# wwPDB EM Validation Summary Report (i)

Nov 28, 2022 – 11:44 AM EST

| | | |
|---|---|---|
| PDB ID | : | 7SPJ |
| EMDB ID | : | EMD-24772 |
| Title | : | Models for C17 reconstruction of Outer Membrane Core Complex (OMCC) of Type IV Secretion System (T4SS) encoded by a plasmid overproducing TraV, TraK and TraB of pED208 |
| Authors | : | Liu, X.; Khara, P.; Baker, M.L.; Christie, P.J.; Hu, B. |
| Deposited on | : | 2021-11-02 |
| Resolution | : | 3.56 Å(reported) |

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

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

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

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

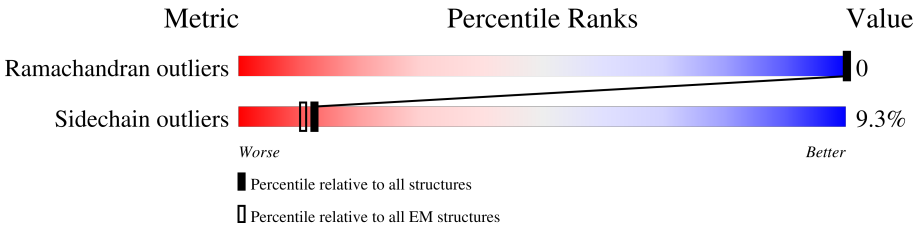
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.56 Å.

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




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

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | AB1 | 204 | 16% · 82% |
| 1 | AB10 | 204 | 16% · 82% |
| 1 | AB11 | 204 | 16% · 82% |
| 1 | AB12 | 204 | 16% · 82% |
| 1 | AB13 | 204 | 16% · 82% |
| 1 | AB14 | 204 | 16% · 82% |
| 1 | AB15 | 204 | 16% · 82% |
| 1 | AB16 | 204 | 16% · 82% |
| 1 | AB17 | 204 | 16% · 82% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | AB2 | 204 | 16% 82% |
| 1 | AB3 | 204 | 16% 82% |
| 1 | AB4 | 204 | 16% 82% |
| 1 | AB5 | 204 | 16% 82% |
| 1 | AB6 | 204 | 16% 82% |
| 1 | AB7 | 204 | 16% 82% |
| 1 | AB8 | 204 | 16% 82% |
| 1 | AB9 | 204 | 16% 82% |
| 2 | EF1 | 453 | 40% 57% |
| 2 | EF10 | 453 | 40% 57% |
| 2 | EF11 | 453 | 40% 57% |
| 2 | EF12 | 453 | 40% 57% |
| 2 | EF13 | 453 | 5% 41% 57% |
| 2 | EF14 | 453 | 40% 57% |
| 2 | EF15 | 453 | 40% 57% |
| 2 | EF16 | 453 | 40% 57% |
| 2 | EF17 | 453 | 40% 57% |
| 2 | EF2 | 453 | 40% 57% |
| 2 | EF3 | 453 | 40% 57% |
| 2 | EF4 | 453 | 40% 57% |
| 2 | EF5 | 453 | 40% 57% |
| 2 | EF6 | 453 | 40% 57% |
| 2 | EF7 | 453 | 40% 57% |
| 2 | EF8 | 453 | 40% 57% |
| 2 | EF9 | 453 | 40% 57% |

## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 29597 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 TraV.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | AB1 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB2 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB3 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB4 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB5 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB6 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB7 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB8 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB9 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB10 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB11 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB12 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB13 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB14 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB15 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB16 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |
| 1 | AB17 | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 261 | 153 | 47 | 56 | 5 | | |

- Molecule 2 is a protein called TraB.

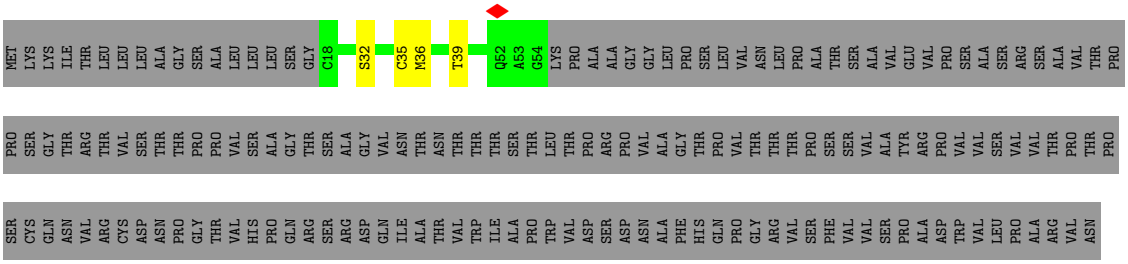
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | EF1 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF2 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF3 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF4 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF5 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF6 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF7 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF8 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF9 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF10 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF11 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF12 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF13 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF14 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF15 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF16 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |
| 2 | EF17 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1480 | 925 | 259 | 290 | 6 | | |

# 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.

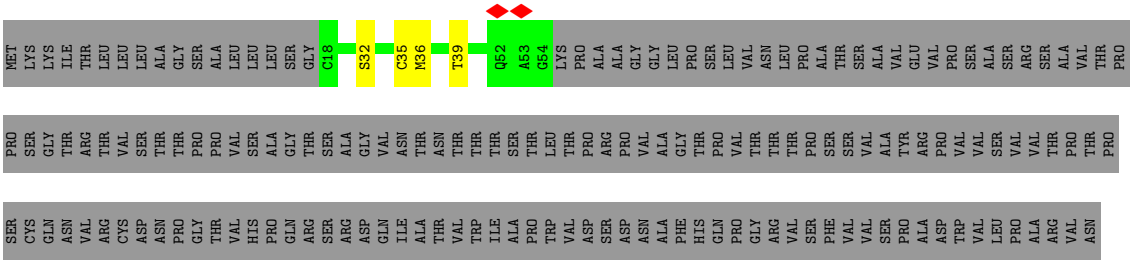
• Molecule 1: TraV

Chain AB1:

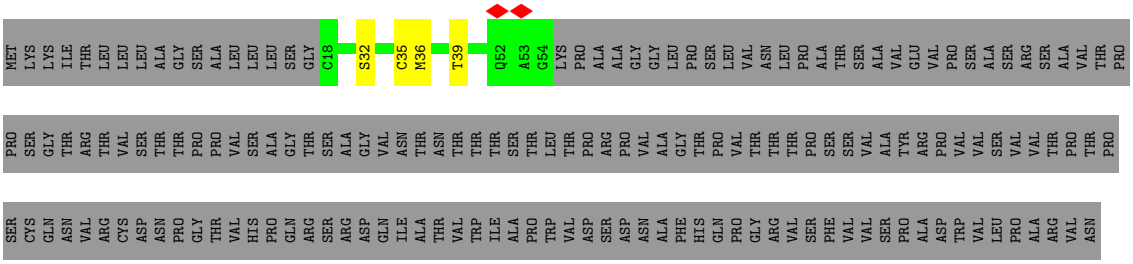

• Molecule 1: TraV

Chain AB2:

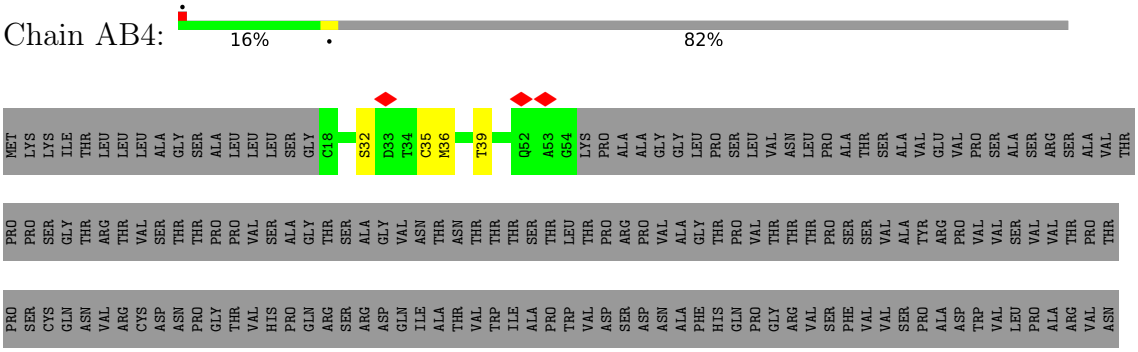

• Molecule 1: TraV

Chain AB3:

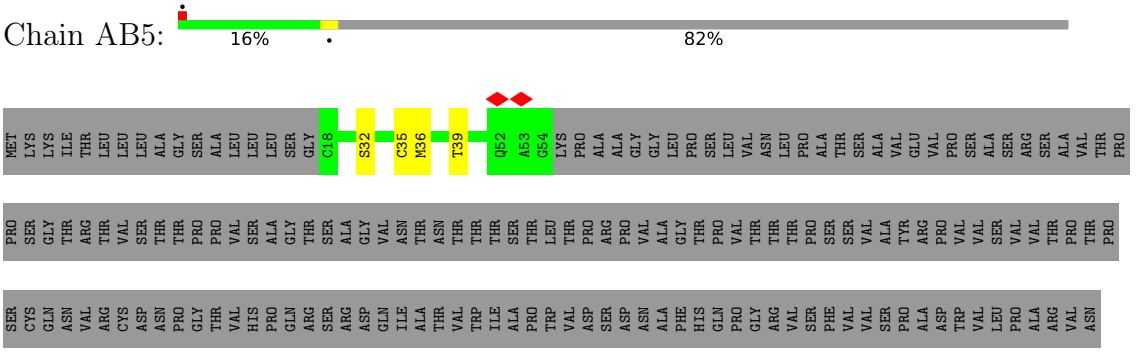

• Molecule 1: TraV

Chain AB4:



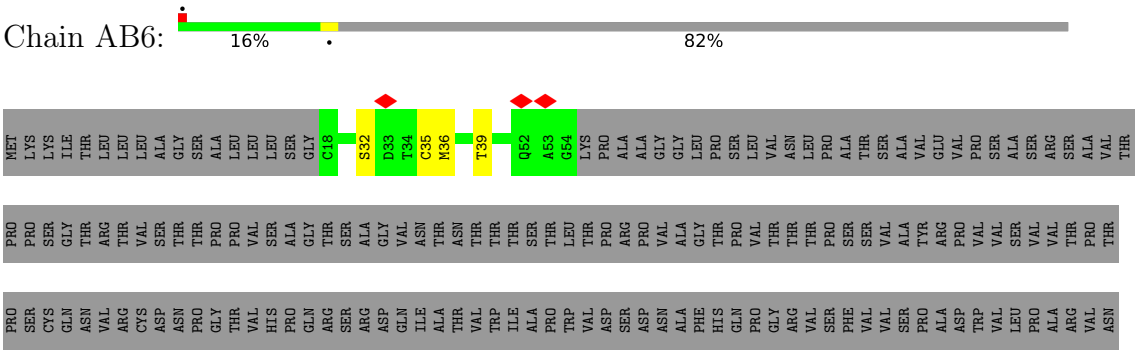

• Molecule 1: TraV

Chain AB5:



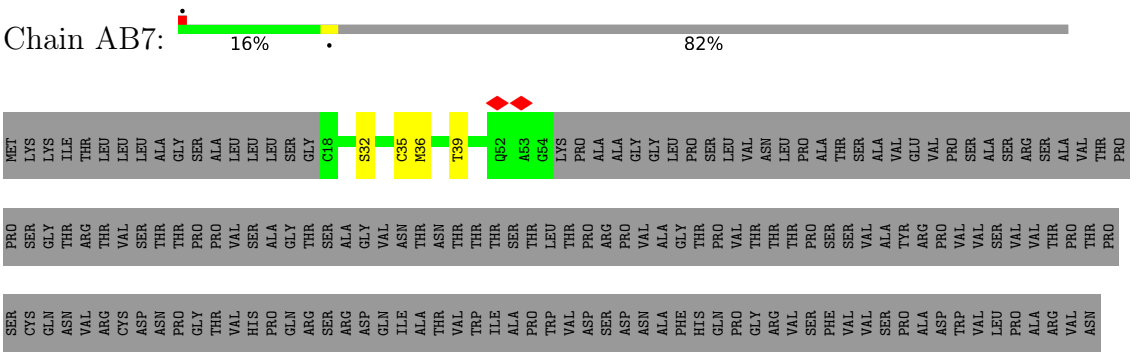

• Molecule 1: TraV

Chain AB6:



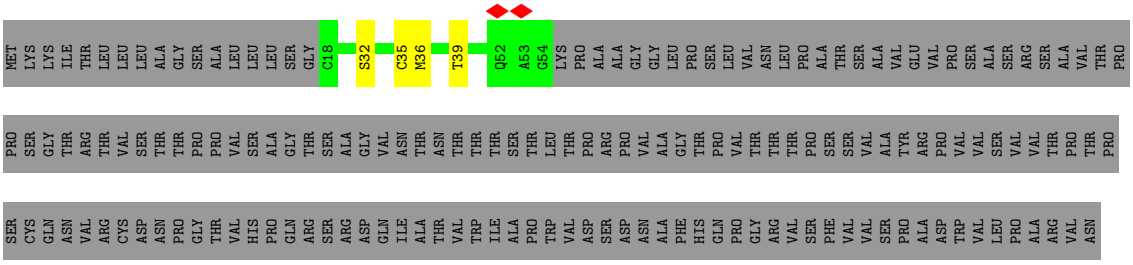

• Molecule 1: TraV

Chain AB7:



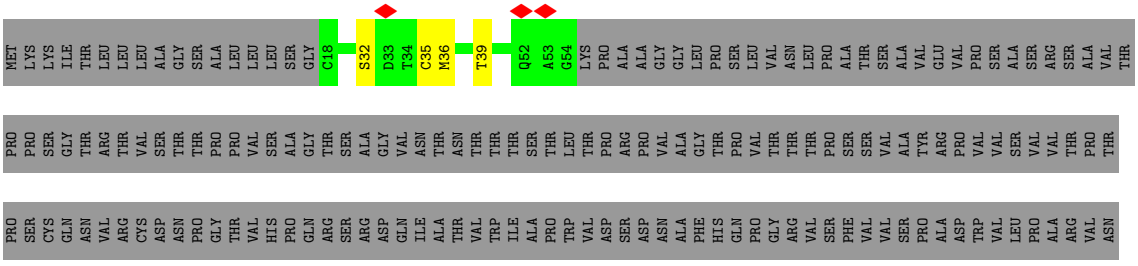

• Molecule 1: TraV

Chain AB8:



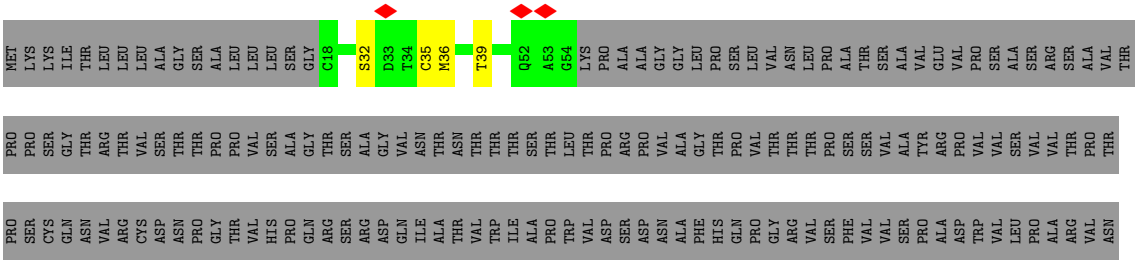

• Molecule 1: TraV

Chain AB9:

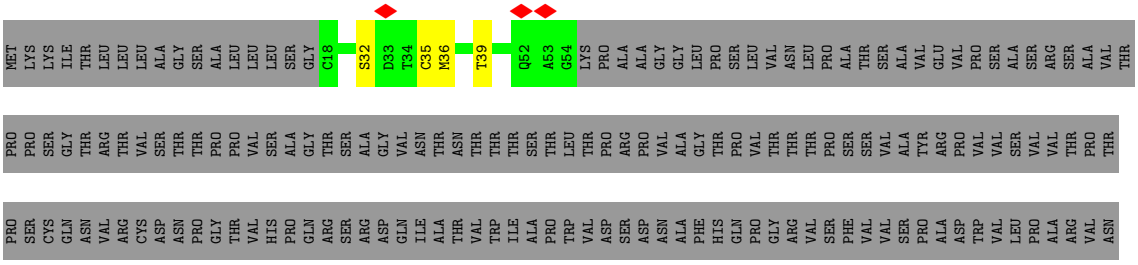

• Molecule 1: TraV

Chain AB10:

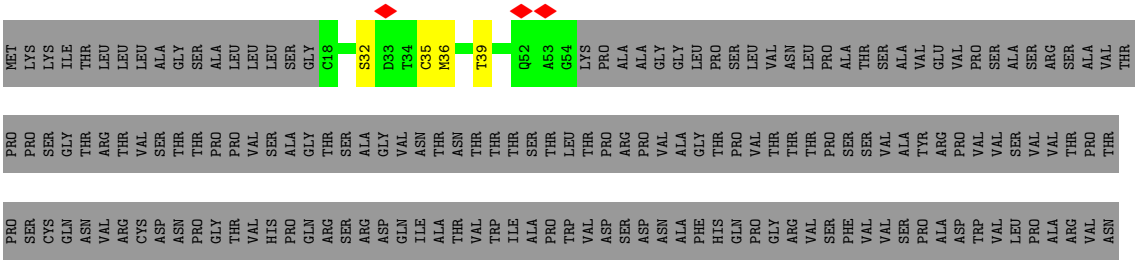

• Molecule 1: TraV

Chain AB11:

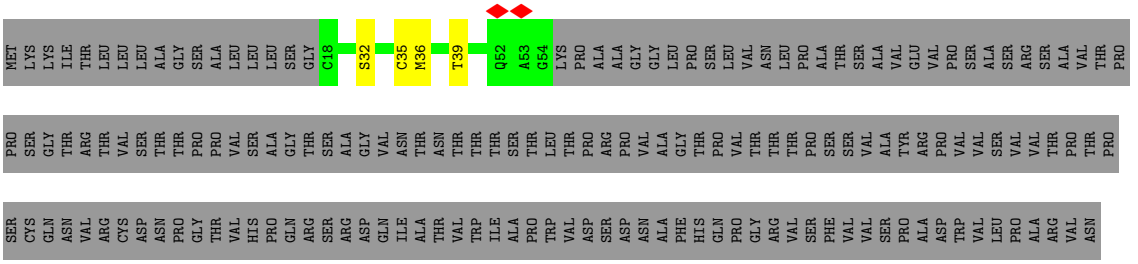

• Molecule 1: TraV

Chain AB12:



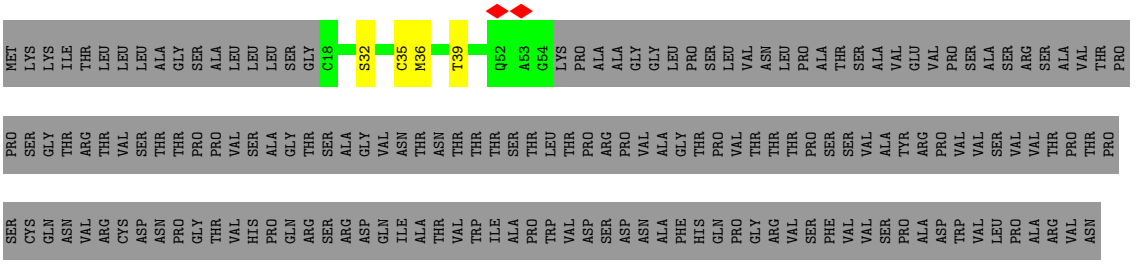

- Molecule 1: TraV

Chain AB13:

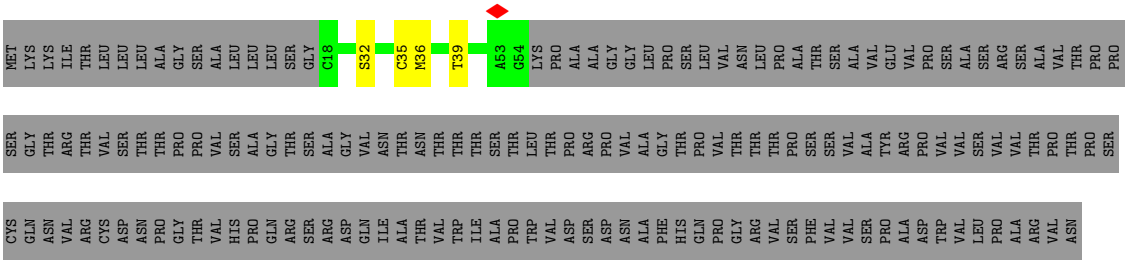

- Molecule 1: TraV

Chain AB14:

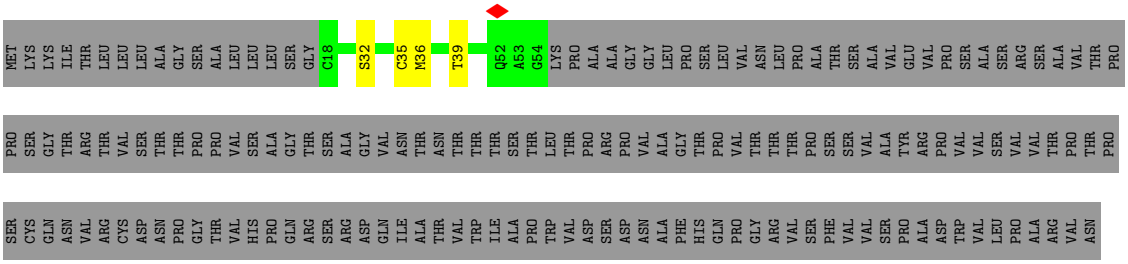

- Molecule 1: TraV

Chain AB15:

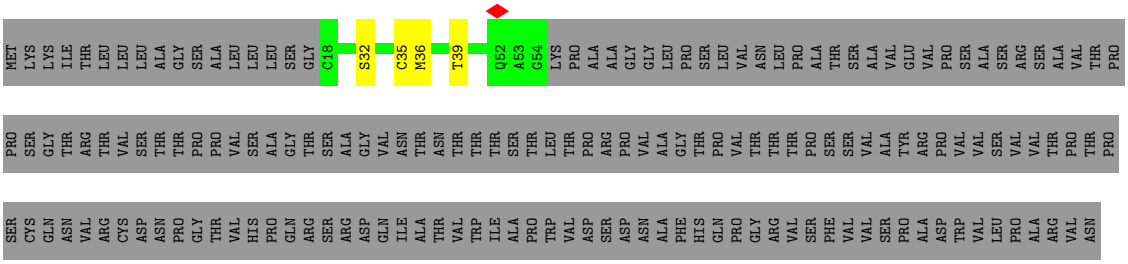

- Molecule 1: TraV

Chain AB16:



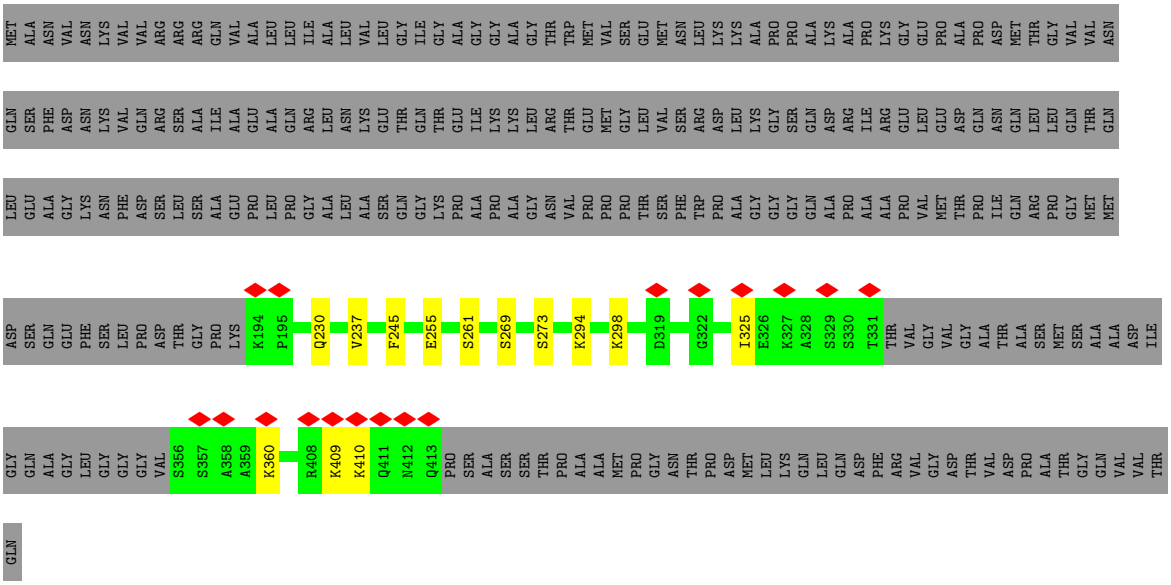
• Molecule 1: TraV

Chain AB17:

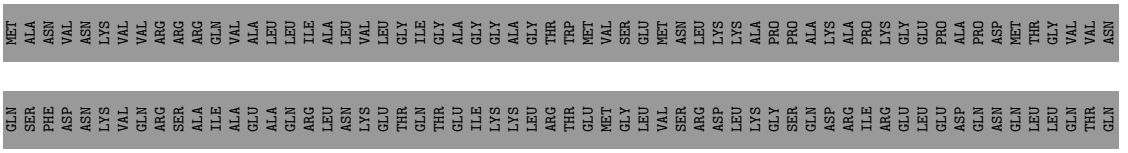
• Molecule 2: TraB

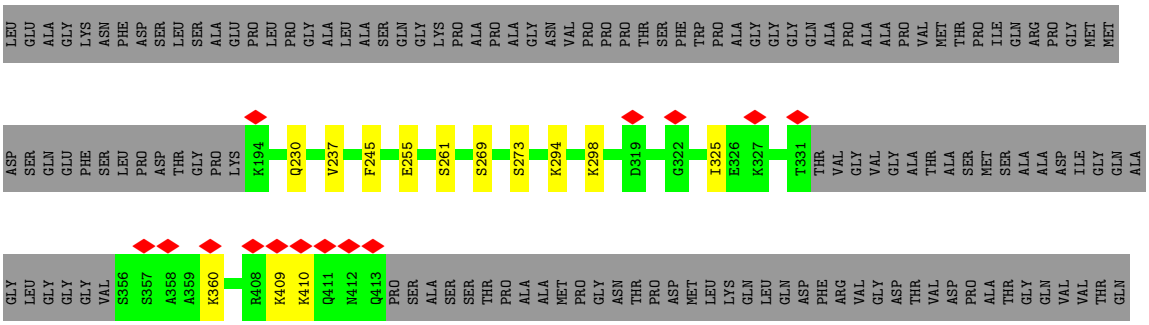
Chain EF1:

• Molecule 2: TraB

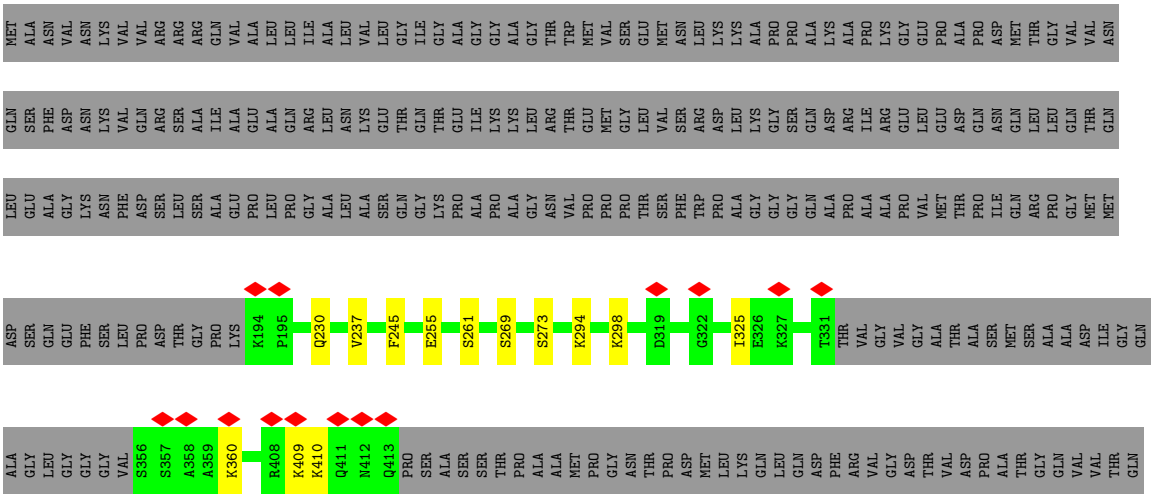
Chain EF2:



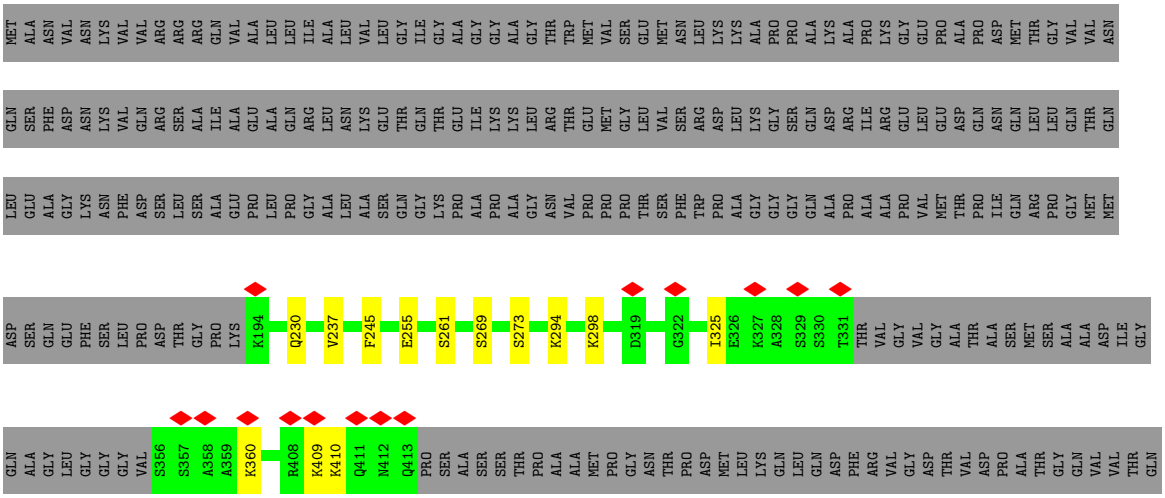

• Molecule 2: TraB

Chain EF3:

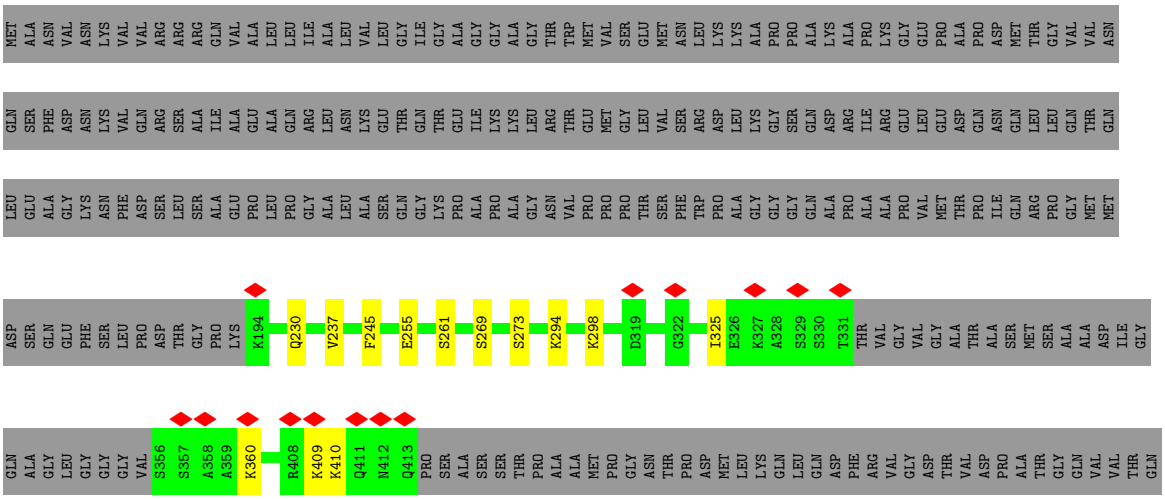

• Molecule 2: TraB

Chain EF4:

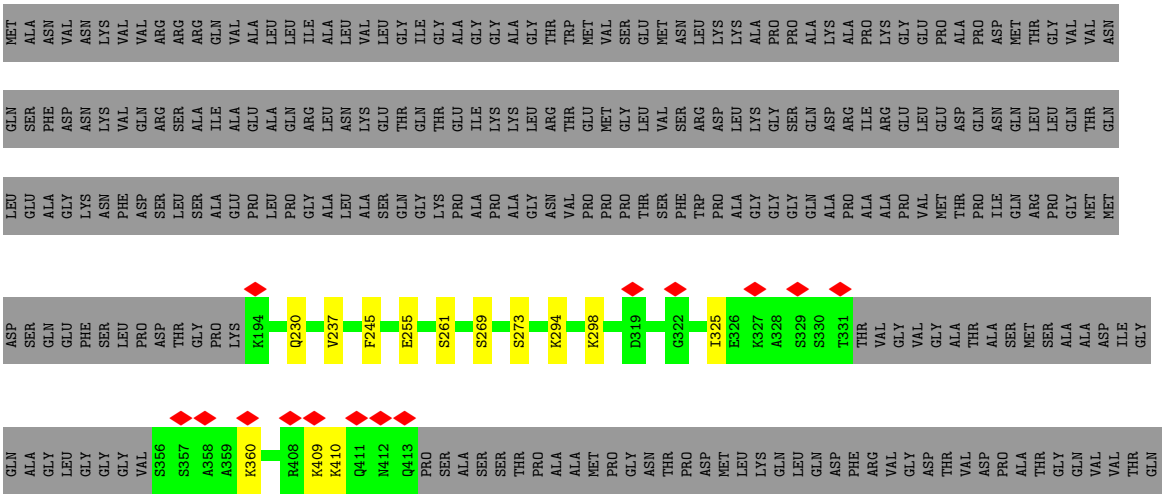

• Molecule 2: TraB

Chain EF5:



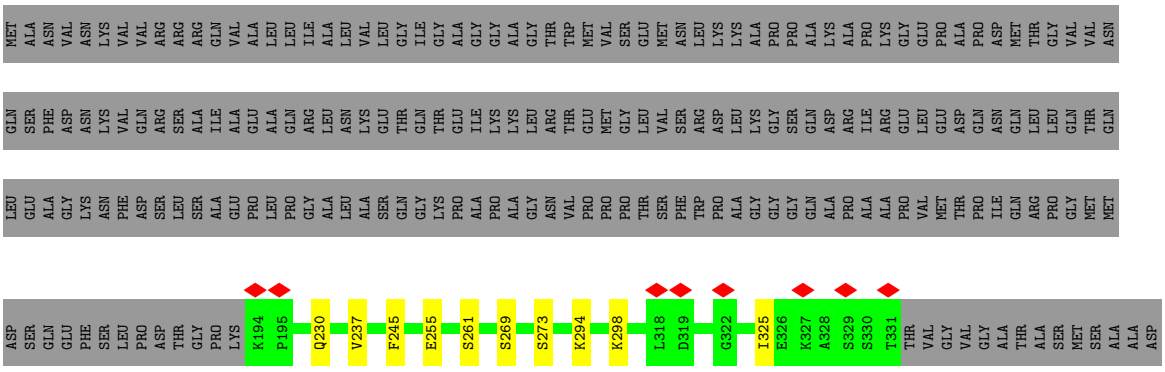

• Molecule 2: TraB

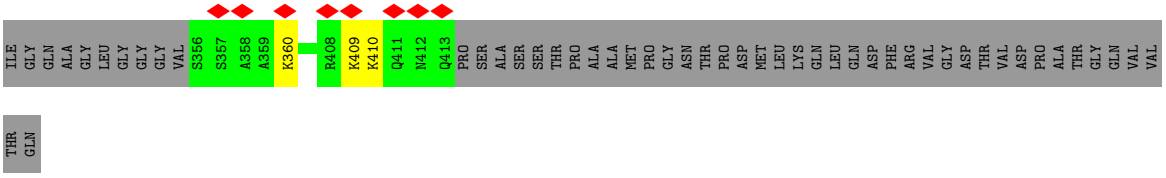
Chain EF6:


• Molecule 2: TraB

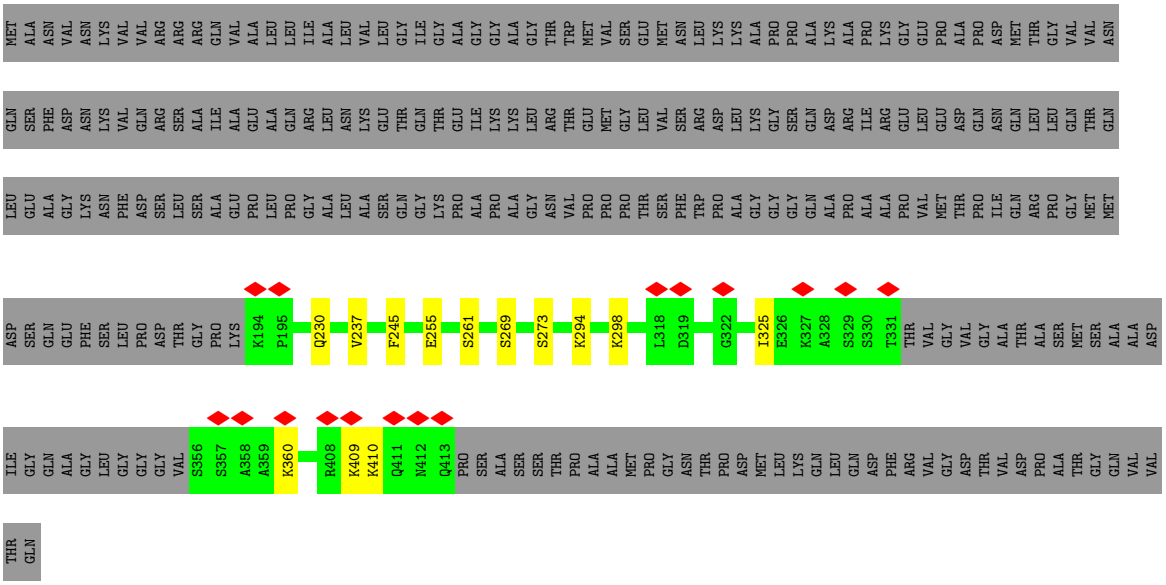
Chain EF7:



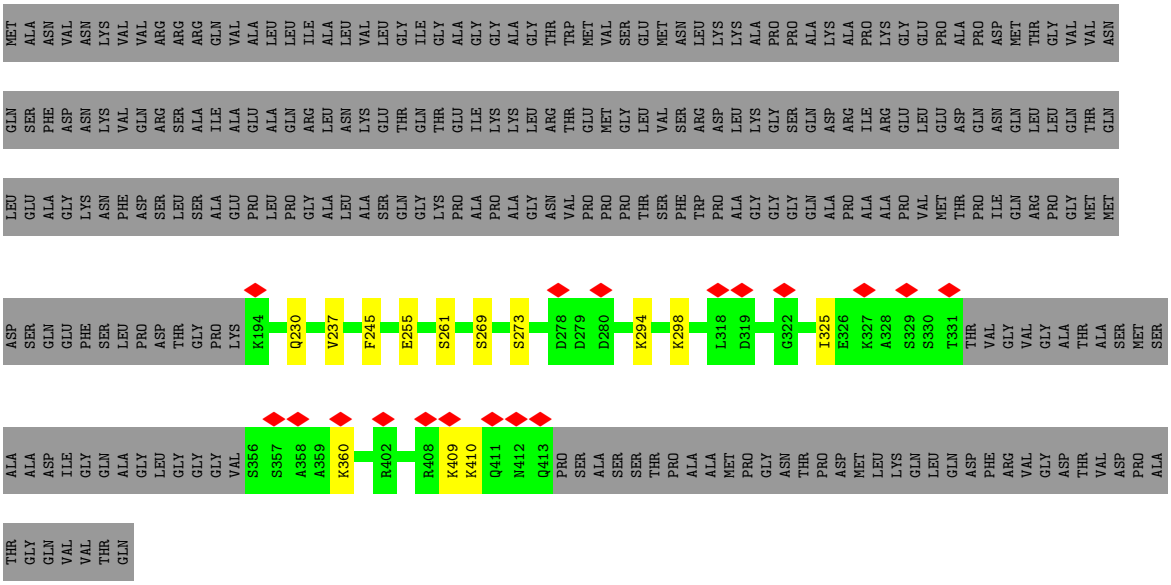

• Molecule 2: TraB

Chain EF8:

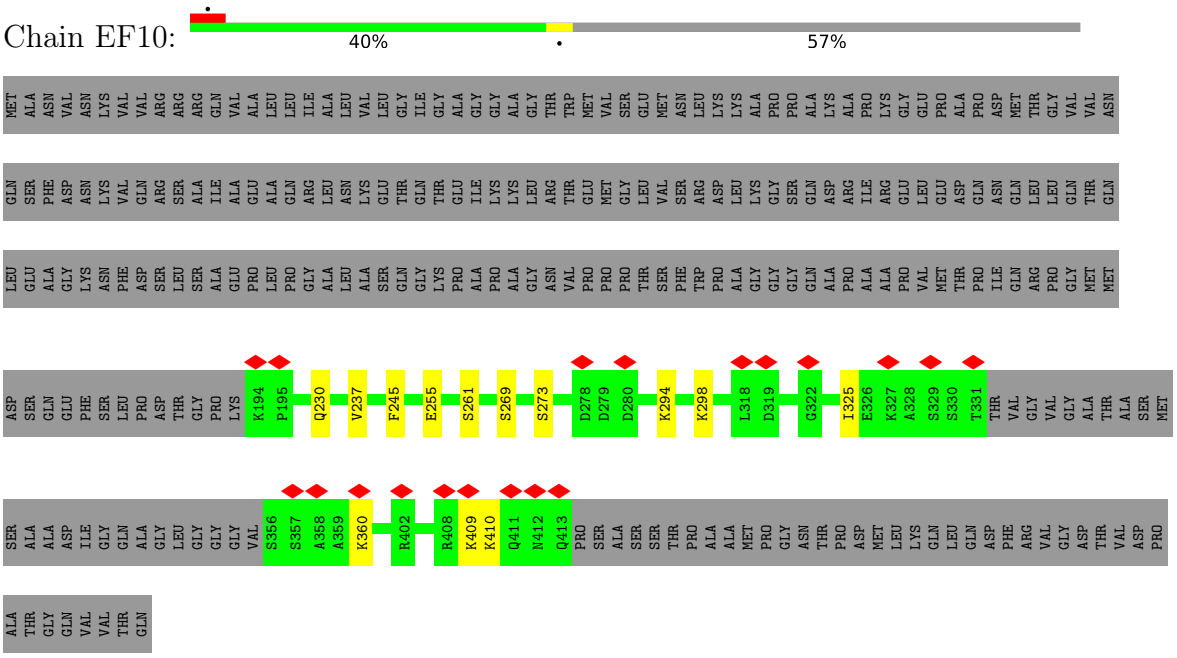

• Molecule 2: TraB

Chain EF9:

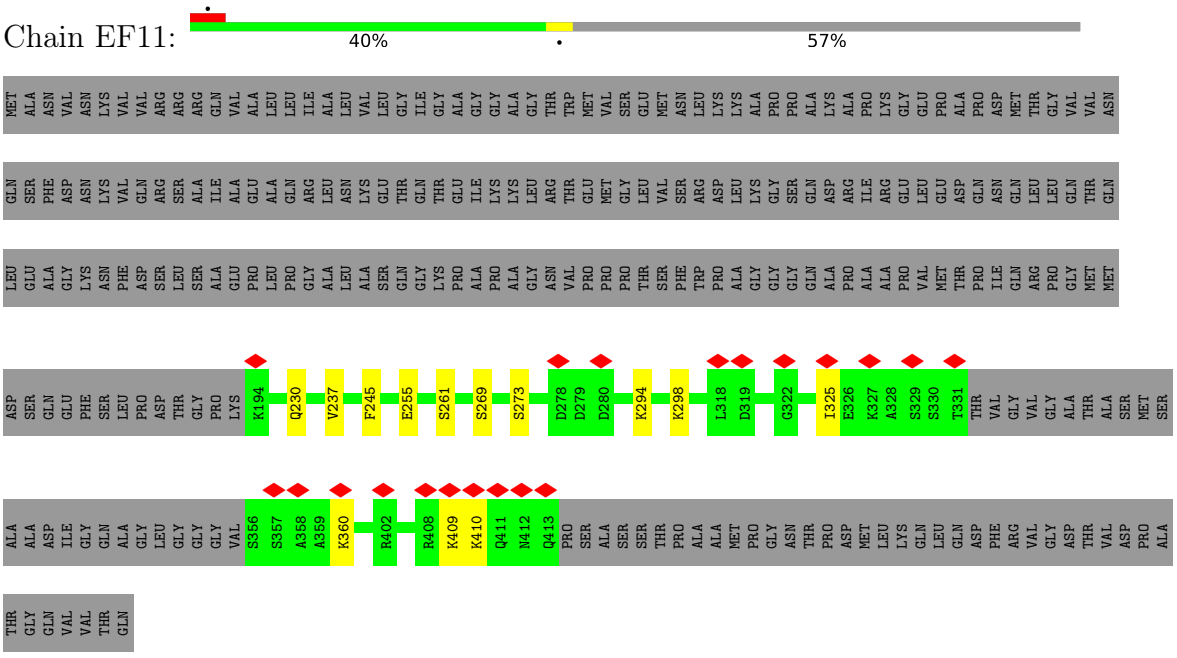

• Molecule 2: TraB

Chain EF10:



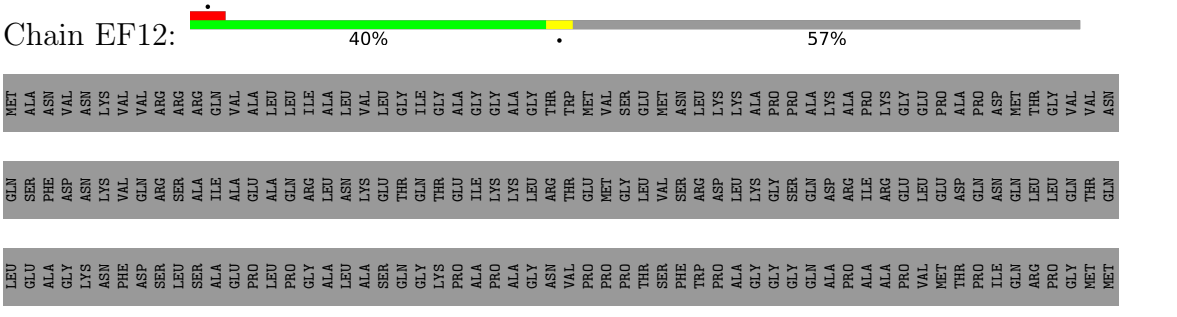

• Molecule 2: TraB

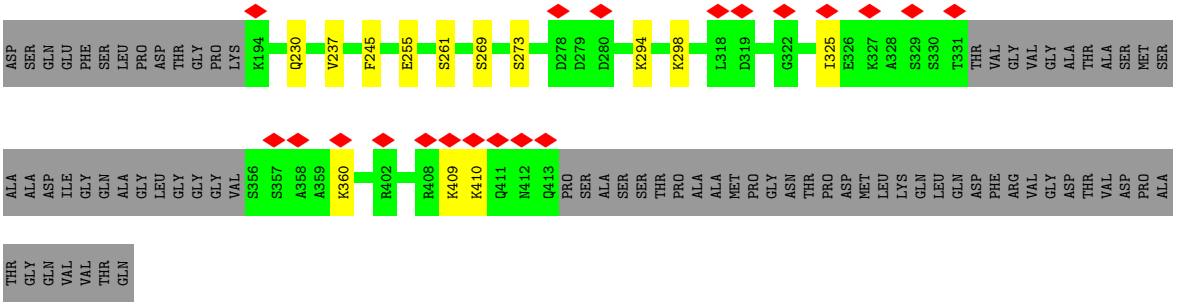
Chain EF11:




• Molecule 2: TraB

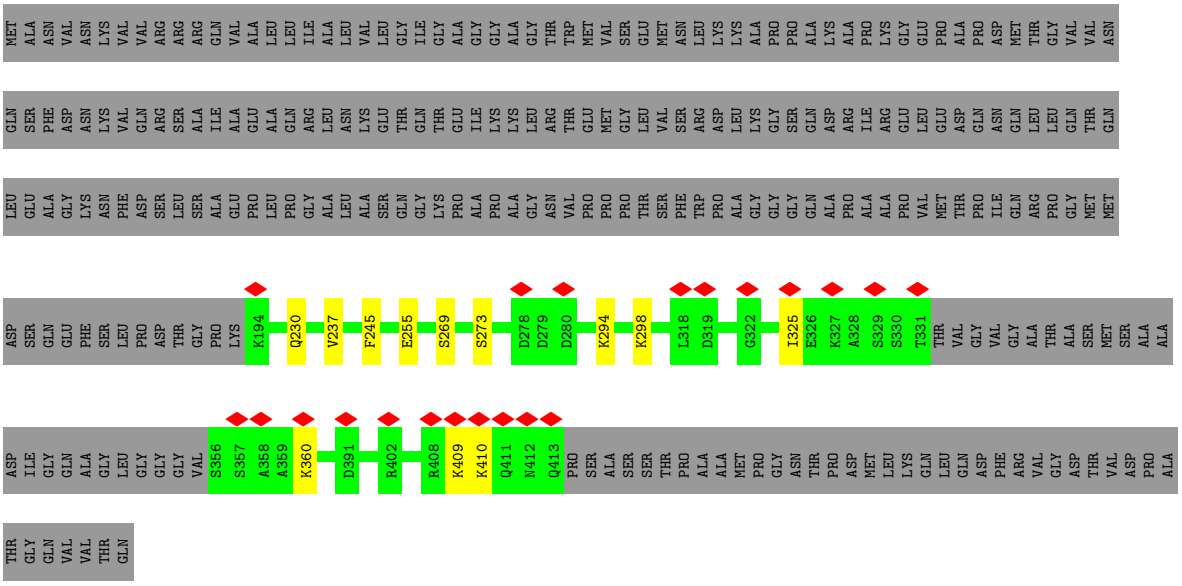
Chain EF12:





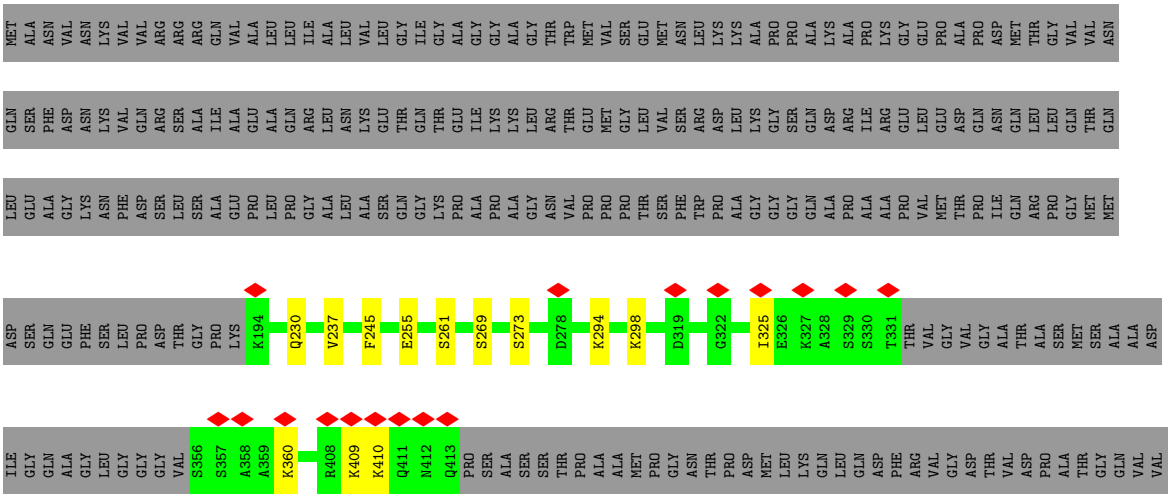
• Molecule 2: TraB

Chain EF13:

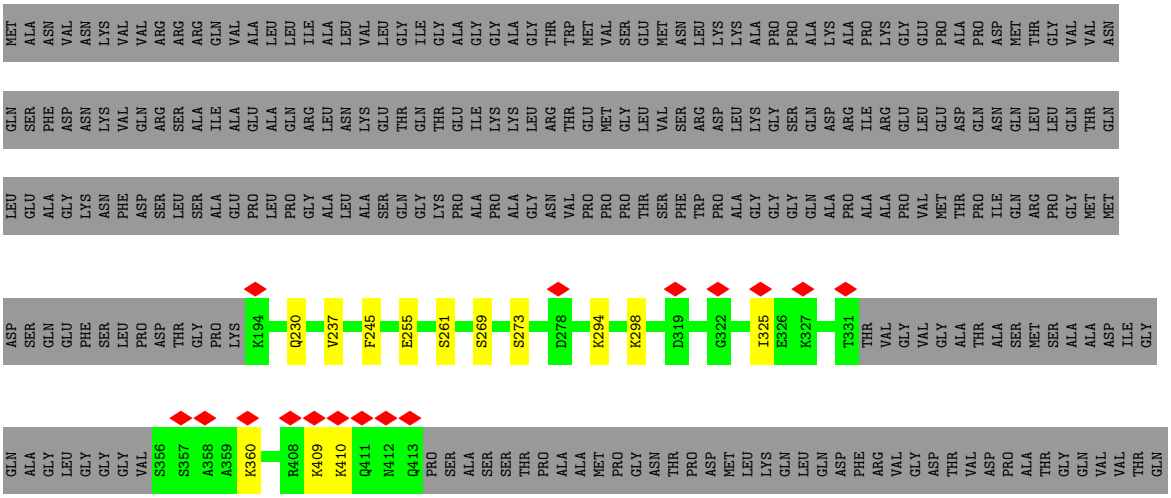
• Molecule 2: TraB

Chain EF14:

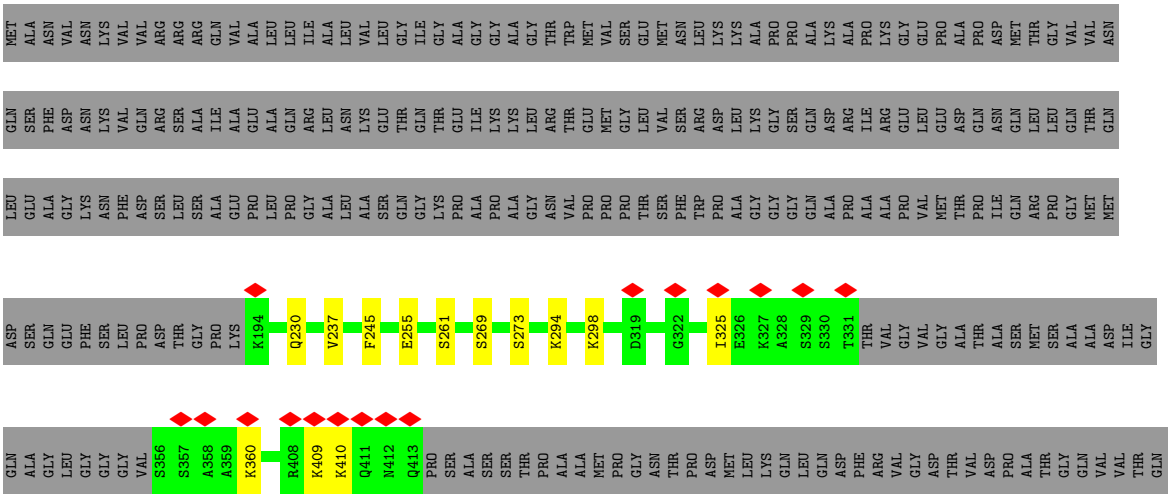

• Molecule 2: TraB

Chain EF15:

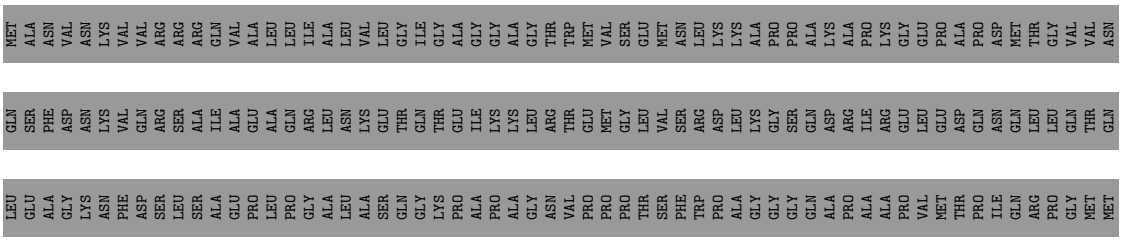

• Molecule 2: TraB

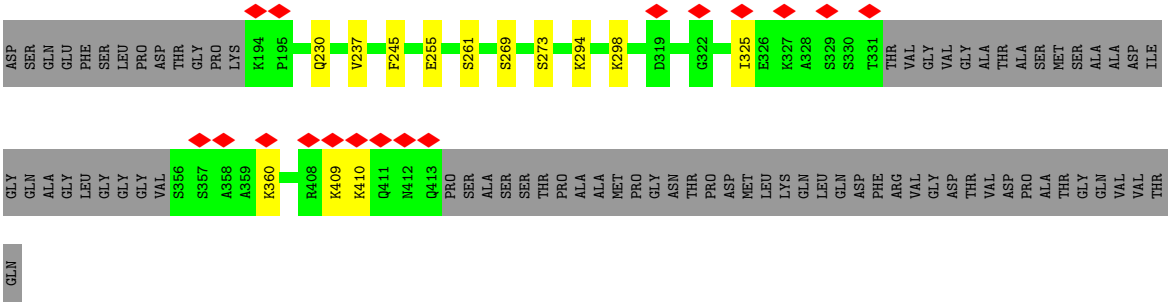
Chain EF16:


• Molecule 2: TraB

Chain EF17:


ASP SER GLN GLU PHE SER LEU PRO ASP THR GLY PRO LYS K194 P195 Q230 V237 F245 E255 S261 S269 S273 K294 K298 D319 G322 I325 E326 K327 A328 S329 S330 T331 THR VAL GLY VAL GLY ALA THR ALA SER MET SER ALA ALA ASP ILE
GLY GLN ALA GLY LEU GLY GLY GLY VAL S356 S357 A358 A359 K360 R408 K409 K410 Q411 N412 Q413 PRO SER ALA SER SER THR PRO ALA ALA MET PRO GLY ASN THR PRO ASP MET LEU LYS GLN LEU GLN ASP PHE ARG VAL GLY ASP THR VAL ASP PRO ALA THR GLY GLN VAL VAL THR
GLN

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C17 | Depositor |
| Number of particles used | 26000 | 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 ($e^-/Å^2$) | 40 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 1.908 | Depositor |
| Minimum map value | -0.933 | Depositor |
| Average map value | 0.005 | Depositor |
| Map value standard deviation | 0.059 | Depositor |
| Recommended contour level | 0.38 | Depositor |
| Map size (Å) | 426.08, 426.08, 426.08 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.0652, 1.0652, 1.0652 | 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 | AB1 | 0.50 | 0/261 | 0.67 | 0/348 |
| 1 | AB10 | 0.49 | 0/261 | 0.67 | 0/348 |
| 1 | AB11 | 0.50 | 0/261 | 0.67 | 0/348 |
| 1 | AB12 | 0.50 | 0/261 | 0.67 | 0/348 |
| 1 | AB13 | 0.49 | 0/261 | 0.67 | 0/348 |
| 1 | AB14 | 0.50 | 0/261 | 0.67 | 0/348 |
| 1 | AB15 | 0.50 | 0/261 | 0.67 | 0/348 |
| 1 | AB16 | 0.50 | 0/261 | 0.67 | 0/348 |
| 1 | AB17 | 0.50 | 0/261 | 0.67 | 0/348 |
| 1 | AB2 | 0.50 | 0/261 | 0.67 | 0/348 |
| 1 | AB3 | 0.49 | 0/261 | 0.67 | 0/348 |
| 1 | AB4 | 0.50 | 0/261 | 0.67 | 0/348 |
| 1 | AB5 | 0.50 | 0/261 | 0.67 | 0/348 |
| 1 | AB6 | 0.49 | 0/261 | 0.67 | 0/348 |
| 1 | AB7 | 0.50 | 0/261 | 0.67 | 0/348 |
| 1 | AB8 | 0.50 | 0/261 | 0.67 | 0/348 |
| 1 | AB9 | 0.50 | 0/261 | 0.67 | 0/348 |
| 2 | EF1 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF10 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF11 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF12 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF13 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF14 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF15 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF16 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF17 | 0.52 | 0/1502 | 0.67 | 0/2021 |
| 2 | EF2 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF3 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF4 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF5 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF6 | 0.52 | 0/1502 | 0.67 | 0/2021 |
| 2 | EF7 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF8 | 0.52 | 0/1502 | 0.66 | 0/2021 |
| 2 | EF9 | 0.52 | 0/1502 | 0.66 | 0/2021 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| All | All | 0.52 | 0/29971 | 0.67 | 0/40273 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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 | AB1 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB10 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB11 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB12 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB13 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB14 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB15 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB16 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB17 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB2 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB3 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB4 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | AB5 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB6 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB7 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB8 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 1 | AB9 | 35/204 (17%) | 32 (91%) | 3 (9%) | 0 | 100 | 100 |
| 2 | EF1 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF10 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF11 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF12 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF13 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF14 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF15 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF16 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF17 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF2 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF3 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF4 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF5 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF6 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF7 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF8 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | EF9 | 192/453 (42%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| All | All | 3859/11169 (35%) | 3706 (96%) | 153 (4%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | AB1 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB10 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB11 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB12 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB13 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB14 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB15 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB16 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB17 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB2 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB3 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB4 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB5 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB6 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB7 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB8 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 1 | AB9 | 28/168 (17%) | 24 (86%) | 4 (14%) | 3 | 21 |
| 2 | EF1 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |
| 2 | EF10 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |
| 2 | EF11 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |
| 2 | EF12 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |
| 2 | EF13 | 155/353 (44%) | 143 (92%) | 12 (8%) | 13 | 44 |
| 2 | EF14 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |
| 2 | EF15 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |
| 2 | EF16 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |
| 2 | EF17 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |
| 2 | EF2 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |
| 2 | EF3 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |
| 2 | EF4 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |
| 2 | EF5 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |
| 2 | EF6 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |
| 2 | EF7 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 | 41 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 2 | EF8 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 41 |
| 2 | EF9 | 155/353 (44%) | 142 (92%) | 13 (8%) | 11 41 |
| All | All | 3111/8857 (35%) | 2823 (91%) | 288 (9%) | 12 38 |

5 of 288 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | EF13 | 298 | LYS |
| 2 | EF17 | 409 | LYS |
| 2 | EF14 | 245 | PHE |
| 2 | EF15 | 409 | LYS |
| 2 | EF3 | 255 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides 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.

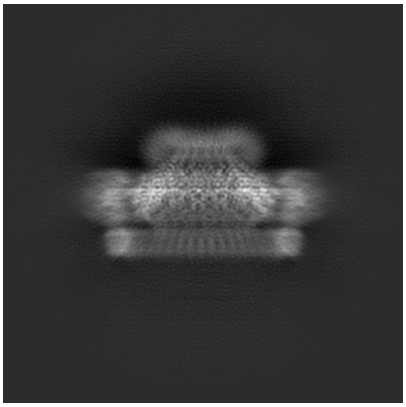
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24772. These allow visual inspection of the internal detail of the map and identification of artifacts.

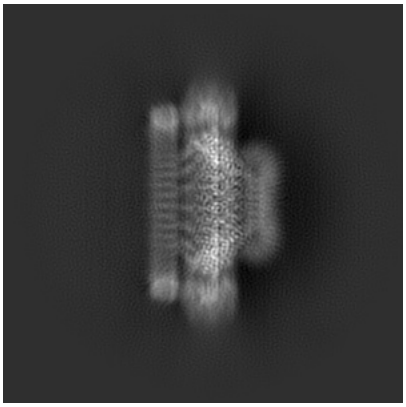
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

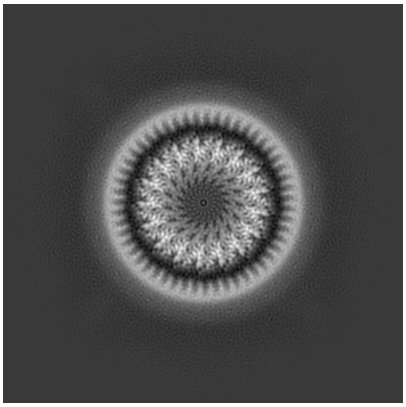
### 6.1.1 Primary map



X



Y

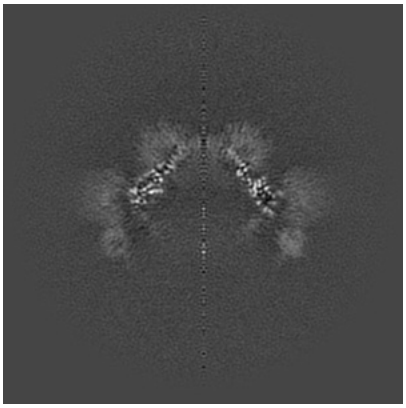


Z

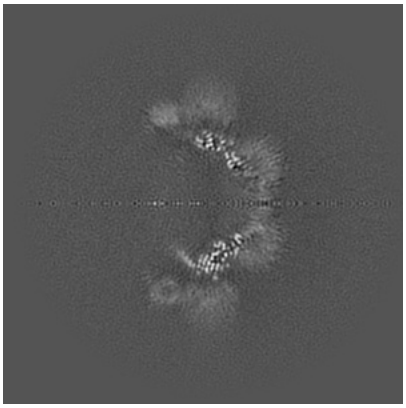
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

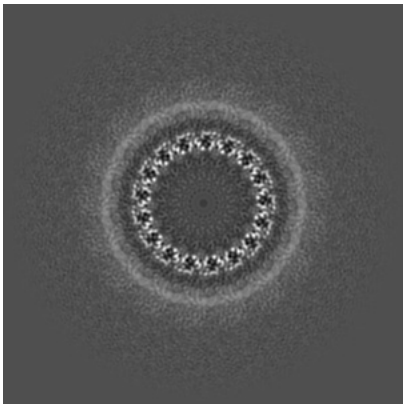
### 6.2.1 Primary map



X Index: 200



Y Index: 200

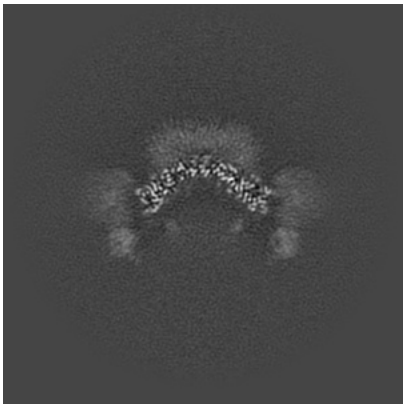


Z Index: 200

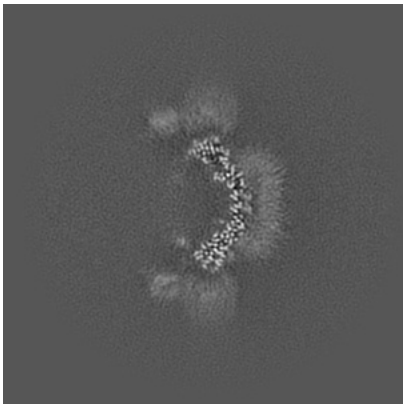
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

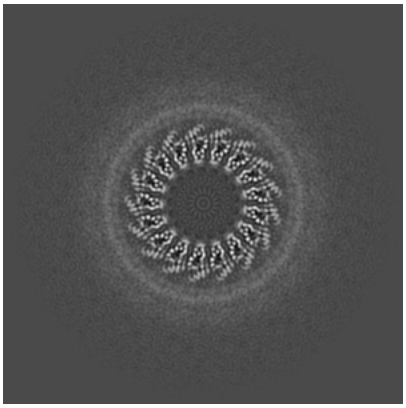
### 6.3.1 Primary map



X Index: 166



Y Index: 167



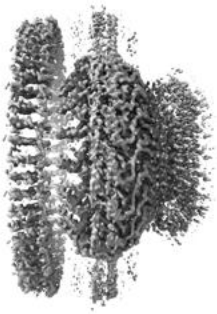
Z Index: 212

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

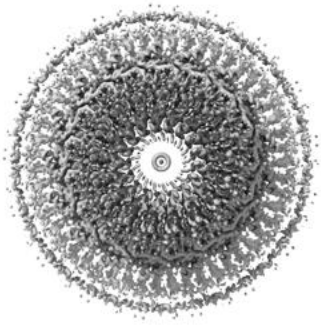
## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

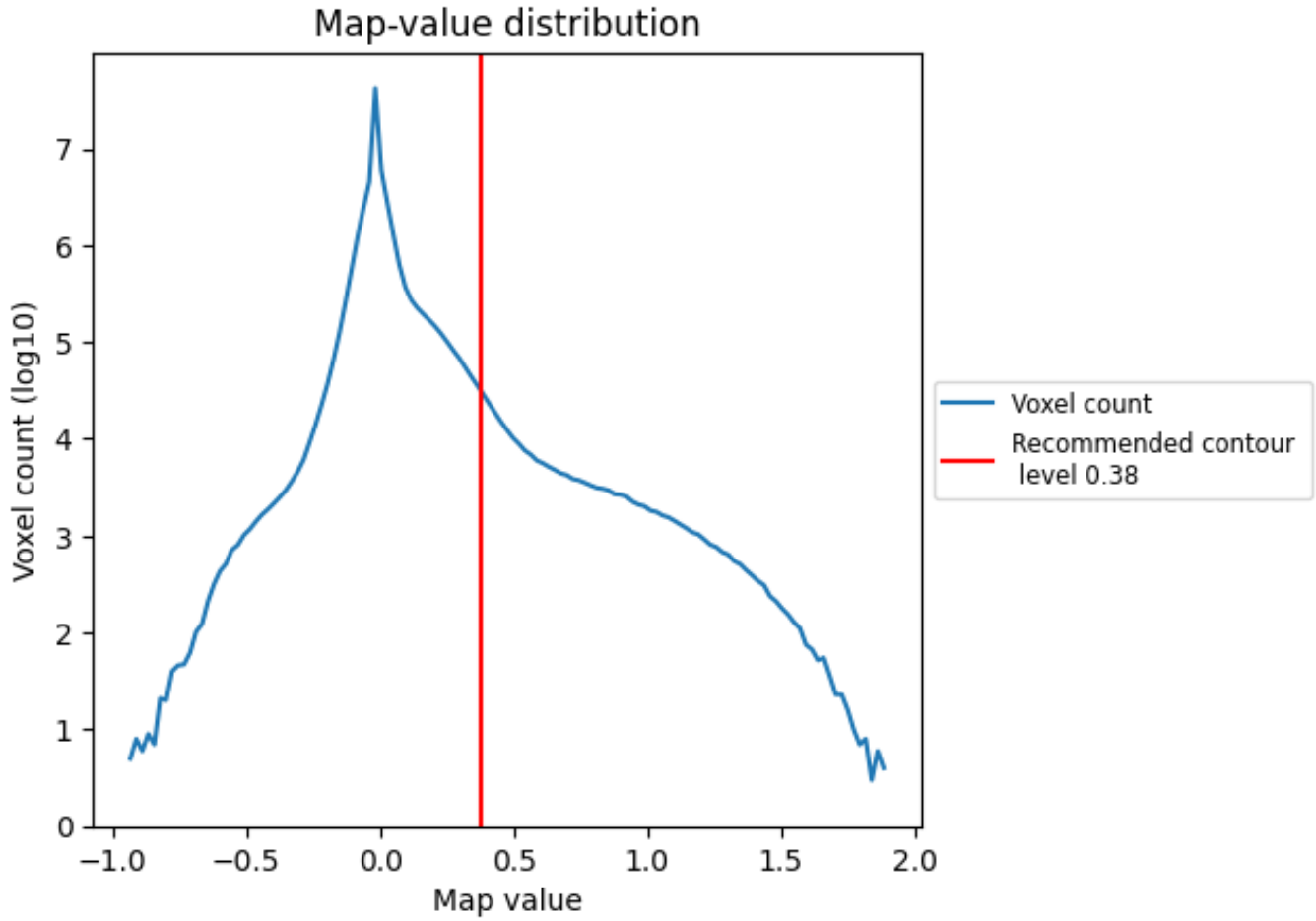
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

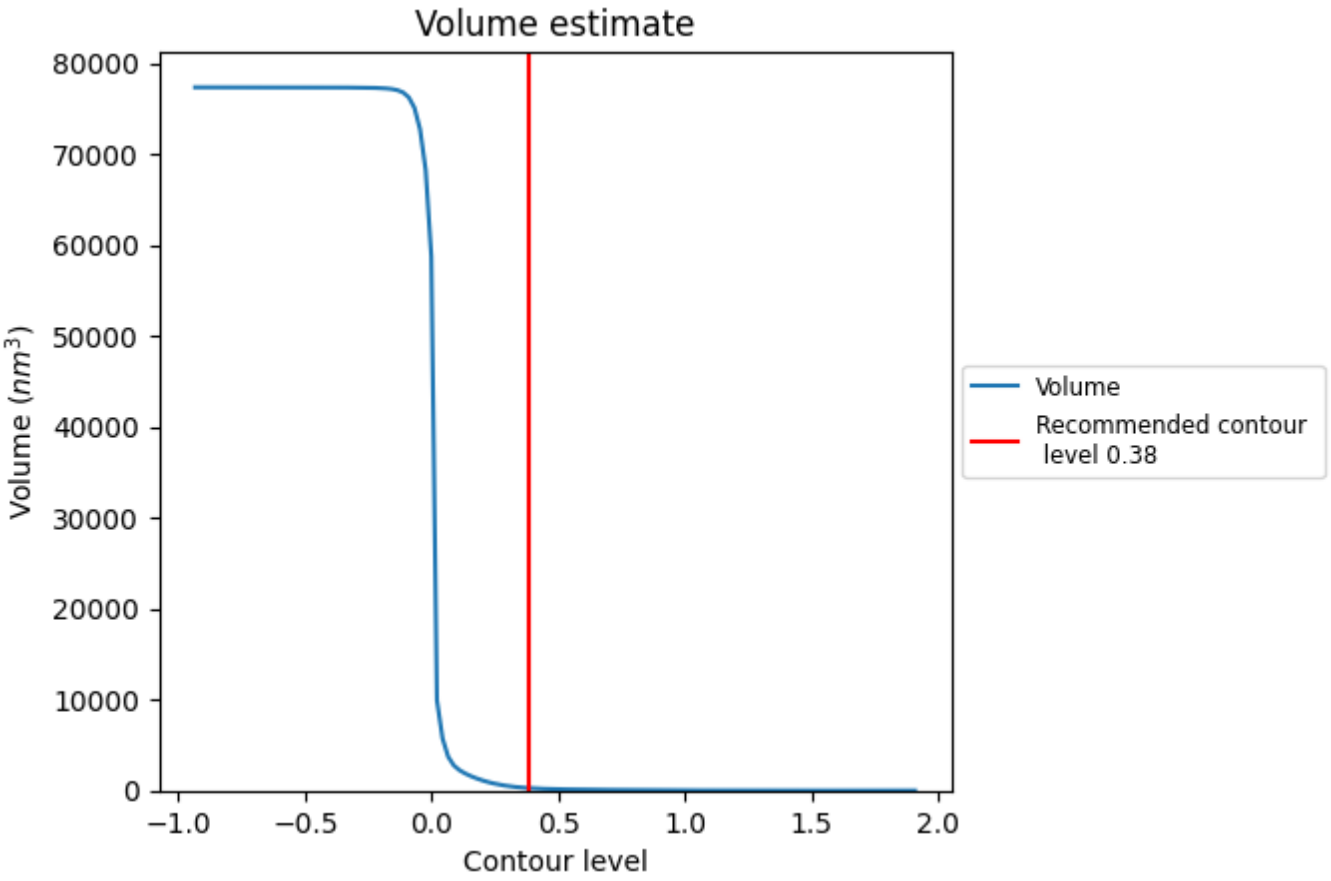
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

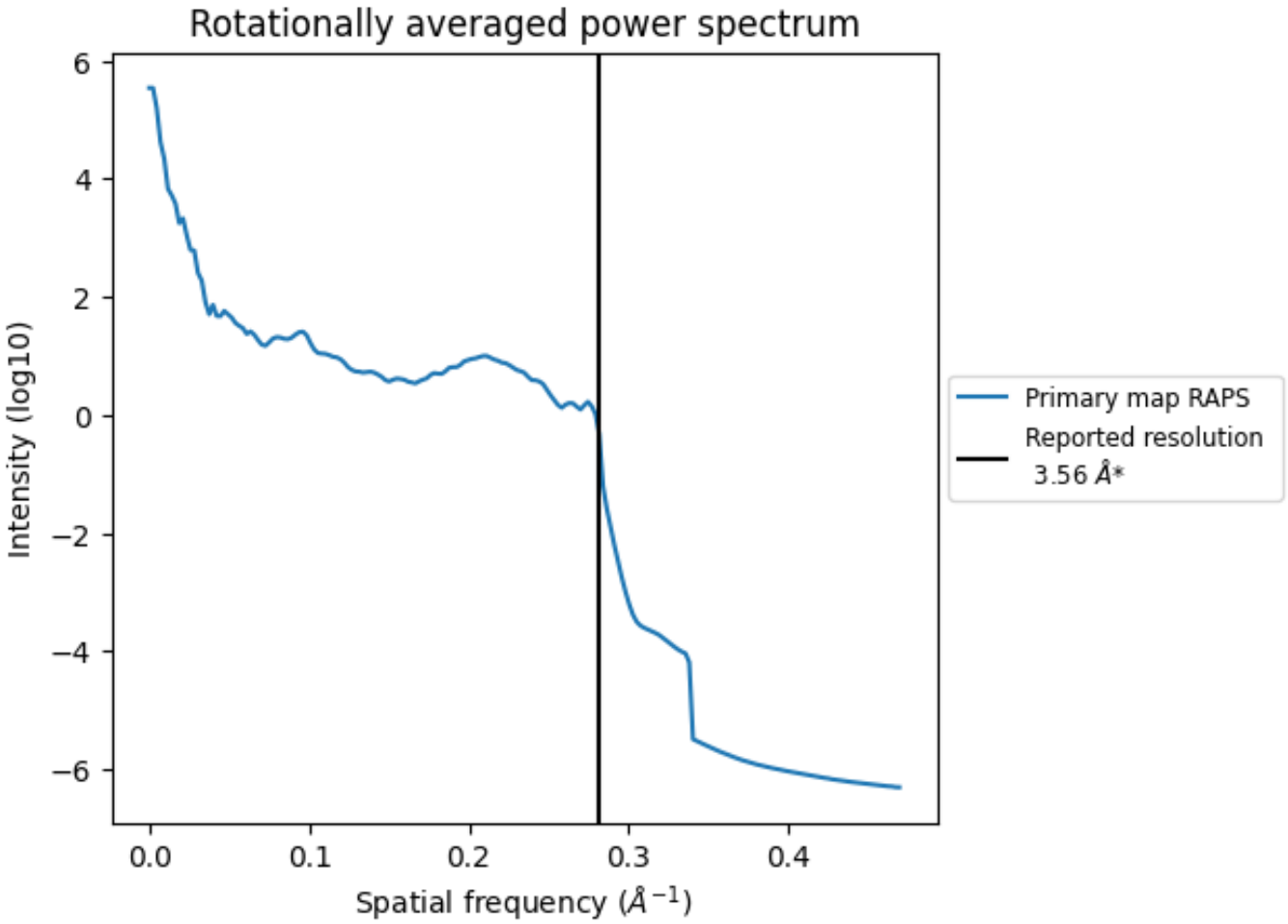
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 279 $nm^3$; this corresponds to an approximate mass of 252 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 0.281 Å$^{-1}$

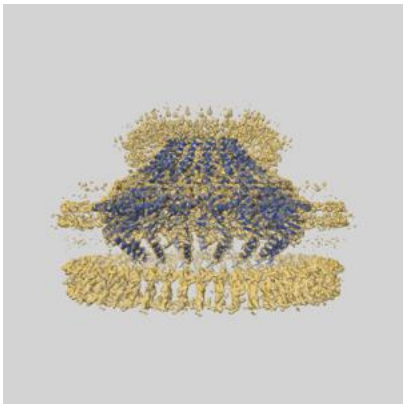
# 8 Fourier-Shell correlation

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

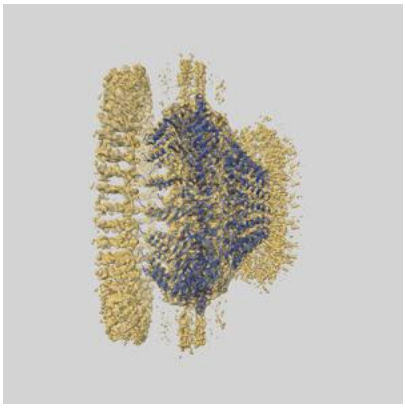
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24772 and PDB model 7SPJ. Per-residue inclusion information can be found in section 3 on page 6.

## 9.1 Map-model overlay



X

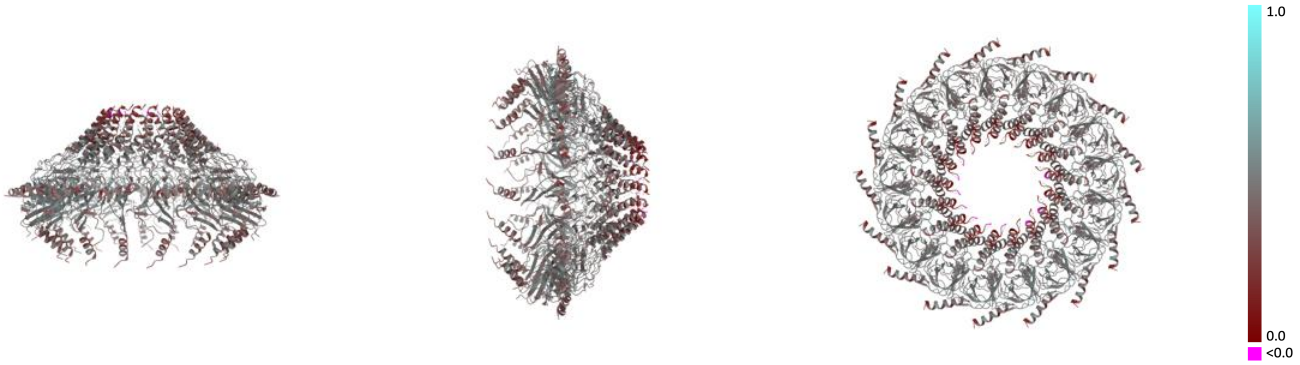


Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.38 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.

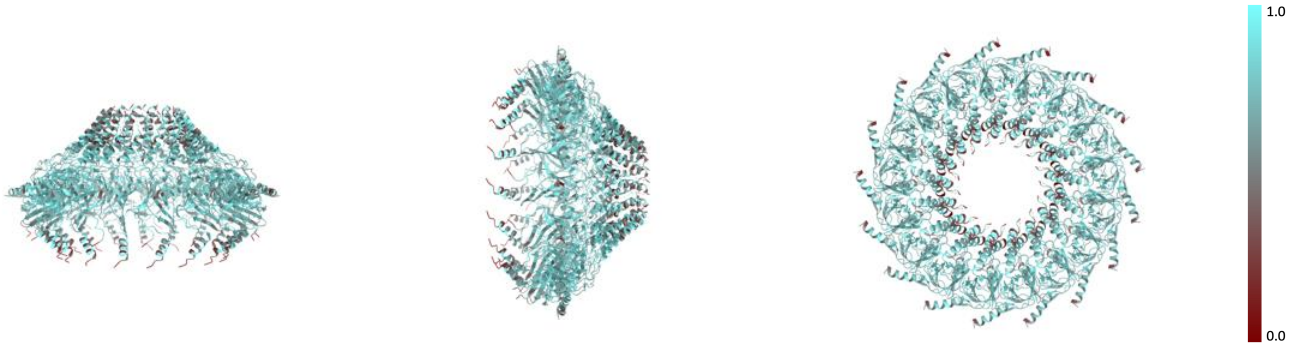
## 9.2 Q-score mapped to coordinate model




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.

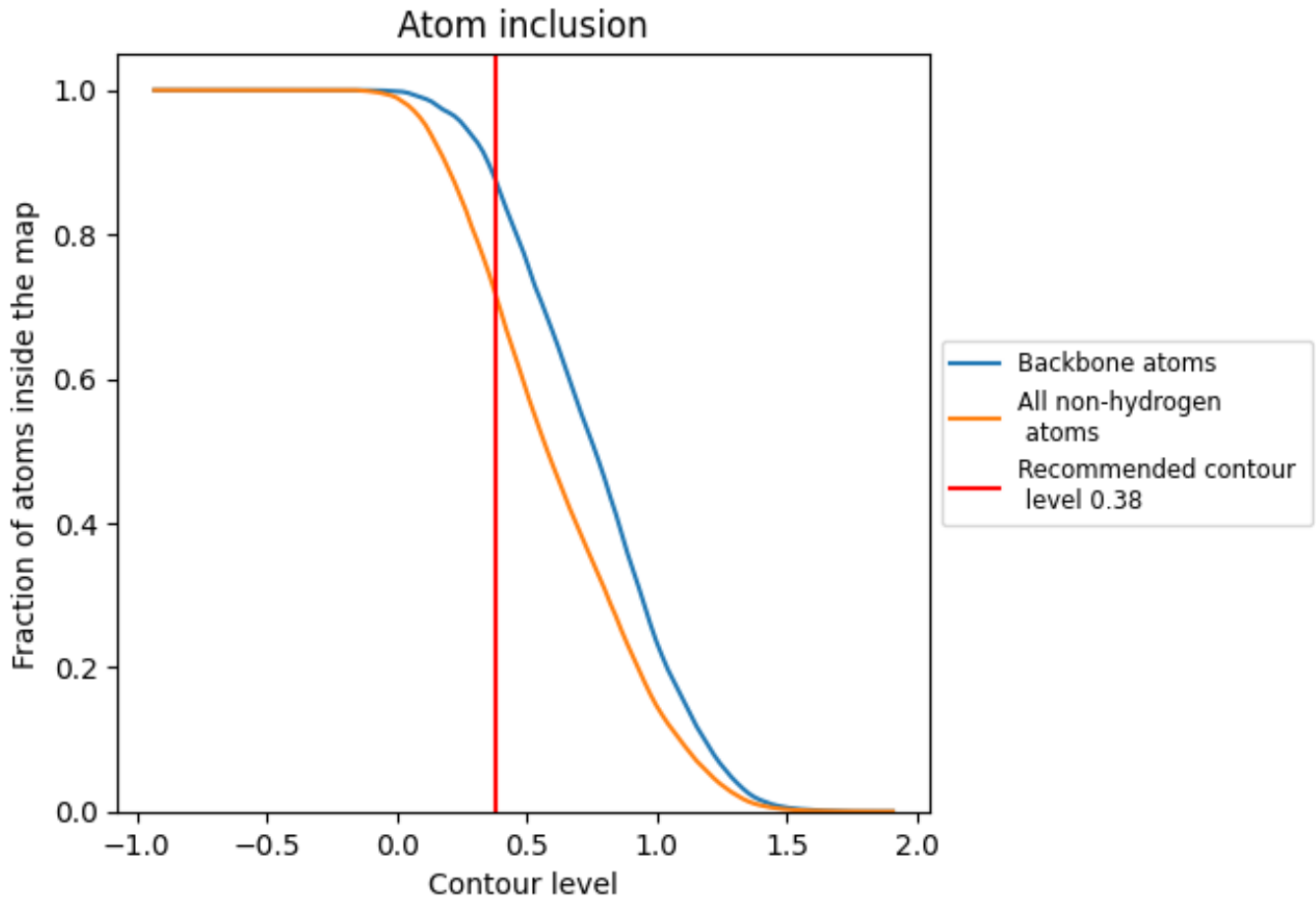
## 9.3 Atom inclusion mapped to coordinate model




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 (0.38).

## 9.4 Atom inclusion (i)




At the recommended contour level, 87% of all backbone atoms, 72% 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 (0.38) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7162 | 0.4300 |
| AB1 | 0.7066 | 0.4350 |
| AB10 | 0.6988 | 0.4060 |
| AB11 | 0.7066 | 0.4110 |
| AB12 | 0.6988 | 0.4130 |
| AB13 | 0.7027 | 0.4210 |
| AB14 | 0.7027 | 0.4260 |
| AB15 | 0.7181 | 0.4280 |
| AB16 | 0.7181 | 0.4330 |
| AB17 | 0.7220 | 0.4330 |
| AB2 | 0.6950 | 0.4330 |
| AB3 | 0.6873 | 0.4290 |
| AB4 | 0.6795 | 0.4290 |
| AB5 | 0.6911 | 0.4230 |
| AB6 | 0.6795 | 0.4170 |
| AB7 | 0.6834 | 0.4130 |
| AB8 | 0.6911 | 0.4120 |
| AB9 | 0.6911 | 0.4080 |
| EF1 | 0.7315 | 0.4490 |
| EF10 | 0.7074 | 0.4170 |
| EF11 | 0.7040 | 0.4170 |
| EF12 | 0.7115 | 0.4220 |
| EF13 | 0.7088 | 0.4270 |
| EF14 | 0.7163 | 0.4330 |
| EF15 | 0.7280 | 0.4400 |
| EF16 | 0.7315 | 0.4450 |
| EF17 | 0.7349 | 0.4500 |
| EF2 | 0.7342 | 0.4470 |
| EF3 | 0.7239 | 0.4430 |
| EF4 | 0.7218 | 0.4360 |
| EF5 | 0.7260 | 0.4310 |
| EF6 | 0.7184 | 0.4250 |
| EF7 | 0.7170 | 0.4220 |
| EF8 | 0.7081 | 0.4180 |
| EF9 | 0.7054 | 0.4140 |