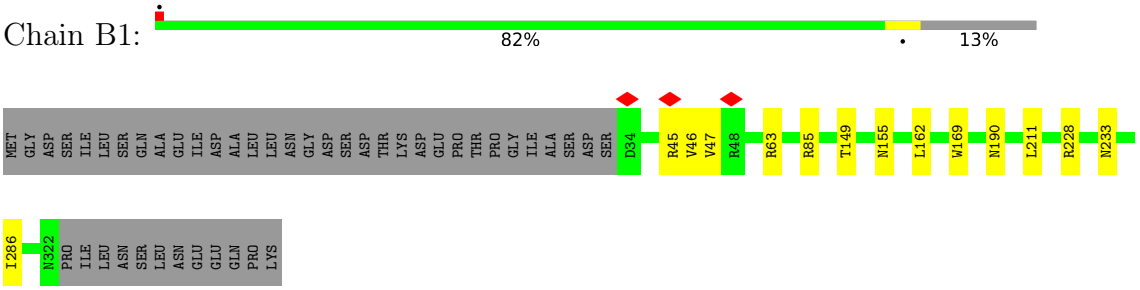

• Molecule 3: Flagellar motor switch protein FliM

Chain Bu:



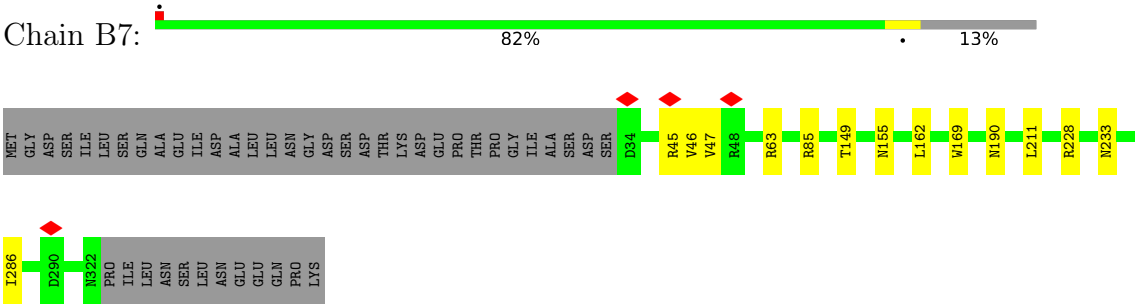

• Molecule 3: Flagellar motor switch protein FliM

Chain B1:



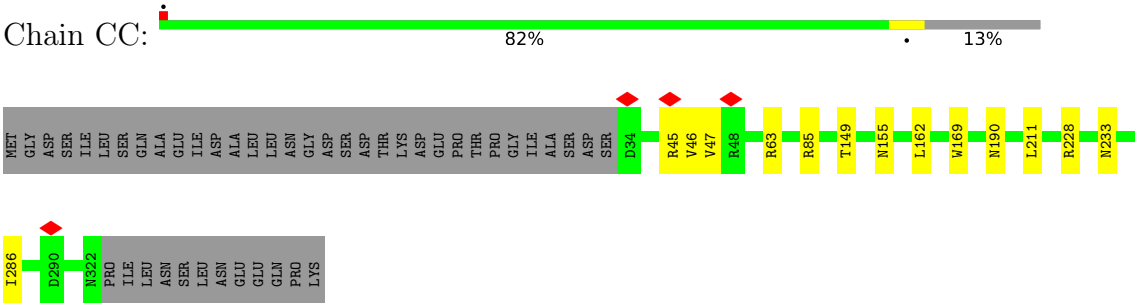

• Molecule 3: Flagellar motor switch protein FliM

Chain B7:



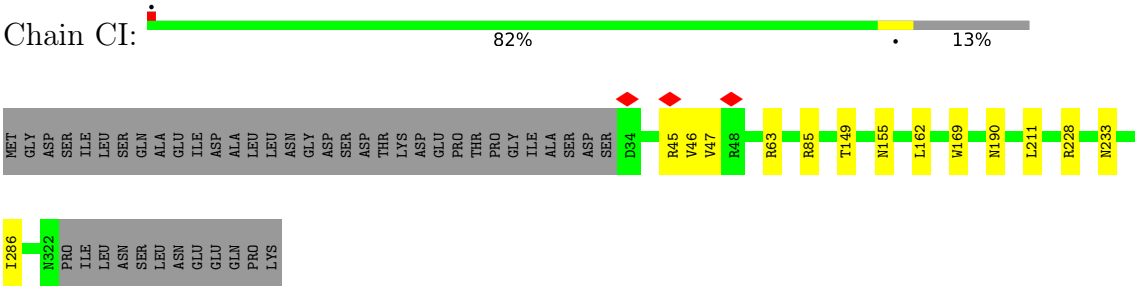

• Molecule 3: Flagellar motor switch protein FliM

Chain CC:



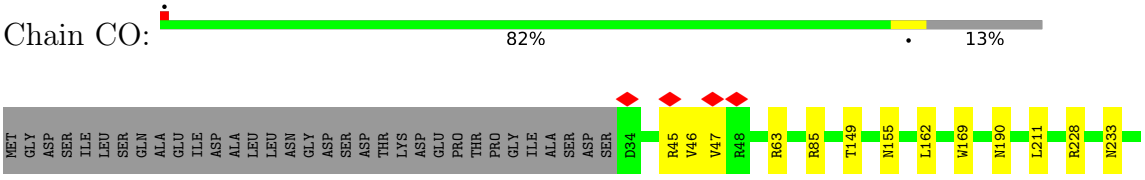

• Molecule 3: Flagellar motor switch protein FliM

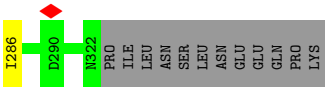
Chain CI:




• Molecule 3: Flagellar motor switch protein FliM

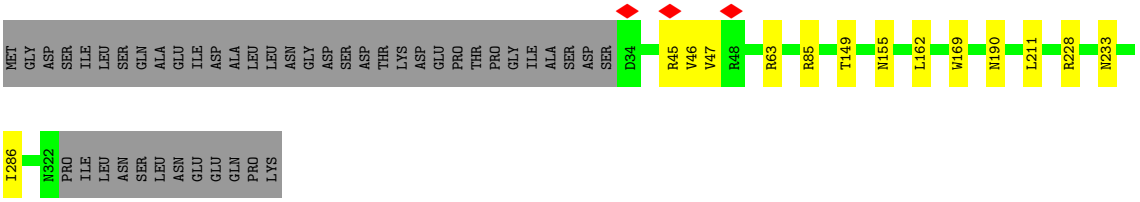
Chain CO:





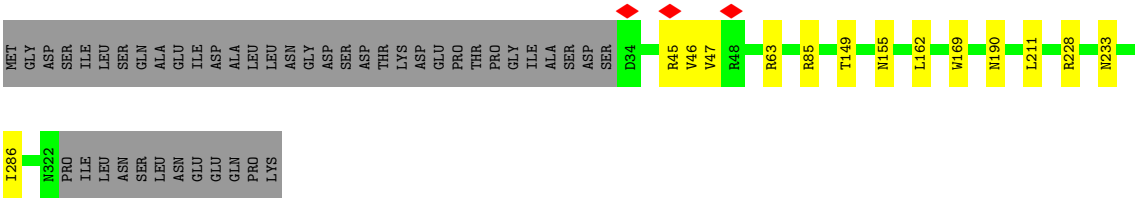

• Molecule 3: Flagellar motor switch protein FliM

Chain CU:



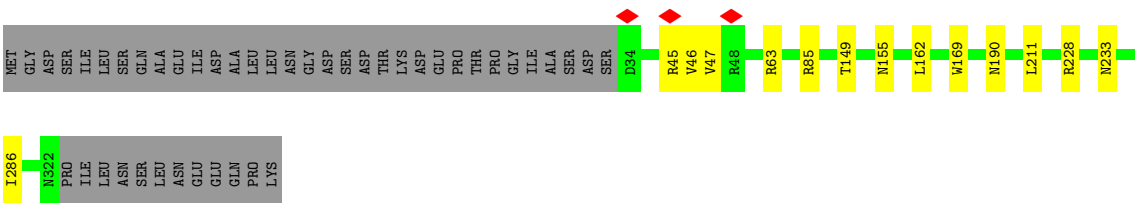

• Molecule 3: Flagellar motor switch protein FliM

Chain Ca:



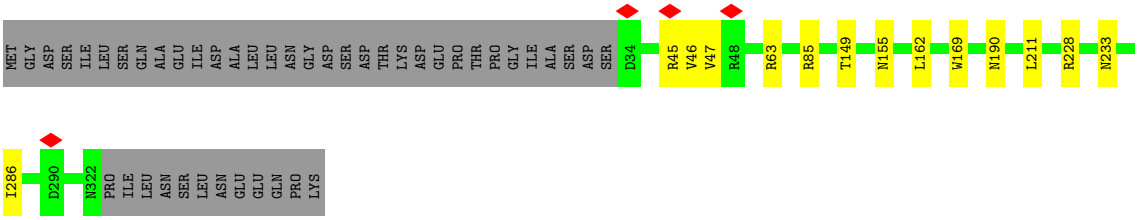

• Molecule 3: Flagellar motor switch protein FliM

Chain Cg:



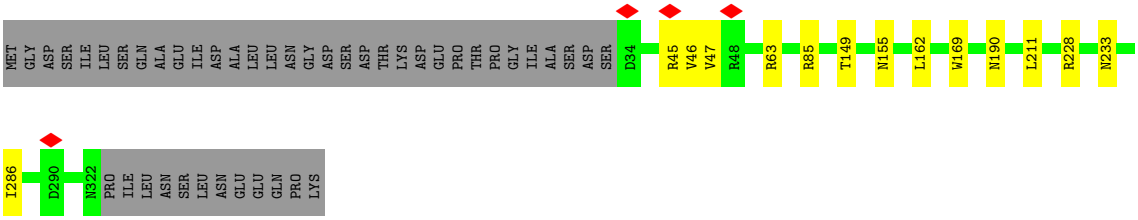

• Molecule 3: Flagellar motor switch protein FliM

Chain Cm:



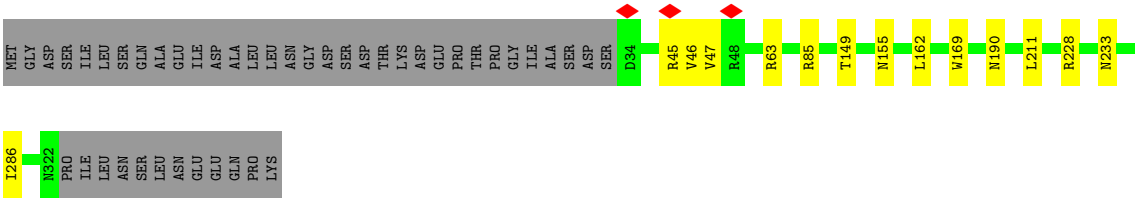

• Molecule 3: Flagellar motor switch protein FliM

Chain Cs:



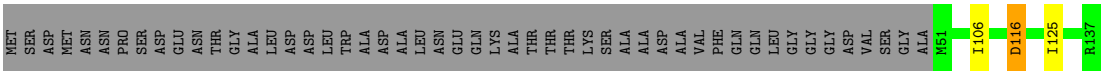

• Molecule 3: Flagellar motor switch protein FliM

Chain Cy:



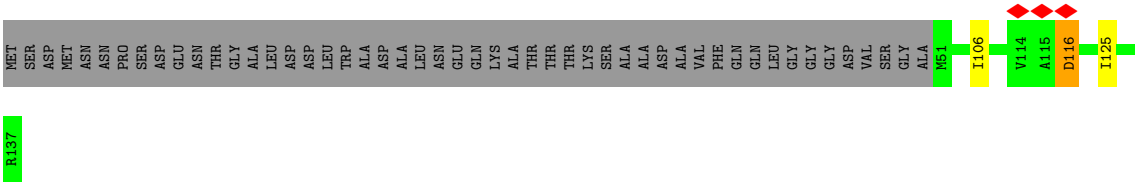

• Molecule 4: Flagellar motor switch protein FliN

Chain n:



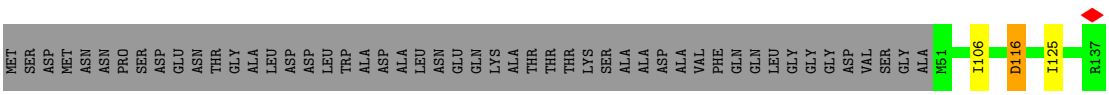

• Molecule 4: Flagellar motor switch protein FliN

Chain o:



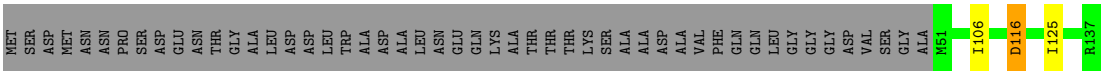

• Molecule 4: Flagellar motor switch protein FliN

Chain p:



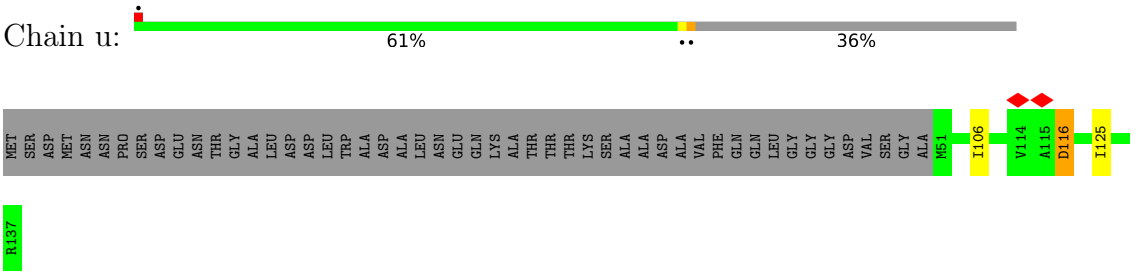

• Molecule 4: Flagellar motor switch protein FliN

Chain t:



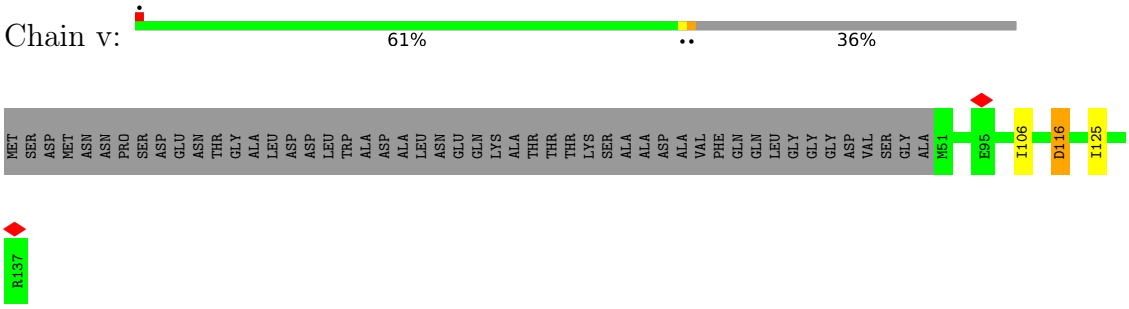
• Molecule 4: Flagellar motor switch protein FliN

Chain u:



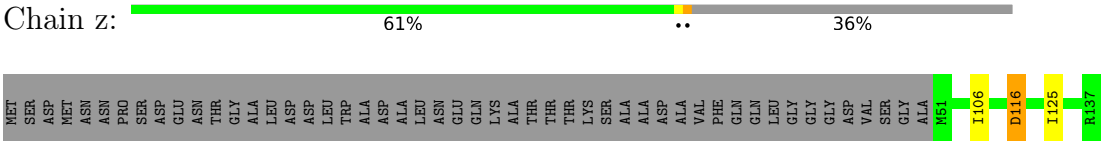

• Molecule 4: Flagellar motor switch protein FliN

Chain v:



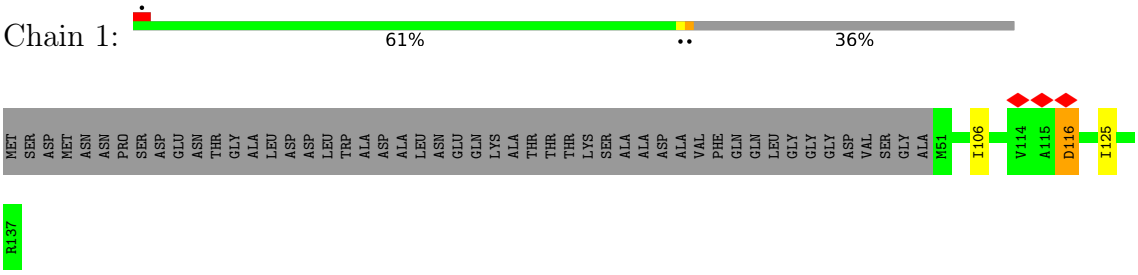

• Molecule 4: Flagellar motor switch protein FliN

Chain z:



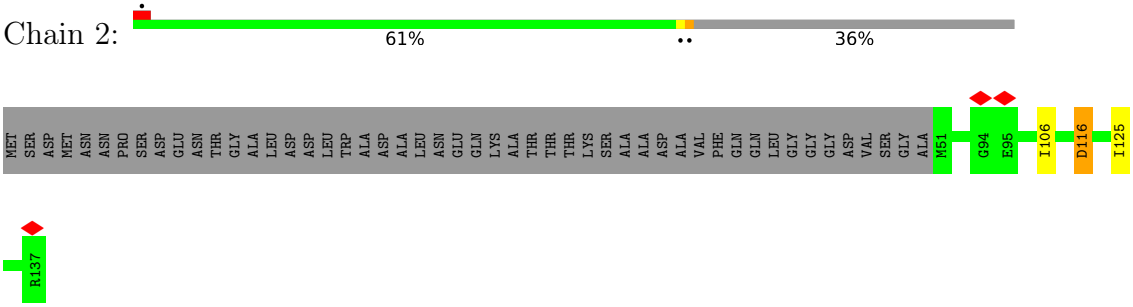

• Molecule 4: Flagellar motor switch protein FliN

Chain 1:



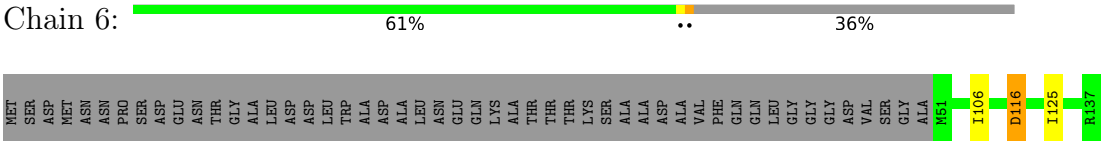

• Molecule 4: Flagellar motor switch protein FliN

Chain 2:



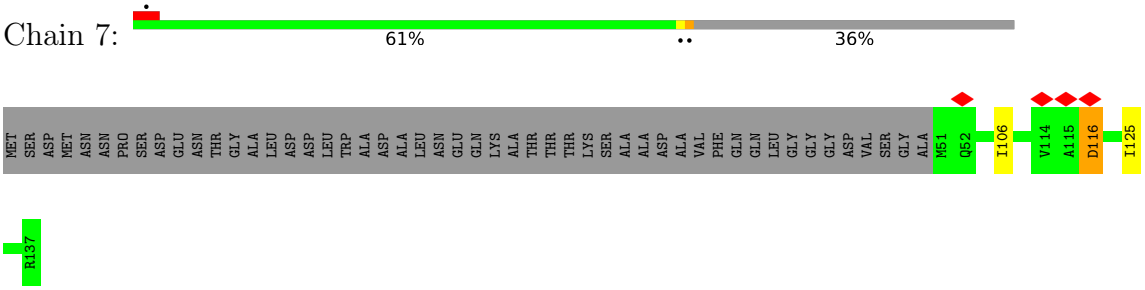
• Molecule 4: Flagellar motor switch protein FliN

Chain 6:



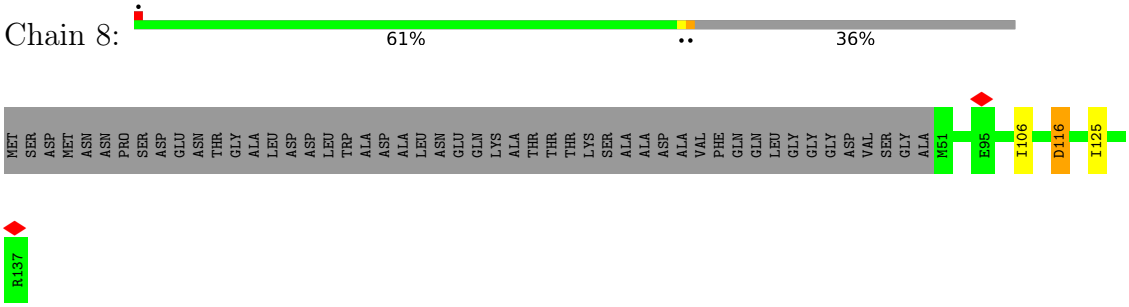

• Molecule 4: Flagellar motor switch protein FliN

Chain 7:



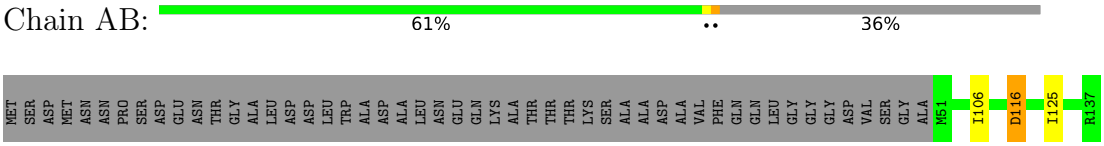

• Molecule 4: Flagellar motor switch protein FliN

Chain 8:



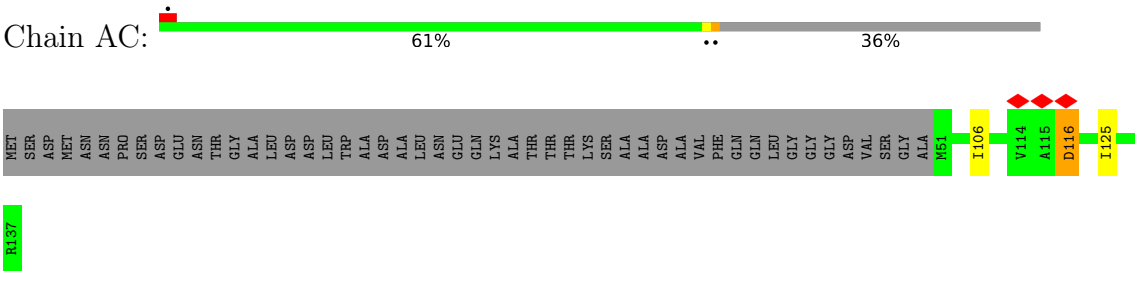

• Molecule 4: Flagellar motor switch protein FliN

Chain AB:



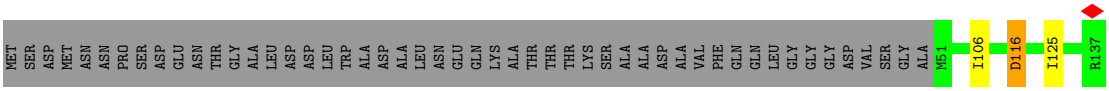

• Molecule 4: Flagellar motor switch protein FliN

Chain AC:

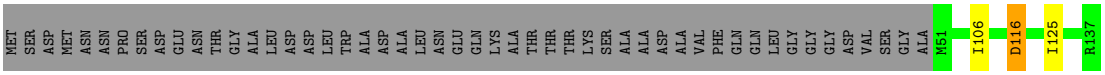



• Molecule 4: Flagellar motor switch protein FliN

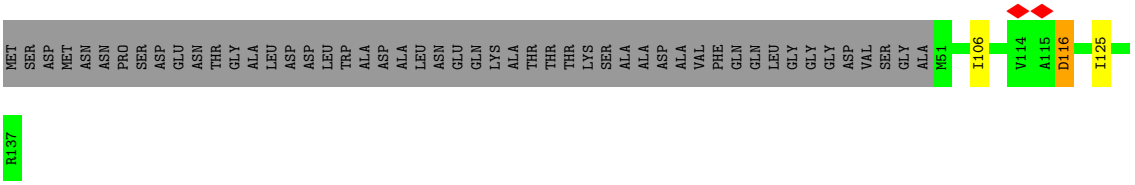
Chain AD:



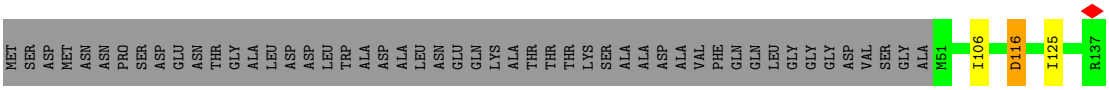

• Molecule 4: Flagellar motor switch protein FliN



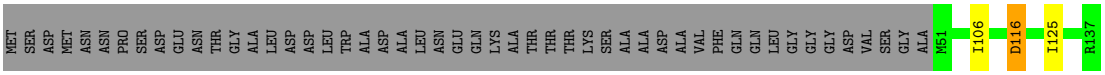

• Molecule 4: Flagellar motor switch protein FliN



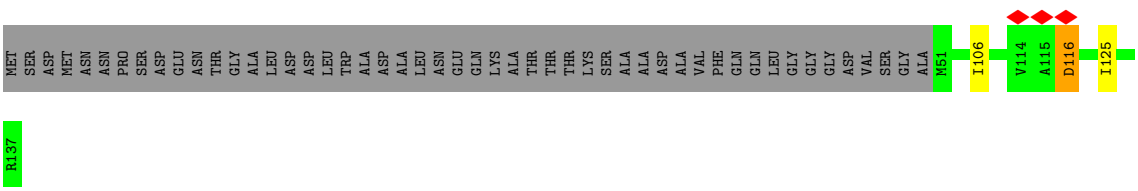

• Molecule 4: Flagellar motor switch protein FliN



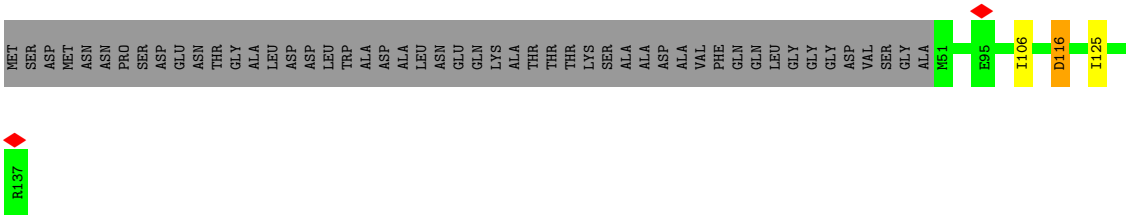

• Molecule 4: Flagellar motor switch protein FliN



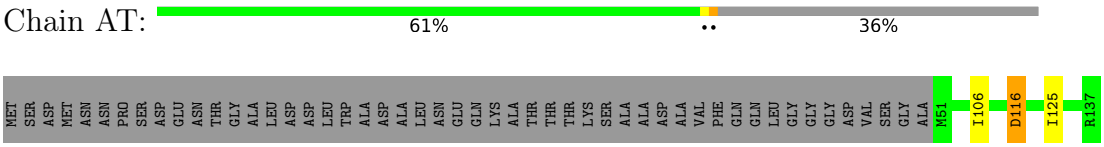

• Molecule 4: Flagellar motor switch protein FliN



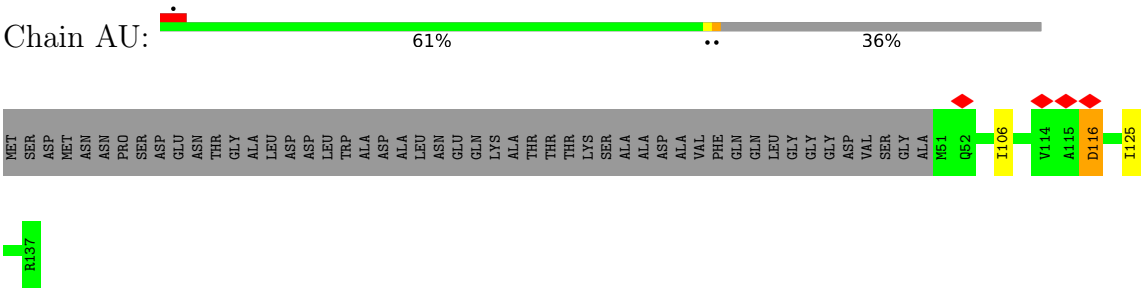

• Molecule 4: Flagellar motor switch protein FliN



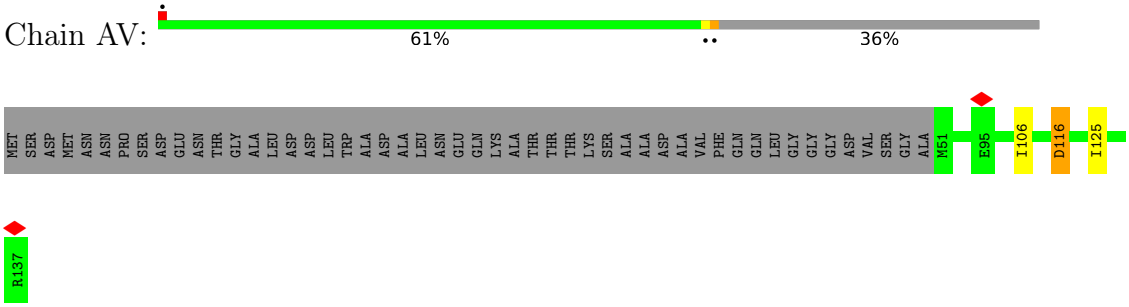

• Molecule 4: Flagellar motor switch protein FliN



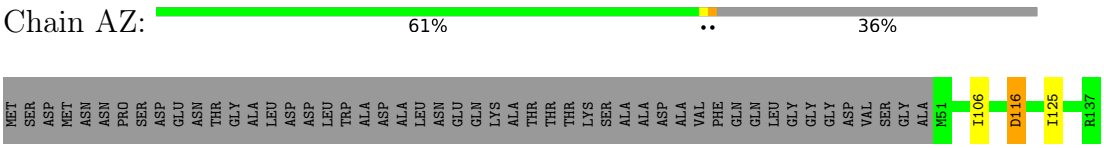

• Molecule 4: Flagellar motor switch protein FliN



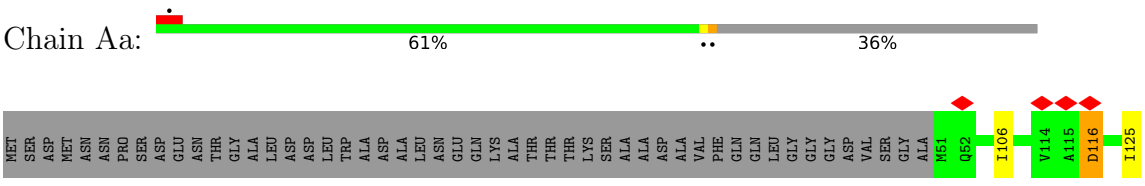

• Molecule 4: Flagellar motor switch protein FliN




• Molecule 4: Flagellar motor switch protein FliN

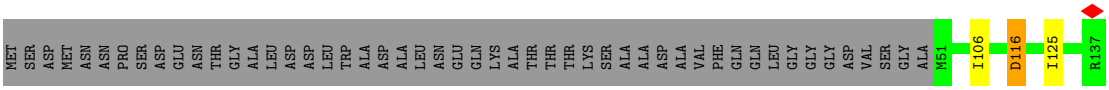



• Molecule 4: Flagellar motor switch protein FliN



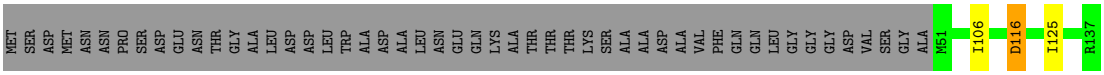
• Molecule 4: Flagellar motor switch protein FliN

Chain Ab:



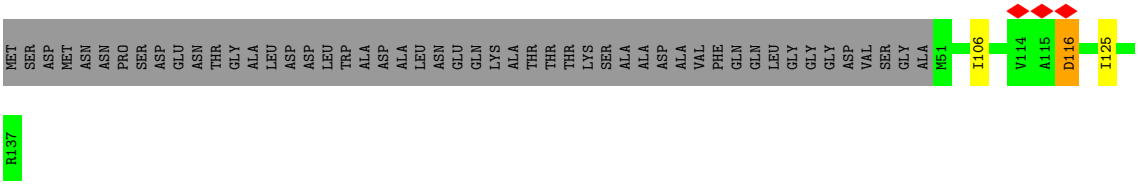

• Molecule 4: Flagellar motor switch protein FliN

Chain Af:



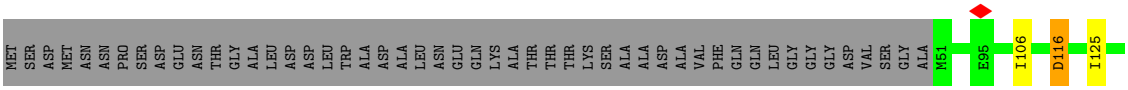

• Molecule 4: Flagellar motor switch protein FliN

Chain Ag:



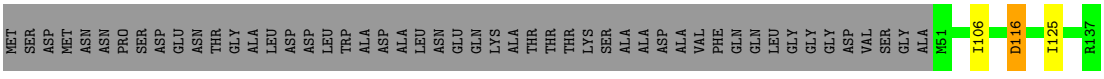

• Molecule 4: Flagellar motor switch protein FliN

Chain Ah:



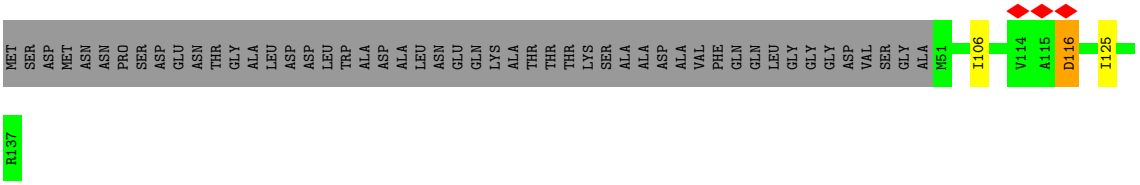

• Molecule 4: Flagellar motor switch protein FliN

Chain Al:



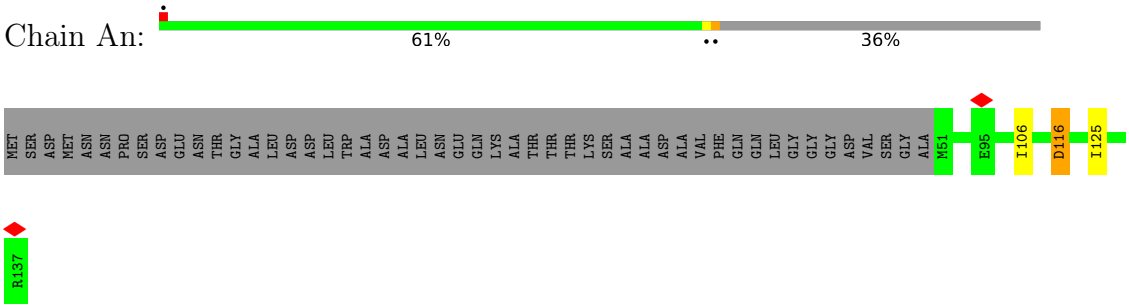

• Molecule 4: Flagellar motor switch protein FliN

Chain Am:



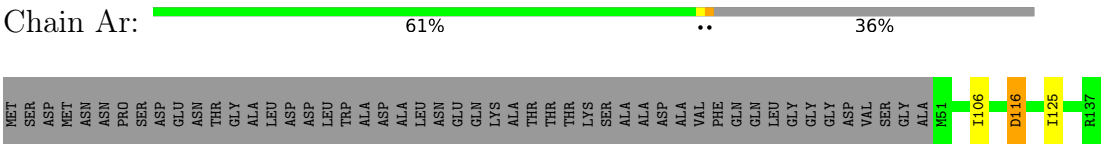

• Molecule 4: Flagellar motor switch protein FliN

Chain An:



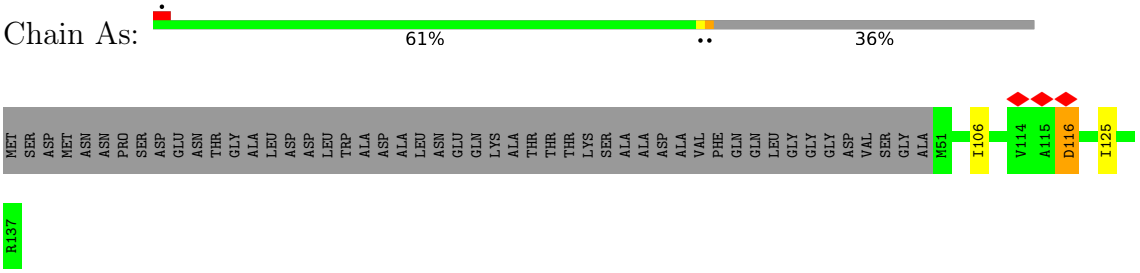

• Molecule 4: Flagellar motor switch protein FliN

Chain Ar:



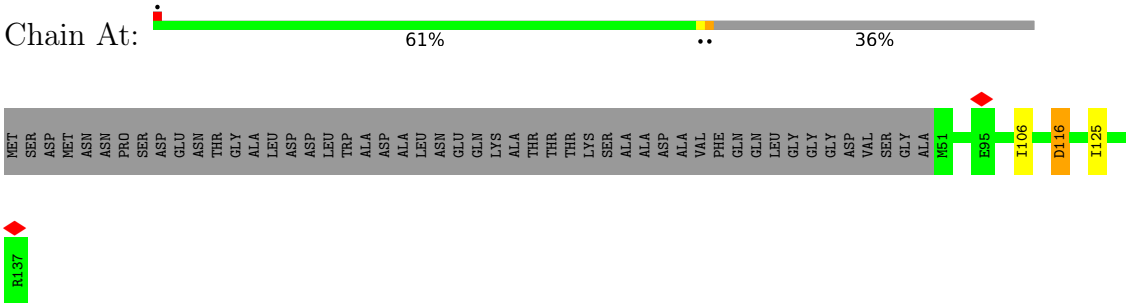

• Molecule 4: Flagellar motor switch protein FliN

Chain As:



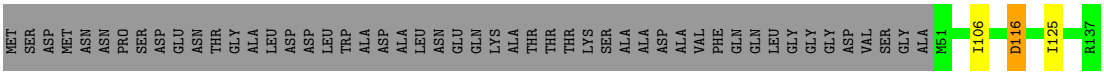

• Molecule 4: Flagellar motor switch protein FliN

Chain At:

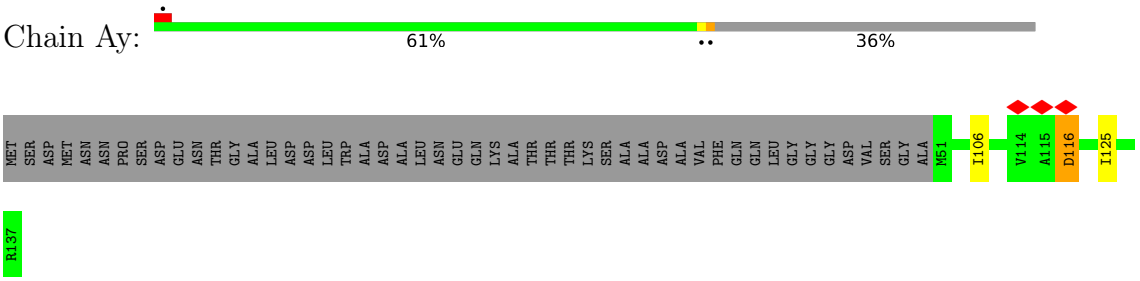



• Molecule 4: Flagellar motor switch protein FliN

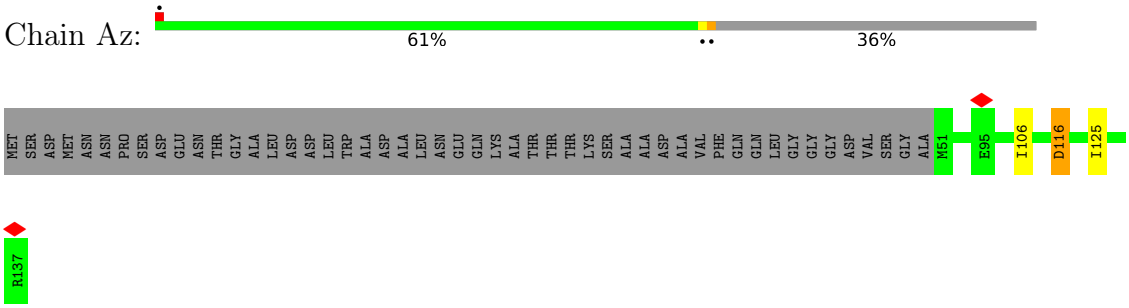
Chain Ax:




• Molecule 4: Flagellar motor switch protein FliN

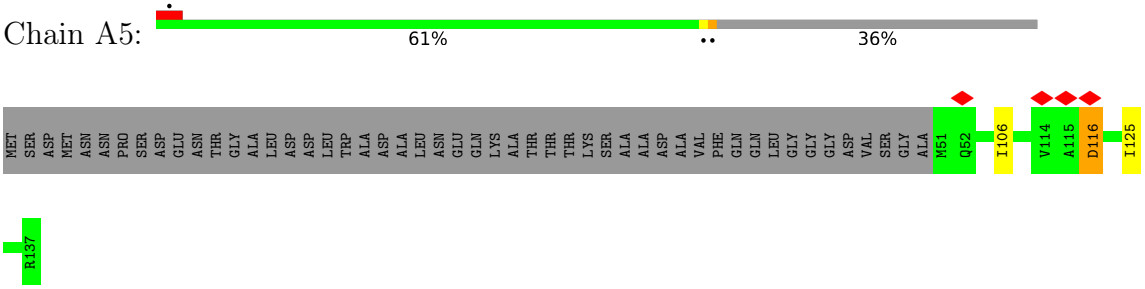



• Molecule 4: Flagellar motor switch protein FliN

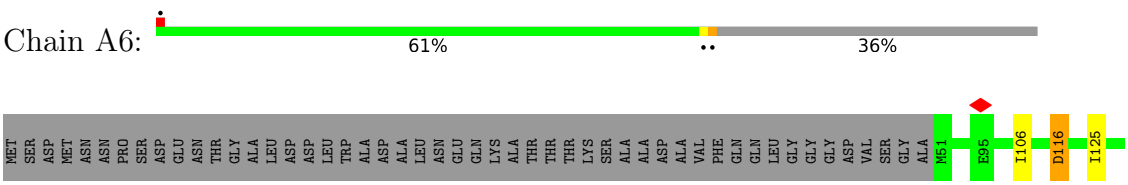



• Molecule 4: Flagellar motor switch protein FliN

• Molecule 4: Flagellar motor switch protein FliN

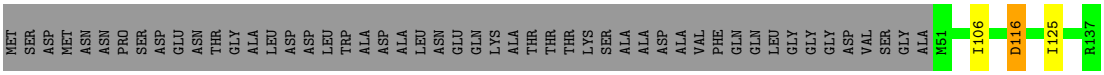



• Molecule 4: Flagellar motor switch protein FliN



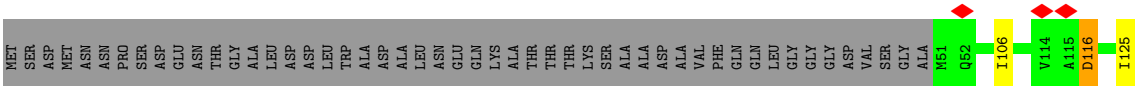
• Molecule 4: Flagellar motor switch protein FliN

Chain A0:



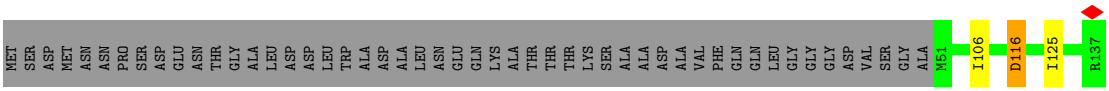

• Molecule 4: Flagellar motor switch protein FliN

Chain BA:



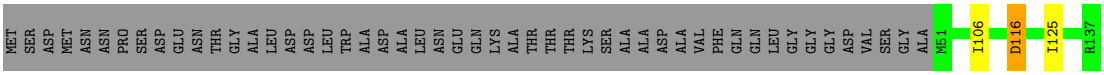
• Molecule 4: Flagellar motor switch protein FliN

Chain BB:



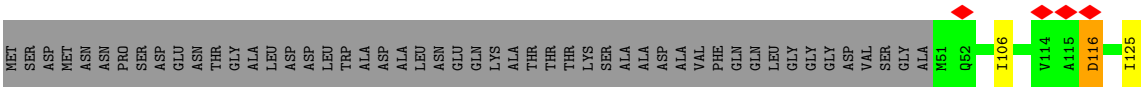

• Molecule 4: Flagellar motor switch protein FliN

Chain BF:



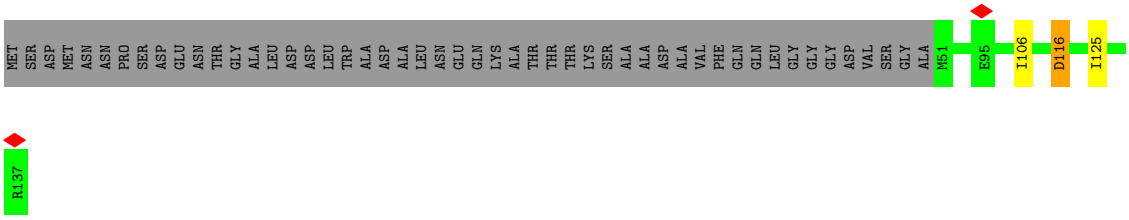

• Molecule 4: Flagellar motor switch protein FliN

Chain BG:

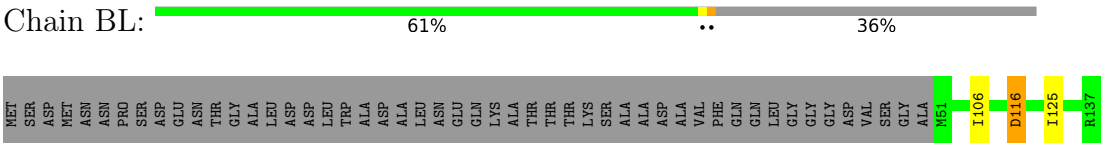


• Molecule 4: Flagellar motor switch protein FliN

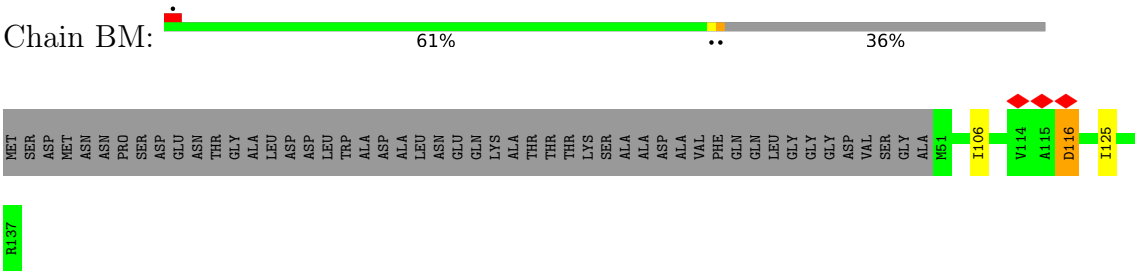
Chain BH:



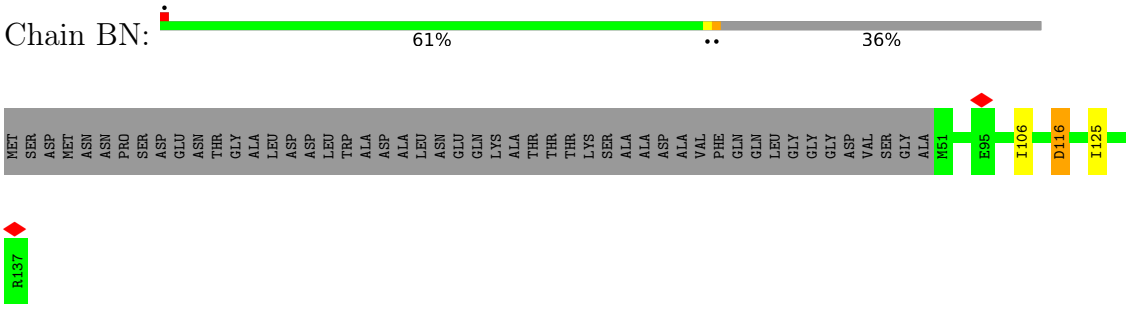

• Molecule 4: Flagellar motor switch protein FliN



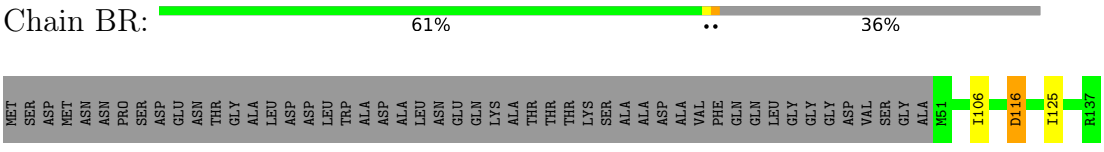

• Molecule 4: Flagellar motor switch protein FliN



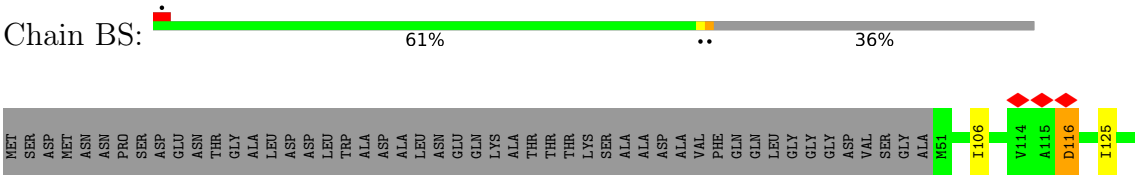

• Molecule 4: Flagellar motor switch protein FliN




• Molecule 4: Flagellar motor switch protein FliN

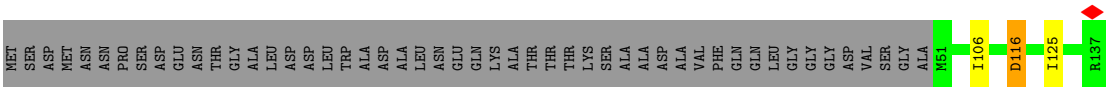



• Molecule 4: Flagellar motor switch protein FliN



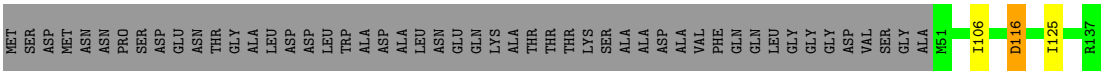
• Molecule 4: Flagellar motor switch protein FliN

Chain BT:



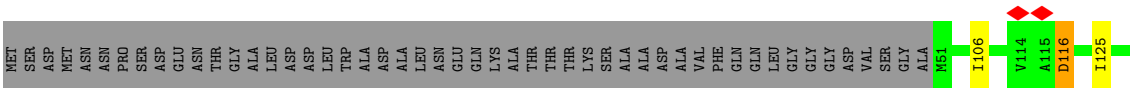

• Molecule 4: Flagellar motor switch protein FliN

Chain BX:



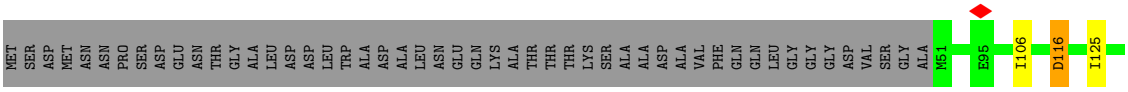

• Molecule 4: Flagellar motor switch protein FliN

Chain BY:



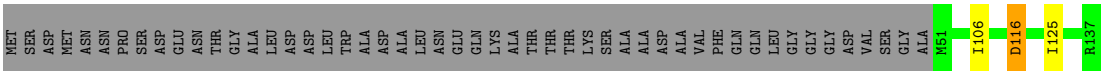
• Molecule 4: Flagellar motor switch protein FliN

Chain BZ:



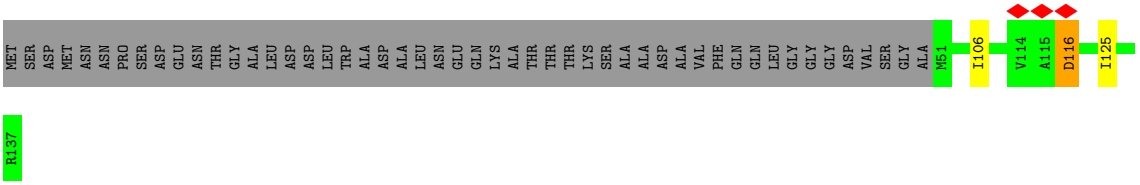
• Molecule 4: Flagellar motor switch protein FliN

Chain Bd:



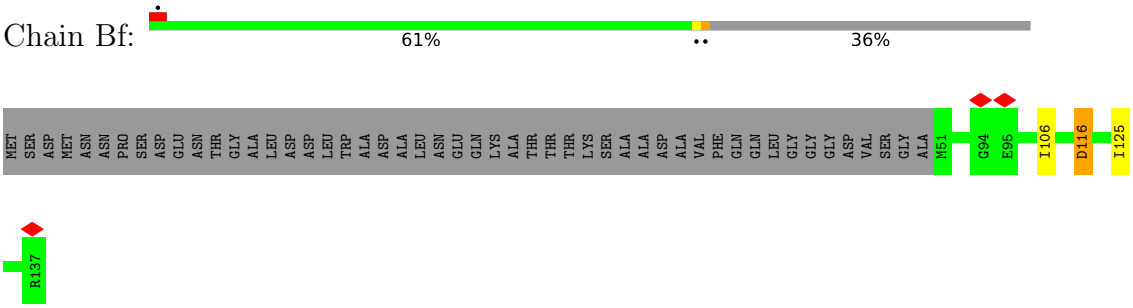

• Molecule 4: Flagellar motor switch protein FliN

Chain Be:



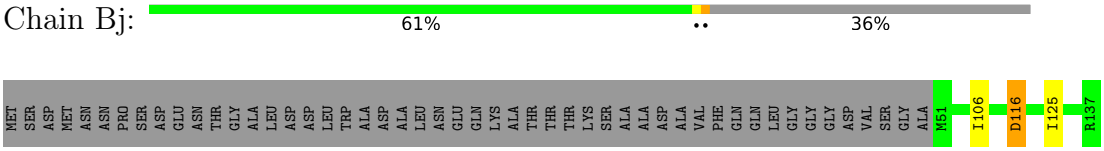

• Molecule 4: Flagellar motor switch protein FliN

Chain Bf:



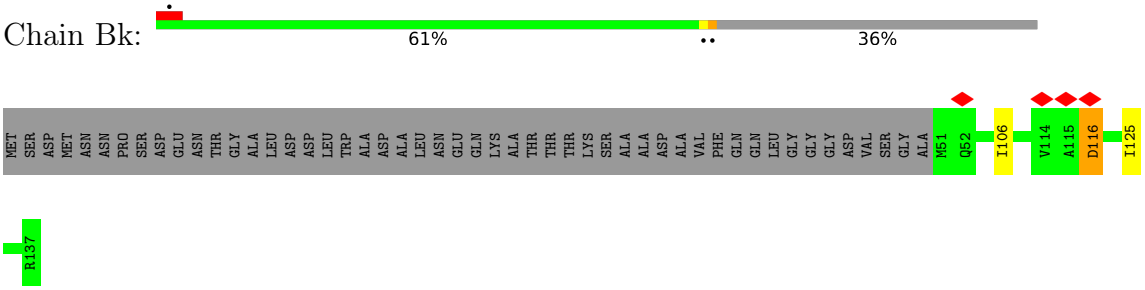

• Molecule 4: Flagellar motor switch protein FliN

Chain Bj:



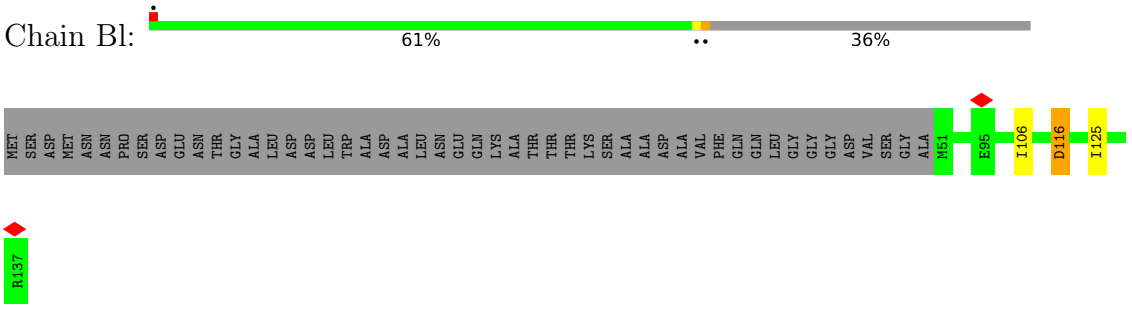

• Molecule 4: Flagellar motor switch protein FliN

Chain Bk:



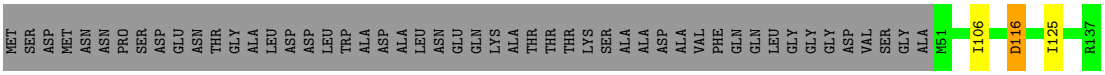

• Molecule 4: Flagellar motor switch protein FliN

Chain Bl:



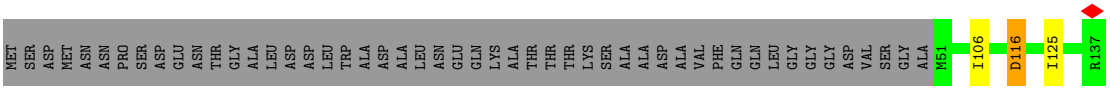

• Molecule 4: Flagellar motor switch protein FliN

Chain Bp:

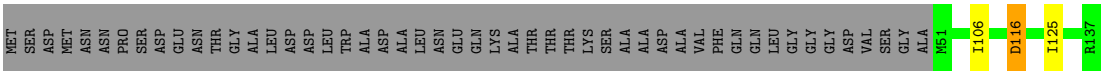



• Molecule 4: Flagellar motor switch protein FliN

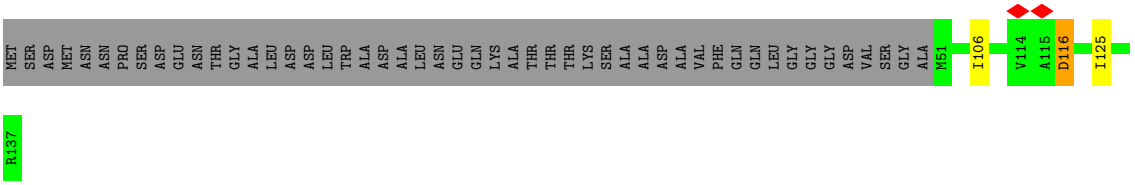
• Molecule 4: Flagellar motor switch protein FliN



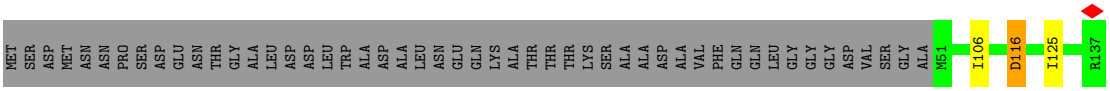

• Molecule 4: Flagellar motor switch protein FliN



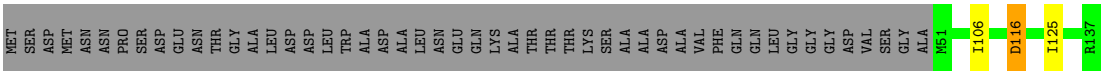

• Molecule 4: Flagellar motor switch protein FliN




• Molecule 4: Flagellar motor switch protein FliN

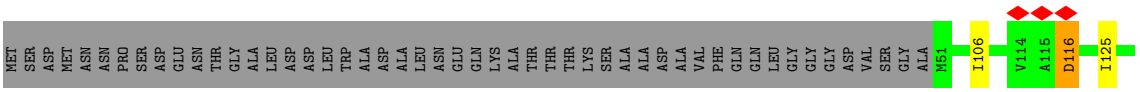



• Molecule 4: Flagellar motor switch protein FliN



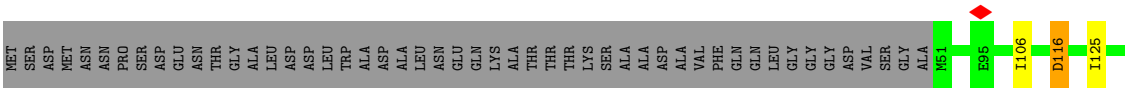

• Molecule 4: Flagellar motor switch protein FliN

Chain B3:



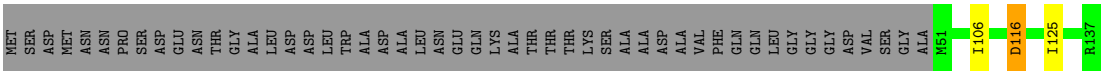

• Molecule 4: Flagellar motor switch protein FliN

Chain B4:



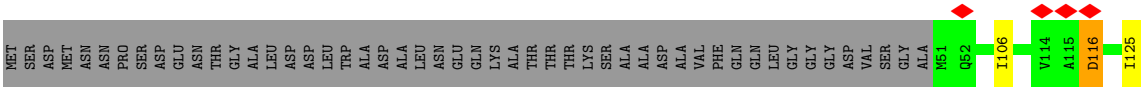

• Molecule 4: Flagellar motor switch protein FliN

Chain B8:



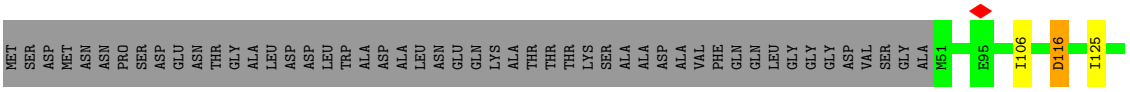

• Molecule 4: Flagellar motor switch protein FliN

Chain B9:



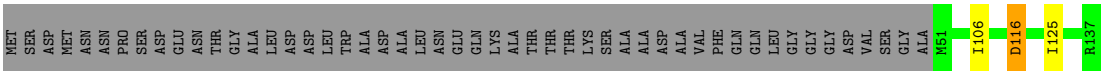

• Molecule 4: Flagellar motor switch protein FliN

Chain B0:



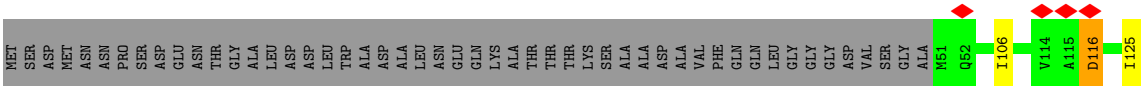
• Molecule 4: Flagellar motor switch protein FliN

Chain CD:



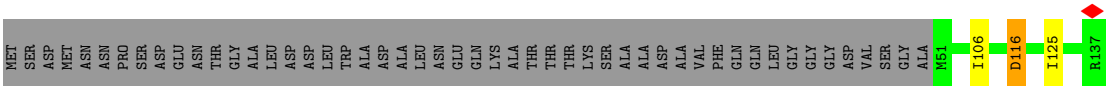

• Molecule 4: Flagellar motor switch protein FliN

Chain CE:



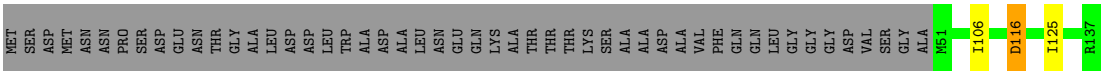
• Molecule 4: Flagellar motor switch protein FliN

Chain CF:



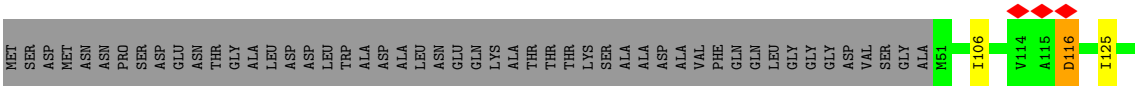

• Molecule 4: Flagellar motor switch protein FliN

Chain CJ:



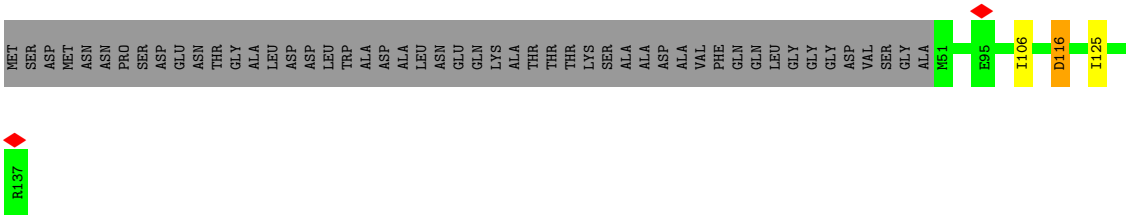

• Molecule 4: Flagellar motor switch protein FliN

Chain CK:



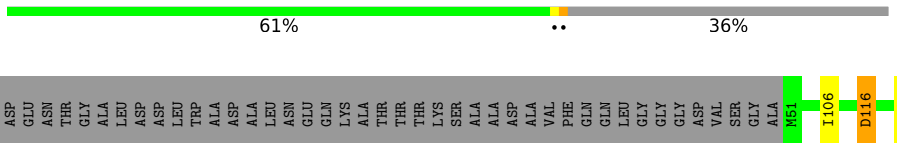
• Molecule 4: Flagellar motor switch protein FliN

Chain CL:



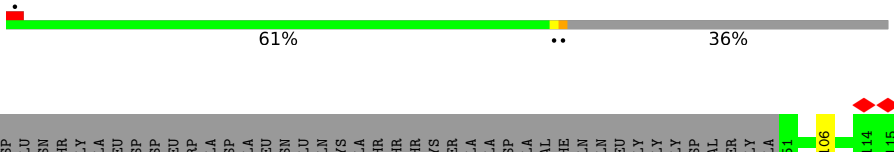

• Molecule 4: Flagellar motor switch protein FliN

Chain CP:



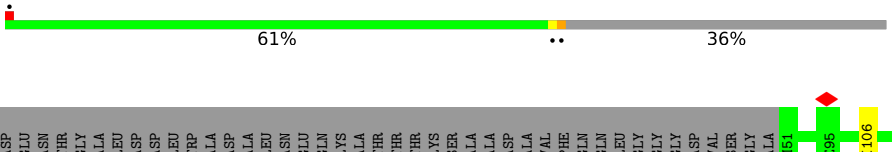

• Molecule 4: Flagellar motor switch protein FliN

Chain CQ:



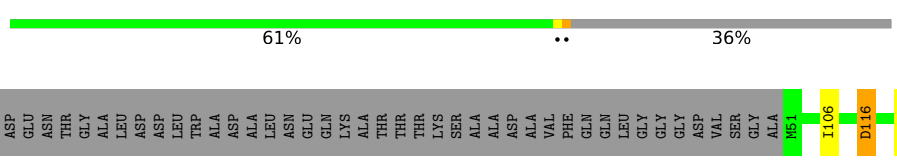

• Molecule 4: Flagellar motor switch protein FliN

Chain CR:



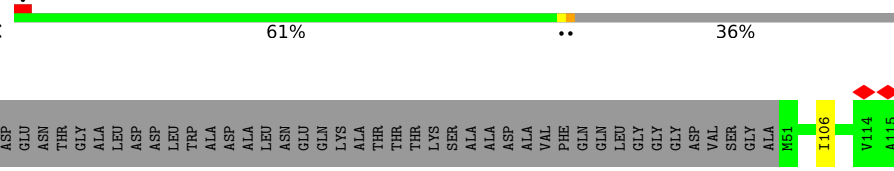

• Molecule 4: Flagellar motor switch protein FliN

Chain CV:



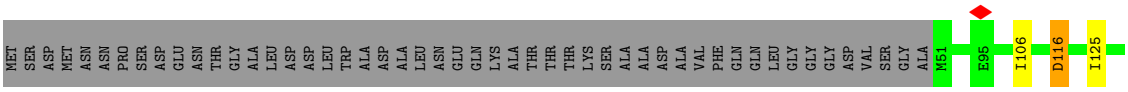

• Molecule 4: Flagellar motor switch protein FliN

Chain CW:



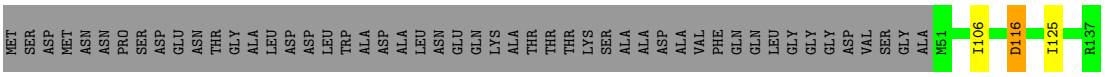
• Molecule 4: Flagellar motor switch protein FliN

Chain CX:



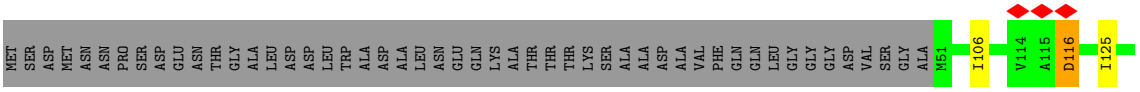
• Molecule 4: Flagellar motor switch protein FliN

Chain Cb:



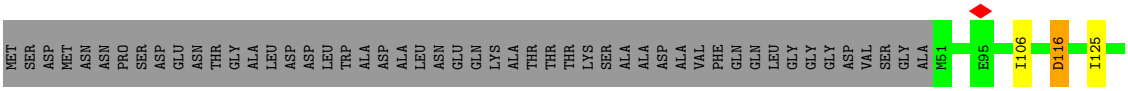

• Molecule 4: Flagellar motor switch protein FliN

Chain Cc:



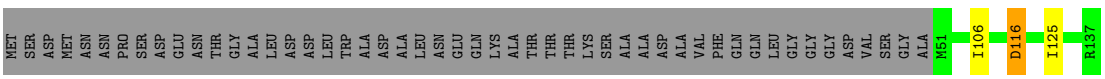
• Molecule 4: Flagellar motor switch protein FliN

Chain Cd:



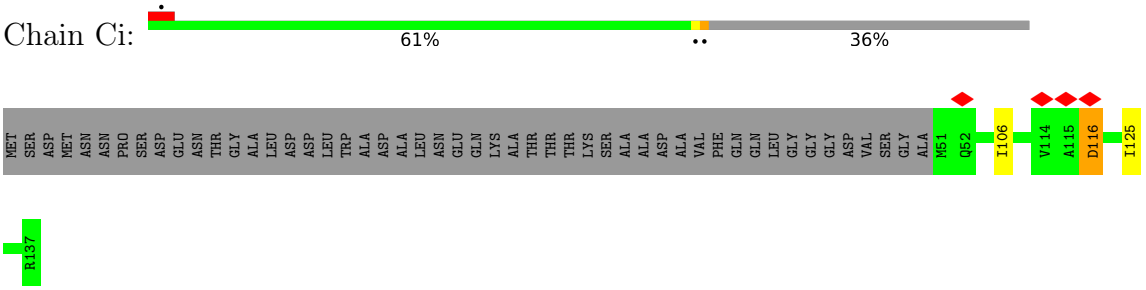
• Molecule 4: Flagellar motor switch protein FliN

Chain Ch:



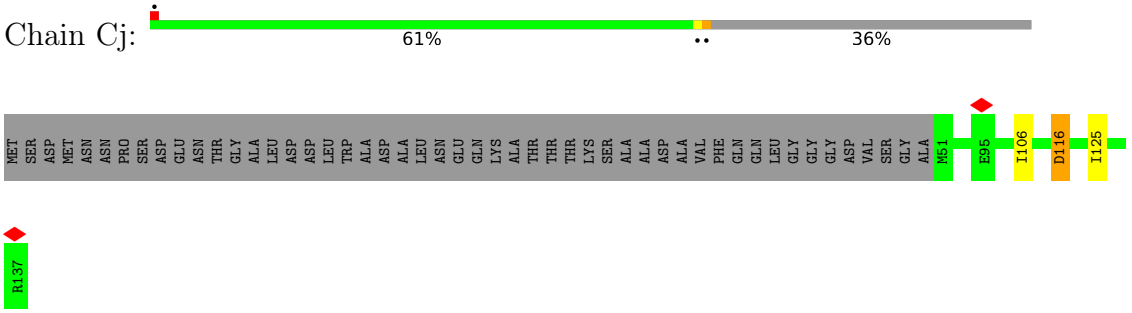

• Molecule 4: Flagellar motor switch protein FliN

Chain Ci:



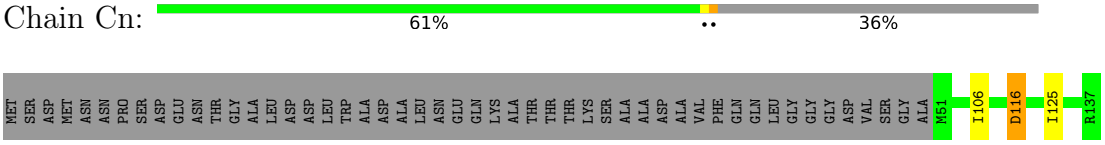

• Molecule 4: Flagellar motor switch protein FliN

Chain Cj:



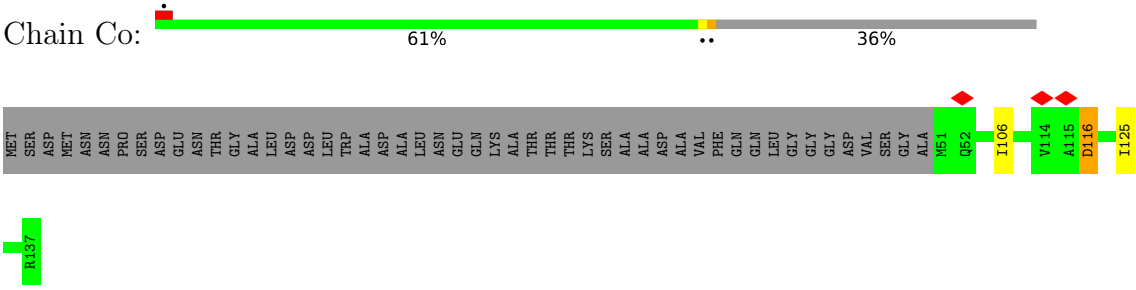

• Molecule 4: Flagellar motor switch protein FliN

Chain Cn:



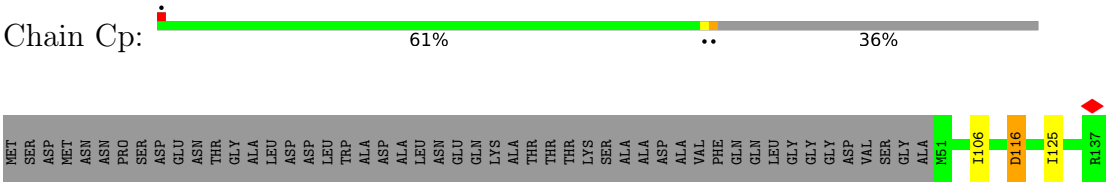

• Molecule 4: Flagellar motor switch protein FliN

Chain Co:



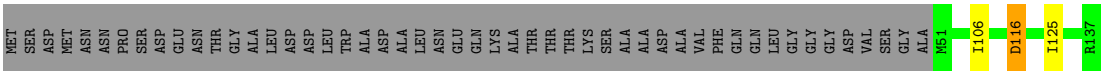

• Molecule 4: Flagellar motor switch protein FliN

Chain Cp:



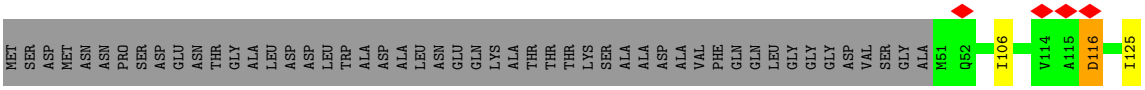

• Molecule 4: Flagellar motor switch protein FliN

Chain Ct:



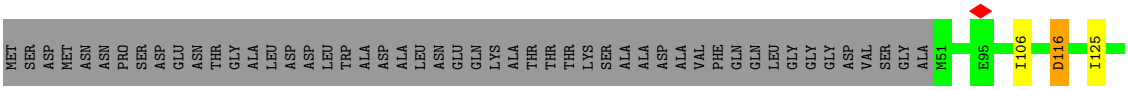

• Molecule 4: Flagellar motor switch protein FliN

Chain Cu:



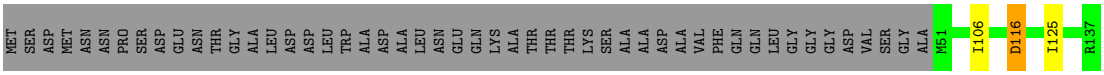
• Molecule 4: Flagellar motor switch protein FliN

Chain Cv:



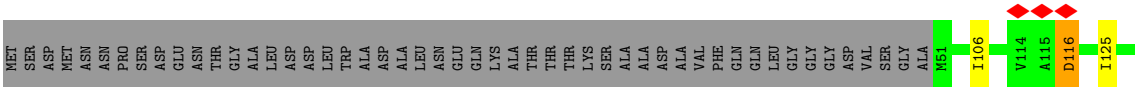
• Molecule 4: Flagellar motor switch protein FliN

Chain Cz:



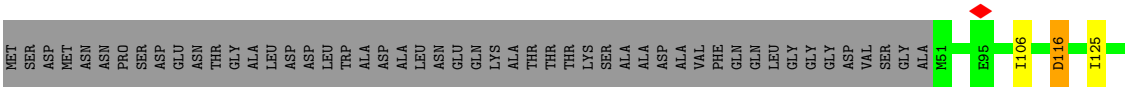

• Molecule 4: Flagellar motor switch protein FliN

Chain C1:



• Molecule 4: Flagellar motor switch protein FliN

Chain C2:



R137

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C34 | Depositor |
| Number of particles used | 19627 | 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 ($e^-/Å^2$) | 41 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 1800 | Depositor |
| Magnification | 81000 | Depositor |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.498 | Depositor |
| Minimum map value | -0.276 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.030 | Depositor |
| Recommended contour level | 0.13 | Depositor |
| Map size (Å) | 660.0, 660.0, 660.0 | wwPDB |
| Map dimensions | 600, 600, 600 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.1, 1.1, 1.1 | 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 | 3 | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | 9 | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | A1 | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | A7 | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | AE | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | AK | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | AQ | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | AW | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | Ac | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | Ai | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | Ao | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | Au | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | B5 | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | BC | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | BI | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | BO | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | BU | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | Ba | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | Bg | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | Bm | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | Bs | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | By | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | CA | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | CG | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | CM | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | CS | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | CY | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | Ce | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | Ck | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | Cq | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | Cw | 0.28 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | k | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | q | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |
| 1 | w | 0.27 | 0/2481 | 0.48 | 1/3344 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 2 | 0 | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | 4 | 0.22 | 0/226 | 0.48 | 0/303 |
| 2 | A2 | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | A8 | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | AF | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | AL | 0.22 | 0/226 | 0.48 | 0/303 |
| 2 | AR | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | AX | 0.22 | 0/226 | 0.48 | 0/303 |
| 2 | Ad | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | Aj | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | Ap | 0.22 | 0/226 | 0.48 | 0/303 |
| 2 | Av | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | B6 | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | BD | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | BJ | 0.22 | 0/226 | 0.48 | 0/303 |
| 2 | BP | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | BV | 0.22 | 0/226 | 0.48 | 0/303 |
| 2 | Bb | 0.22 | 0/226 | 0.48 | 0/303 |
| 2 | Bh | 0.22 | 0/226 | 0.48 | 0/303 |
| 2 | Bn | 0.22 | 0/226 | 0.50 | 0/303 |
| 2 | Bt | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | Bz | 0.22 | 0/226 | 0.48 | 0/303 |
| 2 | CB | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | CH | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | CN | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | CT | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | CZ | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | Cf | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | Cl | 0.22 | 0/226 | 0.48 | 0/303 |
| 2 | Cr | 0.22 | 0/226 | 0.48 | 0/303 |
| 2 | Cx | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | l | 0.22 | 0/226 | 0.49 | 0/303 |
| 2 | r | 0.22 | 0/226 | 0.48 | 0/303 |
| 2 | x | 0.22 | 0/226 | 0.48 | 0/303 |
| 3 | 5 | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | A3 | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | A9 | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | AA | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | AG | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | AM | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | AS | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | AY | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | Ae | 0.25 | 0/2393 | 0.50 | 0/3255 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 3 | Ak | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | Aq | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | Aw | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | B1 | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | B7 | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | BE | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | BK | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | BQ | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | BW | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | Bc | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | Bi | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | Bo | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | Bu | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | CC | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | CI | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | CO | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | CU | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | Ca | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | Cg | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | Cm | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | Cs | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | Cy | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | m | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | s | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 3 | y | 0.25 | 0/2393 | 0.50 | 0/3255 |
| 4 | 1 | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | 2 | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | 6 | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | 7 | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | 8 | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | A0 | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | A4 | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | A5 | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | A6 | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | AB | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | AC | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | AD | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | AH | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | AI | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | AJ | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | AN | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | AO | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | AP | 0.23 | 0/679 | 0.53 | 0/917 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 4 | AT | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | AU | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | AV | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | AZ | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Aa | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | Ab | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Af | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Ag | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | Ah | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Al | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Am | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | An | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Ar | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | As | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | At | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Ax | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | Ay | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Az | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | B0 | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | B2 | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | B3 | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | B4 | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | B8 | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | B9 | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | BA | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | BB | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | BF | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | BG | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | BH | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | BL | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | BM | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | BN | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | BR | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | BS | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | BT | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | BX | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | BY | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | BZ | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Bd | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Be | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | Bf | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Bj | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Bk | 0.23 | 0/679 | 0.52 | 0/917 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 4 | Bl | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Bp | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Bq | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Br | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Bv | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Bw | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | Bx | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | C1 | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | C2 | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | CD | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | CE | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | CF | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | CJ | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | CK | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | CL | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | CP | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | CQ | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | CR | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | CV | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | CW | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | CX | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Cb | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Cc | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | Cd | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Ch | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Ci | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | Cj | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Cn | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Co | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Cp | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Ct | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | Cu | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | Cv | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | Cz | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | n | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | o | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | p | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | t | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | u | 0.23 | 0/679 | 0.52 | 0/917 |
| 4 | v | 0.23 | 0/679 | 0.53 | 0/917 |
| 4 | z | 0.23 | 0/679 | 0.53 | 0/917 |
| All | All | 0.25 | 0/242658 | 0.50 | 34/328202 (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 | 3 | 0 | 2 |
| 1 | 9 | 0 | 2 |
| 1 | A1 | 0 | 2 |
| 1 | A7 | 0 | 2 |
| 1 | AE | 0 | 2 |
| 1 | AK | 0 | 2 |
| 1 | AQ | 0 | 2 |
| 1 | AW | 0 | 2 |
| 1 | Ac | 0 | 2 |
| 1 | Ai | 0 | 2 |
| 1 | Ao | 0 | 2 |
| 1 | Au | 0 | 2 |
| 1 | B5 | 0 | 2 |
| 1 | BC | 0 | 2 |
| 1 | BI | 0 | 2 |
| 1 | BO | 0 | 2 |
| 1 | BU | 0 | 2 |
| 1 | Ba | 0 | 2 |
| 1 | Bg | 0 | 2 |
| 1 | Bm | 0 | 2 |
| 1 | Bs | 0 | 2 |
| 1 | By | 0 | 2 |
| 1 | CA | 0 | 2 |
| 1 | CG | 0 | 2 |
| 1 | CM | 0 | 2 |
| 1 | CS | 0 | 2 |
| 1 | CY | 0 | 2 |
| 1 | Ce | 0 | 2 |
| 1 | Ck | 0 | 2 |
| 1 | Cq | 0 | 2 |
| 1 | Cw | 0 | 2 |
| 1 | k | 0 | 2 |
| 1 | q | 0 | 2 |
| 1 | w | 0 | 2 |
| All | All | 0 | 68 |

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Ac | 66 | PHE | C-N-CA | 5.15 | 134.58 | 121.70 |
| 1 | CG | 66 | PHE | C-N-CA | 5.15 | 134.58 | 121.70 |
| 1 | AK | 66 | PHE | C-N-CA | 5.15 | 134.57 | 121.70 |
| 1 | By | 66 | PHE | C-N-CA | 5.15 | 134.57 | 121.70 |
| 1 | q | 66 | PHE | C-N-CA | 5.14 | 134.56 | 121.70 |

There are no chirality outliers.

5 of 68 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | k | 206 | MET | Mainchain |
| 1 | k | 219 | ARG | Sidechain |
| 1 | q | 206 | MET | Mainchain |
| 1 | q | 219 | ARG | Sidechain |
| 1 | w | 206 | MET | Mainchain |

## 5.2 Too-close contacts (i)

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

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | 3 | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | 9 | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | A1 | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | A7 | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | AE | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | AK | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | AQ | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | AW | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | Ac | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | Ai | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | Ao | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | Au | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | B5 | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | BC | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | BI | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | BO | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | BU | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | Ba | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | Bg | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | Bm | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | Bs | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | By | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | CA | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | CG | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | CM | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | CS | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | CY | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | Ce | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | Ck | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | Cq | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | Cw | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | k | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | q | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 1 | w | 311/331 (94%) | 302 (97%) | 7 (2%) | 2 (1%) | 22 | 61 |
| 2 | 0 | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | 4 | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | A2 | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | A8 | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 2 | AF | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | AL | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | AR | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | AX | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | Ad | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | Aj | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | Ap | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | Av | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | B6 | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | BD | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | BJ | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | BP | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | BV | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | Bb | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | Bh | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | Bn | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | Bt | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | Bz | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | CB | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | CH | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | CN | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | CT | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | CZ | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | Cf | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | Cl | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | Cr | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | Cx | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | l | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | r | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 2 | x | 25/560 (4%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 3 | 5 | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 3 | A3 | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | A9 | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | AA | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | AG | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | AM | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | AS | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | AY | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | Ae | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | Ak | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | Aq | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | Aw | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | B1 | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | B7 | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | BE | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | BK | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | BQ | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | BW | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | Bc | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | Bi | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | Bo | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | Bu | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | CC | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | CI | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | CO | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | CU | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | Ca | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | Cg | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | Cm | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | Cs | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | Cy | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | m | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 3 | s | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 3 | y | 287/334 (86%) | 276 (96%) | 9 (3%) | 2 (1%) | 19 | 57 |
| 4 | 1 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | 2 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | 6 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | 7 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | 8 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | A0 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | A4 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | A5 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | A6 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | AB | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | AC | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | AD | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | AH | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | AI | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | AJ | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | AN | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | AO | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | AP | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | AT | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | AU | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | AV | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | AZ | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Aa | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Ab | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Af | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Ag | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Ah | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Al | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Am | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 4 | An | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Ar | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | As | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | At | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Ax | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Ay | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Az | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | B0 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | B2 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | B3 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | B4 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | B8 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | B9 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BA | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BB | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BF | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BG | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BH | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BL | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BM | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BN | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BR | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BS | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BT | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BX | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BY | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | BZ | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Bd | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Be | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Bf | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Bj | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 4 | Bk | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Bl | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Bp | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Bq | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Br | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Bv | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Bw | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Bx | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | C1 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | C2 | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | CD | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | CE | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | CF | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | CJ | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | CK | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | CL | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | CP | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | CQ | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | CR | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | CV | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | CW | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | CX | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Cb | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Cc | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Cd | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Ch | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Ci | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Cj | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Cn | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Co | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Cp | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 4 | Ct | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Cu | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Cv | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | Cz | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | n | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | o | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | p | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | t | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | u | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | v | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| 4 | z | 85/137 (62%) | 79 (93%) | 5 (6%) | 1 (1%) | 11 | 44 |
| All | All | 29852/55624 (54%) | 28526 (96%) | 1088 (4%) | 238 (1%) | 19 | 55 |

5 of 238 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | n | 116 | ASP |
| 4 | o | 116 | ASP |
| 4 | p | 116 | ASP |
| 4 | t | 116 | ASP |
| 4 | u | 116 | ASP |

### 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 | 3 | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | 9 | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | A1 | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | A7 | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | AE | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | AK | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | AQ | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | AW | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | Ac | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | Ai | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | Ao | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | Au | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | B5 | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | BC | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | BI | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | BO | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | BU | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | Ba | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | Bg | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | Bm | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | Bs | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | By | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | CA | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | CG | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | CM | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | CS | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | CY | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | Ce | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | Ck | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | Cq | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | Cw | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | k | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | q | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 1 | w | 268/282 (95%) | 265 (99%) | 3 (1%) | 70 | 80 |
| 2 | 0 | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | 4 | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 2 | A2 | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | A8 | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | AF | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | AL | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | AR | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | AX | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | Ad | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | Aj | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | Ap | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | Av | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | B6 | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | BD | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | BJ | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | BP | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | BV | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | Bb | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | Bh | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | Bn | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | Bt | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | Bz | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | CB | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | CH | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | CN | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | CT | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | CZ | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | Cf | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | Cl | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | Cr | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | Cx | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | l | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 2 | r | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 2 | x | 26/467 (6%) | 26 (100%) | 0 | 100 | 100 |
| 3 | 5 | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | A3 | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | A9 | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | AA | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | AG | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | AM | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | AS | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | AY | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | Ae | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | Ak | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | Aq | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | Aw | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | B1 | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | B7 | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | BE | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | BK | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | BQ | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | BW | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | Bc | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | Bi | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | Bo | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | Bu | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | CC | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | CI | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | CO | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | CU | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | Ca | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | Cg | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | Cm | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | Cs | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 3 | Cy | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | m | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | s | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 3 | y | 262/301 (87%) | 250 (95%) | 12 (5%) | 23 | 44 |
| 4 | 1 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | 2 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | 6 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | 7 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | 8 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | A0 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | A4 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | A5 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | A6 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | AB | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | AC | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | AD | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | AH | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | AI | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | AJ | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | AN | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | AO | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | AP | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | AT | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | AU | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | AV | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | AZ | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Aa | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Ab | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Af | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Ag | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Ah | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 4 | Al | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Am | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | An | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Ar | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | As | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | At | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Ax | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Ay | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Az | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | B0 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | B2 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | B3 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | B4 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | B8 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | B9 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BA | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BB | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BF | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BG | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BH | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BL | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BM | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BN | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BR | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BS | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BT | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BX | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BY | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | BZ | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Bd | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Be | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 4 | Bf | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Bj | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Bk | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Bl | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Bp | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Bq | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Br | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Bv | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Bw | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Bx | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | C1 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | C2 | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | CD | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | CE | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | CF | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | CJ | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | CK | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | CL | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | CP | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | CQ | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | CR | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | CV | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | CW | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | CX | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Cb | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Cc | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Cd | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Ch | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Ci | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Cj | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Cn | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 4 | Co | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Cp | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Ct | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Cu | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Cv | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | Cz | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | n | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | o | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | p | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | t | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | u | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | v | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| 4 | z | 76/113 (67%) | 73 (96%) | 3 (4%) | 27 | 48 |
| All | All | 26656/47226 (56%) | 25840 (97%) | 816 (3%) | 37 | 54 |

5 of 816 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | Bc | 149 | THR |
| 4 | B4 | 106 | ILE |
| 3 | Cy | 149 | THR |
| 4 | Be | 125 | ILE |
| 3 | Bc | 85 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 320 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B5 | 46 | GLN |
| 1 | Ce | 49 | ASN |
| 4 | B0 | 83 | GLN |
| 1 | CM | 180 | ASN |
| 4 | Co | 102 | ASN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

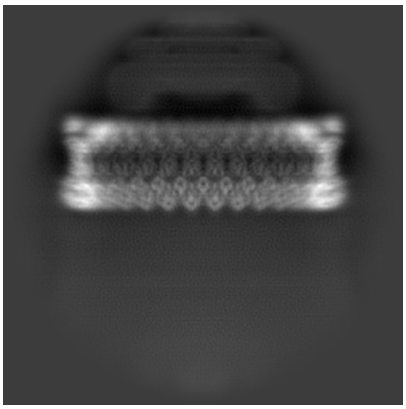
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39349. These allow visual inspection of the internal detail of the map and identification of artifacts.

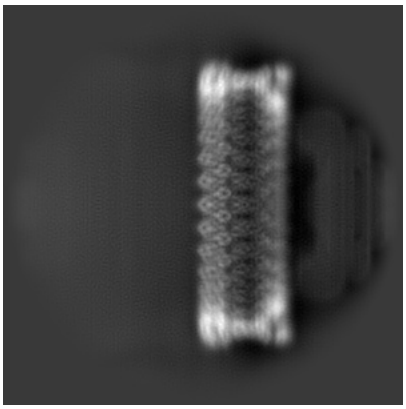
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

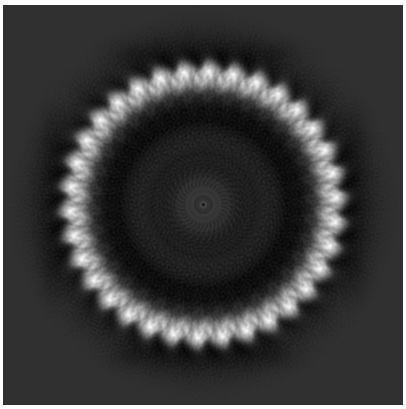
### 6.1.1 Primary map



X

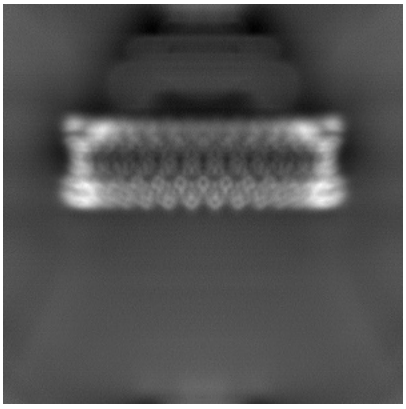


Y

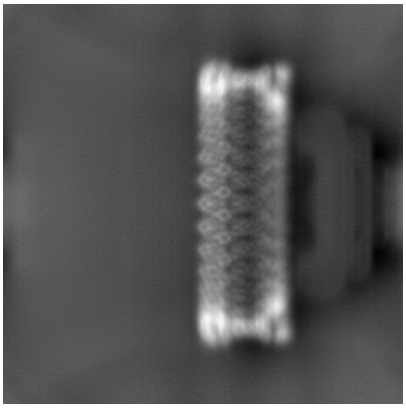


Z

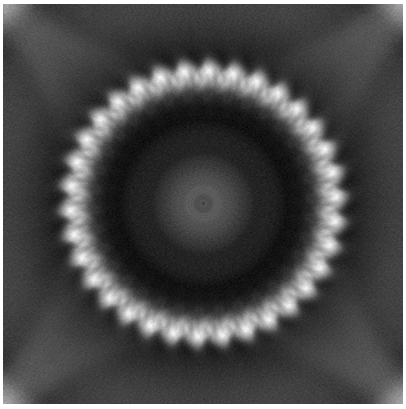
### 6.1.2 Raw map



X



Y

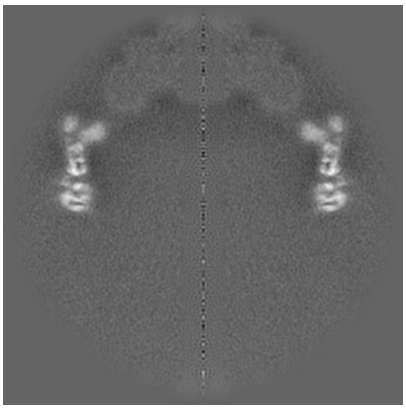


Z

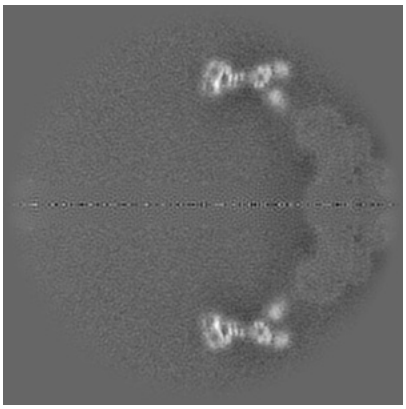
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

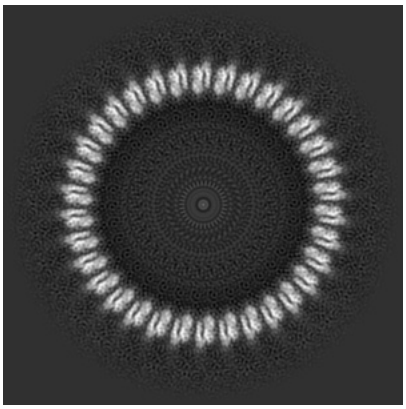
### 6.2.1 Primary map



X Index: 300

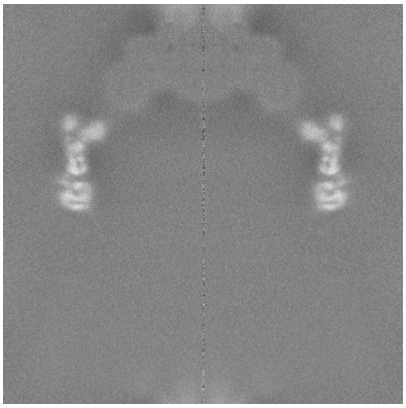


Y Index: 300

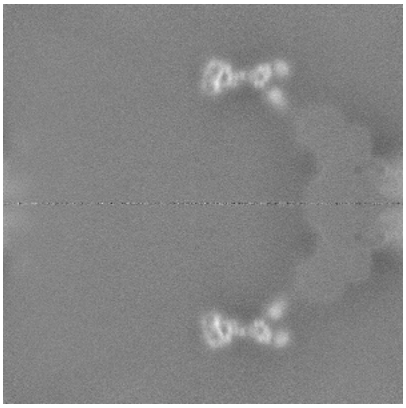


Z Index: 300

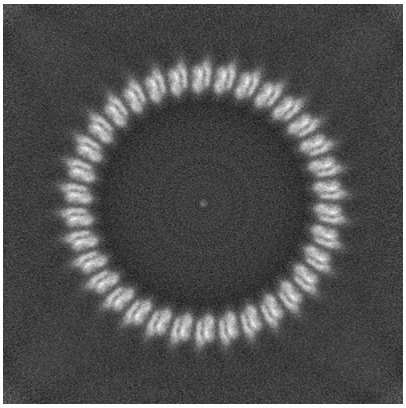
### 6.2.2 Raw map



X Index: 300



Y Index: 300

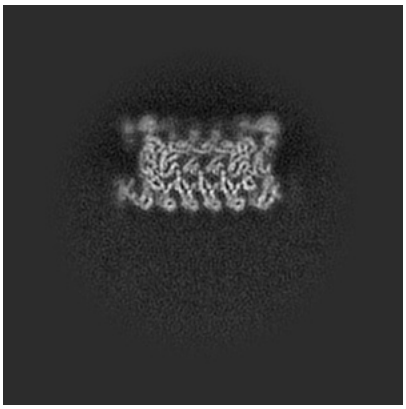


Z Index: 300

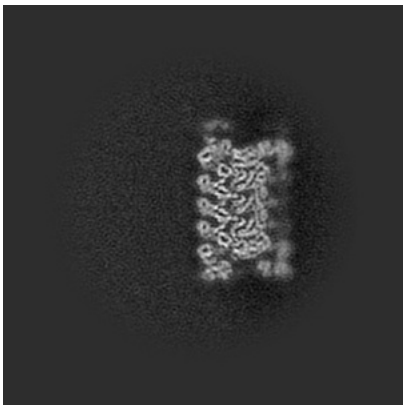
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

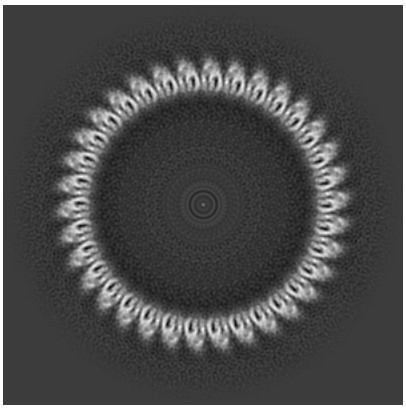
### 6.3.1 Primary map



X Index: 120

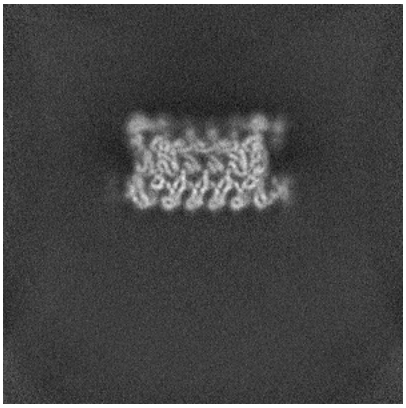


Y Index: 483

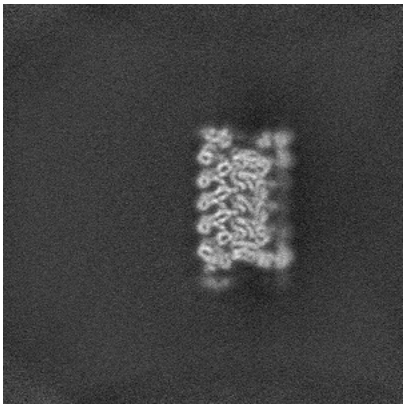


Z Index: 328

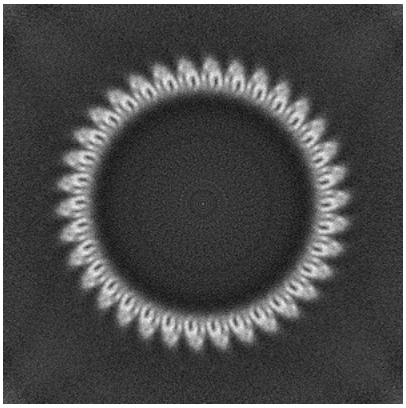
### 6.3.2 Raw map



X Index: 480



Y Index: 117

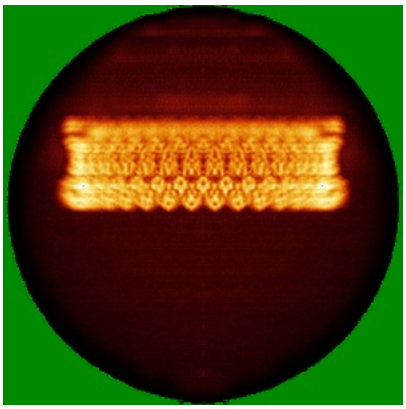


Z Index: 327

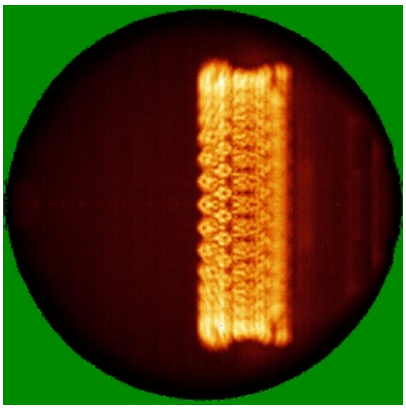
The images above show the largest variance slices of the map in three orthogonal directions.

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

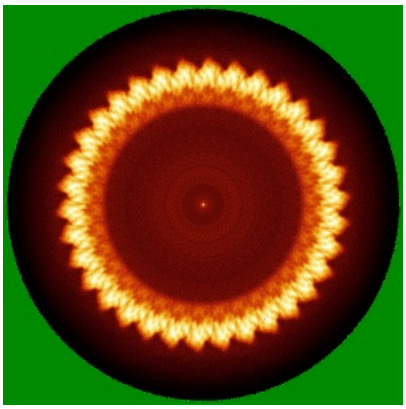
### 6.4.1 Primary map



X

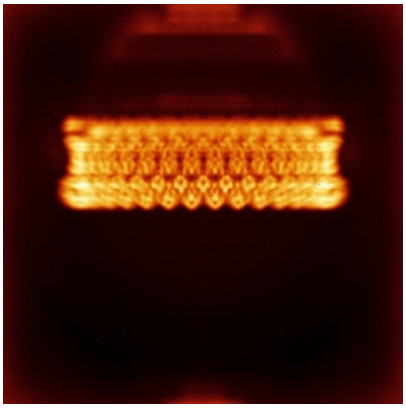


Y

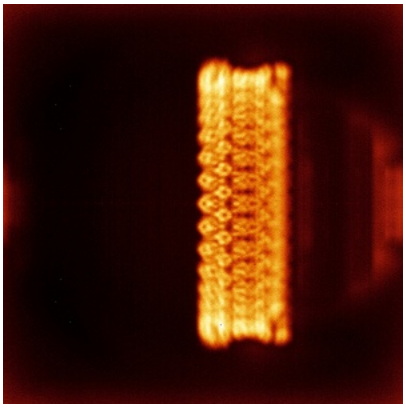


Z

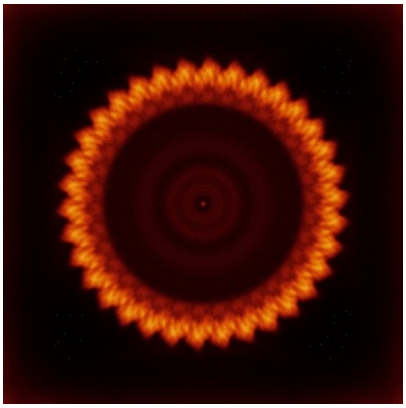
### 6.4.2 Raw map



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.

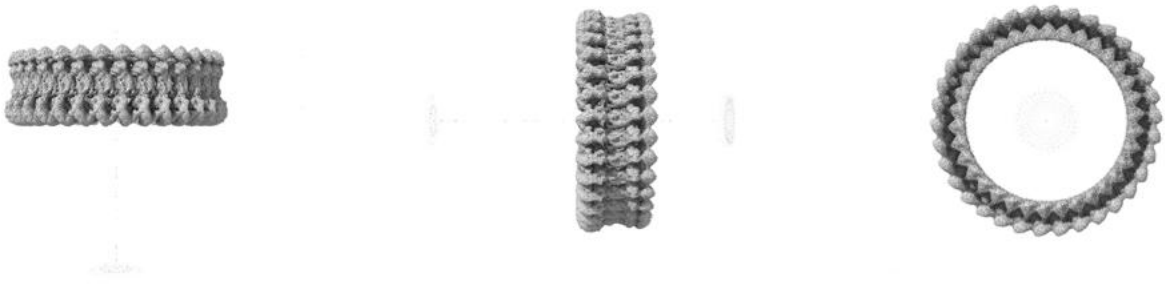
## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

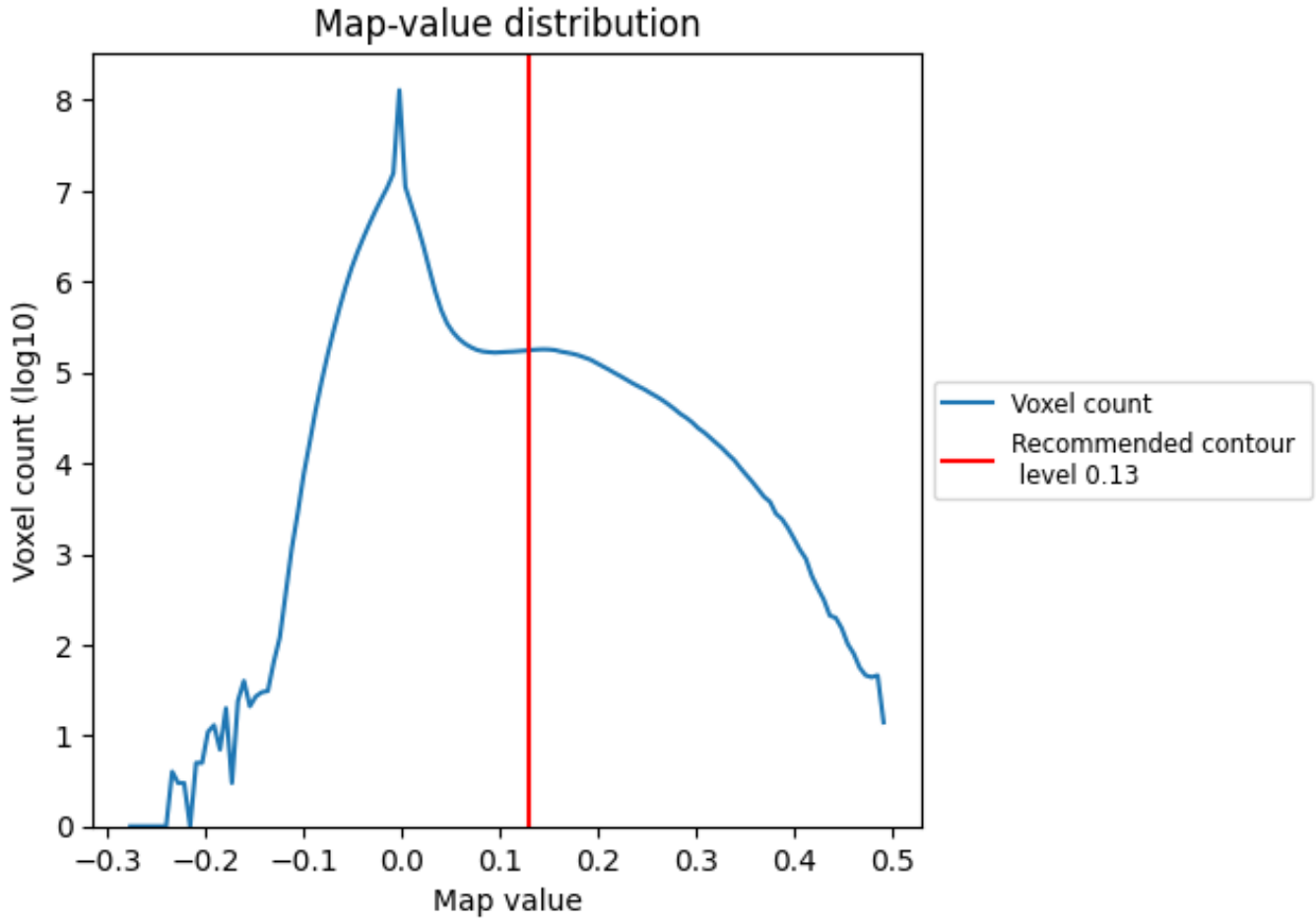
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

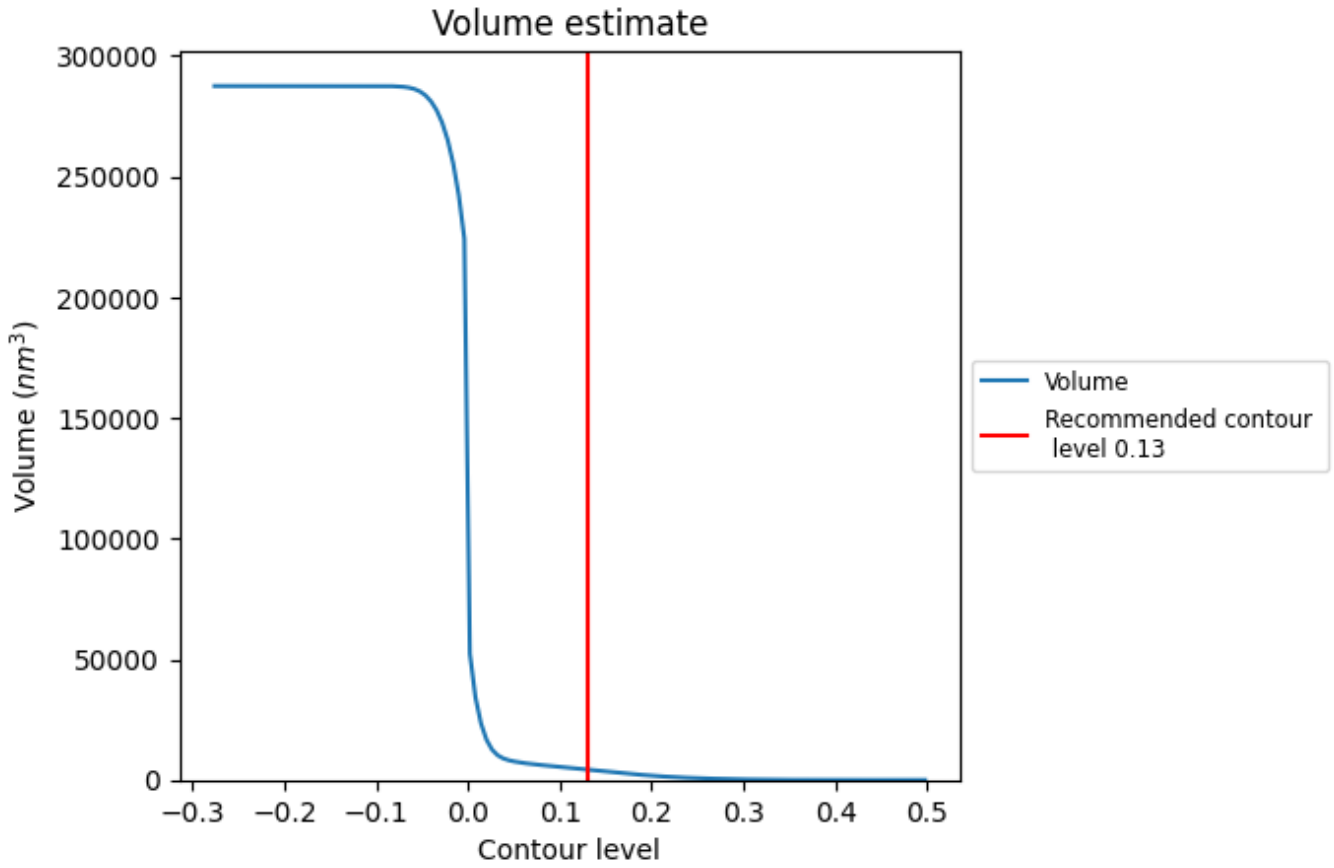
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

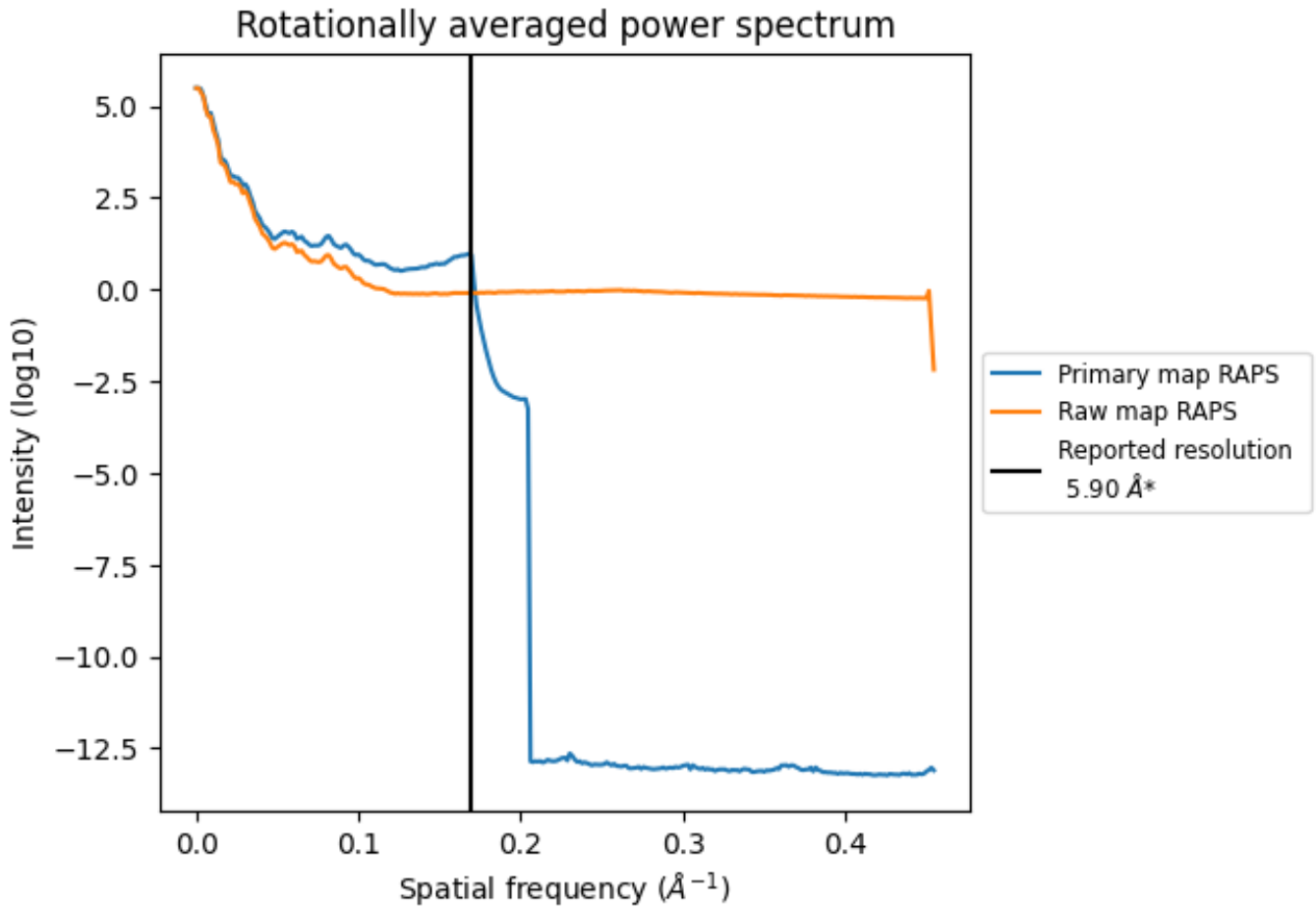
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 4303 $nm^3$; this corresponds to an approximate mass of 3887 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)

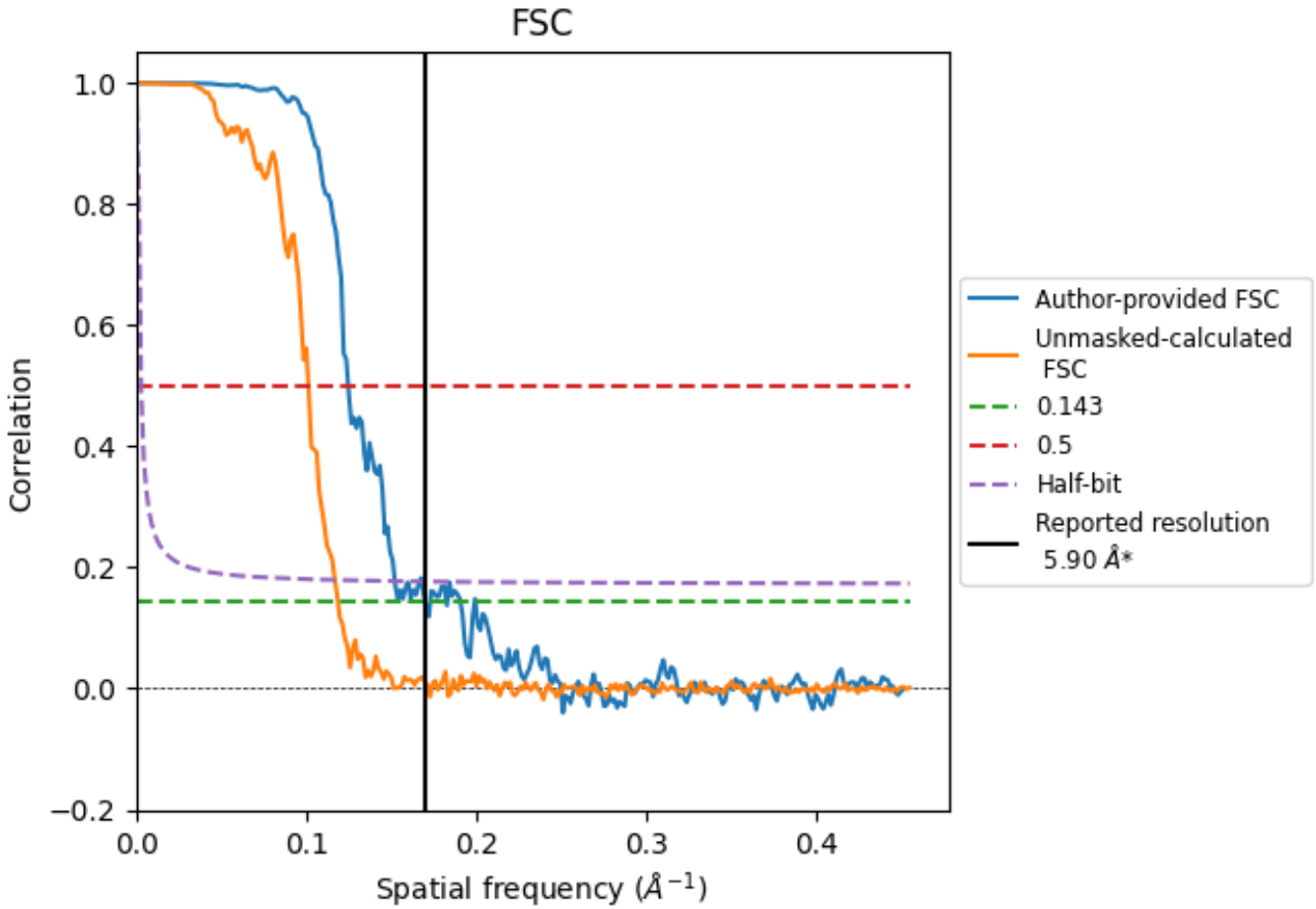



*Reported resolution corresponds to spatial frequency of 0.169 $Å^{-1}$

# 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 0.169 $Å^{-1}$

## 8.2 Resolution estimates (i)

| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 5.90 | - | - |
| Author-provided FSC curve | 5.89 | 8.03 | 6.58 |
| Unmasked-calculated* | 8.43 | 9.87 | 8.56 |

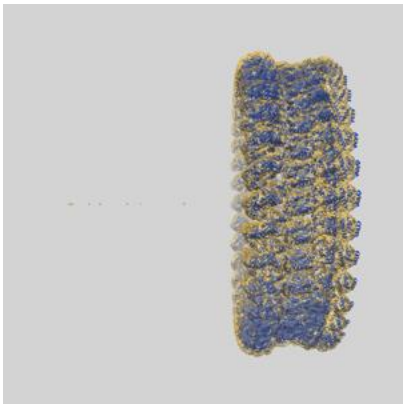
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.43 differs from the reported value 5.9 by more than 10 %

# 9 Map-model fit

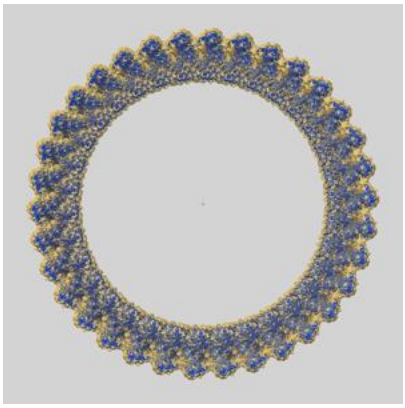
This section contains information regarding the fit between EMDB map EMD-39349 and PDB model 8YJT. Per-residue inclusion information can be found in section 3 on page 22.

## 9.1 Map-model overlay

X



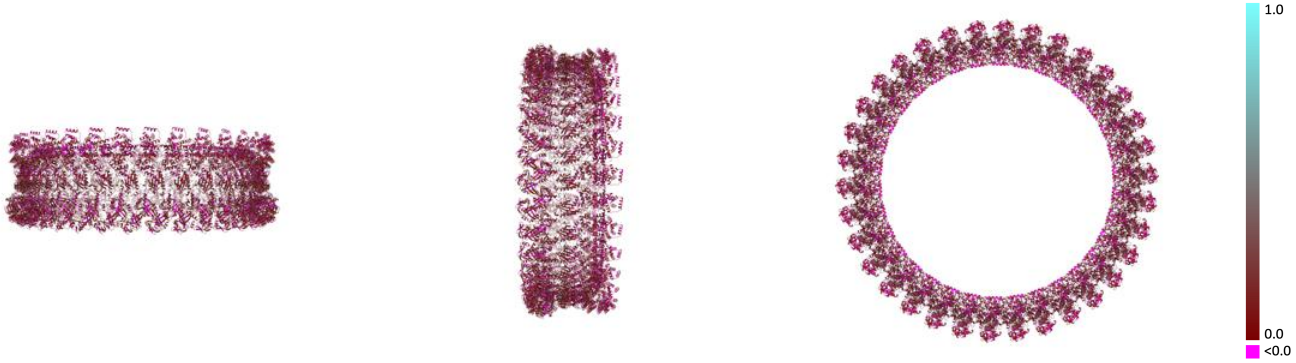
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

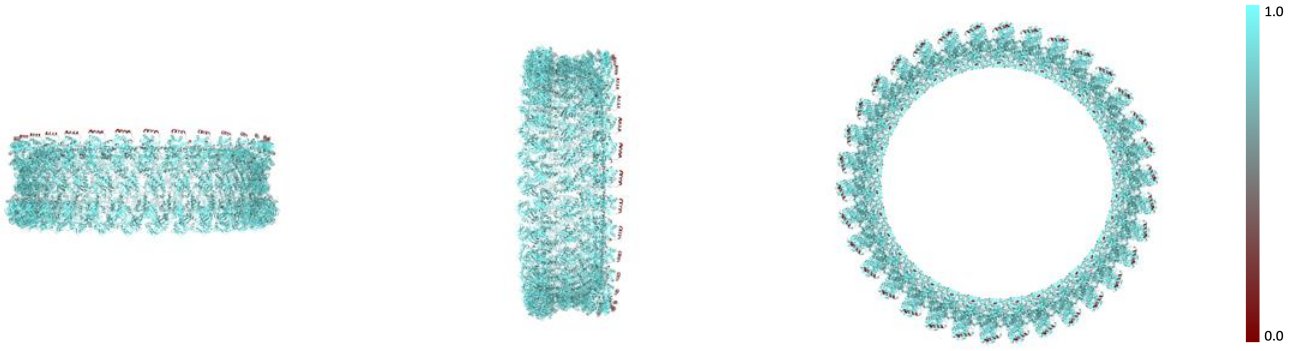
## 9.2 Q-score mapped to coordinate model (i)




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.

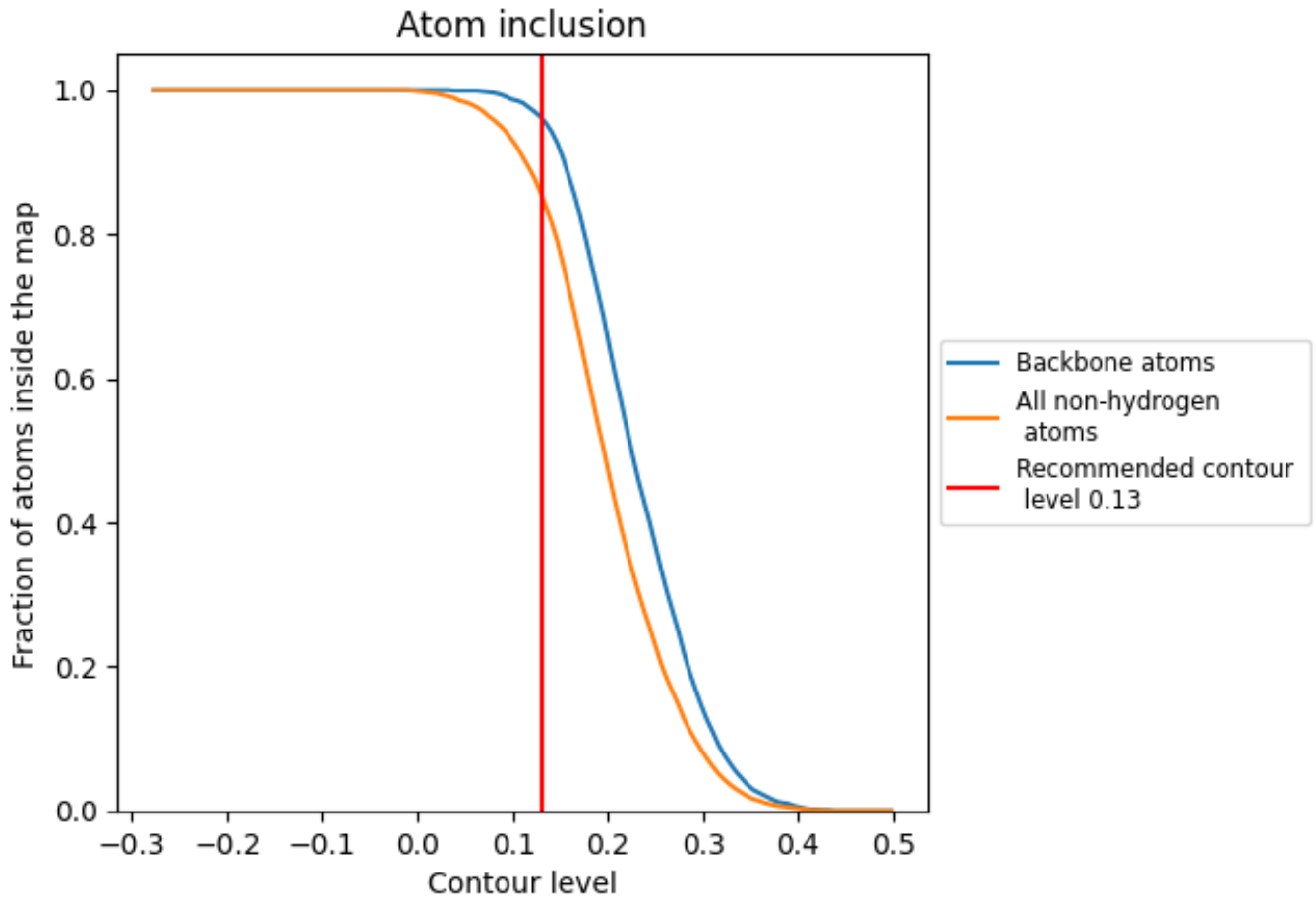
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.13).

## 9.4 Atom inclusion (i)




At the recommended contour level, 96% of all backbone atoms, 86% 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 (0.13) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8560 | 0.1470 |
| 0 | 0.7670 | 0.1200 |
| 1 | 0.8620 | 0.1690 |
| 2 | 0.8680 | 0.1500 |
| 3 | 0.8380 | 0.1240 |
| 4 | 0.7810 | 0.1120 |
| 5 | 0.8650 | 0.1660 |
| 6 | 0.8860 | 0.1530 |
| 7 | 0.8570 | 0.1660 |
| 8 | 0.8690 | 0.1530 |
| 9 | 0.8390 | 0.1260 |
| A0 | 0.8840 | 0.1500 |
| A1 | 0.8380 | 0.1260 |
| A2 | 0.7770 | 0.1110 |
| A3 | 0.8700 | 0.1660 |
| A4 | 0.8830 | 0.1520 |
| A5 | 0.8620 | 0.1690 |
| A6 | 0.8770 | 0.1500 |
| A7 | 0.8400 | 0.1240 |
| A8 | 0.7810 | 0.1160 |
| A9 | 0.8680 | 0.1650 |
| AA | 0.8700 | 0.1650 |
| AB | 0.8840 | 0.1530 |
| AC | 0.8650 | 0.1650 |
| AD | 0.8750 | 0.1530 |
| AE | 0.8400 | 0.1270 |
| AF | 0.7810 | 0.1160 |
| AG | 0.8690 | 0.1650 |
| AH | 0.8830 | 0.1520 |
| AI | 0.8580 | 0.1670 |
| AJ | 0.8780 | 0.1510 |
| AK | 0.8420 | 0.1250 |
| AL | 0.7770 | 0.1130 |
| AM | 0.8660 | 0.1650 |
| AN | 0.8800 | 0.1530 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| AO | 0.8600 | 0.1660 |
| AP | 0.8770 | 0.1510 |
| AQ | 0.8390 | 0.1270 |
| AR | 0.7770 | 0.1160 |
| AS | 0.8660 | 0.1660 |
| AT | 0.8800 | 0.1520 |
| AU | 0.8580 | 0.1670 |
| AV | 0.8750 | 0.1500 |
| AW | 0.8360 | 0.1250 |
| AX | 0.7770 | 0.1130 |
| AY | 0.8650 | 0.1630 |
| AZ | 0.8830 | 0.1520 |
| Aa | 0.8580 | 0.1660 |
| Ab | 0.8830 | 0.1520 |
| Ac | 0.8410 | 0.1250 |
| Ad | 0.7720 | 0.1160 |
| Ae | 0.8700 | 0.1650 |
| Af | 0.8860 | 0.1510 |
| Ag | 0.8600 | 0.1650 |
| Ah | 0.8720 | 0.1530 |
| Ai | 0.8420 | 0.1260 |
| Aj | 0.7770 | 0.1200 |
| Ak | 0.8690 | 0.1650 |
| Al | 0.8840 | 0.1500 |
| Am | 0.8580 | 0.1660 |
| An | 0.8680 | 0.1520 |
| Ao | 0.8410 | 0.1240 |
| Ap | 0.7860 | 0.1150 |
| Aq | 0.8680 | 0.1650 |
| Ar | 0.8860 | 0.1520 |
| As | 0.8570 | 0.1660 |
| At | 0.8710 | 0.1510 |
| Au | 0.8390 | 0.1250 |
| Av | 0.7860 | 0.1120 |
| Aw | 0.8670 | 0.1660 |
| Ax | 0.8800 | 0.1530 |
| Ay | 0.8600 | 0.1690 |
| Az | 0.8750 | 0.1520 |
| B0 | 0.8750 | 0.1540 |
| B1 | 0.8660 | 0.1670 |
| B2 | 0.8800 | 0.1540 |
| B3 | 0.8600 | 0.1690 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| B4 | 0.8770 | 0.1560 |
| B5 | 0.8390 | 0.1260 |
| B6 | 0.7770 | 0.1140 |
| B7 | 0.8660 | 0.1670 |
| B8 | 0.8800 | 0.1520 |
| B9 | 0.8580 | 0.1700 |
| BA | 0.8570 | 0.1690 |
| BB | 0.8740 | 0.1530 |
| BC | 0.8400 | 0.1230 |
| BD | 0.7670 | 0.1170 |
| BE | 0.8660 | 0.1660 |
| BF | 0.8800 | 0.1520 |
| BG | 0.8570 | 0.1700 |
| BH | 0.8750 | 0.1550 |
| BI | 0.8330 | 0.1250 |
| BJ | 0.7860 | 0.1160 |
| BK | 0.8660 | 0.1670 |
| BL | 0.8770 | 0.1500 |
| BM | 0.8620 | 0.1690 |
| BN | 0.8780 | 0.1560 |
| BO | 0.8400 | 0.1240 |
| BP | 0.7670 | 0.1140 |
| BQ | 0.8690 | 0.1660 |
| BR | 0.8870 | 0.1530 |
| BS | 0.8580 | 0.1710 |
| BT | 0.8770 | 0.1570 |
| BU | 0.8410 | 0.1230 |
| BV | 0.7770 | 0.1100 |
| BW | 0.8690 | 0.1660 |
| BX | 0.8840 | 0.1500 |
| BY | 0.8580 | 0.1690 |
| BZ | 0.8680 | 0.1570 |
| Ba | 0.8430 | 0.1240 |
| Bb | 0.7770 | 0.1080 |
| Bc | 0.8660 | 0.1650 |
| Bd | 0.8800 | 0.1540 |
| Be | 0.8620 | 0.1740 |
| Bf | 0.8680 | 0.1550 |
| Bg | 0.8380 | 0.1240 |
| Bh | 0.7810 | 0.1100 |
| Bi | 0.8650 | 0.1660 |
| Bj | 0.8860 | 0.1520 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| Bk | 0.8570 | 0.1700 |
| Bl | 0.8690 | 0.1580 |
| Bm | 0.8390 | 0.1250 |
| Bn | 0.7670 | 0.1210 |
| Bo | 0.8700 | 0.1660 |
| Bp | 0.8840 | 0.1520 |
| Bq | 0.8650 | 0.1690 |
| Br | 0.8750 | 0.1570 |
| Bs | 0.8400 | 0.1260 |
| Bt | 0.7810 | 0.1150 |
| Bu | 0.8690 | 0.1660 |
| Bv | 0.8830 | 0.1520 |
| Bw | 0.8580 | 0.1700 |
| Bx | 0.8780 | 0.1580 |
| By | 0.8420 | 0.1240 |
| Bz | 0.7770 | 0.1130 |
| C1 | 0.8620 | 0.1660 |
| C2 | 0.8780 | 0.1520 |
| CA | 0.8360 | 0.1240 |
| CB | 0.7770 | 0.1130 |
| CC | 0.8650 | 0.1640 |
| CD | 0.8830 | 0.1530 |
| CE | 0.8580 | 0.1680 |
| CF | 0.8830 | 0.1560 |
| CG | 0.8410 | 0.1240 |
| CH | 0.7720 | 0.1130 |
| CI | 0.8700 | 0.1650 |
| CJ | 0.8860 | 0.1500 |
| CK | 0.8600 | 0.1690 |
| CL | 0.8720 | 0.1560 |
| CM | 0.8420 | 0.1250 |
| CN | 0.7770 | 0.1160 |
| CO | 0.8690 | 0.1650 |
| CP | 0.8840 | 0.1520 |
| CQ | 0.8580 | 0.1670 |
| CR | 0.8680 | 0.1550 |
| CS | 0.8410 | 0.1240 |
| CT | 0.7860 | 0.1110 |
| CU | 0.8680 | 0.1640 |
| CV | 0.8860 | 0.1530 |
| CW | 0.8570 | 0.1670 |
| CX | 0.8710 | 0.1540 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| CY | 0.8390 | 0.1240 |
| CZ | 0.7860 | 0.1110 |
| Ca | 0.8670 | 0.1650 |
| Cb | 0.8800 | 0.1540 |
| Cc | 0.8600 | 0.1690 |
| Cd | 0.8750 | 0.1560 |
| Ce | 0.8380 | 0.1260 |
| Cf | 0.7770 | 0.1120 |
| Cg | 0.8700 | 0.1660 |
| Ch | 0.8830 | 0.1520 |
| Ci | 0.8620 | 0.1670 |
| Cj | 0.8770 | 0.1530 |
| Ck | 0.8400 | 0.1250 |
| Cl | 0.7810 | 0.1140 |
| Cm | 0.8680 | 0.1650 |
| Cn | 0.8840 | 0.1510 |
| Co | 0.8570 | 0.1670 |
| Cp | 0.8740 | 0.1560 |
| Cq | 0.8400 | 0.1230 |
| Cr | 0.7670 | 0.1190 |
| Cs | 0.8660 | 0.1640 |
| Ct | 0.8800 | 0.1500 |
| Cu | 0.8570 | 0.1670 |
| Cv | 0.8750 | 0.1540 |
| Cw | 0.8330 | 0.1270 |
| Cx | 0.7860 | 0.1120 |
| Cy | 0.8660 | 0.1650 |
| Cz | 0.8770 | 0.1510 |
| k | 0.8400 | 0.1260 |
| l | 0.7670 | 0.1130 |
| m | 0.8690 | 0.1640 |
| n | 0.8870 | 0.1510 |
| o | 0.8580 | 0.1670 |
| p | 0.8770 | 0.1530 |
| q | 0.8410 | 0.1240 |
| r | 0.7770 | 0.1100 |
| s | 0.8690 | 0.1660 |
| t | 0.8840 | 0.1480 |
| u | 0.8580 | 0.1660 |
| v | 0.8680 | 0.1530 |
| w | 0.8430 | 0.1260 |
| x | 0.7770 | 0.1100 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| y | 0.8660 | 0.1660 |
| z | 0.8800 | 0.1530 |