# wwPDB EM Validation Summary Report (i)

Aug 5, 2026 – 09:47 PM JST

| | | |
|---|---|---|
| PDB ID | : | 8IYL / pdb_00008iyl |
| EMDB ID | : | EMD-35825 |
| Title | : | Tail tip conformation 2 of phage lambda tail |
| Authors | : | Wang, J.W.; Wang, C. |
| Deposited on | : | 2023-04-05 |
| Resolution | : | 3.00 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 (1)) were used in the production of this report:

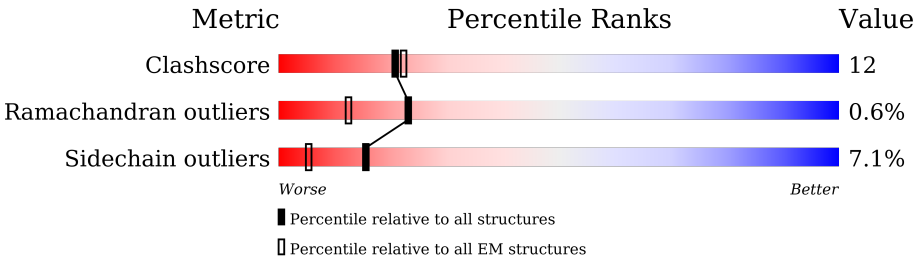
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.50 |

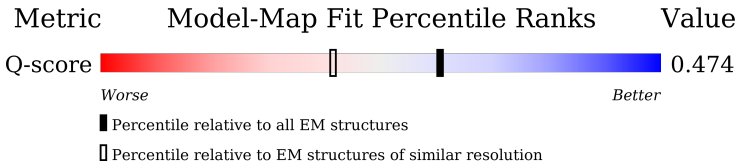
# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 14081 ( 2.50 - 3.50 ) |

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 | D | 109 | 69% 29% • |
| 1 | F | 109 | 72% 27% • |
| 1 | M | 109 | 72% 26% • |
| 1 | X | 109 | 74% 24% • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | Z | 109 | 72% 26% |
| 1 | m | 109 | 74% 26% |
| 2 | E | 1132 | 52% 22% 24% |
| 2 | J | 1132 | 53% 21% 24% |
| 2 | Y | 1132 | 53% 21% 24% |
| 3 | G | 232 | 80% 20% |
| 3 | L | 232 | 78% 21% |
| 3 | d | 232 | 80% 19% |
| 4 | H | 853 | 96% |
| 4 | K | 853 | 96% |
| 4 | e | 853 | 96% |
| 5 | I | 223 | 35% 17% 45% |
| 5 | N | 223 | 34% 17% 45% |
| 5 | f | 223 | 33% 18% 45% |
| 6 | A | 246 | 7% 65% 32% |
| 6 | B | 246 | 11% 67% 29% |
| 6 | C | 246 | 33% 63% 34% |
| 6 | O | 246 | 11% 72% 26% |
| 6 | P | 246 | 13% 70% 28% |
| 6 | Q | 246 | 13% 62% 33% |
| 6 | R | 246 | 15% 72% 25% |
| 6 | S | 246 | 8% 67% 30% |
| 6 | T | 246 | 9% 66% 29% |
| 6 | U | 246 | 33% 65% 31% |
| 6 | V | 246 | 11% 70% 28% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 6 | W | 246 | 33% 70% 28% |
| 6 | a | 246 | 9% 72% 23% |
| 6 | b | 246 | 14% 70% 27% |
| 6 | c | 246 | 33% 71% 26% |
| 6 | g | 246 | 11% 71% 27% |
| 6 | h | 246 | 13% 72% 26% |
| 6 | i | 246 | 12% 65% 30% |
| 6 | j | 246 | 14% 70% 26% |
| 6 | k | 246 | 8% 67% 29% |
| 6 | l | 246 | 9% 67% 30% |
| 6 | n | 246 | 33% 63% 35% |
| 6 | o | 246 | 33% 67% 29% |
| 6 | v | 246 | 13% 69% 28% |

# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 77370 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 Tail tip protein M.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | M | 109 | 884 | 569 | 154 | 157 | 4 | 0 | 0 |
| 1 | m | 109 | 884 | 569 | 154 | 157 | 4 | 0 | 0 |
| 1 | D | 109 | 884 | 569 | 154 | 157 | 4 | 0 | 0 |
| 1 | F | 109 | 884 | 569 | 154 | 157 | 4 | 0 | 0 |
| 1 | X | 109 | 884 | 569 | 154 | 157 | 4 | 0 | 0 |
| 1 | Z | 109 | 884 | 569 | 154 | 157 | 4 | 0 | 0 |

- Molecule 2 is a protein called Tip attachment protein J.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | J | 861 | 6720 | 4212 | 1171 | 1317 | 20 | 0 | 0 |
| 2 | E | 861 | 6720 | 4212 | 1171 | 1317 | 20 | 0 | 0 |
| 2 | Y | 861 | 6720 | 4212 | 1171 | 1317 | 20 | 0 | 0 |

- Molecule 3 is a protein called Tail tip protein L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | L | 232 | 1801 | 1117 | 309 | 362 | 13 | 0 | 0 |
| 3 | G | 232 | 1801 | 1117 | 309 | 362 | 13 | 0 | 0 |
| 3 | d | 232 | 1801 | 1117 | 309 | 362 | 13 | 0 | 0 |

- Molecule 4 is a protein called Tape measure protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | H | 33 | 250 | 154 | 47 | 47 | 2 | 0 | 0 |
| 4 | K | 33 | 250 | 154 | 47 | 47 | 2 | 0 | 0 |
| 4 | e | 33 | 250 | 154 | 47 | 47 | 2 | 0 | 0 |

- Molecule 5 is a protein called Tail tip assembly protein I.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | I | 122 | 865 | 544 | 151 | 165 | 5 | 0 | 0 |
| 5 | N | 122 | 865 | 544 | 151 | 165 | 5 | 0 | 0 |
| 5 | f | 122 | 865 | 544 | 151 | 165 | 5 | 0 | 0 |

- Molecule 6 is a protein called Tail tube protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | V | 243 | 1792 | 1119 | 302 | 366 | 5 | 0 | 0 |
| 6 | v | 243 | 1792 | 1119 | 302 | 366 | 5 | 0 | 0 |
| 6 | B | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | b | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | A | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | a | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | C | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | c | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | O | 243 | 1792 | 1119 | 302 | 366 | 5 | 0 | 0 |
| 6 | P | 243 | 1792 | 1119 | 302 | 366 | 5 | 0 | 0 |
| 6 | Q | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | R | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |

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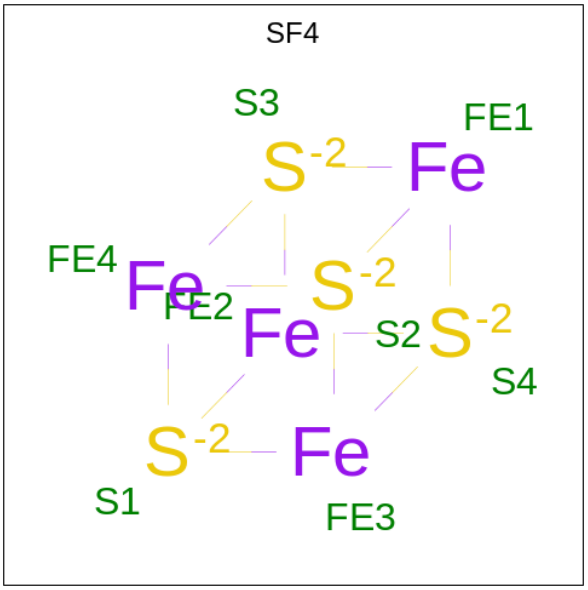
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | S | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | T | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | U | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | W | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | g | 243 | 1792 | 1119 | 302 | 366 | 5 | 0 | 0 |
| 6 | h | 243 | 1792 | 1119 | 302 | 366 | 5 | 0 | 0 |
| 6 | i | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | j | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | k | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | l | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | n | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |
| 6 | o | 244 | 1799 | 1124 | 303 | 367 | 5 | 0 | 0 |

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: $Fe_4S_4$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Fe | S | |
| 7 | L | 1 | 8 | 4 | 4 | 0 |
| | | | Total | Fe | S | |
| 7 | G | 1 | 8 | 4 | 4 | 0 |
| | | | Total | Fe | S | |
| 7 | d | 1 | 8 | 4 | 4 | 0 |

# 3 Residue-property plots (i)

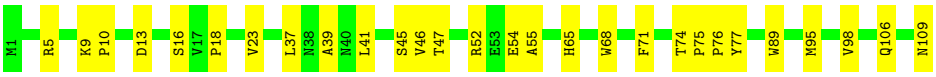
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Tail tip protein M

Chain M: 72% 26%

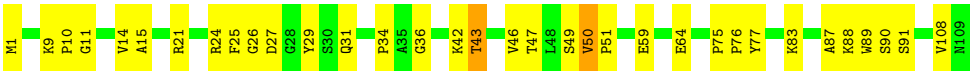
• Molecule 1: Tail tip protein M

Chain m: 74% 26%



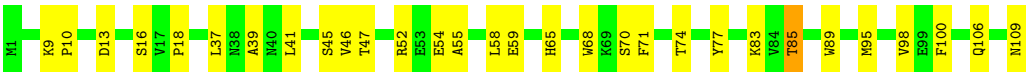

• Molecule 1: Tail tip protein M

Chain D: 69% 29%



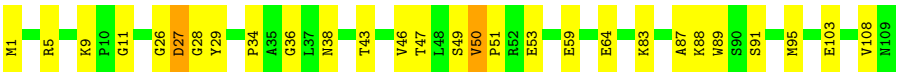

• Molecule 1: Tail tip protein M

Chain F: 72% 27%




• Molecule 1: Tail tip protein M

Chain X: 74% 24%




• Molecule 1: Tail tip protein M

Chain Z: 72% 26% •

M1 K9 P10 D13 S16 V17 P18 L37 N38 A39 N40 L41 S45 V46 T47 R52 E53 E54 A55 L58 H65 W68 F71 T74 Y77 A87 K88 W89 M95 V98 Q106 V107 V108 N109

• Molecule 2: Tip attachment protein J

Chain J: 53% 21% • 24%

M1 G2 K3 S6 T21 Q22 L23 V26 I27 D28 S31 E32 G33 E36 V39 D40 L47 N48 S49 D54 N58 T65 F68 R69 A70 G71 Q75 E82 E87 T88 V89 L90 Y96 D97 T98 P99 I100 T101 R102 T103 I104 T105 S106 A107 N108

I109 L112 R113 F114 G117 V118 L121 V122 R130 S133 E134 V135 R136 L137 L138 V139 Q140 I141 Q142 R143 W147 V148 T149 D152 I153 T154 I155 K158 S161 L164 A165 S166 V167 V168 M169 R175 P176 F177 R180 R183 M184 T185 P186 N195 W199

S200 S201 E204 D207 V208 K209 Q210 P213 N214 T215 A216 L217 V218 G219 D223 S233 Y236 R239 G240 R241 Q244 S247 N248 Y249 S257 G258 I259 W260 D261 G262 T263 F264 K265 N271 M272 A273 W274 W277 Y285 G286 M287 R290 L291 L301

D309 C325 N326 A327 Y328 D341 A345 M346 R347 V351 Q355 Q361 D362 R363 P364 S365 D366 Y371 N372 R373 S374 N375 M378 P379 D380 D381 P384 F385 R386 F389 S390 A391 L392 R395 H396 N397 A398 I404 D405 N408 G409 W410 E411 T412 D419

I423 A424 R425 N429 V430 M433 D434 A435 F436 T439 W450 K453 T461 F464 S465 H473 V474 P475 I479 D484 V495 S500 R503 T504 D508 R509 E510 I511 P514 V535 V538 T539 D540 G541 V542 K543 V544 K545 V546 V549 P550 D551

Y556 S557 V558 W559 E560 L563 L566 E578 T583 Y584 A585 P593 E596 D600 V613 V616 A620 V621 E627 V628 T629 Q636 T643 V646 G649 V650 L667 R679 F680 T681 Q682 L683 A684 Y688 A694 V695 Q700 Q701 G702

D703 L722 T723 P724 G725 Q728 I729 T730 T741 F744 E745 F748 S749 E750 K751 Q752 D755 I756 R757 Q758 V759 T763 L766 G767 T768 A769 L770 Y771 W772 S776 I777 N778 I779 K780 P781 Y785 Y786 V792 K797 A803 A807 E812 L815 D816

F817 F818 K819 G820 K821 I822 T823 H826 L827 G828 K829 E830 L831 L832 L845 D857 N860 A861 MET TRP ALA VAL LYS ILE GLU GLN THR LYS ASP GLY LYS HIS TYR VAL ALA GLY ILE GLY LEU SER MET GLU ASP THR GLU GLU GLY LYS LEU SER GLN PHE LEU VAL ALA ALA

ASN ARG ILE ALA PHE ILE ASP PRO ALA ASN GLY ASN GLU THR PRO MET PHE VAL ALA GLN GLY ASN GLN ILE PHE MET ASN ASP VAL PHE LEU LYS ARG LEU THR ALA PRO THR ILE THR LEU SER GLY GLY ASN PRO PRO ALA PHE SER LEU THR PRO ASP GLY LYS LEU SER GLN LEU THR ALA ALA ASN

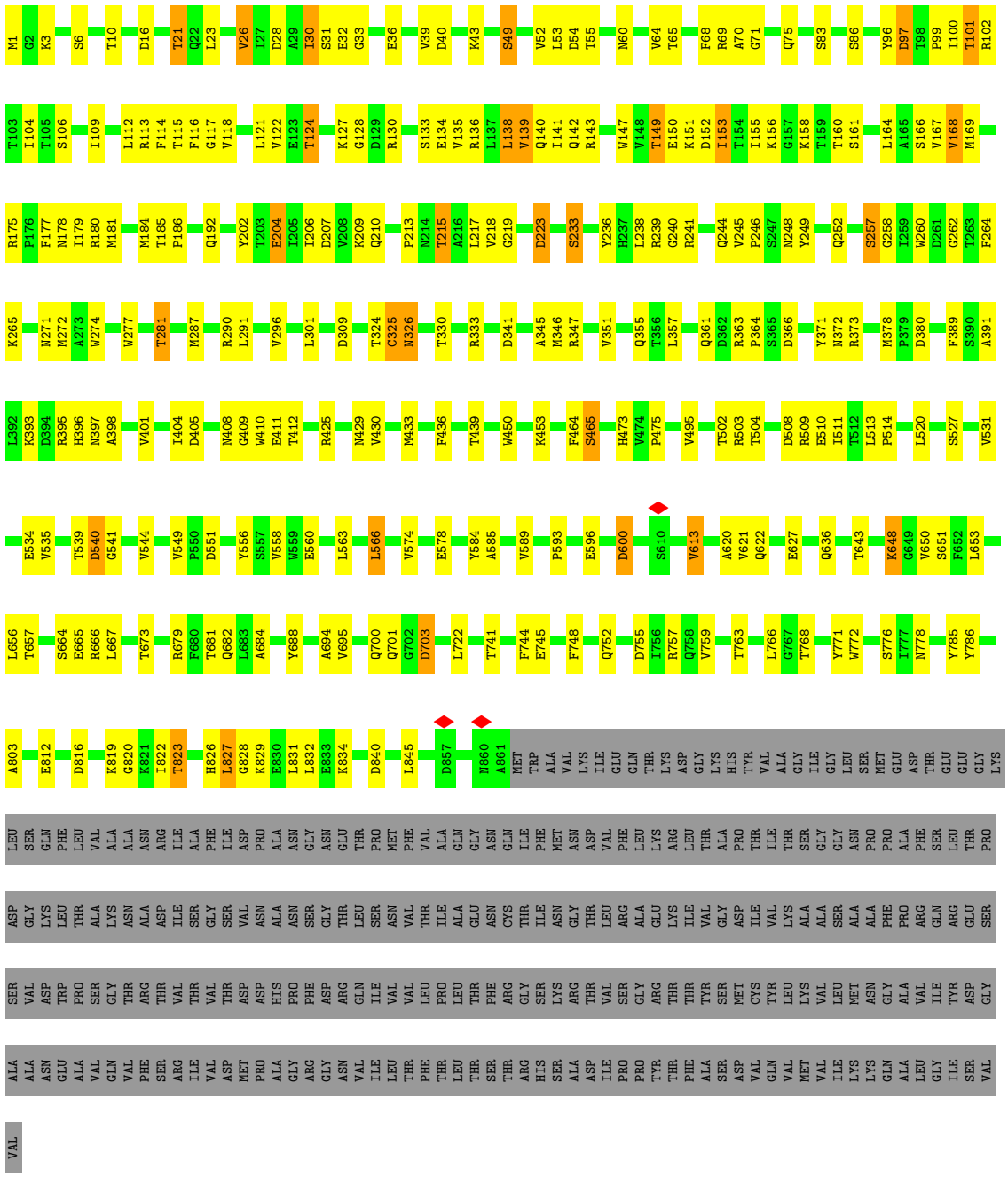
ALA ASP ILE SER GLY SER VAL ASN ALA ASN SER GLY THR ARG GLN ASN ASN ASN THR ILE SER ILE VAL LYS ALA ALA SER ALA ALA PHE PRO ARG GLN ARG GLU SER SER VAL ASP LYS LEU THR PRO SER GLY THR

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

PHE SER ARG ILE VAL ASP MET PRO ALA GLY ARG GLY ASN VAL ILE LEU THR PHE THR LEU THR SER THR ARG HIS SER ALA ASP ILE PRO PRO TYR THR PHE ALA SER ASP VAL GLN VAL MET VAL ILE LYS LYS GLN ALA LEU GLY ILE SER VAL VAL

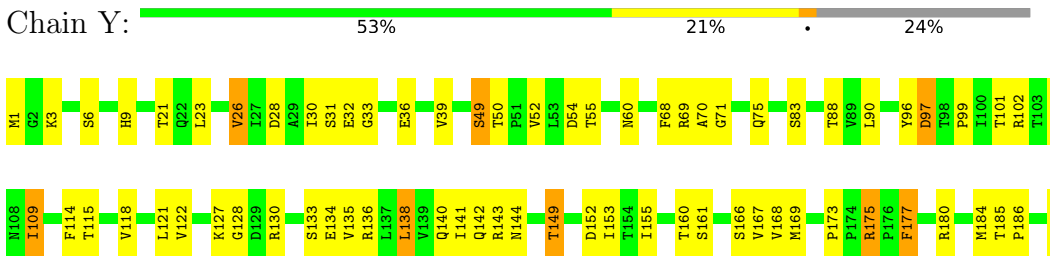
• Molecule 2: Tip attachment protein J

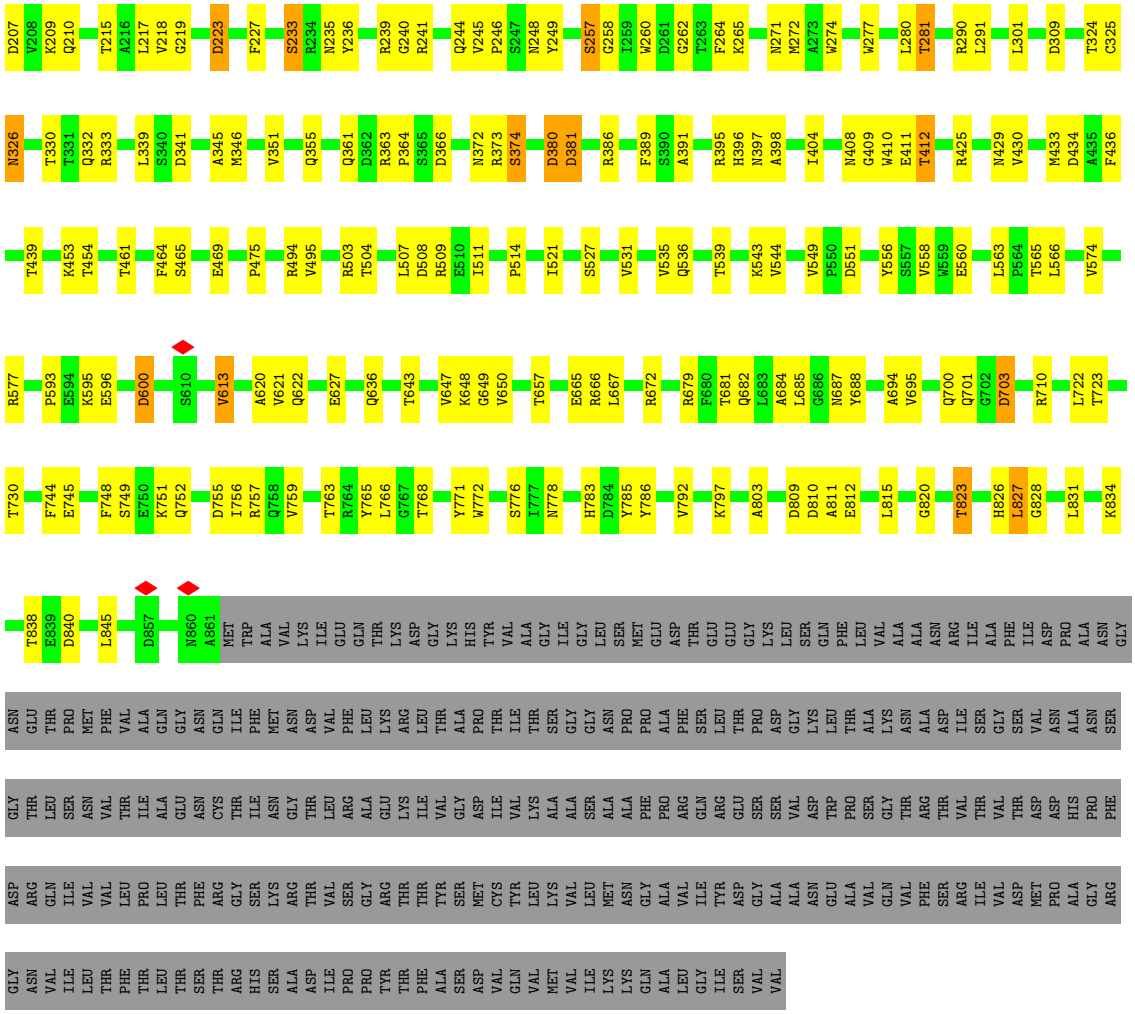
Chain E: 52% 22% • 24%



- Molecule 2: Tip attachment protein J

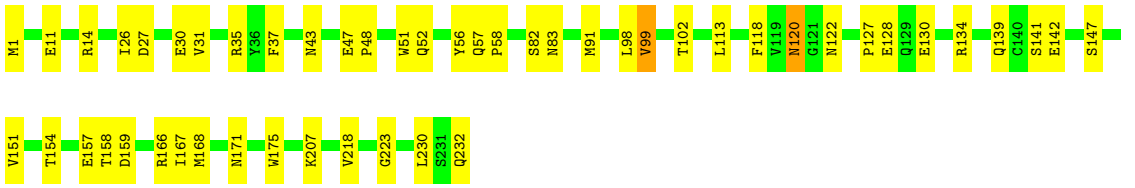
Chain Y:





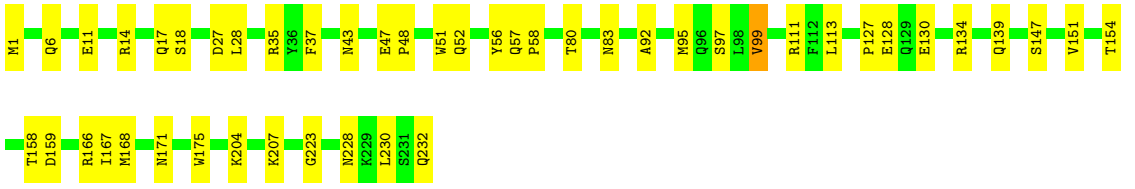

- Molecule 3: Tail tip protein L

Chain L: 78% 21%




- Molecule 3: Tail tip protein L

Chain G: 80% 20%



- Molecule 3: Tail tip protein L

Chain d: 80% 19%

M1 R5 Q6 E11 C12 T13 R14 Q17 D27 G32 R35 Y36 F37 N43 E47 P48 W51 Q52 Y56 Q57 P58 I61 E67 V81 M95 V99 R105 L113 F118 V119 N120 G121 N122 P127 E128 Q129 E130 S133 R134

Q139 E142 D159 R166 T167 M168 L169 A170 N171 W175 D191 K207 G223 Q232

- Molecule 4: Tape measure protein

Chain H: 96%

MET ALA GLU PRO VAL GLY ASP LEU VAL VAL ASP LEU SER LEU ASP ALA ALA ARG PHE ASP GLU GLN MET ALA ARG VAL ARG ARG HIS PHE SER GLY THR GLU SER ASP ALA LYS LYS THR ALA ALA VAL VAL GLU GLN SER LEU SER ARG GLN ALA LEU ALA ALA GLN LYS ALA GLY ILE

SER VAL GLY GLN TYR LYS ALA ALA MET ARG MET LEU PRO ALA GLN PHE THR ASP VAL ALA THR GLN LEU ALA GLY GLY GLN SER PRO TRP LEU ILE LEU LEU GLN GLN GLY GLY GLN VAL LYS ASP SER PHE GLY GLY MET ILE PRO MET PHE ARG GLY LEU ALA GLY ALA ILE THR LEU

PRO MET VAL GLY ALA THR SER LEU ALA VAL ALA ALA THR GLY ALA LEU ALA TYR ALA TRP TYR GLN GLY ASN SER THR LEU SER ASP PHE ASN LYS THR LEU VAL LEU SER GLY ASN GLN ALA GLY LEU THR ALA ASP ARG MET LEU VAL LEU SER ARG ALA GLY GLN ALA ALA GLY LEU THR

PHE ASN GLN THR SER GLU SER LEU SER ALA LEU VAL LYS ALA GLY VAL SER GLY GLU ALA GLN ILE ALA SER ILE SER GLN SER VAL ALA ARG PHE SER SER ALA SER GLY VAL GLU VAL ASP LYS VAL ALA GLU ALA PHE GLY LYS LYS LEU THR THR ASP PRO THR SER GLY LEU THR ALA

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

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

GLU LYS ALA ARG LEU ALA LEU GLU ALA ALA ARG LYS LYS ALA GLU GLN GLN THR GLN GLN ASP LYS ASN ALA GLN GLN GLN SER ASP THR GLU ALA SER ARG LEU LYS TYR THR GLU GLU ALA GLN LYS ALA TYR GLU ARG LEU GLN THR PRO LEU GLU LYS TYR THR ALA ARG GLN GLU

GLU LEU ASN LYS ALA LEU LYS ASP GLY LYS ILE LEU GLN ALA ASP TYR ASN THR LEU MET ALA ALA ALA LYS LYS ASP TYR GLU ALA THR LEU LYS LYS PRO LYS GLN SER SER VAL LYS VAL SER ALA GLY ASP ARG GLN GLU ASP SER ALA HIS LEU ALA ALA LEU LEU THR LEU GLN ALA

GLU LEU ARG THR LEU GLU LYS HIS ALA GLY ALA ASN GLU LYS ILE SER GLN GLU ARG ARG ASP LEU TRP LYS ALA GLU SER GLN PHE ALA VAL LEU GLU LYS ALA ALA GLN GLN GLU LYS SER LEU LEU ALA HIS LYS ASP GLU THR LEU GLU TYR LYS ARG

GLN LEU ALA ALA LEU GLY ASP LYS VAL THR TYR GLN GLU ARG LEU ASN ALA LEU ALA GLN GLN ALA ASP LYS PHE ALA GLN GLN ARG ALA ALA LYS ARG ALA ALA ILE ASP ALA LYS SER ARG GLY LEU THR ASP ARG GLN ALA GLU ARG GLU ALA THR GLU GLN ARG LEU LYS GLU GLN

TYR GLY ASP ASN PRO LEU ALA LEU ASN ASN VAL MET SER GLU GLN LYS LYS THR TRP ALA ALA GLU ASP GLN LEU ARG GLY ASN TRP MET ALA GLY LEU LYS SER GLY TRP SER GLU TRP GLU GLU SER ALA THR ASP SER MET SER GLN VAL LYS SER ALA ALA THR GLN THR PHE ASP

GLY ILE ALA GLN ASN MET ALA ALA MET LEU THR GLY SER GLU GLN ASN TRP ARG SER PHE THR ARG SER VAL LEU SER MET MET THR GLU ILE LEU LEU LYS GLN ALA MET VAL GLY ILE VAL GLY SER ILE GLY SER ALA ILE GLY GLY ALA VAL GLY GLY GLY ALA SER ALA GLY

GLY THR ALA ILE GLN ALA ALA ALA ALA LYS PHE HIS PHE ALA THR GLY GLY PHE THR GLY THR GLY GLY GLY LYS TYR GLU PRO ALA GLY ILE VAL HIS ARG GLY GLU PHE VAL PHE THR LYS GLU ALA THR SER ARG ILE GLY VAL GLY ASN LEU TYR ARG LEU MET ARG GLY TYR ALA THR

GLY GLY TYR VAL GLY THR PRO GLY SER MET ALA ASP SER ARG SER GLN ALA SER GLY THR PHE GLU GLN ASN ASN HIS VAL VAL ASN ASN ASP GLY THR ASN GLY Q817 I818 G819 P820 K824 A825 V826 Y827 D828 M829 A830 D836 E837 S849 GLY GLY GLY ARG

Chain K: 96%

MET ALA GLU PRO VAL GLY ASP LEU VAL VAL ASP LEU SER LEU ASP ALA ALA ARG PHE ASP GLU GLN MET ALA ARG VAL ARG ARG HIS PHE SER GLY THR GLU SER ASP ALA LYS LYS THR ALA ALA VAL VAL GLU GLN SER LEU SER ARG GLN ALA LEU ALA ALA GLN LYS GLY ILE

SER VAL GLY GLN TYR LYS ALA ALA MET ARG MET LEU PRO ALA GLN PHE THR ASP VAL ALA THR GLN LEU ALA GLY GLY GLN SER PRO TRP LEU ILE LEU LEU GLN GLN GLN GLY GLY GLN VAL LYS ASP SER PHE GLY GLY MET ILE PRO MET PHE ARG GLY LEU ALA GLY ALA ILE THR LEU

PRO MET VAL GLY ALA THR SER LEU ALA VAL ALA THR GLY ALA LEU ALA TYR ALA TRP TYR GLN GLY ASN SER THR LEU SER ASP PHE ASN LYS THR LEU VAL LEU SER GLY ASN GLN ALA GLY LEU THR ALA ASP ARG MET LEU VAL LEU SER ARG ALA GLY GLN ALA ALA GLY LEU THR

PHE ASN GLN THR SER GLU SER LEU SER ALA LEU VAL LYS ALA GLY VAL SER GLY GLU ALA GLN ILE ALA SER ILE SER GLN SER VAL ALA ARG PHE SER SER SER ALA GLY VAL GLU VAL ASP LYS VAL ALA GLU ALA PHE GLY LYS LYS LEU THR THR ASP PRO THR SER GLY LEU THR ALA

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

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

GLU LYS ALA ARG LEU ALA LEU GLU GLN ALA ALA ARG LYS LYS ALA GLU GLN GLN THR GLN GLN ASP LYS ASN ALA GLN GLN GLN SER ASP THR GLU ALA ALA SER ARG GLU LYS TYR THR GLU GLU ALA GLN LYS ALA TYR GLU ARG LEU GLN THR PRO LEU GLU LYS TYR THR ALA ARG GLN GLU

GLU LEU ASN LYS ALA LEU LYS ASP GLY LYS ILE LEU GLN ALA ASP TYR ASN THR LEU MET ALA ALA ALA LYS LYS ASP TYR GLU ALA THR LEU LYS LYS LYS PRO LYS GLN SER SER VAL LYS VAL SER ALA GLY ASP ARG GLN GLU ASP SER ALA HIS ALA ALA ALA LEU LEU THR LEU GLN ALA

GLU LEU ARG THR LEU GLU LYS HIS ALA GLY ALA ASN GLU LYS ILE SER GLN GLN ARG ARG ASP LEU TRP LYS ALA GLU SER GLN PHE ALA VAL LEU LEU GLU GLU ALA ALA GLN ARG ARG ARG GLN LEU SER ALA GLN GLU LYS SER LEU LEU ALA HIS LYS ASP GLU THR LEU GLU TYR LYS ARG

GLN LEU ALA ALA LEU GLY ASP LYS VAL THR TYR GLN GLU ARG LEU ASN ALA LEU ALA ALA GLN GLN GLN ARG ALA LYS ARG ALA ALA ALA ILE ASP ALA LYS SER ARG GLY LEU THR ASP ARG GLN ALA GLU ARG GLU ALA THR GLU GLN LEU ARG GLU GLN GLN

TYR GLY ASP ASN PRO LEU ALA LEU ASN ASN VAL MET SER GLU GLN LYS LYS THR TRP ALA ALA GLU ASP GLN LEU ARG GLY ASN TRP MET ALA GLY LEU LYS SER GLY TRP SER GLU TRP GLU GLU SER ALA THR ASP SER MET SER GLN VAL LYS SER ALA ALA THR GLN THR PHE ASP

GLY ILE ALA GLN ASN MET ALA ALA MET LEU THR GLY SER GLU GLN ASN TRP ARG SER PHE THR ARG SER VAL LEU SER MET MET THR GLU ILE LEU LEU LYS GLN ALA MET VAL GLY ILE VAL GLY SER ILE GLY SER ALA ILE GLY GLY ALA VAL GLY GLY GLY ALA SER ALA SER

GLY THR ALA ILE GLN ALA ALA ALA ALA LYS PHE HIS ALA GLY ALA ALA LYS TYR GLU PRO ALA GLY ILE VAL HIS ARG GLY GLU PHE VAL PHE THR LYS GLU ALA THR SER ARG ILE GLY VAL GLY ASN LEU TYR ARG LEU MET ARG GLY TYR ALA THR

GLY GLY TYR VAL GLY THR PRO GLY SER MET ALA ASP SER ARG SER GLN ALA SER GLY THR PHE GLU GLN ASN ASN HIS VAL VAL ILE ASN ASN ASP GLY THR ASN GLY Q817 I818 G819 P820 K824 A825 V826 Y827 D828 M829 A830 R835 D836 S849 GLY GLY GLY ARG

- Molecule 4: Tape measure protein

Chain e: 96%

MET ALA GLU PRO VAL GLY ASP LEU VAL VAL ASP LEU SER LEU ASP ALA ALA ARG PHE ASP GLU GLN MET ALA ARG VAL ARG ARG HIS PHE SER GLY THR GLU SER ASP ALA LYS LYS THR ALA ALA VAL VAL GLU GLN SER LEU SER ARG GLN ALA LEU ALA ALA GLN LYS GLY ILE

SER VAL GLY GLN TYR LYS ALA ALA MET ARG MET LEU PRO ALA GLN PHE THR ASP VAL ALA THR GLN LEU ALA GLY GLY GLN SER PRO TRP LEU ILE LEU LEU GLN GLN GLN GLY GLY GLN VAL LYS ASP SER PHE GLY GLY MET ILE PRO MET PHE ARG GLY LEU ALA GLY ALA ILE THR LEU

PRO MET VAL GLY ALA THR SER LEU ALA VAL ALA THR GLY ALA LEU ALA TYR ALA TRP TYR GLN GLY ASN SER THR LEU SER ASP PHE ASN LYS THR LEU VAL LEU SER GLY ASN GLN ALA GLY LEU THR ALA ASP ARG MET LEU VAL LEU SER ARG ALA GLY GLN ALA ALA GLY LEU THR

PHE ASN GLN THR SER GLU SER LEU SER ALA LEU VAL LYS ALA GLY VAL SER GLY GLU ALA GLN ILE ALA SER ILE SER GLN SER VAL ALA ARG PHE SER SER SER ALA GLY VAL GLU VAL ASP LYS VAL ALA GLU ALA PHE GLY LYS LYS LEU THR THR ASP PRO THR SER GLY LEU THR ALA

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

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

GLU LYS ALA ARG LEU ALA LEU GLU ALA ALA ARG LYS LYS ALA GLU GLN GLN THR GLN GLN ASP LYS ASN ALA GLN GLN GLN SER ASP THR GLU ALA SER ARG LEU LYS TYR THR GLU GLU ALA GLN LYS ALA TYR GLU ARG LEU GLN THR PRO LEU GLU LYS TYR THR ALA ARG GLN GLU

GLU LEU ASN LYS ALA LEU LYS ASP GLY LYS ILE LEU GLN ALA ASP TYR ASN THR LEU MET ALA ALA ALA LYS LYS ASP TYR GLU ALA THR LEU LYS LYS PRO LYS GLN SER SER SER VAL LYS VAL SER ALA GLY ASP ARG GLN GLU ASP SER ALA HIS ALA ALA LEU LEU THR LEU GLU ALA

GLU LEU ARG THR LEU GLU LYS HIS ALA GLY LYS ALA ASN GLU LYS ILE SER GLN GLN ARG ARG ASP LEU TRP LYS ALA GLU SER GLN GLN PHE ALA VAL LEU GLU GLU ALA ALA GLN ARG ARG ARG GLN LEU SER ALA GLN GLU LYS SER LEU LEU ALA HIS LYS ASP GLU THR LEU GLU TYR LYS ARG

GLN LEU ALA ALA LEU GLY ASP LYS VAL THR TYR GLN GLU ARG LEU ASN ALA LEU ALA GLN GLN GLN ARG ALA LYS ARG ALA ALA ILE ASP ALA LYS SER ARG GLY LEU THR ASP ARG GLN ALA GLU ARG GLU ALA THR GLU GLN ARG LEU LYS GLU GLN

TYR GLY ASP ASN PRO LEU ALA LEU ASN ASN VAL MET SER GLU GLN LYS LYS THR TRP ALA ALA GLU ASP GLN LEU ALA GLY ASN TRP MET ALA GLY LEU LYS SER GLY TRP SER GLU TRP GLU GLU SER ALA THR ASP SER SER GLN VAL LYS SER ALA ALA THR GLN THR PHE ASP

GLY ILE ALA GLN ASN MET ALA ALA MET LEU THR GLY SER GLU GLN ASN TRP ARG SER PHE THR ARG SER VAL LEU SER MET MET THR GLU ILE LEU LEU LYS GLN ALA MET VAL GLY ILE VAL GLY SER ILE GLY SER ALA ILE GLY GLY ALA VAL GLY GLY GLY GLY ALA SER ALA SER GLY

GLY THR ALA ILE GLN ALA ALA ALA ALA LYS PHE HIS PHE ALA THR GLY GLY PHE THR GLY THR GLY GLY LYS TYR GLU PRO ALA GLY ILE VAL HIS ARG GLY GLU PHE VAL PHE THR LYS GLU ALA THR SER ARG ILE GLY VAL GLY ASN LEU TYR ARG LEU MET ARG GLY TYR ALA THR

GLY GLY TYR VAL GLY THR PRO GLY SER MET ALA ASP SER ARG SER GLN ALA SER GLY THR PHE GLU GLN ASN ASN HIS VAL VAL ILE ASN ASN ASP GLY THR ASN GLY Q817 I818 G819 P820 K824 A825 V826 Y827 D828 M829 A830 R831 R835 D836 E837 S849 GLY GLY GLY ARG

- Molecule 5: Tail tip assembly protein I

Chain I: 35% 17% 45%

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

GLN VAL ARG ILE ALA GLY ARG ASP VAL SER THR SER GLY LEU THR ALA GLN LEU HIS GLU THR LEU PRO ASP GLY ALA VAL ILE HIS ILE VAL PRO ARG VAL ALA GLY ALA LYS SER GLY GLY V102 F103 Q104 I105 V106 L107 G108 A109 A110 A111 G114 S115 F116 F117 T118 A119 G120 A121

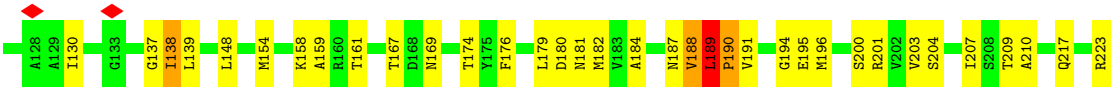
T122 L123 I130 G133 G137 I138 L148 K158 A159 R160 T161 P162 R163 T167 D168 N169 G170 T174 Y175 F176 L179 D180 N181 M182 V183 A184 N187 V188 L189 P190 V191 L192 Y193 G194 E195 M196 S200 R201 I207 S208 T209 A210 Q217 R223

- Molecule 5: Tail tip assembly protein I

Chain N: 34% 17% 45%

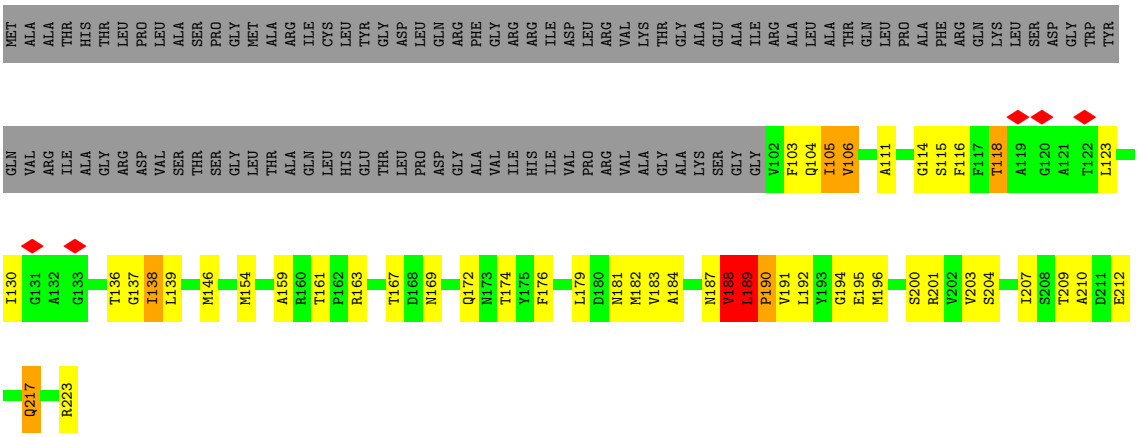
MET ALA ALA THR HIS THR LEU PRO LEU ALA SER PRO GLY MET ALA ARG ILE CYS LEU TYR GLY ASP LEU GLN ARG PHE GLY ARG ARG ILE ASP LEU ARG VAL LYS THR GLY ALA GLU ALA ILE ARG ALA ALA LEU ALA THR GLN LEU PRO ALA PHE ARG GLN LYS LEU SER ASP GLY TRP TYR

GLN VAL ARG ILE ALA GLY ARG ASP VAL SER THR SER GLY LEU THR ALA GLN LEU HIS GLU THR LEU PRO ASP GLY ALA VAL ILE HIS ILE VAL PRO ARG VAL ALA GLY ALA LYS SER GLY GLY V102 F103 Q104 I105 V106 L107 G108 A109 A110 A111 F116 F117 T118 A119 G120 A121 T122 L123



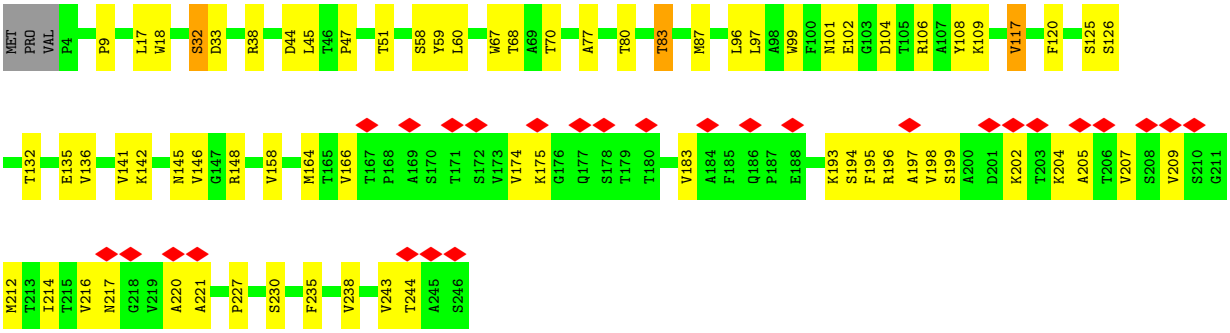

• Molecule 5: Tail tip assembly protein I

Chain f:



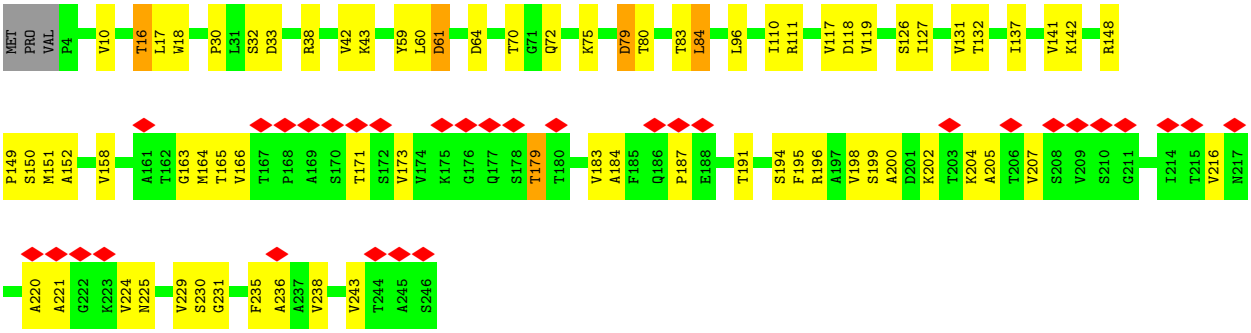

• Molecule 6: Tail tube protein

Chain V:



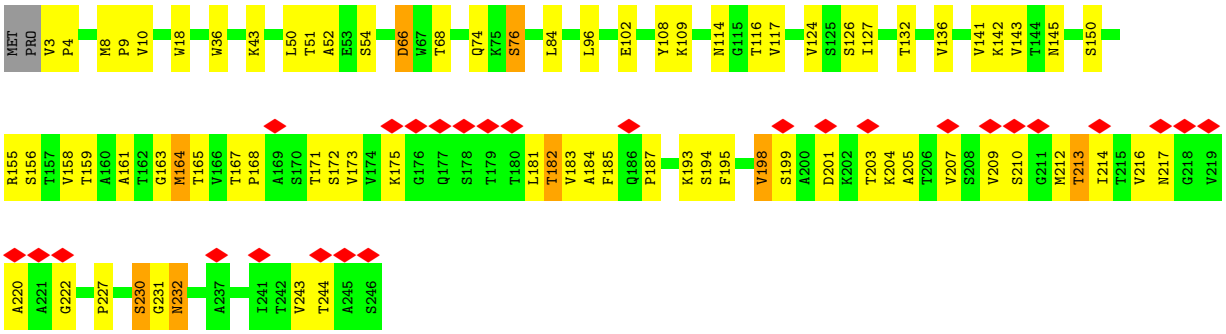

• Molecule 6: Tail tube protein

Chain v:



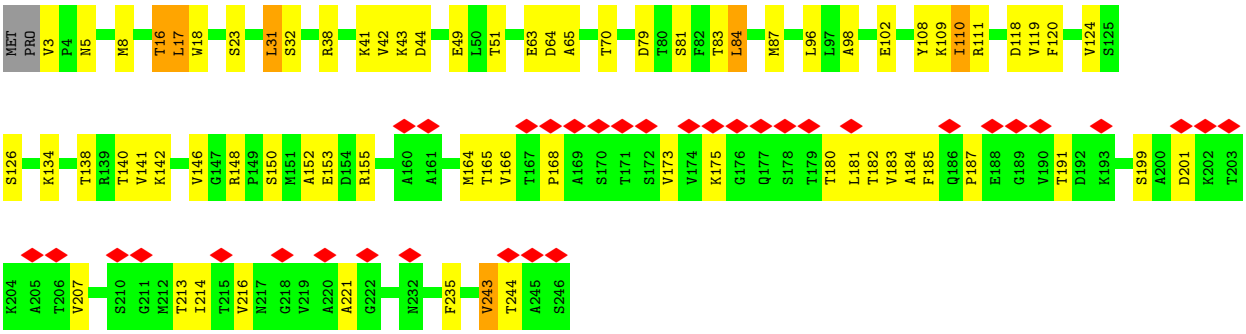

• Molecule 6: Tail tube protein

Chain B:



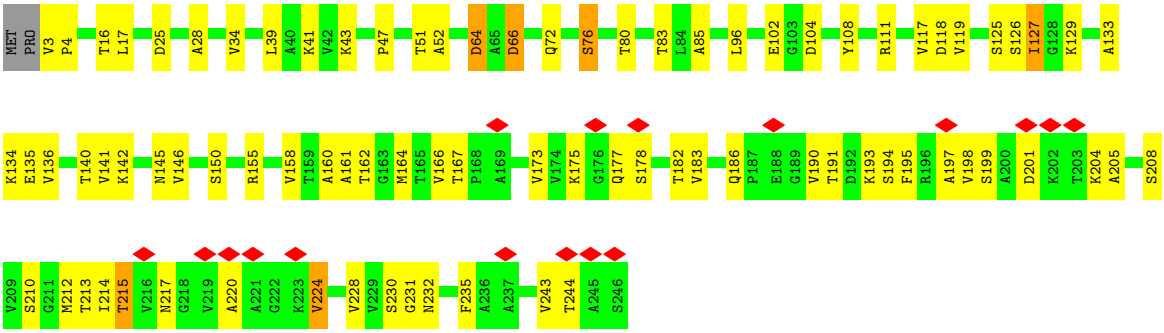

- Molecule 6: Tail tube protein

Chain b:



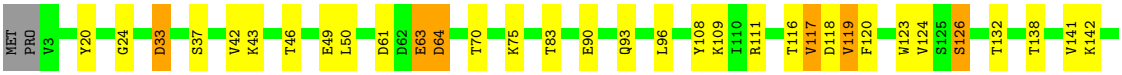

- Molecule 6: Tail tube protein

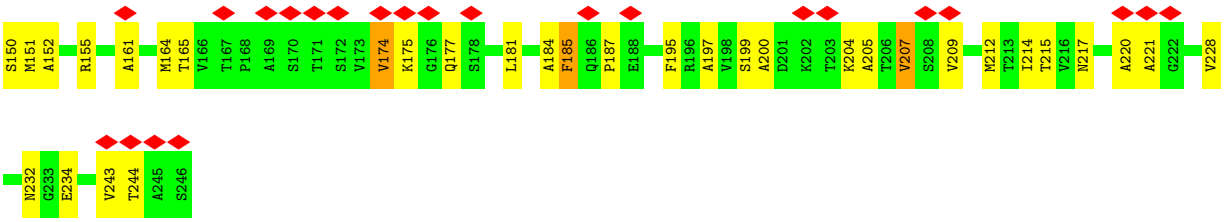
Chain A:




- Molecule 6: Tail tube protein

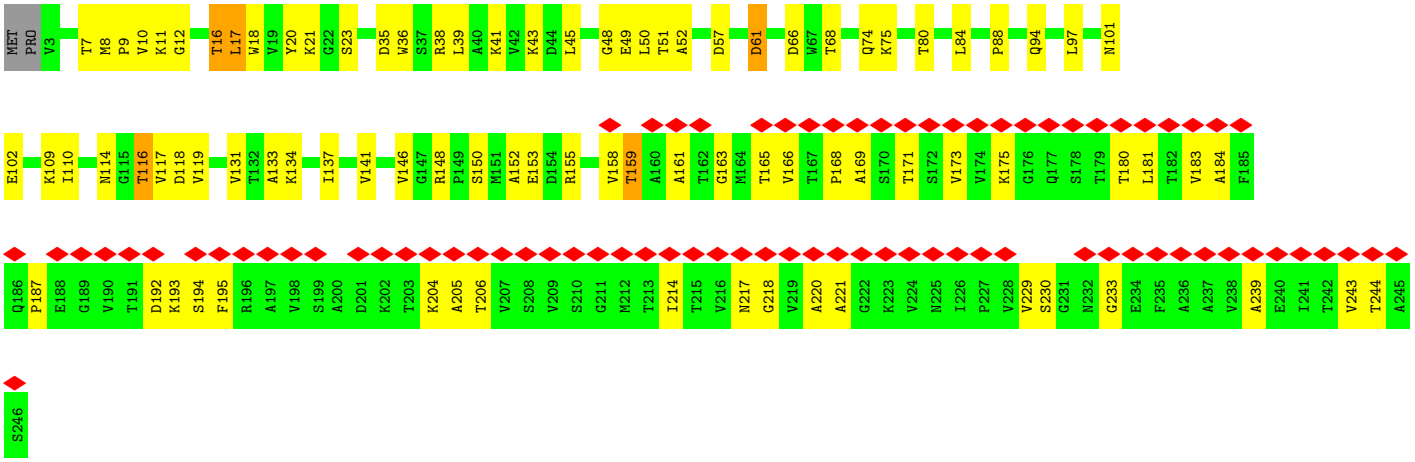
Chain a:





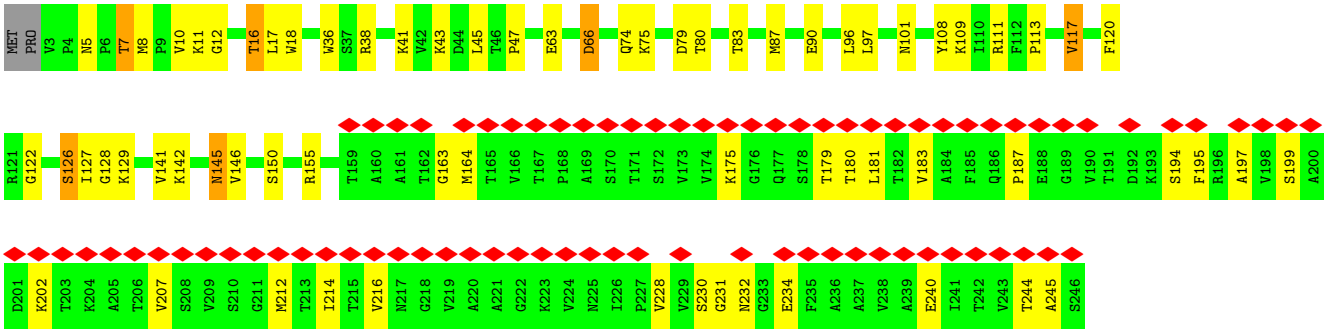

• Molecule 6: Tail tube protein

Chain C:



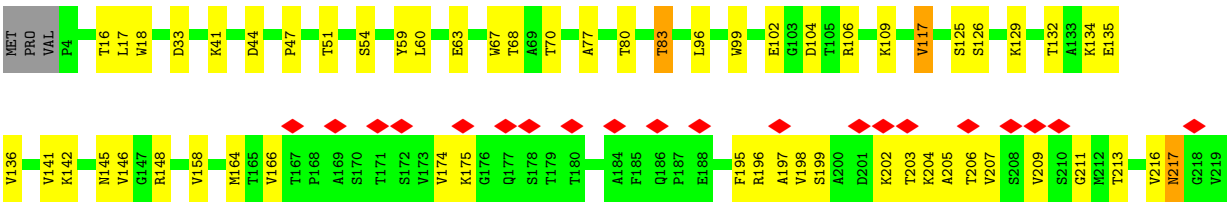

• Molecule 6: Tail tube protein

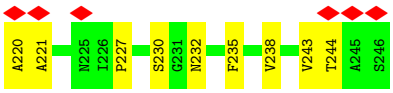
Chain c:




• Molecule 6: Tail tube protein

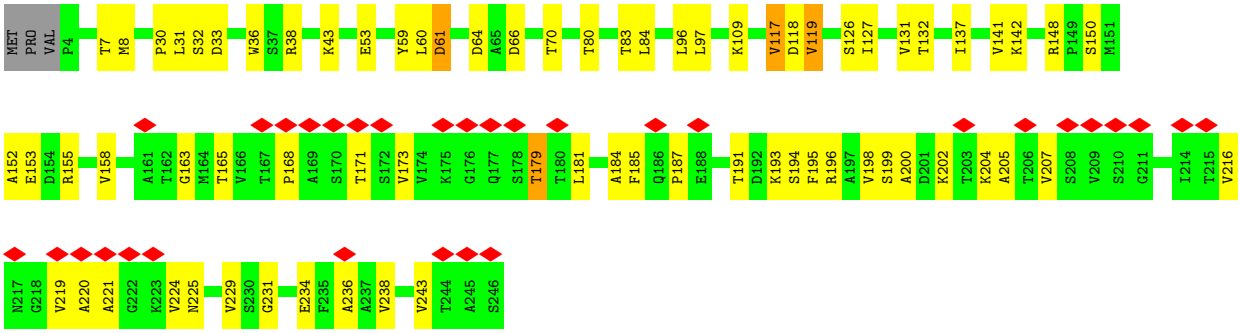
Chain O:





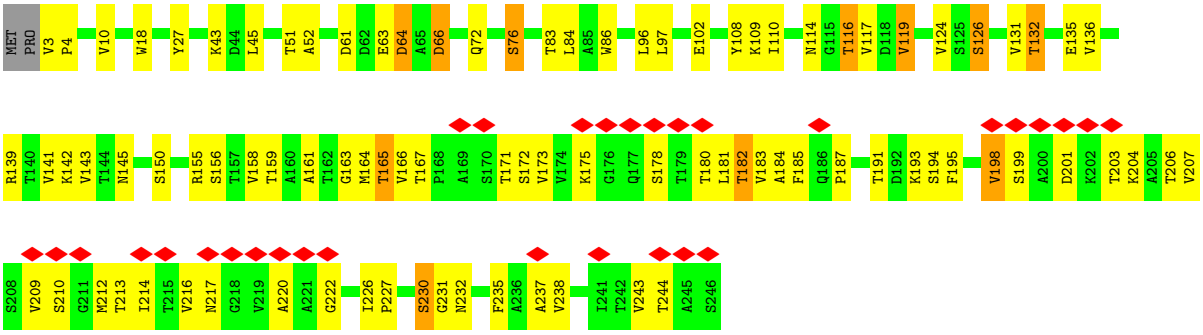

• Molecule 6: Tail tube protein

Chain P:



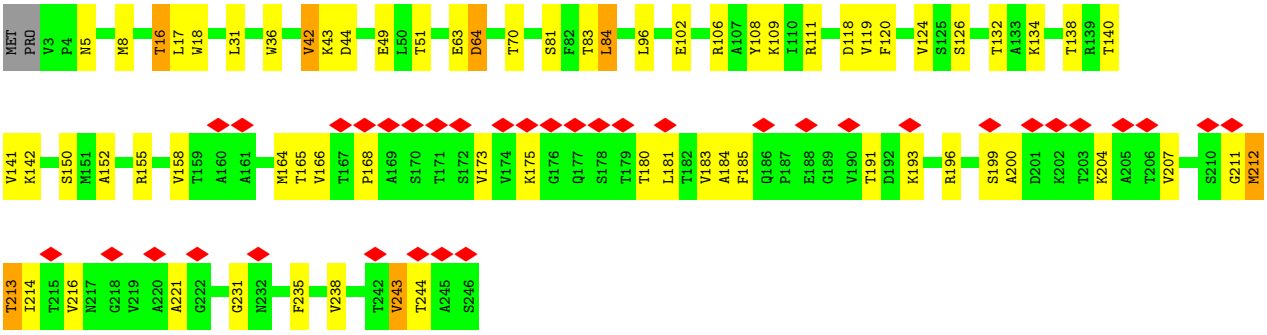

• Molecule 6: Tail tube protein

Chain Q:



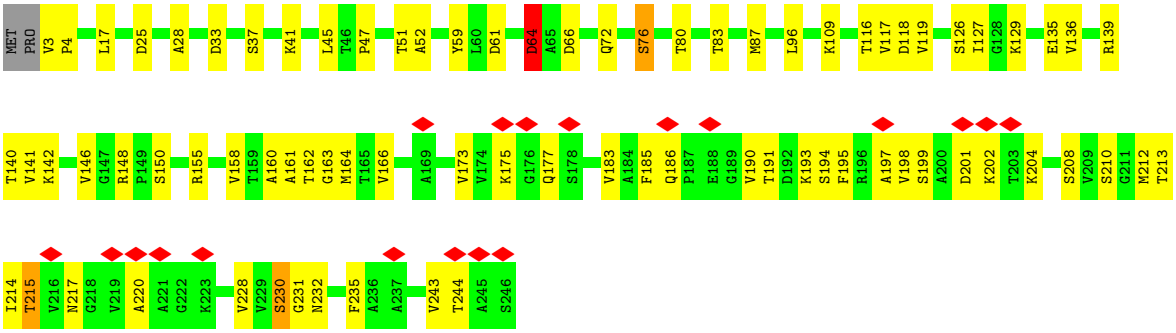

• Molecule 6: Tail tube protein

Chain R:



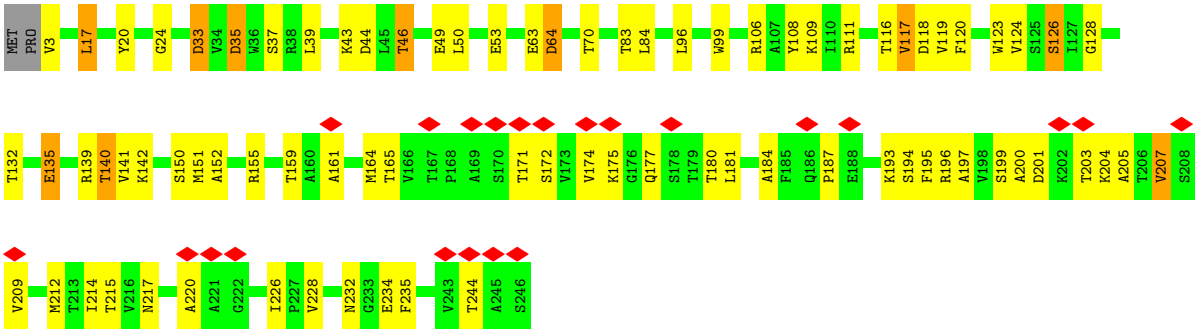

• Molecule 6: Tail tube protein

Chain S:



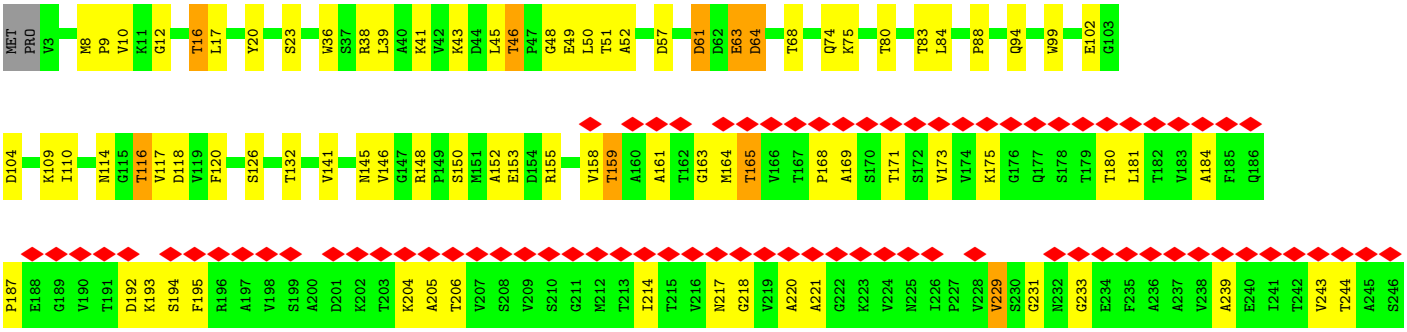

- Molecule 6: Tail tube protein

Chain T:



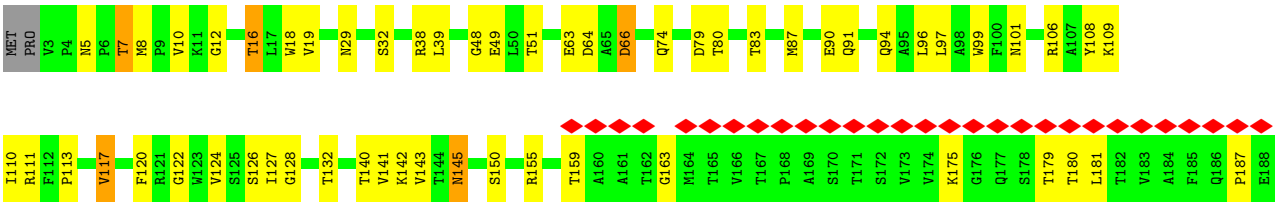

- Molecule 6: Tail tube protein

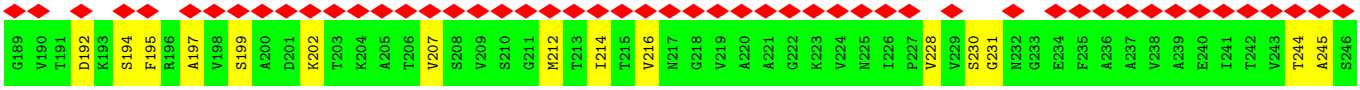
Chain U:




- Molecule 6: Tail tube protein

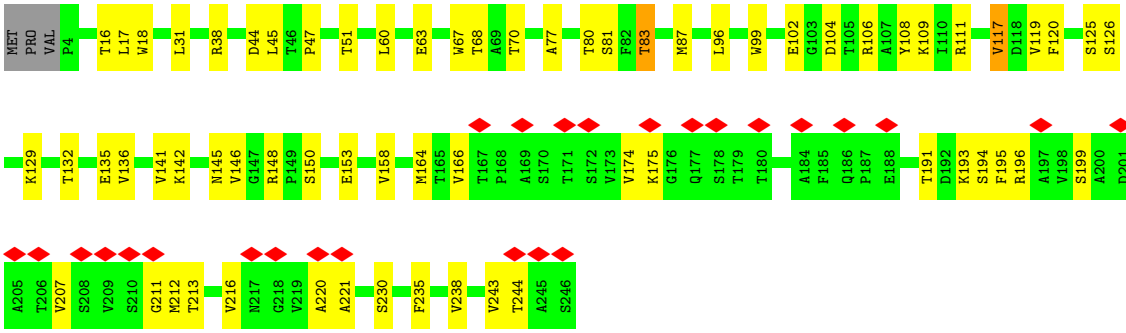
Chain W:





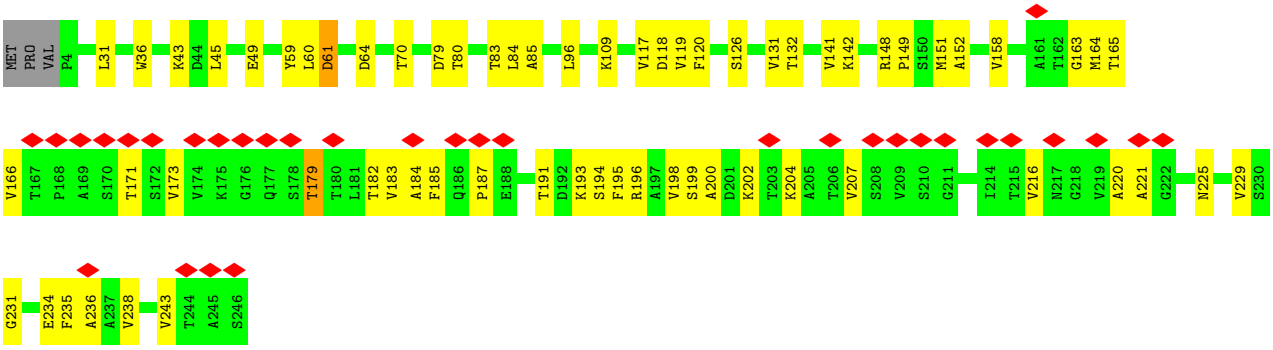

• Molecule 6: Tail tube protein

Chain g:



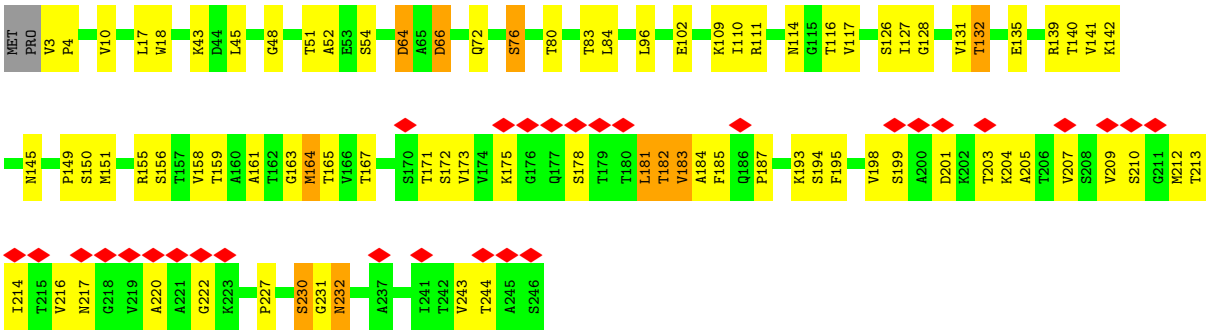

• Molecule 6: Tail tube protein

Chain h:



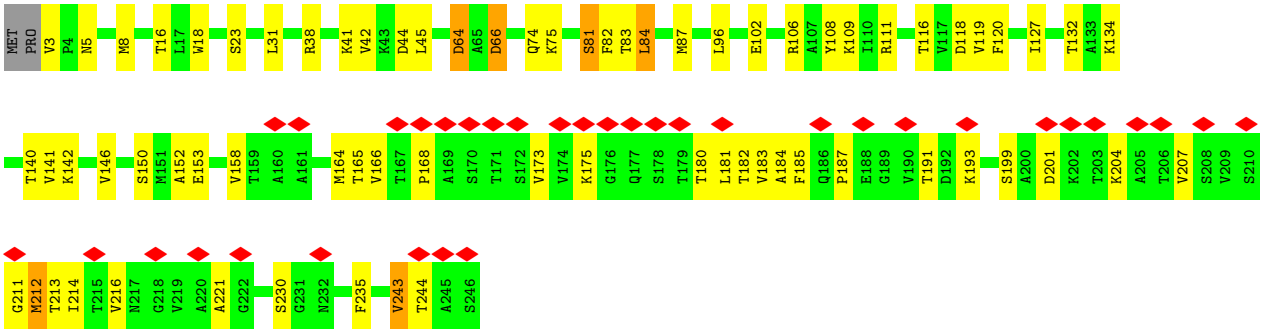

• Molecule 6: Tail tube protein

Chain i:



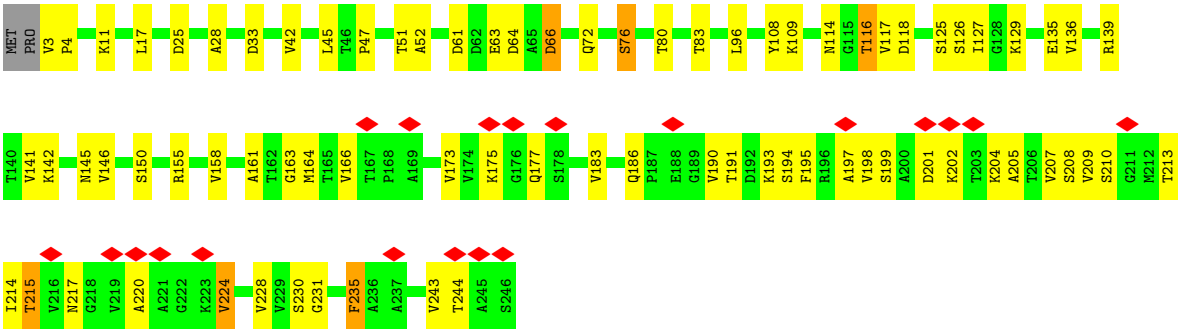

• Molecule 6: Tail tube protein

Chain j:



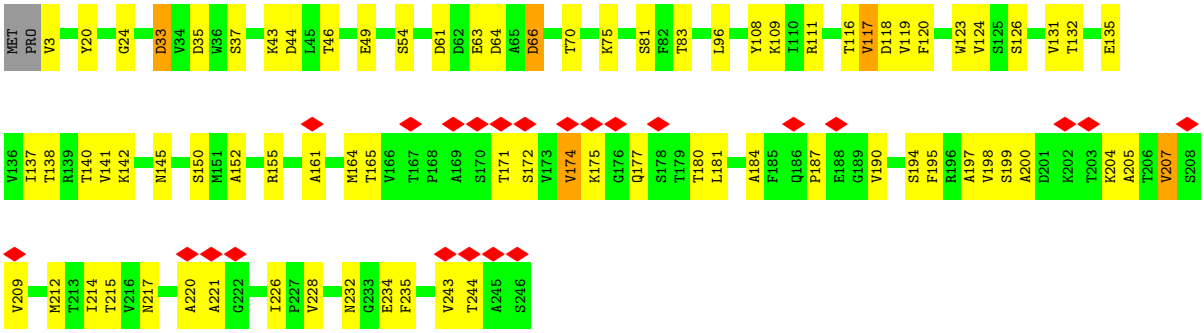

- Molecule 6: Tail tube protein

Chain k:



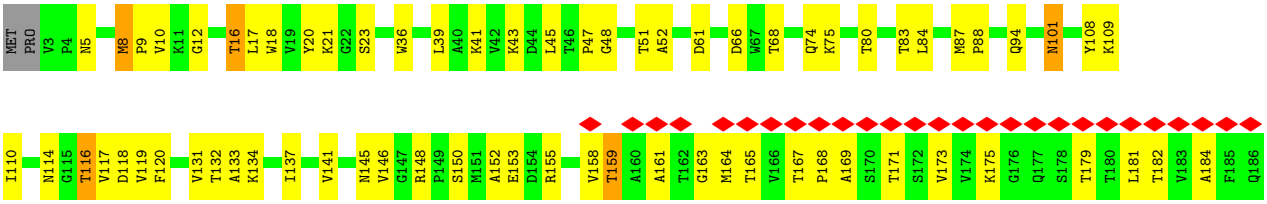

- Molecule 6: Tail tube protein

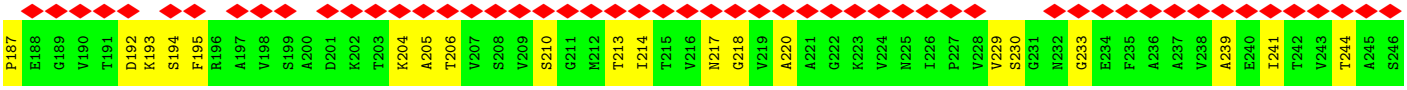
Chain l:




- Molecule 6: Tail tube protein

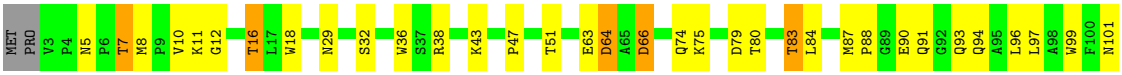
Chain n:

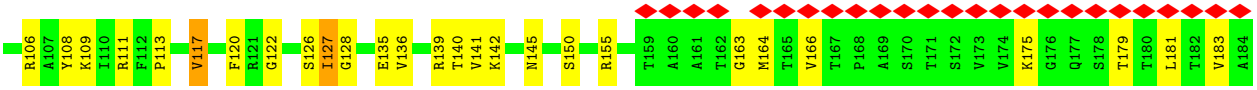





- Molecule 6: Tail tube protein

Chain o:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 54547 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 3.471 | Depositor |
| Minimum map value | -1.590 | Depositor |
| Average map value | -0.001 | Depositor |
| Map value standard deviation | 0.082 | Depositor |
| Recommended contour level | 0.25 | Depositor |
| Map size (Å) | 515.616, 515.616, 515.616 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.0742, 1.0742, 1.0742 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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 | D | 0.19 | 0/909 | 0.42 | 0/1231 |
| 1 | F | 0.18 | 0/909 | 0.41 | 0/1231 |
| 1 | M | 0.19 | 0/909 | 0.41 | 0/1231 |
| 1 | X | 0.19 | 0/909 | 0.41 | 0/1231 |
| 1 | Z | 0.19 | 0/909 | 0.41 | 0/1231 |
| 1 | m | 0.18 | 0/909 | 0.39 | 0/1231 |
| 2 | E | 0.16 | 0/6866 | 0.36 | 0/9348 |
| 2 | J | 0.16 | 0/6866 | 0.36 | 0/9348 |
| 2 | Y | 0.16 | 0/6866 | 0.37 | 0/9348 |
| 3 | G | 0.16 | 0/1836 | 0.27 | 0/2487 |
| 3 | L | 0.16 | 0/1836 | 0.28 | 0/2487 |
| 3 | d | 0.16 | 0/1836 | 0.29 | 0/2487 |
| 4 | H | 0.18 | 0/252 | 0.42 | 0/335 |
| 4 | K | 0.21 | 0/252 | 0.45 | 0/335 |
| 4 | e | 0.23 | 0/252 | 0.43 | 0/335 |
| 5 | I | 0.20 | 0/876 | 0.57 | 0/1186 |
| 5 | N | 0.19 | 0/876 | 0.55 | 0/1186 |
| 5 | f | 0.19 | 0/876 | 0.53 | 0/1186 |
| 6 | A | 0.17 | 0/1834 | 0.39 | 0/2505 |
| 6 | B | 0.16 | 0/1834 | 0.37 | 0/2505 |
| 6 | C | 0.14 | 0/1834 | 0.37 | 0/2505 |
| 6 | O | 0.16 | 0/1827 | 0.34 | 0/2494 |
| 6 | P | 0.16 | 0/1827 | 0.29 | 0/2494 |
| 6 | Q | 0.16 | 0/1834 | 0.38 | 0/2505 |
| 6 | R | 0.16 | 0/1834 | 0.37 | 1/2505 (0.0%) |
| 6 | S | 0.17 | 0/1834 | 0.40 | 0/2505 |
| 6 | T | 0.17 | 0/1834 | 0.35 | 0/2505 |
| 6 | U | 0.13 | 0/1834 | 0.37 | 2/2505 (0.1%) |
| 6 | V | 0.16 | 0/1827 | 0.34 | 0/2494 |
| 6 | W | 0.14 | 0/1834 | 0.34 | 0/2505 |
| 6 | a | 0.17 | 0/1834 | 0.36 | 2/2505 (0.1%) |
| 6 | b | 0.16 | 0/1834 | 0.37 | 0/2505 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 6 | c | 0.15 | 0/1834 | 0.37 | 0/2505 |
| 6 | g | 0.16 | 0/1827 | 0.33 | 0/2494 |
| 6 | h | 0.16 | 0/1827 | 0.29 | 0/2494 |
| 6 | i | 0.16 | 0/1834 | 0.38 | 0/2505 |
| 6 | j | 0.16 | 0/1834 | 0.37 | 1/2505 (0.0%) |
| 6 | k | 0.17 | 0/1834 | 0.40 | 0/2505 |
| 6 | l | 0.17 | 0/1834 | 0.34 | 0/2505 |
| 6 | n | 0.14 | 0/1834 | 0.36 | 0/2505 |
| 6 | o | 0.14 | 0/1834 | 0.35 | 0/2505 |
| 6 | v | 0.16 | 0/1827 | 0.29 | 0/2494 |
| All | All | 0.16 | 0/78918 | 0.37 | 6/107508 (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 |
|---|---|---|---|
| 2 | E | 0 | 1 |
| 2 | J | 0 | 1 |
| 2 | Y | 0 | 1 |
| 5 | I | 0 | 1 |
| 5 | N | 0 | 1 |
| 5 | f | 0 | 1 |
| All | All | 0 | 6 |

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | a | 63 | GLU | CA-C-N | 5.53 | 132.10 | 121.54 |
| 6 | a | 63 | GLU | C-N-CA | 5.53 | 132.10 | 121.54 |
| 6 | j | 212 | MET | CA-CB-CG | 5.19 | 124.47 | 114.10 |
| 6 | U | 63 | GLU | CA-C-N | 5.16 | 131.40 | 121.54 |
| 6 | U | 63 | GLU | C-N-CA | 5.16 | 131.40 | 121.54 |

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | E | 175 | ARG | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 5 | I | 189 | LEU | Peptide |
| 2 | J | 175 | ARG | Peptide |
| 5 | N | 189 | LEU | Peptide |
| 2 | Y | 175 | ARG | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | D | 884 | 0 | 881 | 24 | 0 |
| 1 | F | 884 | 0 | 881 | 20 | 0 |
| 1 | M | 884 | 0 | 881 | 23 | 0 |
| 1 | X | 884 | 0 | 881 | 20 | 0 |
| 1 | Z | 884 | 0 | 881 | 21 | 0 |
| 1 | m | 884 | 0 | 881 | 22 | 0 |
| 2 | E | 6720 | 0 | 6558 | 206 | 0 |
| 2 | J | 6720 | 0 | 6558 | 178 | 0 |
| 2 | Y | 6720 | 0 | 6558 | 177 | 0 |
| 3 | G | 1801 | 0 | 1715 | 30 | 0 |
| 3 | L | 1801 | 0 | 1715 | 32 | 0 |
| 3 | d | 1801 | 0 | 1715 | 34 | 0 |
| 4 | H | 250 | 0 | 251 | 11 | 0 |
| 4 | K | 250 | 0 | 251 | 11 | 0 |
| 4 | e | 250 | 0 | 251 | 14 | 0 |
| 5 | I | 865 | 0 | 874 | 42 | 0 |
| 5 | N | 865 | 0 | 874 | 45 | 0 |
| 5 | f | 865 | 0 | 874 | 49 | 0 |
| 6 | A | 1799 | 0 | 1768 | 49 | 0 |
| 6 | B | 1799 | 0 | 1768 | 48 | 0 |
| 6 | C | 1799 | 0 | 1768 | 57 | 0 |
| 6 | O | 1792 | 0 | 1760 | 32 | 0 |
| 6 | P | 1792 | 0 | 1760 | 39 | 0 |
| 6 | Q | 1799 | 0 | 1768 | 54 | 0 |
| 6 | R | 1799 | 0 | 1768 | 42 | 0 |
| 6 | S | 1799 | 0 | 1768 | 48 | 0 |
| 6 | T | 1799 | 0 | 1768 | 50 | 0 |
| 6 | U | 1799 | 0 | 1768 | 57 | 0 |
| 6 | V | 1792 | 0 | 1760 | 44 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 6 | W | 1799 | 0 | 1768 | 52 | 0 |
| 6 | a | 1799 | 0 | 1768 | 41 | 0 |
| 6 | b | 1799 | 0 | 1768 | 47 | 0 |
| 6 | c | 1799 | 0 | 1768 | 52 | 0 |
| 6 | g | 1792 | 0 | 1760 | 35 | 0 |
| 6 | h | 1792 | 0 | 1760 | 39 | 0 |
| 6 | i | 1799 | 0 | 1768 | 51 | 0 |
| 6 | j | 1799 | 0 | 1768 | 45 | 0 |
| 6 | k | 1799 | 0 | 1768 | 50 | 0 |
| 6 | l | 1799 | 0 | 1768 | 47 | 0 |
| 6 | n | 1799 | 0 | 1768 | 62 | 0 |
| 6 | o | 1799 | 0 | 1768 | 59 | 0 |
| 6 | v | 1792 | 0 | 1760 | 44 | 0 |
| 7 | G | 8 | 0 | 0 | 0 | 0 |
| 7 | L | 8 | 0 | 0 | 0 | 0 |
| 7 | d | 8 | 0 | 0 | 0 | 0 |
| All | All | 77370 | 0 | 75864 | 1837 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 1837 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:Q:183:VAL:HB | 6:Q:212:MET:HE1 | 1.58 | 0.86 |
| 6:B:96:LEU:HD21 | 6:B:141:VAL:HG21 | 1.59 | 0.84 |
| 6:W:87:MET:HB3 | 6:W:90:GLU:HG2 | 1.59 | 0.84 |
| 2:J:240:GLY:HA3 | 5:I:194:GLY:H | 1.43 | 0.83 |
| 1:Z:55:ALA:HB2 | 1:Z:98:VAL:HG11 | 1.60 | 0.83 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | D | 107/109 (98%) | 94 (88%) | 13 (12%) | 0 | 100 | 100 |
| 1 | F | 107/109 (98%) | 93 (87%) | 13 (12%) | 1 (1%) | 14 | 48 |
| 1 | M | 107/109 (98%) | 94 (88%) | 13 (12%) | 0 | 100 | 100 |
| 1 | X | 107/109 (98%) | 94 (88%) | 13 (12%) | 0 | 100 | 100 |
| 1 | Z | 107/109 (98%) | 95 (89%) | 11 (10%) | 1 (1%) | 14 | 48 |
| 1 | m | 107/109 (98%) | 92 (86%) | 14 (13%) | 1 (1%) | 14 | 48 |
| 2 | E | 859/1132 (76%) | 780 (91%) | 75 (9%) | 4 (0%) | 24 | 60 |
| 2 | J | 859/1132 (76%) | 773 (90%) | 82 (10%) | 4 (0%) | 24 | 60 |
| 2 | Y | 859/1132 (76%) | 775 (90%) | 81 (9%) | 3 (0%) | 36 | 70 |
| 3 | G | 230/232 (99%) | 222 (96%) | 8 (4%) | 0 | 100 | 100 |
| 3 | L | 230/232 (99%) | 222 (96%) | 8 (4%) | 0 | 100 | 100 |
| 3 | d | 230/232 (99%) | 224 (97%) | 6 (3%) | 0 | 100 | 100 |
| 4 | H | 31/853 (4%) | 25 (81%) | 6 (19%) | 0 | 100 | 100 |
| 4 | K | 31/853 (4%) | 25 (81%) | 6 (19%) | 0 | 100 | 100 |
| 4 | e | 31/853 (4%) | 26 (84%) | 5 (16%) | 0 | 100 | 100 |
| 5 | I | 120/223 (54%) | 97 (81%) | 17 (14%) | 6 (5%) | 1 | 10 |
| 5 | N | 120/223 (54%) | 97 (81%) | 17 (14%) | 6 (5%) | 1 | 10 |
| 5 | f | 120/223 (54%) | 97 (81%) | 17 (14%) | 6 (5%) | 1 | 10 |
| 6 | A | 242/246 (98%) | 225 (93%) | 14 (6%) | 3 (1%) | 10 | 40 |
| 6 | B | 242/246 (98%) | 223 (92%) | 18 (7%) | 1 (0%) | 30 | 65 |
| 6 | C | 242/246 (98%) | 224 (93%) | 16 (7%) | 2 (1%) | 16 | 50 |
| 6 | O | 241/246 (98%) | 227 (94%) | 13 (5%) | 1 (0%) | 30 | 65 |
| 6 | P | 241/246 (98%) | 229 (95%) | 12 (5%) | 0 | 100 | 100 |
| 6 | Q | 242/246 (98%) | 223 (92%) | 18 (7%) | 1 (0%) | 30 | 65 |
| 6 | R | 242/246 (98%) | 228 (94%) | 13 (5%) | 1 (0%) | 30 | 65 |
| 6 | S | 242/246 (98%) | 224 (93%) | 15 (6%) | 3 (1%) | 10 | 40 |
| 6 | T | 242/246 (98%) | 231 (96%) | 10 (4%) | 1 (0%) | 30 | 65 |
| 6 | U | 242/246 (98%) | 225 (93%) | 14 (6%) | 3 (1%) | 10 | 40 |
| 6 | V | 241/246 (98%) | 228 (95%) | 12 (5%) | 1 (0%) | 30 | 65 |
| 6 | W | 242/246 (98%) | 228 (94%) | 14 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 6 | a | 242/246 (98%) | 232 (96%) | 9 (4%) | 1 (0%) | 30 | 65 |
| 6 | b | 242/246 (98%) | 230 (95%) | 11 (4%) | 1 (0%) | 30 | 65 |
| 6 | c | 242/246 (98%) | 230 (95%) | 12 (5%) | 0 | 100 | 100 |
| 6 | g | 241/246 (98%) | 229 (95%) | 11 (5%) | 1 (0%) | 30 | 65 |
| 6 | h | 241/246 (98%) | 228 (95%) | 13 (5%) | 0 | 100 | 100 |
| 6 | i | 242/246 (98%) | 224 (93%) | 17 (7%) | 1 (0%) | 30 | 65 |
| 6 | j | 242/246 (98%) | 229 (95%) | 12 (5%) | 1 (0%) | 30 | 65 |
| 6 | k | 242/246 (98%) | 224 (93%) | 15 (6%) | 3 (1%) | 10 | 40 |
| 6 | l | 242/246 (98%) | 230 (95%) | 11 (4%) | 1 (0%) | 30 | 65 |
| 6 | n | 242/246 (98%) | 225 (93%) | 15 (6%) | 2 (1%) | 16 | 50 |
| 6 | o | 242/246 (98%) | 229 (95%) | 12 (5%) | 1 (0%) | 30 | 65 |
| 6 | v | 241/246 (98%) | 228 (95%) | 13 (5%) | 0 | 100 | 100 |
| All | All | 10164/13878 (73%) | 9378 (92%) | 725 (7%) | 61 (1%) | 23 | 56 |

5 of 61 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | I | 105 | ILE |
| 5 | I | 188 | VAL |
| 5 | I | 190 | PRO |
| 6 | V | 158 | VAL |
| 6 | B | 158 | VAL |

### 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 | D | 96/96 (100%) | 89 (93%) | 7 (7%) | 13 | 42 |
| 1 | F | 96/96 (100%) | 92 (96%) | 4 (4%) | 26 | 61 |
| 1 | M | 96/96 (100%) | 88 (92%) | 8 (8%) | 10 | 37 |
| 1 | X | 96/96 (100%) | 86 (90%) | 10 (10%) | 7 | 28 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | Z | 96/96 (100%) | 91 (95%) | 5 (5%) | 21 | 55 |
| 1 | m | 96/96 (100%) | 94 (98%) | 2 (2%) | 47 | 75 |
| 2 | E | 734/958 (77%) | 683 (93%) | 51 (7%) | 14 | 45 |
| 2 | J | 734/958 (77%) | 685 (93%) | 49 (7%) | 15 | 46 |
| 2 | Y | 734/958 (77%) | 676 (92%) | 58 (8%) | 11 | 39 |
| 3 | G | 198/198 (100%) | 187 (94%) | 11 (6%) | 19 | 52 |
| 3 | L | 198/198 (100%) | 187 (94%) | 11 (6%) | 19 | 52 |
| 3 | d | 198/198 (100%) | 194 (98%) | 4 (2%) | 48 | 76 |
| 4 | H | 24/648 (4%) | 24 (100%) | 0 | 100 | 100 |
| 4 | K | 24/648 (4%) | 24 (100%) | 0 | 100 | 100 |
| 4 | e | 24/648 (4%) | 24 (100%) | 0 | 100 | 100 |
| 5 | I | 86/162 (53%) | 81 (94%) | 5 (6%) | 18 | 51 |
| 5 | N | 86/162 (53%) | 80 (93%) | 6 (7%) | 14 | 44 |
| 5 | f | 86/162 (53%) | 79 (92%) | 7 (8%) | 11 | 38 |
| 6 | A | 194/196 (99%) | 175 (90%) | 19 (10%) | 7 | 30 |
| 6 | B | 194/196 (99%) | 179 (92%) | 15 (8%) | 12 | 40 |
| 6 | C | 194/196 (99%) | 184 (95%) | 10 (5%) | 21 | 55 |
| 6 | O | 193/196 (98%) | 176 (91%) | 17 (9%) | 9 | 35 |
| 6 | P | 193/196 (98%) | 175 (91%) | 18 (9%) | 8 | 32 |
| 6 | Q | 194/196 (99%) | 173 (89%) | 21 (11%) | 6 | 26 |
| 6 | R | 194/196 (99%) | 179 (92%) | 15 (8%) | 12 | 40 |
| 6 | S | 194/196 (99%) | 178 (92%) | 16 (8%) | 10 | 37 |
| 6 | T | 194/196 (99%) | 178 (92%) | 16 (8%) | 10 | 37 |
| 6 | U | 194/196 (99%) | 182 (94%) | 12 (6%) | 16 | 49 |
| 6 | V | 193/196 (98%) | 182 (94%) | 11 (6%) | 18 | 52 |
| 6 | W | 194/196 (99%) | 182 (94%) | 12 (6%) | 16 | 49 |
| 6 | a | 194/196 (99%) | 181 (93%) | 13 (7%) | 15 | 46 |
| 6 | b | 194/196 (99%) | 179 (92%) | 15 (8%) | 12 | 40 |
| 6 | c | 194/196 (99%) | 182 (94%) | 12 (6%) | 16 | 49 |
| 6 | g | 193/196 (98%) | 179 (93%) | 14 (7%) | 13 | 42 |
| 6 | h | 193/196 (98%) | 180 (93%) | 13 (7%) | 15 | 46 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 6 | i | 194/196 (99%) | 176 (91%) | 18 (9%) | 8 | 32 |
| 6 | j | 194/196 (99%) | 178 (92%) | 16 (8%) | 10 | 37 |
| 6 | k | 194/196 (99%) | 179 (92%) | 15 (8%) | 12 | 40 |
| 6 | l | 194/196 (99%) | 176 (91%) | 18 (9%) | 8 | 32 |
| 6 | n | 194/196 (99%) | 183 (94%) | 11 (6%) | 18 | 52 |
| 6 | o | 194/196 (99%) | 184 (95%) | 10 (5%) | 21 | 55 |
| 6 | v | 193/196 (98%) | 177 (92%) | 16 (8%) | 10 | 37 |
| All | All | 8352/11178 (75%) | 7761 (93%) | 591 (7%) | 15 | 43 |

5 of 591 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Z | 98 | VAL |
| 6 | n | 83 | THR |
| 6 | g | 51 | THR |
| 1 | Z | 74 | THR |
| 6 | i | 232 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | E | 407 | ASN |
| 5 | f | 169 | ASN |
| 5 | N | 185 | GLN |
| 4 | e | 841 | GLN |
| 6 | l | 225 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 7 | SF4 | L | 301 | 3 | 0,12,12 | - | - | - | | |
| 7 | SF4 | G | 301 | 3 | 0,12,12 | - | - | - | | |
| 7 | SF4 | d | 301 | 3 | 0,12,12 | - | - | - | | |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 7 | SF4 | L | 301 | 3 | - | - | 0/6/5/5 |
| 7 | SF4 | G | 301 | 3 | - | - | 0/6/5/5 |
| 7 | SF4 | d | 301 | 3 | - | - | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

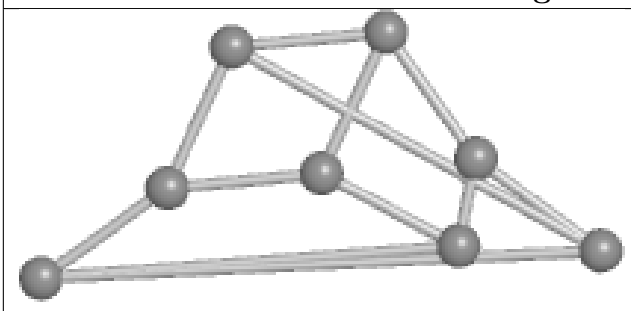
There are no ring outliers.

No monomer is involved in short contacts.

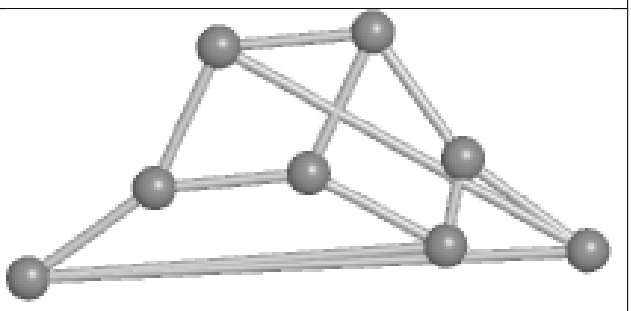
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

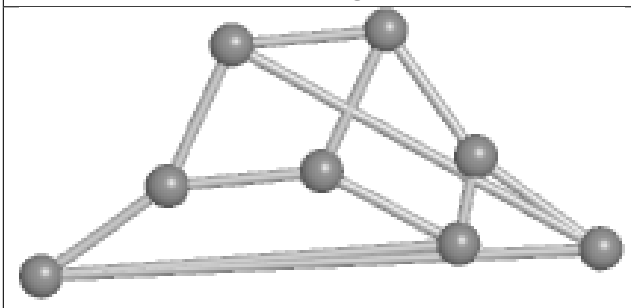
**Ligand SF4 L 301**



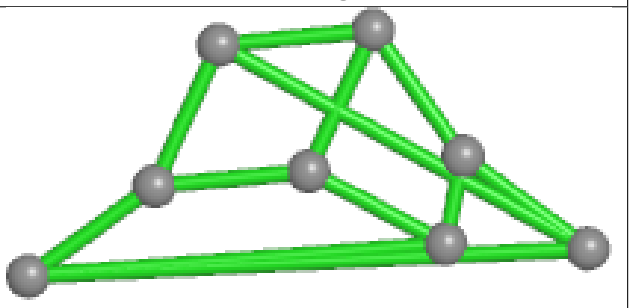
**Bond lengths**



**Bond angles**

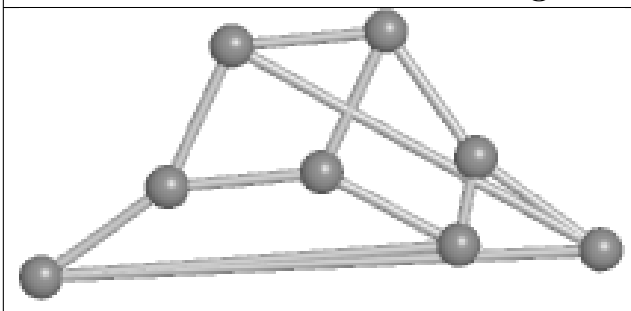


**Torsions**

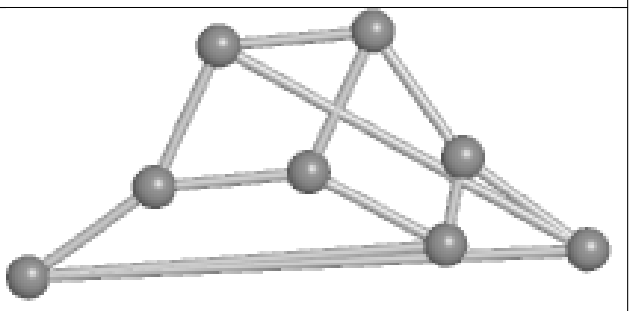


**Rings**

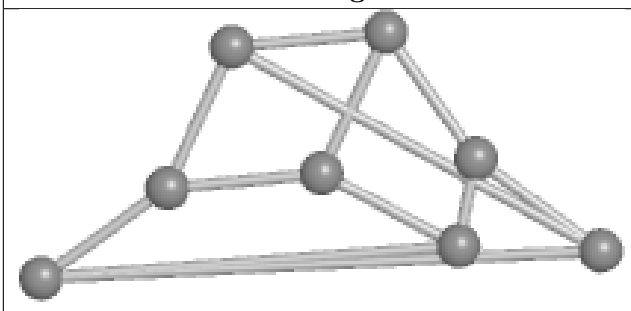
**Ligand SF4 G 301**



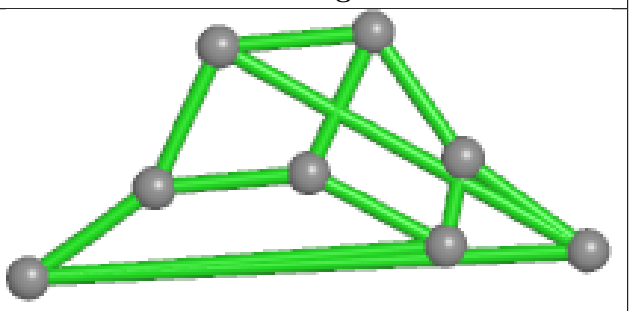
**Bond lengths**



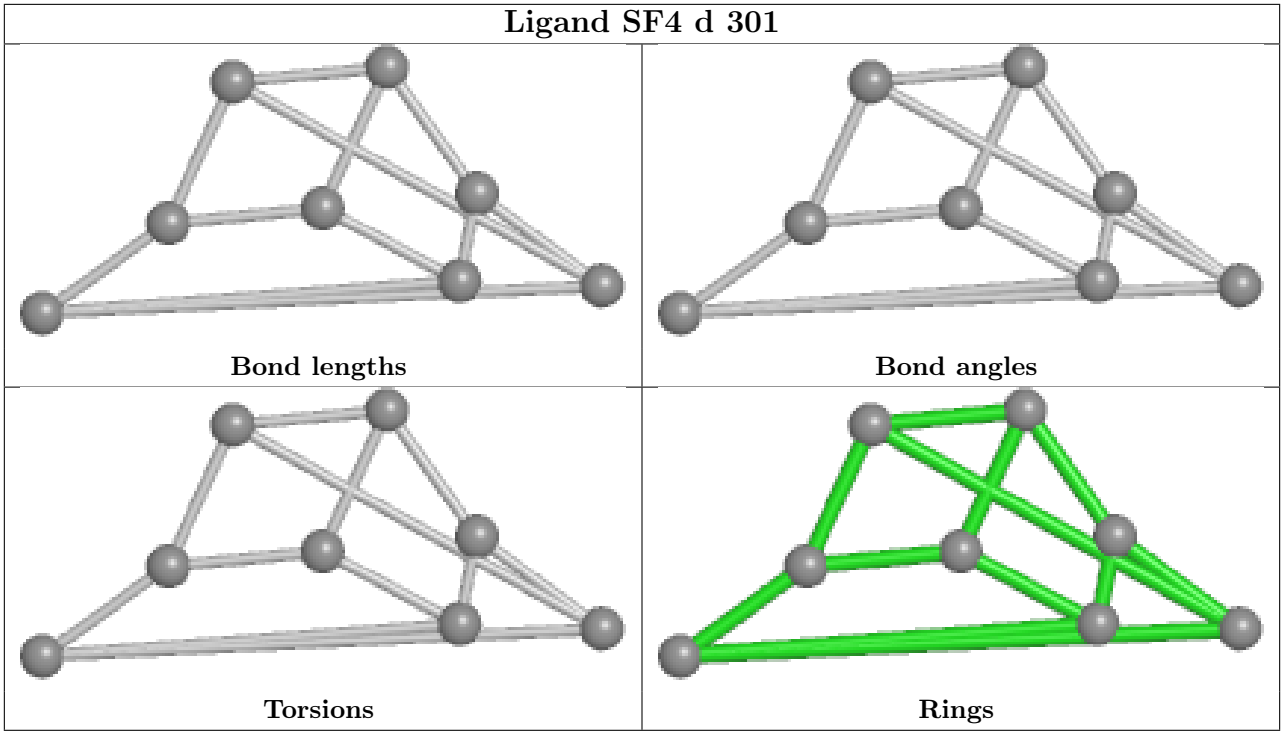
**Bond angles**



**Torsions**



**Rings**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

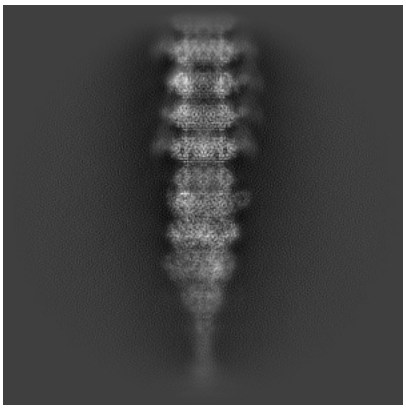
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-35825. These allow visual inspection of the internal detail of the map and identification of artifacts.

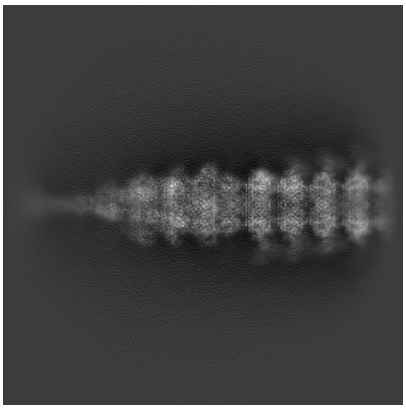
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

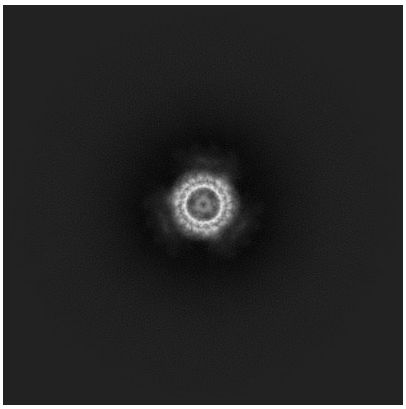
### 6.1.1 Primary map



X

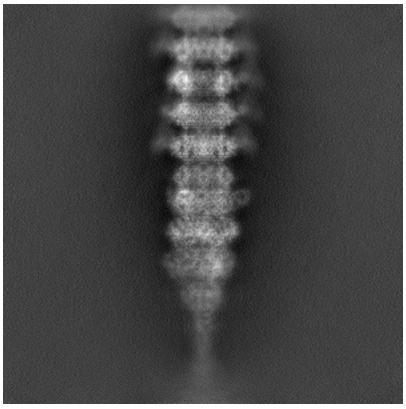


Y

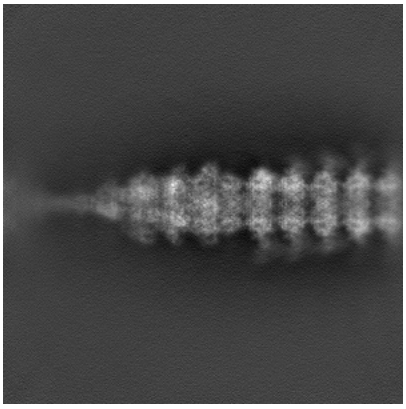


Z

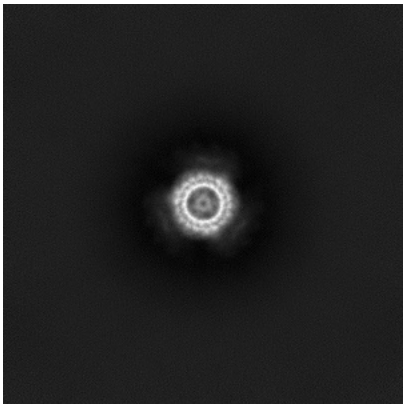
### 6.1.2 Raw map



X



Y

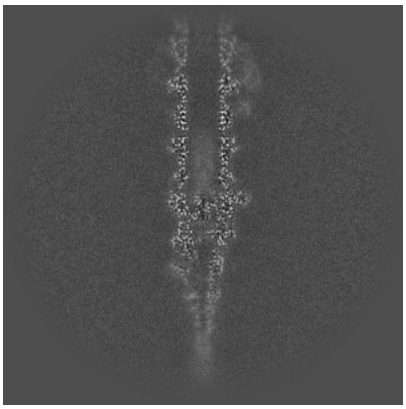


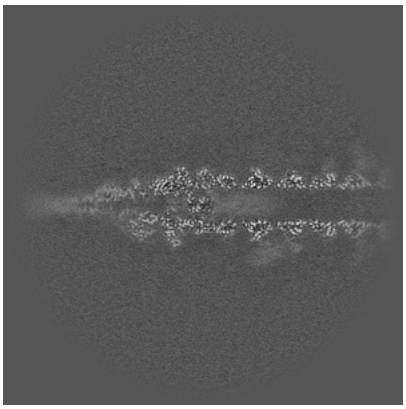
Z

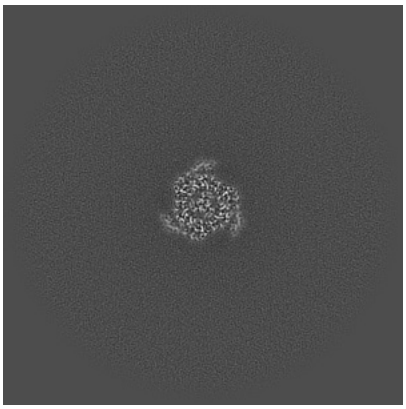
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

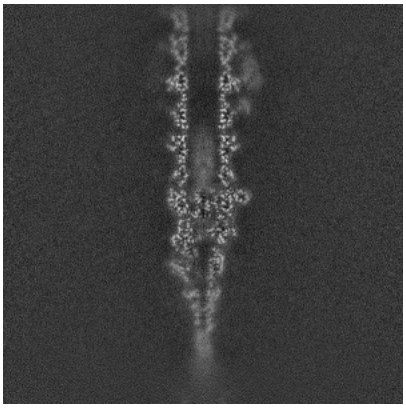
### 6.2.1 Primary map

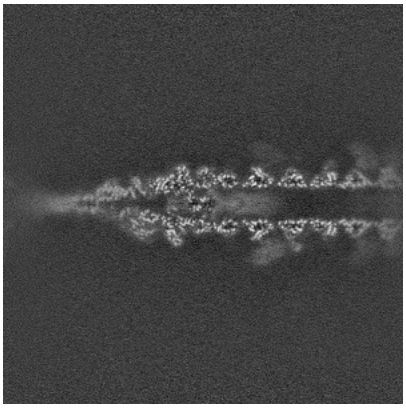

X Index: 240

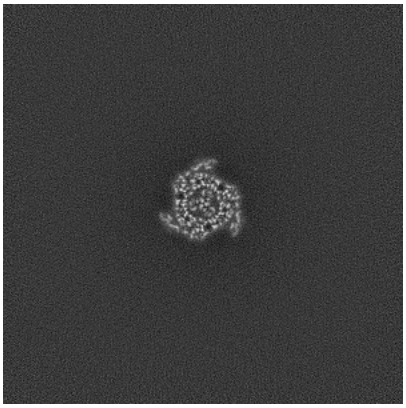

Y Index: 240


Z Index: 240

### 6.2.2 Raw map


X Index: 240

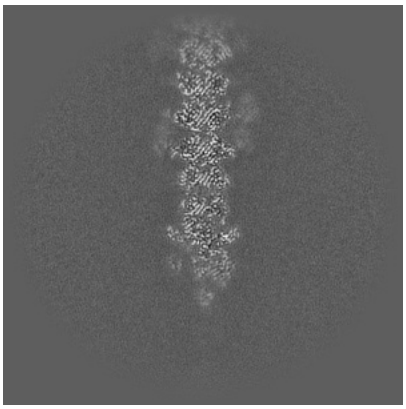

Y Index: 240

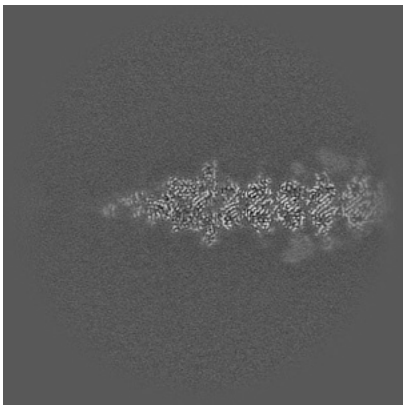

Z Index: 240

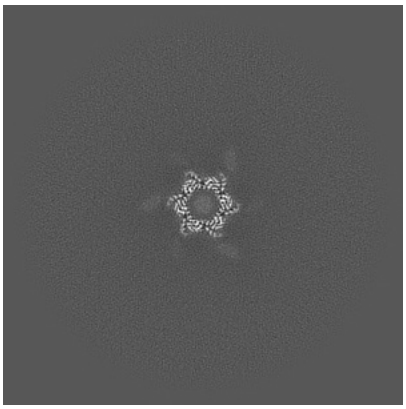
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

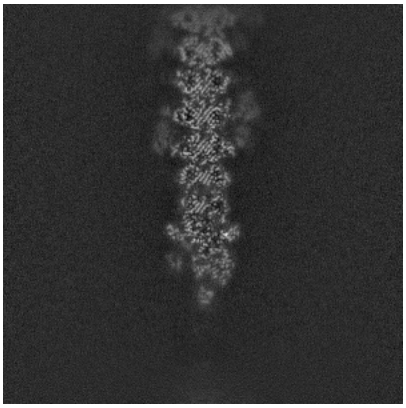
### 6.3.1 Primary map

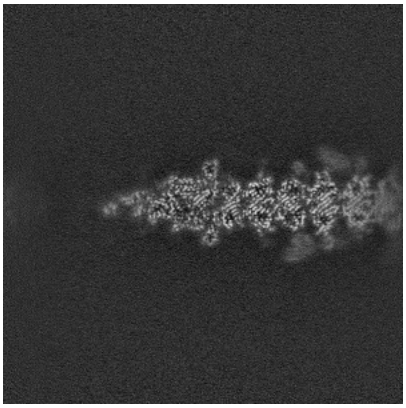

X Index: 261

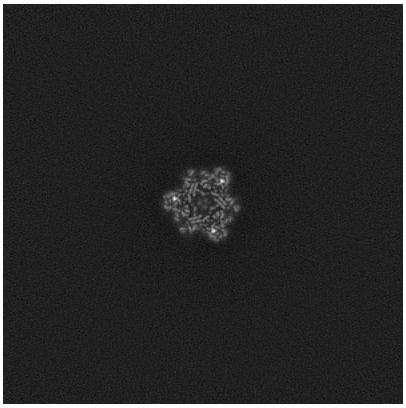

Y Index: 219


Z Index: 299

### 6.3.2 Raw map


X Index: 261

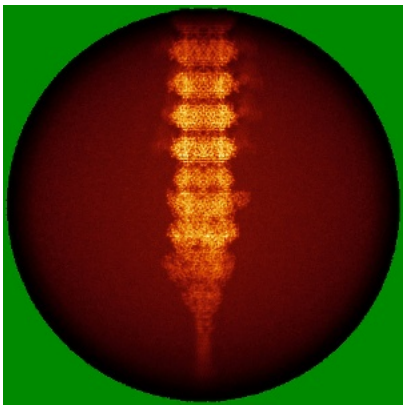

Y Index: 219

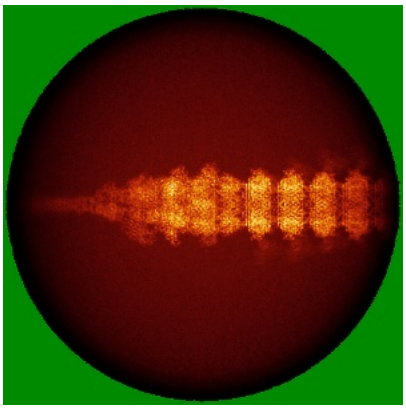

Z Index: 203

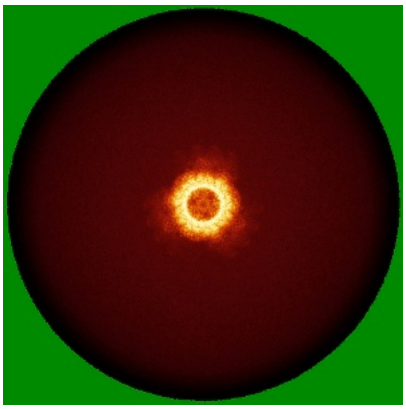
The images above show the largest variance slices of the map in three orthogonal directions.

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

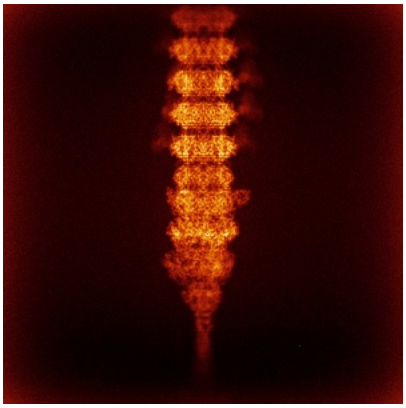
### 6.4.1 Primary map

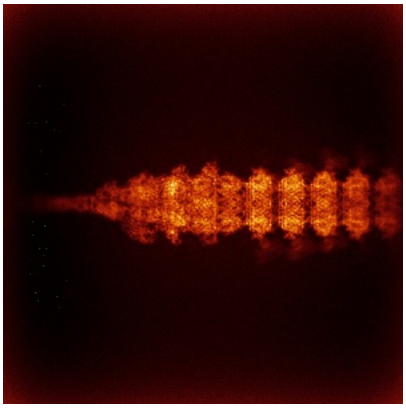

X

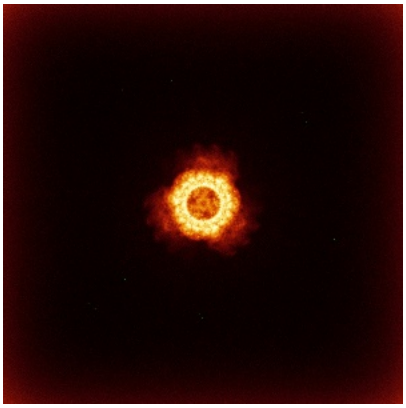

Y


Z

### 6.4.2 Raw map


X

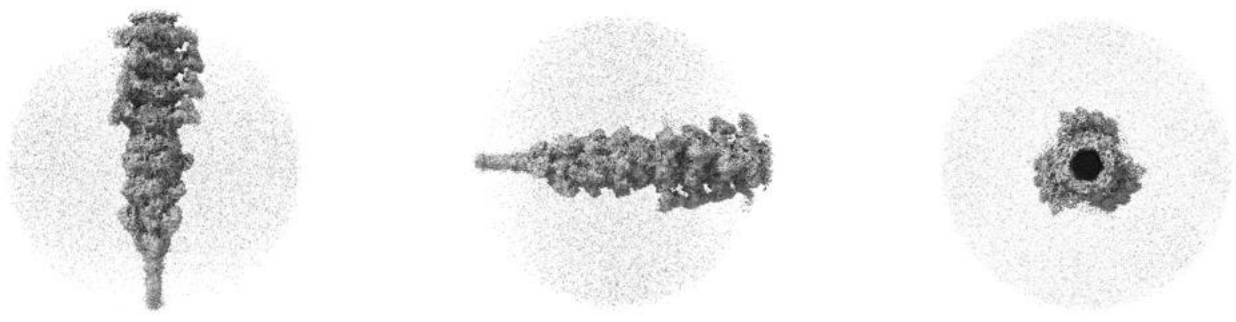

Y


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 0.25. 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.

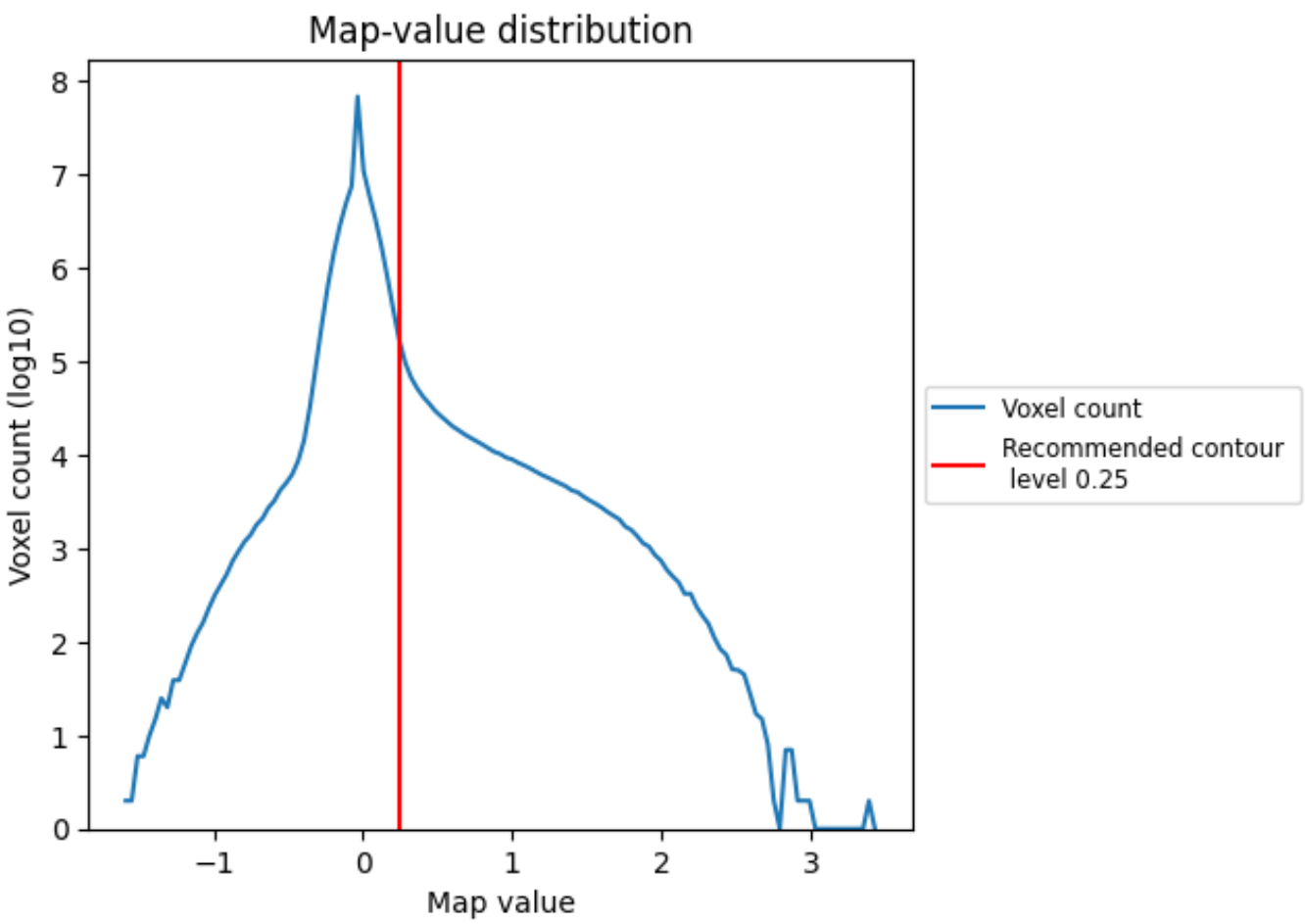
## 6.6 Mask visualisation (i)

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

# 7 Map analysis (i)

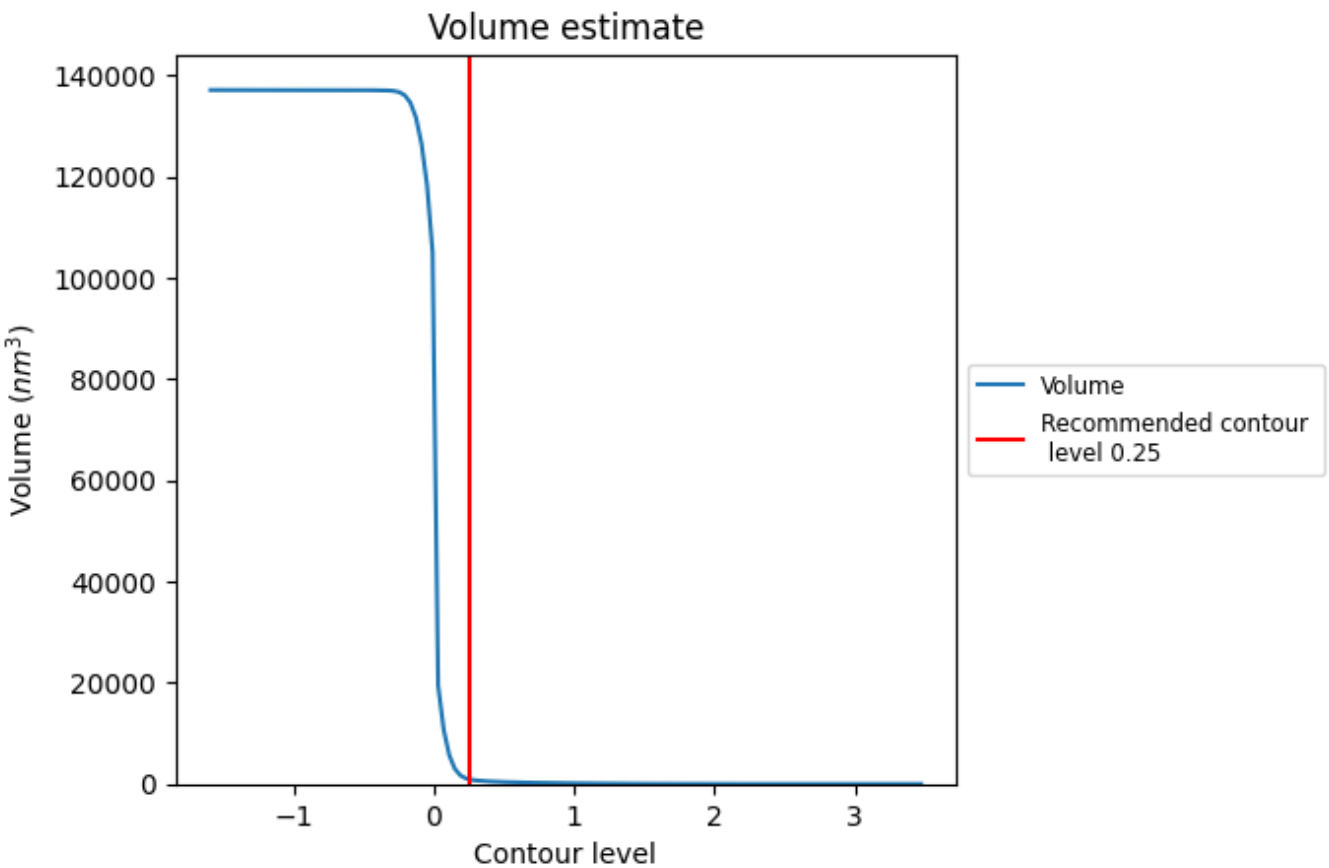
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

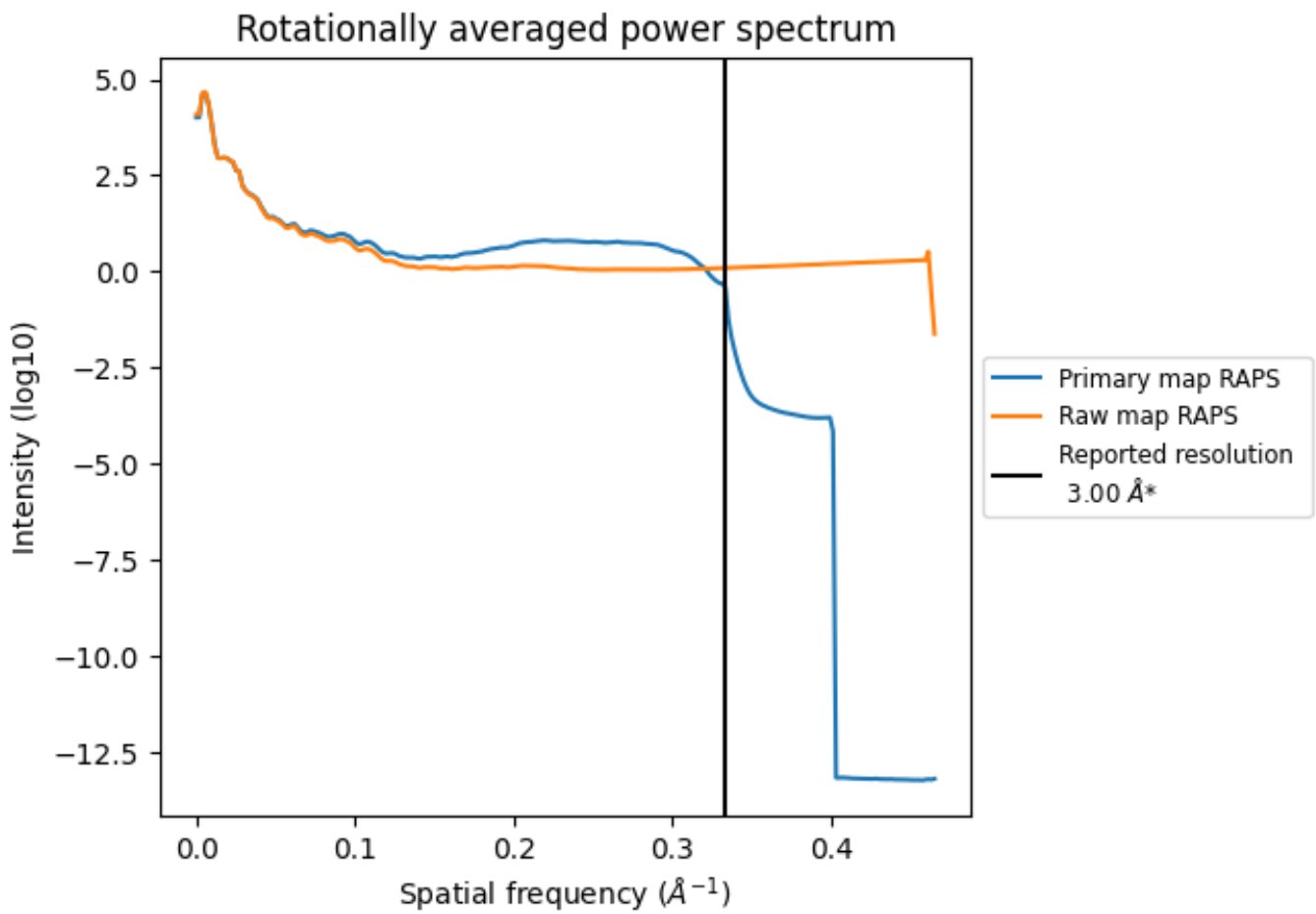
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 959 $nm^3$; this corresponds to an approximate mass of 867 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)

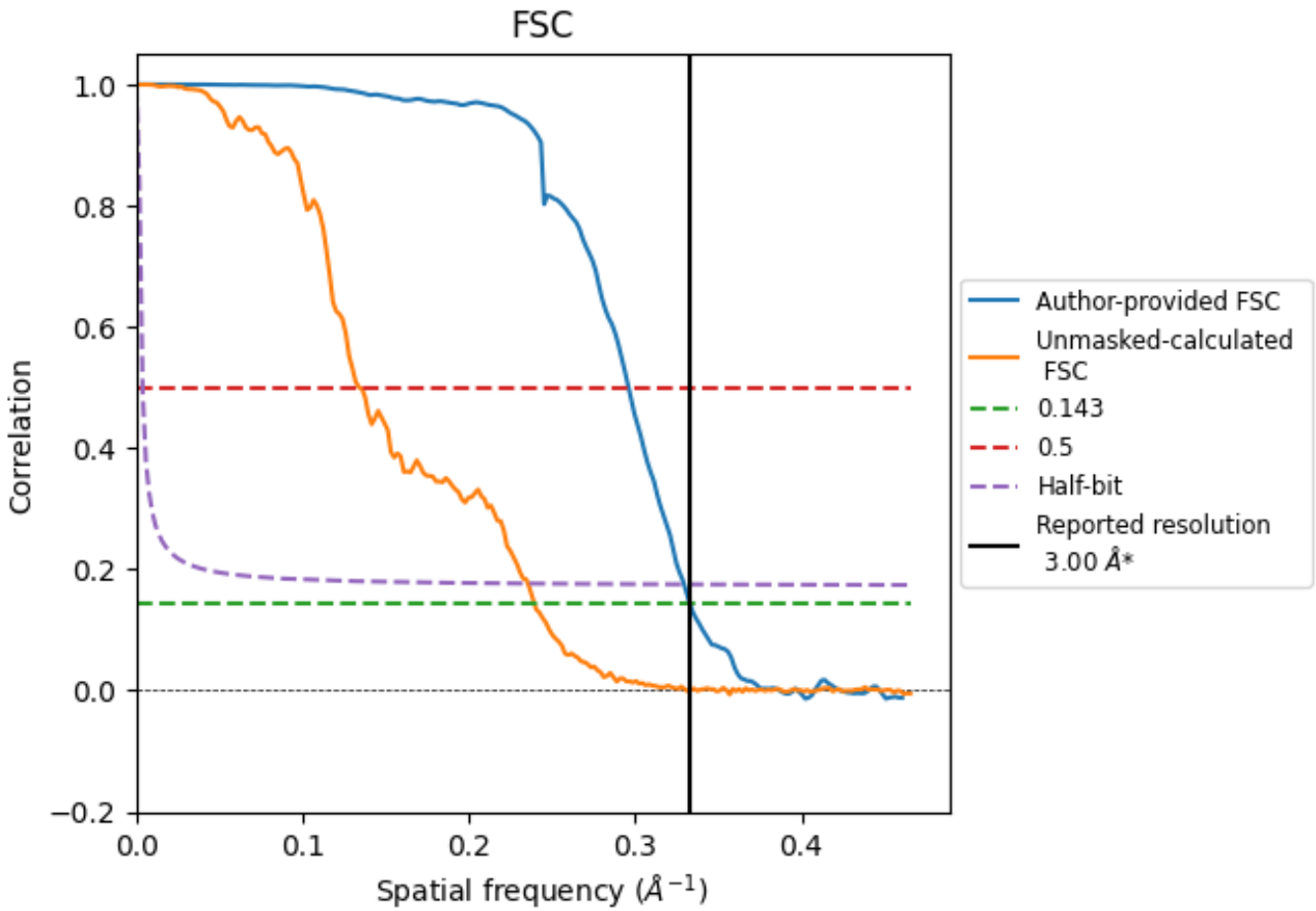



*Reported resolution corresponds to spatial frequency of 0.333 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

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 (i)




*Reported resolution corresponds to spatial frequency of 0.333 Å$^{-1}$

## 8.2 Resolution estimates (i)

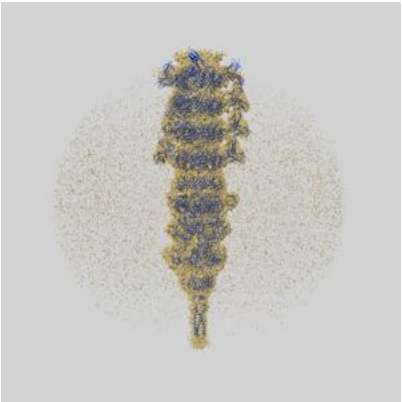
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.00 | - | - |
| Author-provided FSC curve | 3.00 | 3.38 | 3.04 |
| Unmasked-calculated* | 4.18 | 7.46 | 4.24 |

*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 4.18 differs from the reported value 3.0 by more than 10 %

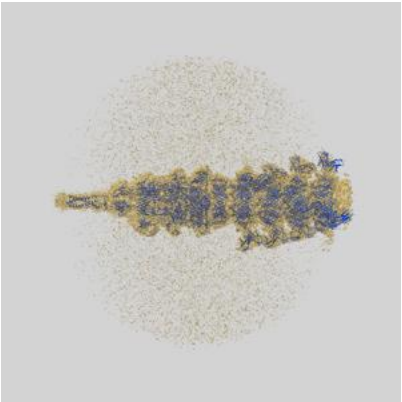
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-35825 and PDB model 8IYL. Per-residue inclusion information can be found in section 3 on page 9.

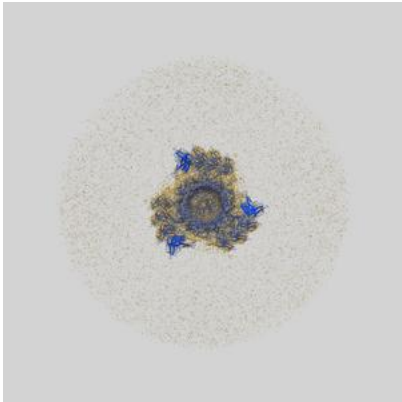
## 9.1 Map-model overlay (i)



X



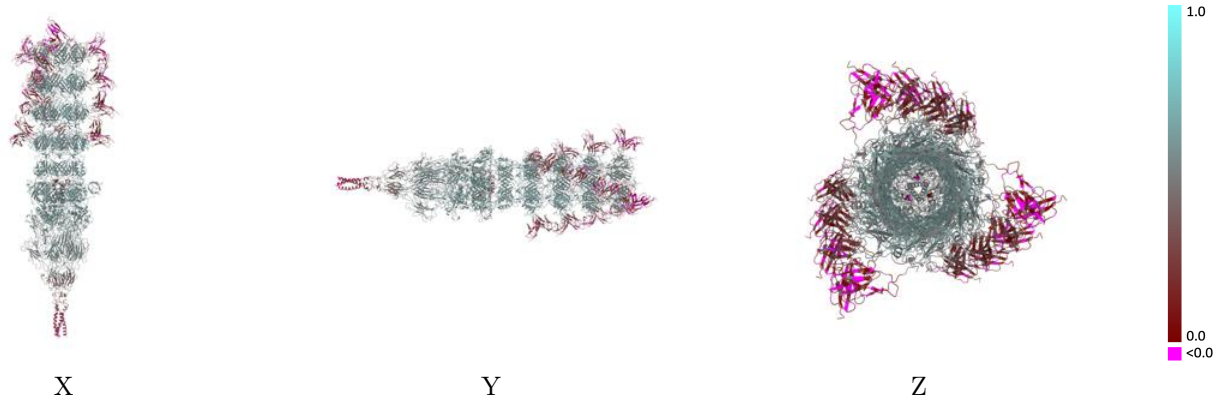
Y



Z

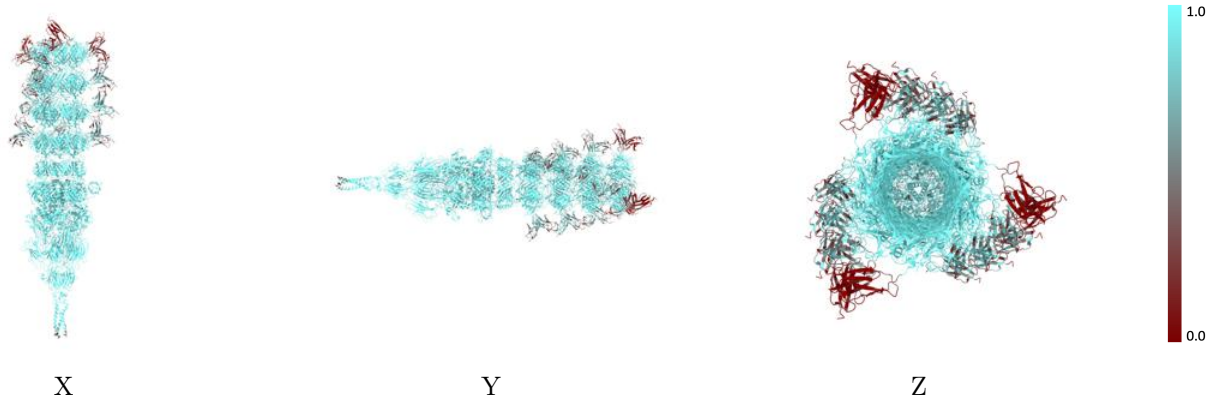
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



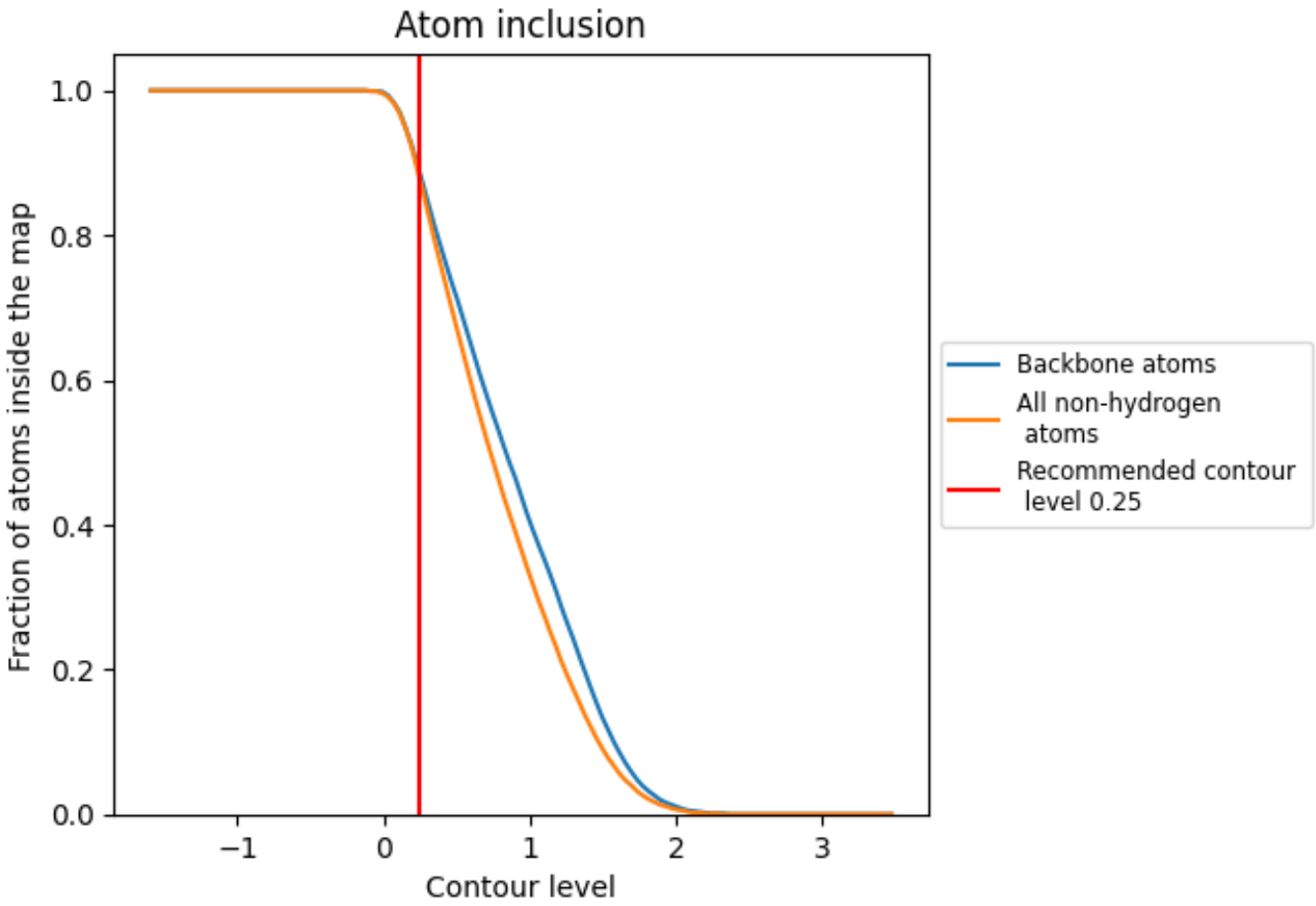

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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




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 (0.25).

## 9.4 Atom inclusion (i)




At the recommended contour level, 88% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8760 | 0.4740 |
| A | 0.8720 | 0.4660 |
| B | 0.8360 | 0.4360 |
| C | 0.6960 | 0.3720 |
| D | 0.9880 | 0.5630 |
| E | 0.9700 | 0.5070 |
| F | 0.9860 | 0.5690 |
| G | 0.9840 | 0.5690 |
| H | 0.9470 | 0.5320 |
| I | 0.9150 | 0.4910 |
| J | 0.9720 | 0.5070 |
| K | 0.9510 | 0.5240 |
| L | 0.9840 | 0.5670 |
| M | 0.9910 | 0.5640 |
| N | 0.9050 | 0.4850 |
| O | 0.8370 | 0.4680 |
| P | 0.8230 | 0.4600 |
| Q | 0.8330 | 0.4370 |
| R | 0.8270 | 0.4420 |
| S | 0.8660 | 0.4650 |
| T | 0.8530 | 0.4610 |
| U | 0.6920 | 0.3750 |
| V | 0.8360 | 0.4650 |
| W | 0.6700 | 0.3730 |
| X | 0.9910 | 0.5650 |
| Y | 0.9730 | 0.5070 |
| Z | 0.9830 | 0.5700 |
| a | 0.8570 | 0.4600 |
| b | 0.8320 | 0.4420 |
| c | 0.6710 | 0.3720 |
| d | 0.9860 | 0.5650 |
| e | 0.9550 | 0.5260 |
| f | 0.9070 | 0.4880 |
| g | 0.8350 | 0.4680 |
| h | 0.8230 | 0.4600 |

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*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| i | 0.8320 | 0.4350 |
| j | 0.8310 | 0.4410 |
| k | 0.8670 | 0.4650 |
| l | 0.8540 | 0.4590 |
| m | 0.9800 | 0.5710 |
| n | 0.6880 | 0.3710 |
| o | 0.6690 | 0.3710 |
| v | 0.8200 | 0.4620 |