



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 09:17 PM EST

PDB ID : 7MUY
EMDB ID : EMD-24026
Title : Reconstruction of the Legionella pneumophila Dot/Icm T4SS 3DVA Map 5
Authors : Sheedlo, M.J.; Durie, C.L.; Swanson, M.; Lacy, D.B.; Ohi, M.D.
Deposited on : 2021-05-14
Resolution : 4.60 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

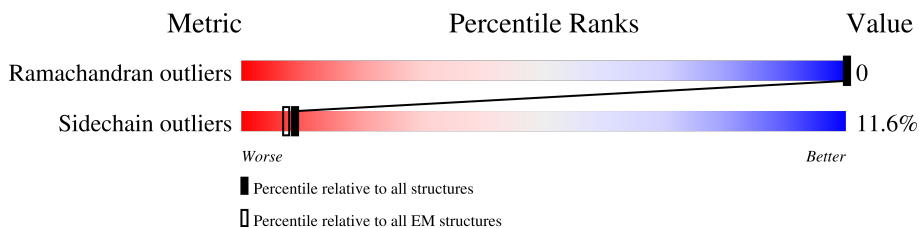
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 4.60 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.



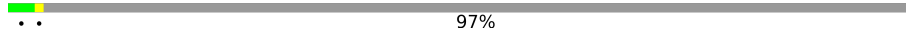

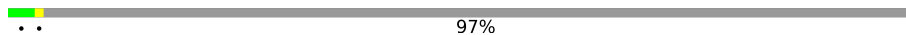
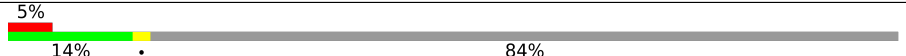
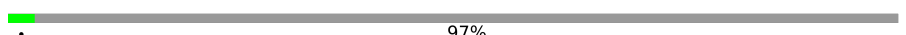
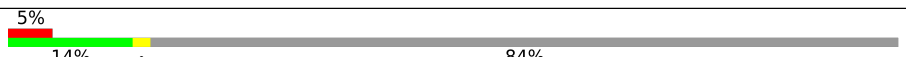
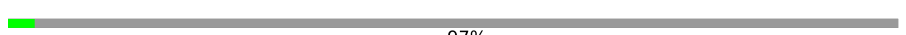
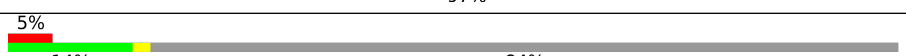

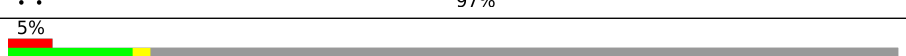

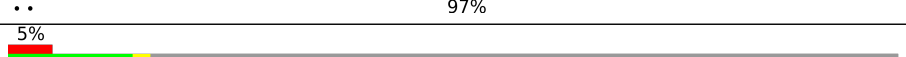

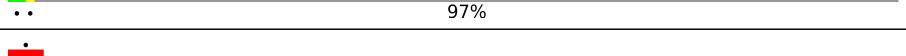
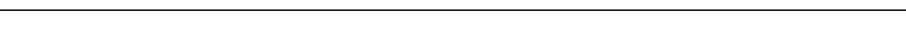
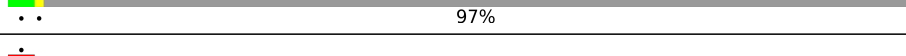

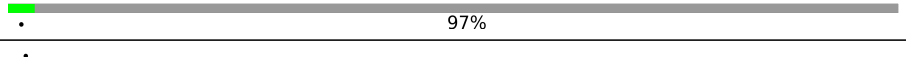




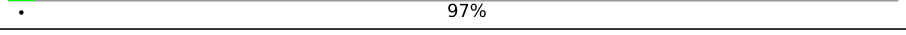
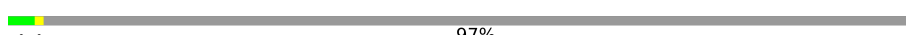
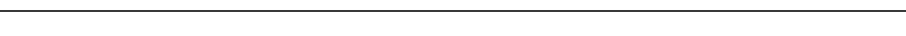
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 $\leq 5\%$. 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 | AG | 1048 | 14% 84% |
| 1 | Ag | 1048 | 97% |
| 1 | BG | 1048 | 14% 84% |
| 1 | Bg | 1048 | 97% |
| 1 | CG | 1048 | 14% 84% |
| 1 | Cg | 1048 | 97% |
| 1 | DG | 1048 | 14% 84% |
| 1 | Dg | 1048 | 97% |
| 1 | EG | 1048 | 14% 84% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | Eg | 1048 |  97% |
| 1 | FG | 1048 |  84% |
| 1 | Fg | 1048 |  97% |
| 1 | GG | 1048 |  84% |
| 1 | Gg | 1048 |  97% |
| 1 | HG | 1048 |  84% |
| 1 | Hg | 1048 |  97% |
| 1 | IG | 1048 |  84% |
| 1 | Ig | 1048 |  97% |
| 1 | JG | 1048 |  84% |
| 1 | Jg | 1048 |  97% |
| 1 | KG | 1048 |  84% |
| 1 | Kg | 1048 |  97% |
| 1 | LG | 1048 |  84% |
| 1 | Lg | 1048 |  97% |
| 1 | MG | 1048 |  84% |
| 1 | Mg | 1048 |  97% |
| 1 | NG | 1048 |  84% |
| 1 | OG | 1048 |  84% |
| 1 | PG | 1048 |  84% |
| 1 | VG | 1048 |  97% |
| 1 | WG | 1048 |  97% |
| 1 | XG | 1048 |  97% |
| 1 | YG | 1048 |  97% |
| 1 | ZG | 1048 |  97% |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | AD | 163 | 77% 9% 14% |
| 2 | Ad | 163 | 77% 7% 16% |
| 2 | BD | 163 | 81% 5% 14% |
| 2 | Bd | 163 | 77% 7% 16% |
| 2 | CD | 163 | 76% 10% 14% |
| 2 | Cd | 163 | 75% 9% 16% |
| 2 | DD | 163 | 80% 6% 14% |
| 2 | Dd | 163 | 77% 7% 16% |
| 2 | ED | 163 | 82% 14% |
| 2 | Ed | 163 | 77% 7% 16% |
| 2 | FD | 163 | 76% 10% 14% |
| 2 | Fd | 163 | 79% 6% 16% |
| 2 | GD | 163 | 79% 7% 14% |
| 2 | Gd | 163 | 77% 7% 16% |
| 2 | HD | 163 | 79% 7% 14% |
| 2 | Hd | 163 | 79% 5% 16% |
| 2 | ID | 163 | 80% 6% 14% |
| 2 | Id | 163 | 78% 6% 16% |
| 2 | JD | 163 | 80% 6% 14% |
| 2 | Jd | 163 | 79% 5% 16% |
| 2 | KD | 163 | 79% 7% 14% |
| 2 | Kd | 163 | 78% 6% 16% |
| 2 | LD | 163 | 77% 9% 14% |
| 2 | Ld | 163 | 78% 6% 16% |
| 2 | MD | 163 | 77% 9% 14% |









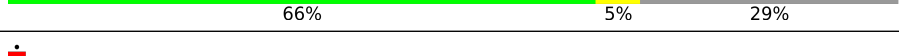
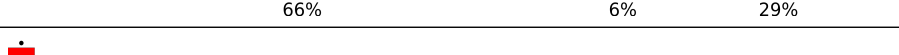
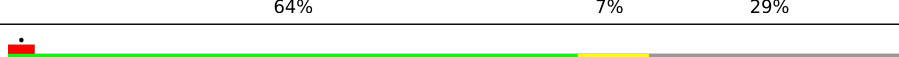
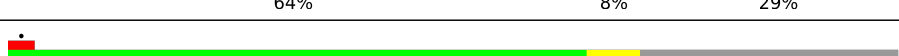

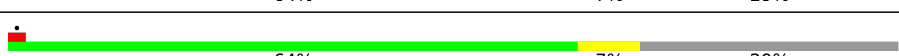
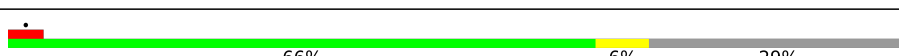
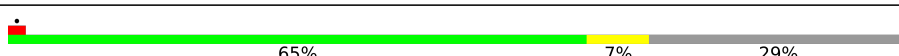





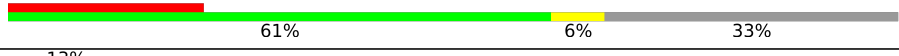

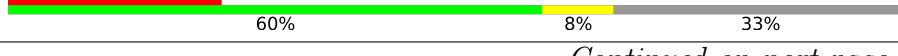

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 2 | Md | 163 |  77% 7% 16% |
| 3 | AF | 269 |  21% 77% |
| 3 | Af | 269 |  20% 78% |
| 3 | BF | 269 |  20% 77% |
| 3 | Bf | 269 |  20% 78% |
| 3 | CF | 269 |  22% 77% |
| 3 | Cf | 269 |  19% 78% |
| 3 | DF | 269 |  20% 77% |
| 3 | Df | 269 |  21% 78% |
| 3 | EF | 269 |  21% 77% |
| 3 | Ef | 269 |  22% 78% |
| 3 | FF | 269 |  20% 77% |
| 3 | Ff | 269 |  20% 78% |
| 3 | GF | 269 |  21% 77% |
| 3 | Gf | 269 |  20% 78% |
| 3 | HF | 269 |  20% 77% |
| 3 | Hf | 269 |  20% 78% |
| 3 | IF | 269 |  21% 77% |
| 3 | If | 269 |  20% 78% |
| 3 | JF | 269 |  20% 77% |
| 3 | Jf | 269 |  21% 78% |
| 3 | KF | 269 |  22% 77% |
| 3 | Kf | 269 |  21% 78% |
| 3 | LF | 269 |  21% 77% |
| 3 | Lf | 269 |  18% 78% |



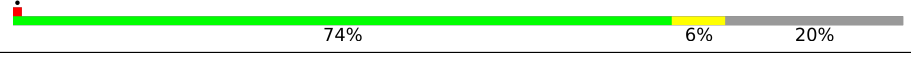
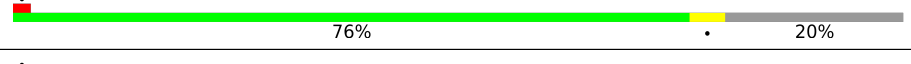
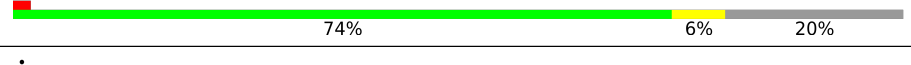



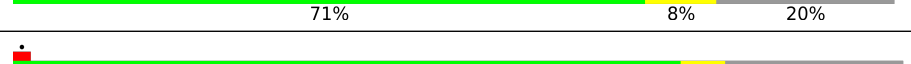
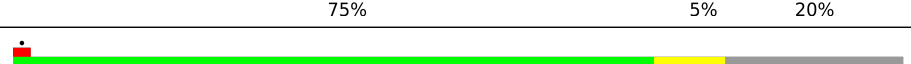
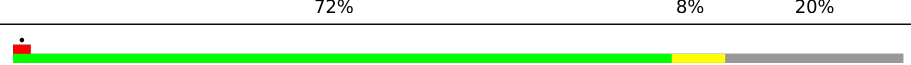
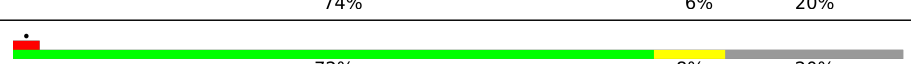
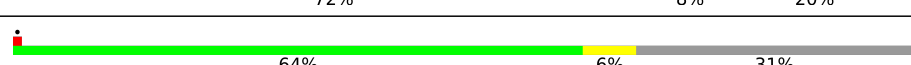
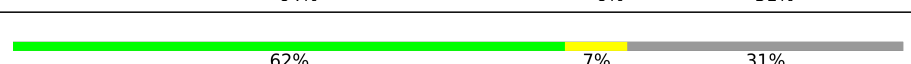
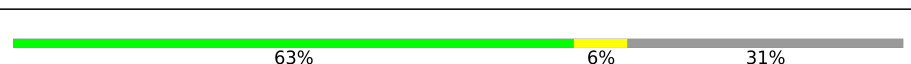
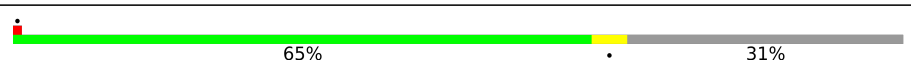
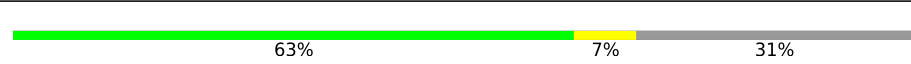


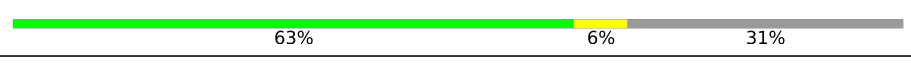

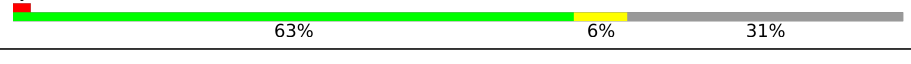



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 3 | MF | 269 |  20% 77% |
| 3 | Mf | 269 |  20% 78% |
| 3 | VF | 269 |  22% 77% |
| 3 | WF | 269 |  21% 77% |
| 3 | XF | 269 |  22% 77% |
| 3 | YF | 269 |  21% 77% |
| 3 | ZF | 269 |  22% 77% |
| 4 | AH | 361 |  64% 8% 29% |
| 4 | BH | 361 |  66% 5% 29% |
| 4 | CH | 361 |  66% 6% 29% |
| 4 | DH | 361 |  64% 7% 29% |
| 4 | EH | 361 |  64% 8% 29% |
| 4 | FH | 361 |  65% 6% 29% |
| 4 | GH | 361 |  64% 7% 29% |
| 4 | HH | 361 |  64% 7% 29% |
| 4 | IH | 361 |  66% 6% 29% |
| 4 | JH | 361 |  65% 7% 29% |
| 4 | KH | 361 |  66% 6% 29% |
| 4 | LH | 361 |  65% 6% 29% |
| 4 | MH | 361 |  65% 7% 29% |
| 4 | VH | 361 |  9% 60% 8% 33% |
| 4 | WH | 361 |  15% 58% 9% 33% |
| 4 | XH | 361 |  22% 61% 6% 33% |
| 4 | YH | 361 |  13% 60% 7% 33% |
| 4 | ZH | 361 |  24% 60% 8% 33% |











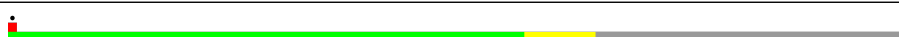


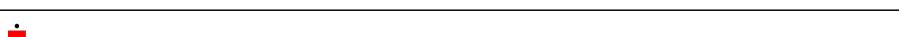
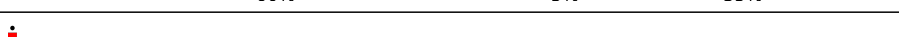
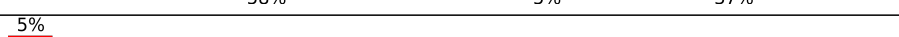



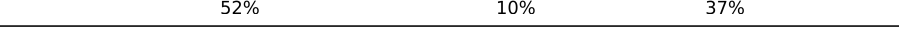





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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | AK | 189 |  |
| 5 | BK | 189 |  |
| 5 | CK | 189 |  |
| 5 | DK | 189 |  |
| 5 | EK | 189 |  |
| 5 | FK | 189 |  |
| 5 | GK | 189 |  |
| 5 | HK | 189 |  |
| 5 | IK | 189 |  |
| 5 | JK | 189 |  |
| 5 | KK | 189 |  |
| 5 | LK | 189 |  |
| 5 | MK | 189 |  |
| 6 | AL | 249 |  |
| 6 | BL | 249 |  |
| 6 | CL | 249 |  |
| 6 | DL | 249 |  |
| 6 | EL | 249 |  |
| 6 | FL | 249 |  |
| 6 | GL | 249 |  |
| 6 | HL | 249 |  |
| 6 | IL | 249 |  |
| 6 | JL | 249 |  |
| 6 | KL | 249 |  |
| 6 | LL | 249 |  |

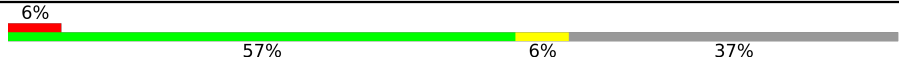
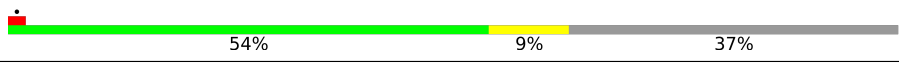
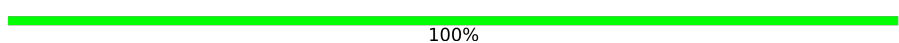

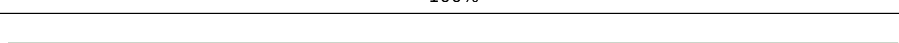
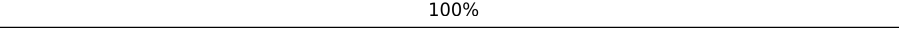
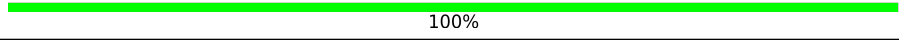
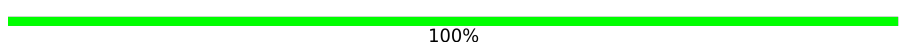

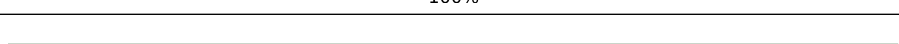
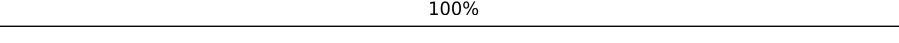
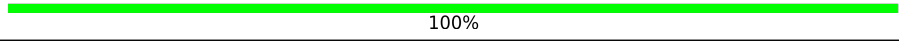
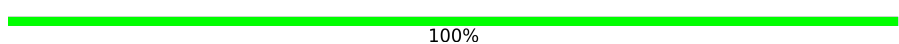

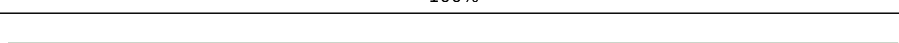
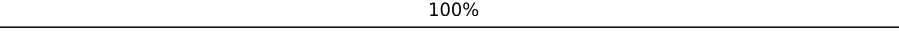
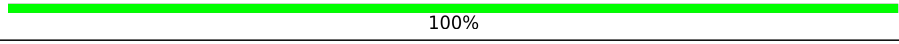
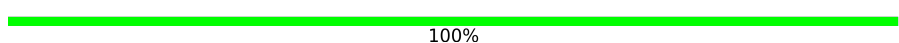

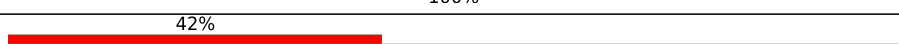
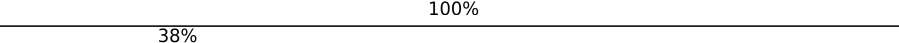
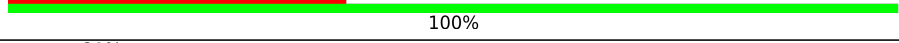
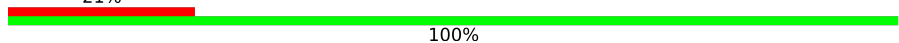
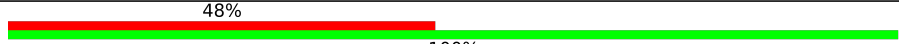
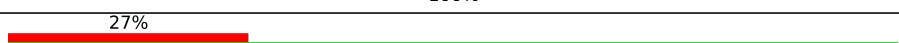
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 6 | ML | 249 |  63% 6% 31% |
| 7 | AM | 320 |  60% 5% 35% |
| 7 | BM | 320 |  56% 9% 35% |
| 7 | CM | 320 |  57% 8% 35% |
| 7 | DM | 320 |  58% 7% 35% |
| 7 | EM | 320 |  57% 8% 35% |
| 7 | FM | 320 |  58% 7% 35% |
| 7 | GM | 320 |  58% 7% 35% |
| 7 | HM | 320 |  58% 7% 35% |
| 7 | IM | 320 |  57% 8% 35% |
| 7 | JM | 320 |  58% 8% 35% |
| 7 | KM | 320 |  57% 8% 35% |
| 7 | LM | 320 |  58% 7% 35% |
| 7 | MM | 320 |  60% 5% 35% |
| 8 | AN | 124 |  58% 5% 37% |
| 8 | BN | 124 |  5% 52% 10% 37% |
| 8 | CN | 124 |  6% 60% 37% |
| 8 | DN | 124 |  54% 9% 37% |
| 8 | EN | 124 |  52% 10% 37% |
| 8 | FN | 124 |  53% 10% 37% |
| 8 | GN | 124 |  6% 56% 7% 37% |
| 8 | HN | 124 |  5% 52% 10% 37% |
| 8 | IN | 124 |  56% 7% 37% |
| 8 | JN | 124 |  6% 58% 5% 37% |
| 8 | KN | 124 |  7% 56% 6% 37% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 8 | LN | 124 |  6% 57% 6% 37% |
| 8 | MN | 124 |  1% 54% 9% 37% |
| 9 | AU | 9 |  100% |
| 9 | BU | 9 |  100% |
| 9 | CU | 9 |  100% |
| 9 | DU | 9 |  100% |
| 9 | EU | 9 |  100% |
| 9 | FU | 9 |  100% |
| 9 | GU | 9 |  100% |
| 9 | HU | 9 |  100% |
| 9 | IU | 9 |  100% |
| 9 | JU | 9 |  100% |
| 9 | KU | 9 |  100% |
| 9 | LU | 9 |  100% |
| 9 | MU | 9 |  100% |
| 10 | AX | 48 |  38% 100% |
| 10 | BX | 48 |  42% 100% |
| 10 | CX | 48 |  38% 100% |
| 10 | DX | 48 |  21% 100% |
| 10 | EX | 48 |  48% 100% |
| 10 | FX | 48 |  27% 100% |
| 10 | GX | 48 |  17% 100% |
| 10 | HX | 48 |  33% 100% |
| 10 | IX | 48 |  42% 100% |
| 10 | JX | 48 |  40% 100% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 10 | KX | 48 | |
| 10 | LX | 48 | |
| 10 | MX | 48 | |
| 10 | VX | 48 | |
| 10 | WX | 48 | |
| 10 | XX | 48 | |
| 10 | YX | 48 | |
| 10 | ZX | 48 | |
| 11 | AC | 303 | |
| 11 | BC | 303 | |
| 11 | CC | 303 | |
| 11 | DC | 303 | |
| 11 | EC | 303 | |
| 11 | FC | 303 | |
| 11 | GC | 303 | |
| 11 | HC | 303 | |
| 11 | IC | 303 | |
| 11 | JC | 303 | |
| 11 | KC | 303 | |
| 11 | LC | 303 | |
| 11 | MC | 303 | |

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 192370 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 IcmE protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | AG | 165 | 1229 | 780 | 203 | 242 | 4 | 0 | 0 |
| 1 | Eg | 34 | 276 | 168 | 47 | 60 | 1 | 0 | 0 |
| 1 | Fg | 34 | 276 | 168 | 47 | 60 | 1 | 0 | 0 |
| 1 | BG | 165 | 1229 | 780 | 203 | 242 | 4 | 0 | 0 |
| 1 | Gg | 34 | 276 | 168 | 47 | 60 | 1 | 0 | 0 |
| 1 | Hg | 34 | 276 | 168 | 47 | 60 | 1 | 0 | 0 |
| 1 | CG | 165 | 1229 | 780 | 203 | 242 | 4 | 0 | 0 |
| 1 | Bg | 34 | 276 | 168 | 47 | 60 | 1 | 0 | 0 |
| 1 | Ig | 34 | 276 | 168 | 47 | 60 | 1 | 0 | 0 |
| 1 | Jg | 34 | 276 | 168 | 47 | 60 | 1 | 0 | 0 |
| 1 | DG | 165 | 1229 | 780 | 203 | 242 | 4 | 0 | 0 |
| 1 | Kg | 34 | 276 | 168 | 47 | 60 | 1 | 0 | 0 |
| 1 | Lg | 34 | 276 | 168 | 47 | 60 | 1 | 0 | 0 |
| 1 | EG | 165 | 1229 | 780 | 203 | 242 | 4 | 0 | 0 |
| 1 | Mg | 34 | 276 | 168 | 47 | 60 | 1 | 0 | 0 |
| 1 | VG | 34 | 276 | 168 | 47 | 60 | 1 | 0 | 0 |
| 1 | WG | 34 | 276 | 168 | 47 | 60 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | XG | 34 | Total | C | N | O | S | 0 | 0 |
| | | | 276 | 168 | 47 | 60 | 1 | | |
| 1 | FG | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 780 | 203 | 242 | 4 | | |
| 1 | YG | 34 | Total | C | N | O | S | 0 | 0 |
| | | | 276 | 168 | 47 | 60 | 1 | | |
| 1 | ZG | 34 | Total | C | N | O | S | 0 | 0 |
| | | | 276 | 168 | 47 | 60 | 1 | | |
| 1 | GG | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 780 | 203 | 242 | 4 | | |
| 1 | Cg | 34 | Total | C | N | O | S | 0 | 0 |
| | | | 276 | 168 | 47 | 60 | 1 | | |
| 1 | Dg | 34 | Total | C | N | O | S | 0 | 0 |
| | | | 276 | 168 | 47 | 60 | 1 | | |
| 1 | HG | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 780 | 203 | 242 | 4 | | |
| 1 | IG | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 780 | 203 | 242 | 4 | | |
| 1 | JG | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 780 | 203 | 242 | 4 | | |
| 1 | KG | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 780 | 203 | 242 | 4 | | |
| 1 | LG | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 780 | 203 | 242 | 4 | | |
| 1 | MG | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 780 | 203 | 242 | 4 | | |
| 1 | NG | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 780 | 203 | 242 | 4 | | |
| 1 | OG | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 780 | 203 | 242 | 4 | | |
| 1 | PG | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 780 | 203 | 242 | 4 | | |
| 1 | Ag | 34 | Total | C | N | O | S | 0 | 0 |
| | | | 276 | 168 | 47 | 60 | 1 | | |

- Molecule 2 is a protein called DotD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | ED | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1086 | 692 | 185 | 206 | 3 | | |
| 2 | Ed | 137 | Total | C | N | O | S | 0 | 0 |
| | | | 1058 | 672 | 182 | 202 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | FD | 140 | 1086 | 692 | 185 | 206 | 3 | 0 | 0 |
| 2 | Fd | 137 | 1058 | 672 | 182 | 202 | 2 | 0 | 0 |
| 2 | GD | 140 | 1086 | 692 | 185 | 206 | 3 | 0 | 0 |
| 2 | Gd | 137 | 1058 | 672 | 182 | 202 | 2 | 0 | 0 |
| 2 | HD | 140 | 1086 | 692 | 185 | 206 | 3 | 0 | 0 |
| 2 | Hd | 137 | 1058 | 672 | 182 | 202 | 2 | 0 | 0 |
| 2 | ID | 140 | 1086 | 692 | 185 | 206 | 3 | 0 | 0 |
| 2 | Id | 137 | 1058 | 672 | 182 | 202 | 2 | 0 | 0 |
| 2 | JD | 140 | 1086 | 692 | 185 | 206 | 3 | 0 | 0 |
| 2 | Jd | 137 | 1058 | 672 | 182 | 202 | 2 | 0 | 0 |
| 2 | KD | 140 | 1086 | 692 | 185 | 206 | 3 | 0 | 0 |
| 2 | Kd | 137 | 1058 | 672 | 182 | 202 | 2 | 0 | 0 |
| 2 | LD | 140 | 1086 | 692 | 185 | 206 | 3 | 0 | 0 |
| 2 | Ld | 137 | 1058 | 672 | 182 | 202 | 2 | 0 | 0 |
| 2 | MD | 140 | 1086 | 692 | 185 | 206 | 3 | 0 | 0 |
| 2 | Md | 137 | 1058 | 672 | 182 | 202 | 2 | 0 | 0 |
| 2 | Ad | 137 | 1058 | 672 | 182 | 202 | 2 | 0 | 0 |
| 2 | BD | 140 | 1086 | 692 | 185 | 206 | 3 | 0 | 0 |
| 2 | Bd | 137 | 1058 | 672 | 182 | 202 | 2 | 0 | 0 |
| 2 | CD | 140 | 1086 | 692 | 185 | 206 | 3 | 0 | 0 |
| 2 | Cd | 137 | 1058 | 672 | 182 | 202 | 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | DD | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1086 | 692 | 185 | 206 | 3 | | |
| 2 | Dd | 137 | Total | C | N | O | S | 0 | 0 |
| | | | 1058 | 672 | 182 | 202 | 2 | | |
| 2 | AD | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1086 | 692 | 185 | 206 | 3 | | |

- Molecule 3 is a protein called DotF.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3 | EF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | Ef | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 290 | 77 | 81 | 1 | | |
| 3 | FF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | Ff | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 290 | 77 | 81 | 1 | | |
| 3 | AF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | GF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | Gf | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 290 | 77 | 81 | 1 | | |
| 3 | HF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | Hf | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 290 | 77 | 81 | 1 | | |
| 3 | IF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | If | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 290 | 77 | 81 | 1 | | |
| 3 | JF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | Jf | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 290 | 77 | 81 | 1 | | |
| 3 | KF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | Kf | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 290 | 77 | 81 | 1 | | |
| 3 | LF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3 | Lf | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 290 | 77 | 81 | 1 | | |
| 3 | MF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | Mf | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 290 | 77 | 81 | 1 | | |
| 3 | VF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | WF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | XF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | YF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | ZF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | Af | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 290 | 77 | 81 | 1 | | |
| 3 | BF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | Bf | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 290 | 77 | 81 | 1 | | |
| 3 | CF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | Cf | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 290 | 77 | 81 | 1 | | |
| 3 | DF | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 483 | 308 | 84 | 90 | 1 | | |
| 3 | Df | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 290 | 77 | 81 | 1 | | |

- Molecule 4 is a protein called Type IV secretion protein IcmK.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | EH | 258 | Total | C | N | O | S | 0 | 0 |
| | | | 1983 | 1268 | 336 | 371 | 8 | | |
| 4 | FH | 258 | Total | C | N | O | S | 0 | 0 |
| | | | 1983 | 1268 | 336 | 371 | 8 | | |
| 4 | GH | 258 | Total | C | N | O | S | 0 | 0 |
| | | | 1983 | 1268 | 336 | 371 | 8 | | |
| 4 | HH | 258 | Total | C | N | O | S | 0 | 0 |
| | | | 1983 | 1268 | 336 | 371 | 8 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | IH | 258 | Total 1983 | C 1268 | N 336 | O 371 | S 8 | 0 | 0 |
| 4 | JH | 258 | Total 1983 | C 1268 | N 336 | O 371 | S 8 | 0 | 0 |
| 4 | AH | 258 | Total 1983 | C 1268 | N 336 | O 371 | S 8 | 0 | 0 |
| 4 | KH | 258 | Total 1983 | C 1268 | N 336 | O 371 | S 8 | 0 | 0 |
| 4 | LH | 258 | Total 1983 | C 1268 | N 336 | O 371 | S 8 | 0 | 0 |
| 4 | MH | 258 | Total 1983 | C 1268 | N 336 | O 371 | S 8 | 0 | 0 |
| 4 | VH | 243 | Total 1875 | C 1201 | N 319 | O 348 | S 7 | 0 | 0 |
| 4 | WH | 243 | Total 1875 | C 1201 | N 319 | O 348 | S 7 | 0 | 0 |
| 4 | XH | 243 | Total 1875 | C 1201 | N 319 | O 348 | S 7 | 0 | 0 |
| 4 | YH | 243 | Total 1875 | C 1201 | N 319 | O 348 | S 7 | 0 | 0 |
| 4 | ZH | 243 | Total 1875 | C 1201 | N 319 | O 348 | S 7 | 0 | 0 |
| 4 | BH | 258 | Total 1983 | C 1268 | N 336 | O 371 | S 8 | 0 | 0 |
| 4 | CH | 258 | Total 1983 | C 1268 | N 336 | O 371 | S 8 | 0 | 0 |
| 4 | DH | 258 | Total 1983 | C 1268 | N 336 | O 371 | S 8 | 0 | 0 |

- Molecule 5 is a protein called Inner membrane lipoprotein YiaD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| | | | Total | C | N | O | S | | |
| 5 | EK | 151 | Total 1175 | C 747 | N 209 | O 215 | S 4 | 0 | 0 |
| 5 | FK | 151 | Total 1175 | C 747 | N 209 | O 215 | S 4 | 0 | 0 |
| 5 | GK | 151 | Total 1175 | C 747 | N 209 | O 215 | S 4 | 0 | 0 |
| 5 | HK | 151 | Total 1175 | C 747 | N 209 | O 215 | S 4 | 0 | 0 |
| 5 | IK | 151 | Total 1175 | C 747 | N 209 | O 215 | S 4 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | JK | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1175 | 747 | 209 | 215 | 4 | | |
| 5 | KK | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1175 | 747 | 209 | 215 | 4 | | |
| 5 | LK | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1175 | 747 | 209 | 215 | 4 | | |
| 5 | AK | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1175 | 747 | 209 | 215 | 4 | | |
| 5 | MK | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1175 | 747 | 209 | 215 | 4 | | |
| 5 | BK | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1175 | 747 | 209 | 215 | 4 | | |
| 5 | CK | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1175 | 747 | 209 | 215 | 4 | | |
| 5 | DK | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1175 | 747 | 209 | 215 | 4 | | |

- Molecule 6 is a protein called Outer membrane protein, OmpA family protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | EL | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 877 | 253 | 253 | 5 | | |
| 6 | FL | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 877 | 253 | 253 | 5 | | |
| 6 | GL | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 877 | 253 | 253 | 5 | | |
| 6 | HL | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 877 | 253 | 253 | 5 | | |
| 6 | IL | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 877 | 253 | 253 | 5 | | |
| 6 | JL | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 877 | 253 | 253 | 5 | | |
| 6 | KL | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 877 | 253 | 253 | 5 | | |
| 6 | LL | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 877 | 253 | 253 | 5 | | |
| 6 | ML | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 877 | 253 | 253 | 5 | | |
| 6 | AL | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 877 | 253 | 253 | 5 | | |
| 6 | BL | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 877 | 253 | 253 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | CL | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 877 | 253 | 253 | 5 | | |
| 6 | DL | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 877 | 253 | 253 | 5 | | |

- Molecule 7 is a protein called DUF2807 domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7 | EM | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1046 | 293 | 308 | 3 | | |
| 7 | FM | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1046 | 293 | 308 | 3 | | |
| 7 | GM | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1046 | 293 | 308 | 3 | | |
| 7 | HM | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1046 | 293 | 308 | 3 | | |
| 7 | IM | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1046 | 293 | 308 | 3 | | |
| 7 | JM | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1046 | 293 | 308 | 3 | | |
| 7 | KM | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1046 | 293 | 308 | 3 | | |
| 7 | LM | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1046 | 293 | 308 | 3 | | |
| 7 | MM | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1046 | 293 | 308 | 3 | | |
| 7 | AM | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1046 | 293 | 308 | 3 | | |
| 7 | BM | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1046 | 293 | 308 | 3 | | |
| 7 | CM | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1046 | 293 | 308 | 3 | | |
| 7 | DM | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1650 | 1046 | 293 | 308 | 3 | | |

- Molecule 8 is a protein called Neurogenic locus notch.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 8 | EN | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 357 | 99 | 113 | 13 | | |
| 8 | FN | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 357 | 99 | 113 | 13 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 8 | GN | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 357 | 99 | 113 | 13 | | |
| 8 | HN | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 357 | 99 | 113 | 13 | | |
| 8 | IN | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 357 | 99 | 113 | 13 | | |
| 8 | JN | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 357 | 99 | 113 | 13 | | |
| 8 | KN | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 357 | 99 | 113 | 13 | | |
| 8 | LN | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 357 | 99 | 113 | 13 | | |
| 8 | MN | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 357 | 99 | 113 | 13 | | |
| 8 | AN | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 357 | 99 | 113 | 13 | | |
| 8 | BN | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 357 | 99 | 113 | 13 | | |
| 8 | CN | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 357 | 99 | 113 | 13 | | |
| 8 | DN | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 357 | 99 | 113 | 13 | | |

- Molecule 9 is a protein called Unknown protein fragment.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|-------|
| 9 | EU | 9 | Total | C | N | O | 0 | 0 |
| | | | 45 | 27 | 9 | 9 | | |
| 9 | FU | 9 | Total | C | N | O | 0 | 0 |
| | | | 45 | 27 | 9 | 9 | | |
| 9 | GU | 9 | Total | C | N | O | 0 | 0 |
| | | | 45 | 27 | 9 | 9 | | |
| 9 | HU | 9 | Total | C | N | O | 0 | 0 |
| | | | 45 | 27 | 9 | 9 | | |
| 9 | IU | 9 | Total | C | N | O | 0 | 0 |
| | | | 45 | 27 | 9 | 9 | | |
| 9 | JU | 9 | Total | C | N | O | 0 | 0 |
| | | | 45 | 27 | 9 | 9 | | |
| 9 | KU | 9 | Total | C | N | O | 0 | 0 |
| | | | 45 | 27 | 9 | 9 | | |
| 9 | LU | 9 | Total | C | N | O | 0 | 0 |
| | | | 45 | 27 | 9 | 9 | | |

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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|-------|
| | | | Total | C | N | O | | |
| 9 | MU | 9 | 45 | 27 | 9 | 9 | 0 | 0 |
| 9 | AU | 9 | 45 | 27 | 9 | 9 | 0 | 0 |
| 9 | BU | 9 | 45 | 27 | 9 | 9 | 0 | 0 |
| 9 | CU | 9 | 45 | 27 | 9 | 9 | 0 | 0 |
| 9 | DU | 9 | 45 | 27 | 9 | 9 | 0 | 0 |

- Molecule 10 is a protein called Unknown protein fragment.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 10 | EX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |
| 10 | FX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |
| 10 | GX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |
| 10 | HX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |
| 10 | IX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |
| 10 | JX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |
| 10 | KX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |
| 10 | LX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |
| 10 | MX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |
| 10 | VX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |
| 10 | WX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |
| 10 | XX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |
| 10 | YX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |
| 10 | ZX | 48 | 240 | 144 | 48 | 48 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10 | AX | 48 | Total | C | N | O | 0 | 0 |
| | | | 240 | 144 | 48 | 48 | | |
| 10 | BX | 48 | Total | C | N | O | 0 | 0 |
| | | | 240 | 144 | 48 | 48 | | |
| 10 | CX | 48 | Total | C | N | O | 0 | 0 |
| | | | 240 | 144 | 48 | 48 | | |
| 10 | DX | 48 | Total | C | N | O | 0 | 0 |
| | | | 240 | 144 | 48 | 48 | | |

- Molecule 11 is a protein called DotC.

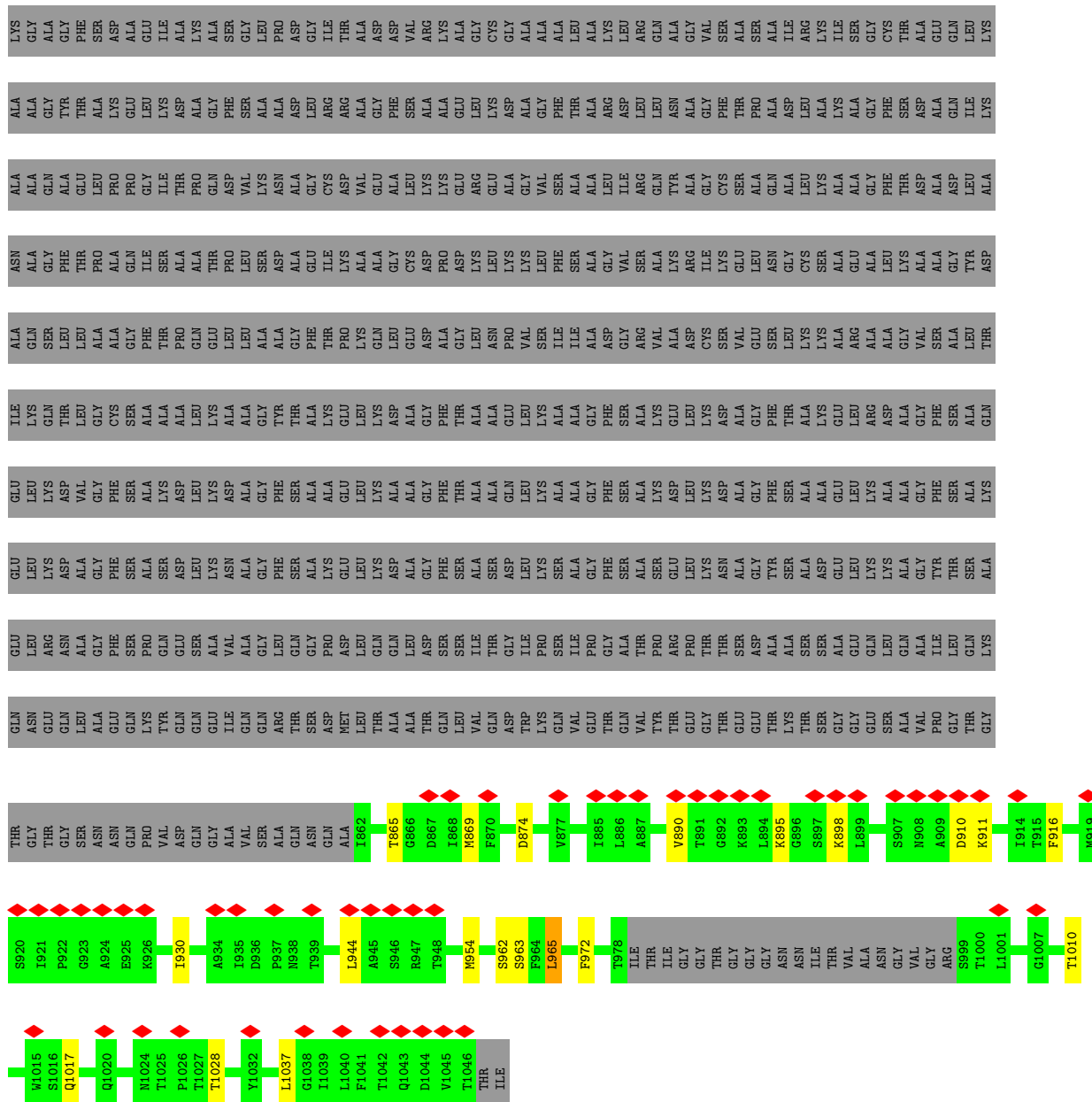
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11 | CC | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 1921 | 1216 | 340 | 357 | 8 | | |
| 11 | BC | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 1921 | 1216 | 340 | 357 | 8 | | |
| 11 | GC | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 1921 | 1216 | 340 | 357 | 8 | | |
| 11 | KC | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 1921 | 1216 | 340 | 357 | 8 | | |
| 11 | DC | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1061 | 292 | 309 | 5 | | |
| 11 | EC | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1061 | 292 | 309 | 5 | | |
| 11 | FC | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 1921 | 1216 | 340 | 357 | 8 | | |
| 11 | HC | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1061 | 292 | 309 | 5 | | |
| 11 | IC | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1061 | 292 | 309 | 5 | | |
| 11 | JC | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1061 | 292 | 309 | 5 | | |
| 11 | LC | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1061 | 292 | 309 | 5 | | |
| 11 | MC | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1061 | 292 | 309 | 5 | | |
| 11 | AC | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1061 | 292 | 309 | 5 | | |

Table with 19 rows of amino acid sequences. The sequence in the 12th row contains highlighted residues: Q791, E792, E793, E794, Q795, L808, Q814, E816, T817, Q818, V819, T824.

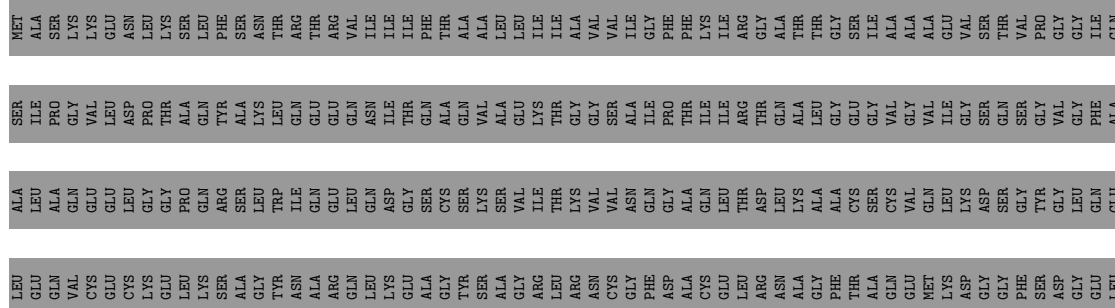
● Molecule 1: IcmE protein

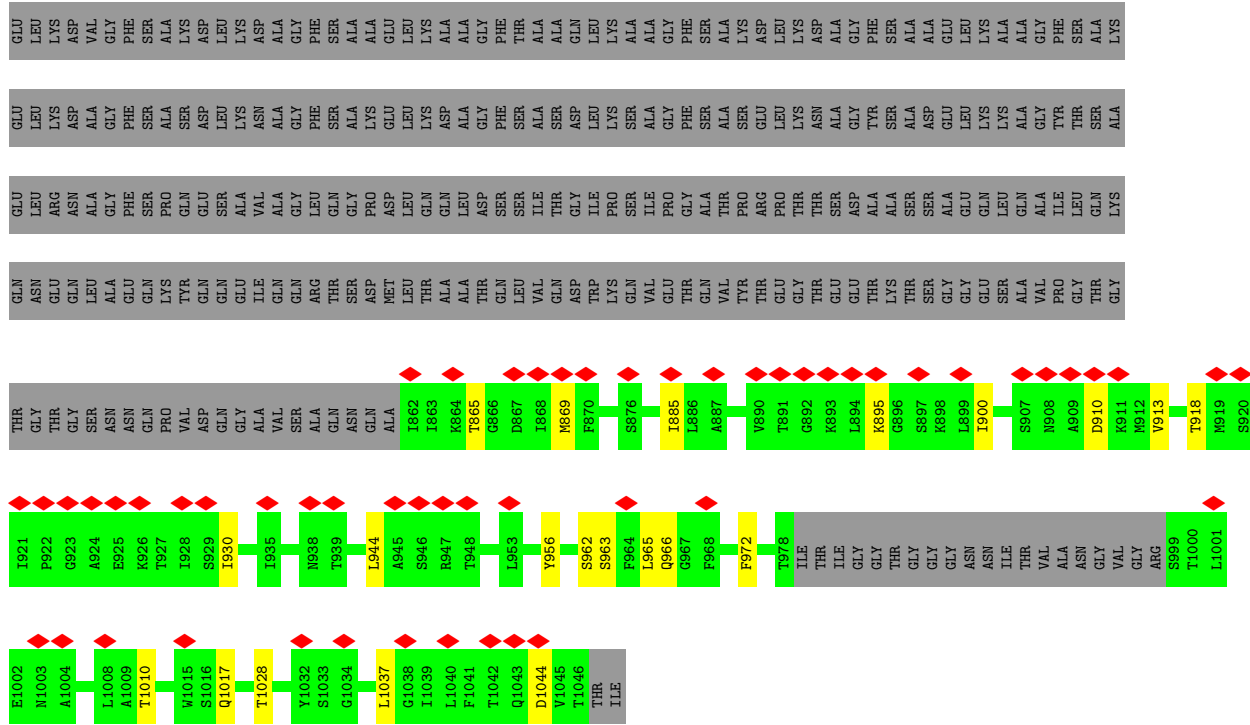


Table with 2 rows of amino acid sequences.



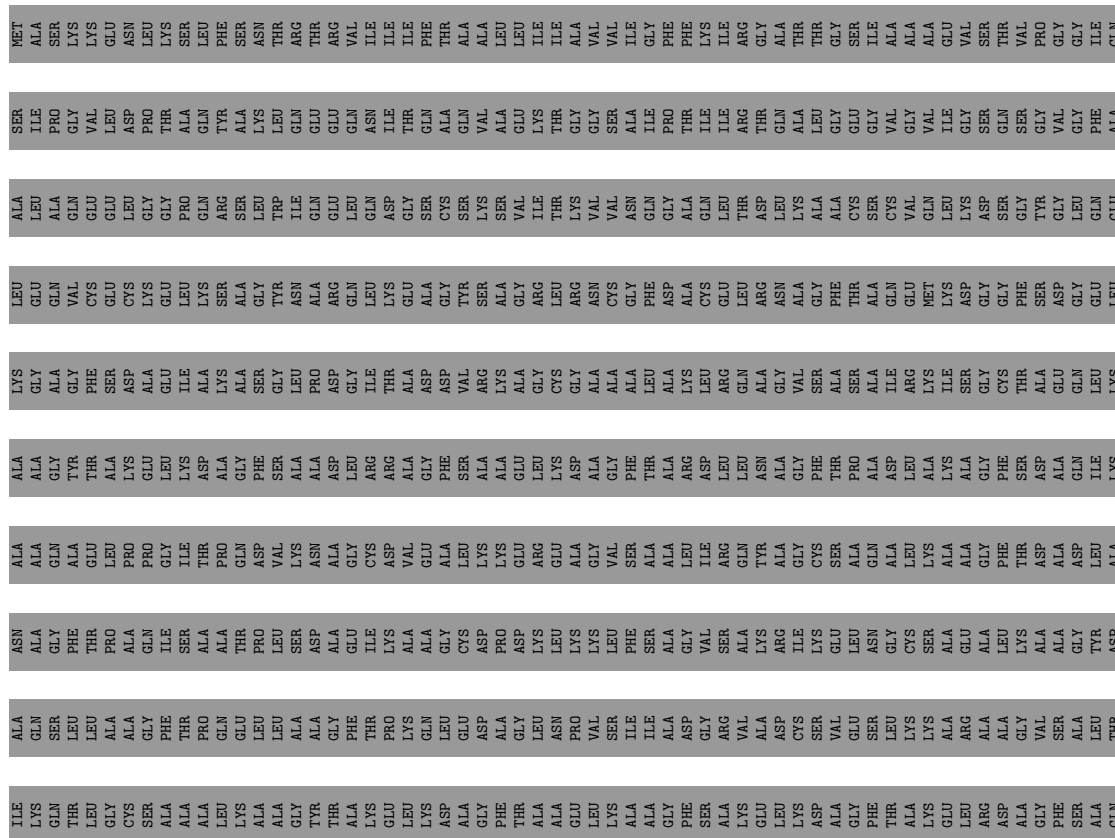
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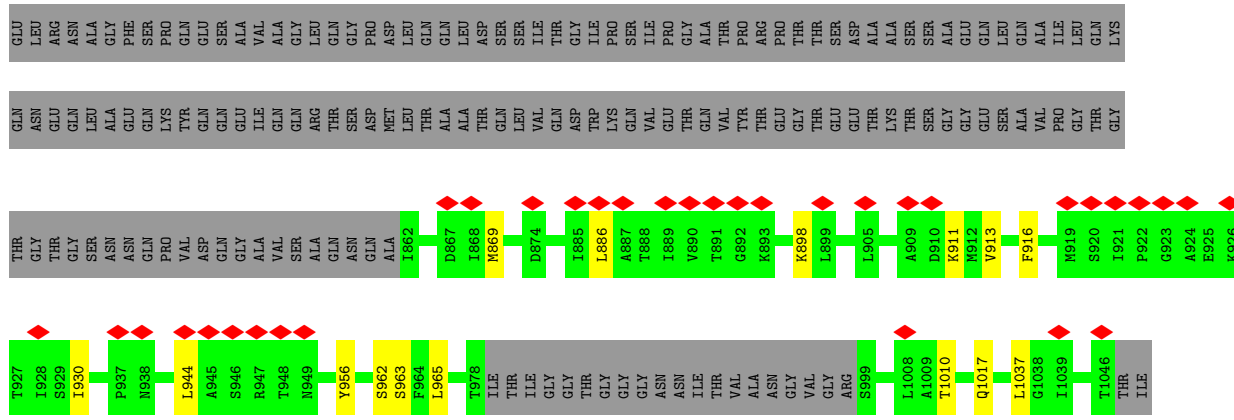




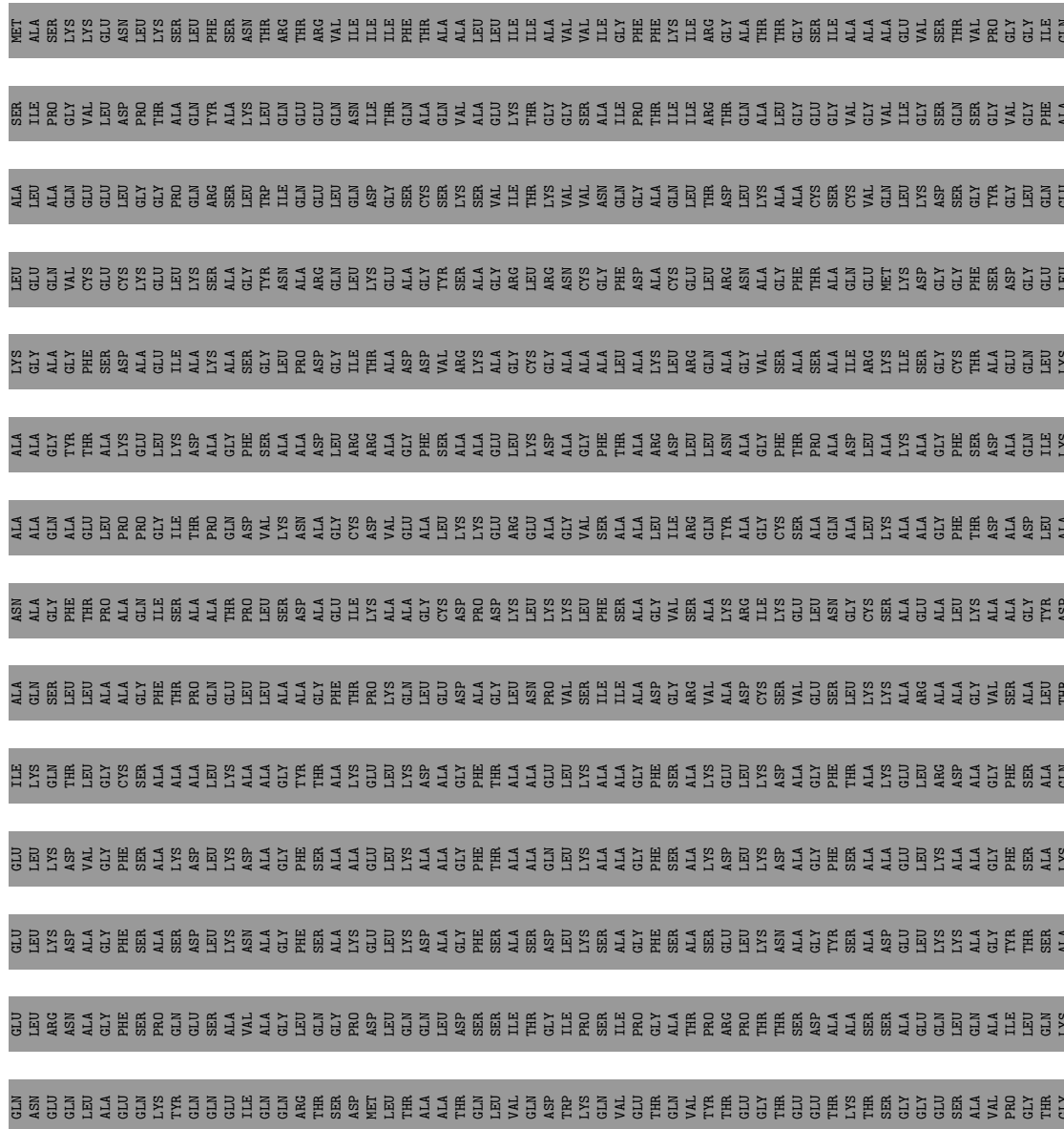
● Molecule 1: IcmE protein

Chain Cg: 97%



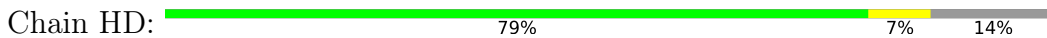


Molecule 1: IcmE protein

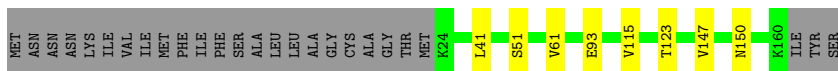
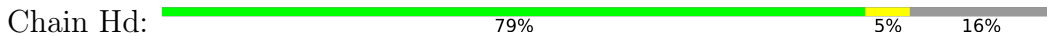




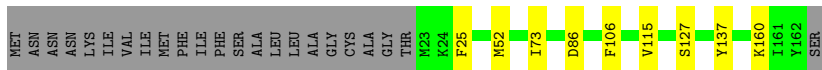
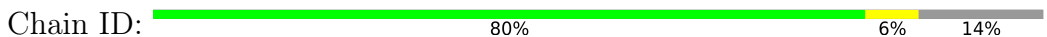
● Molecule 2: DotD



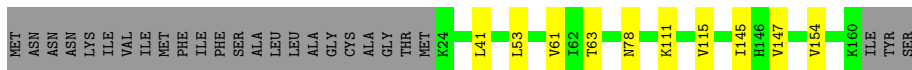
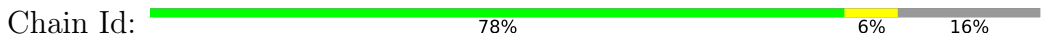
● Molecule 2: DotD



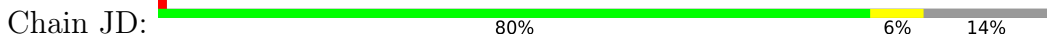
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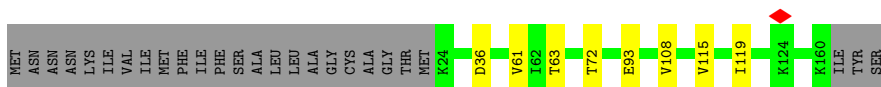
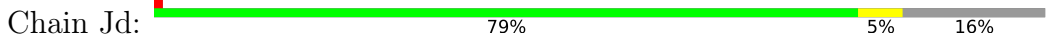
● Molecule 2: DotD



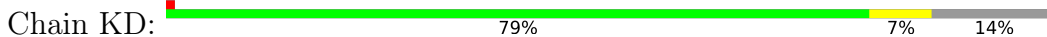
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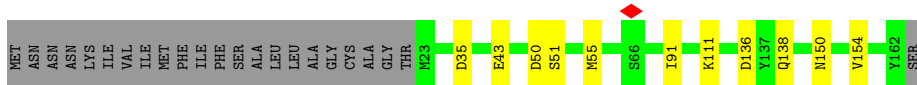


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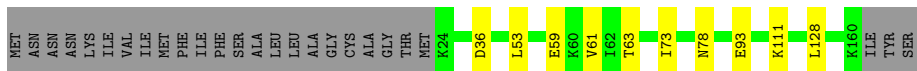
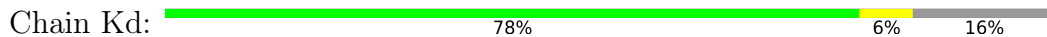


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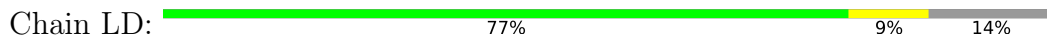




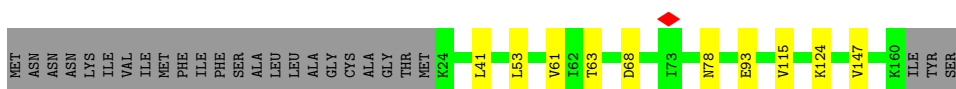
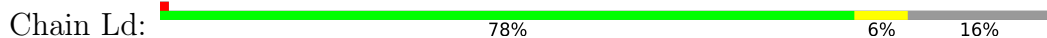
• Molecule 2: DotD



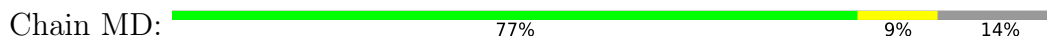
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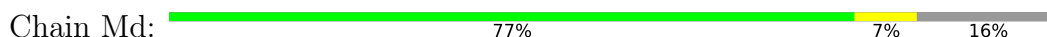
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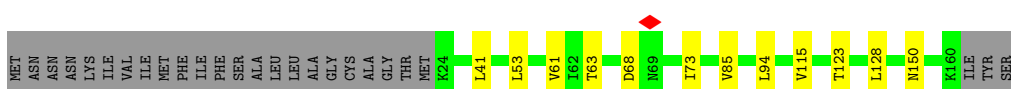
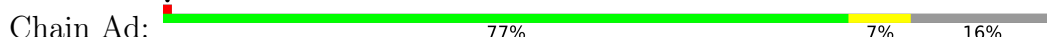
• Molecule 2: DotD



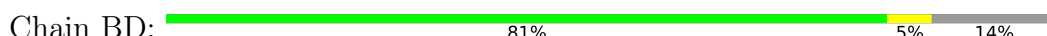
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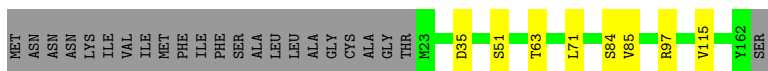


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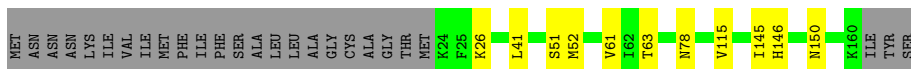
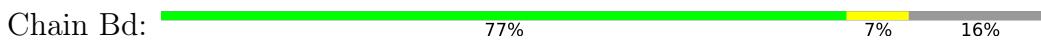


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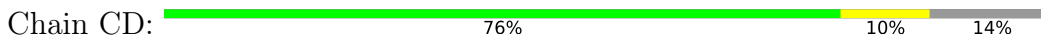




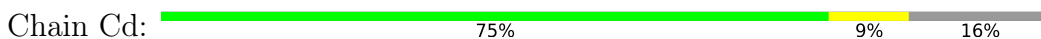
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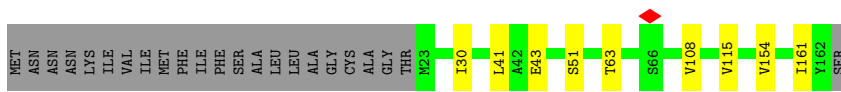
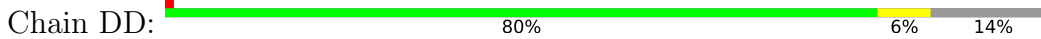
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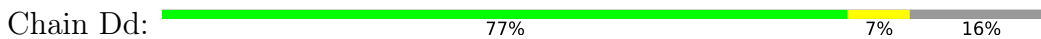
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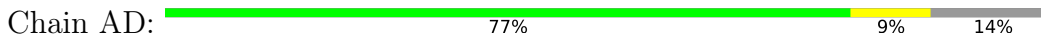
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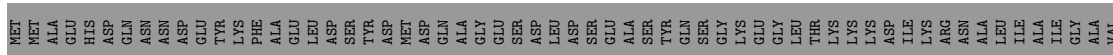
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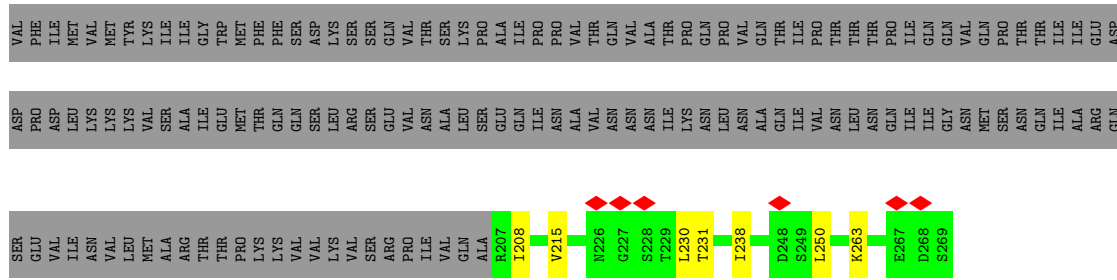


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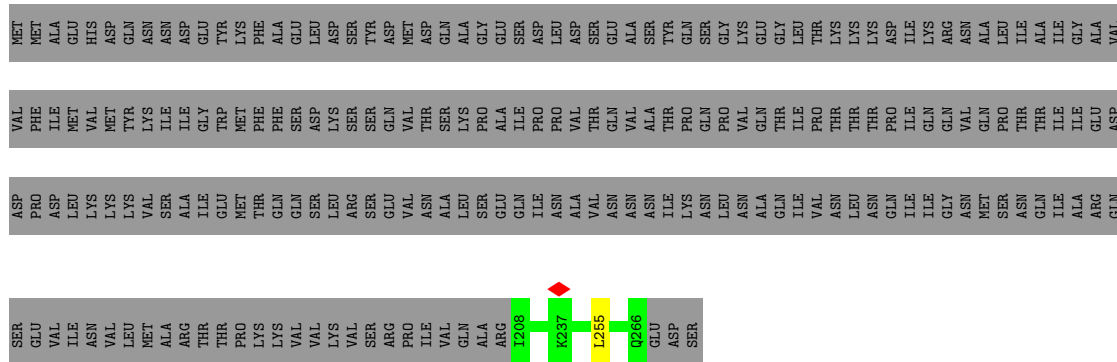


• Molecule 3: DotF

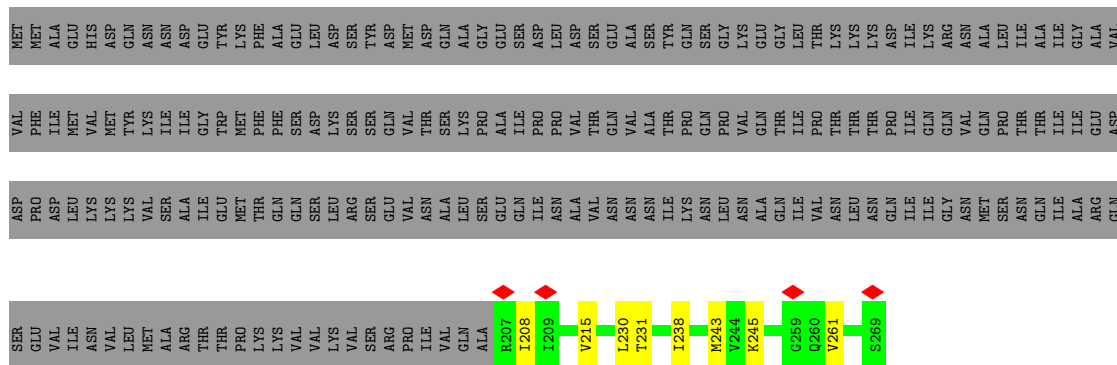




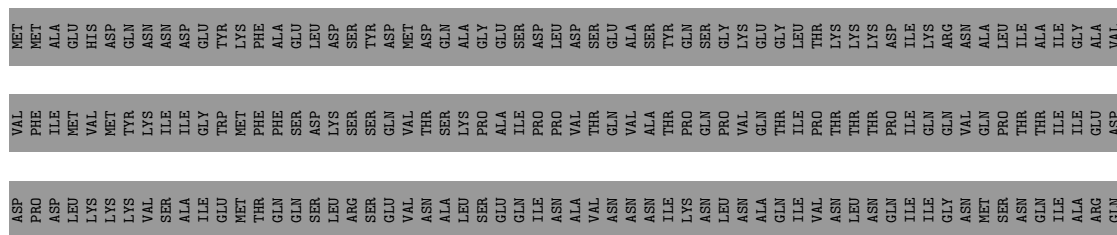
• Molecule 3: DotF



• Molecule 3: DotF



• Molecule 3: DotF





| | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | MET | ALA | GLU | HIS | ASP | GLN | ASN | ASN | GLU | GLY | TYR | PHE | PHE | ALA | GLN | GLU | LEU | ASP | LEU | ASP | SER | TYR | GLN | GLN | GLY | VAL |
| VAL | PHE | ILE | LEU | MET | VAL | TYR | LYS | ILE | ILE | GLY | TRP | MET | PHE | PHE | GLN | SER | ASP | ASP | LEU | LEU | SER | SER | GLN | VAL | ALA | ASP |
| ASP | PRO | ASP | LEU | GLU | LYS | LYS | VAL | SER | ALA | ASP | ILE | GLY | TRP | GLU | THR | GLN | GLN | LEU | LEU | ARG | SER | GLU | VAL | VAL | ALA | GLN |
| SER | GLU | VAL | ILE | ASN | VAL | LEU | MET | ALA | ARG | THR | THR | PRO | MET | LYS | LYS | VAL | VAL | LEU | LEU | VAL | SER | ARG | PRO | ILE | ALA | GLN |
| R207 | V215 | N226 | G227 | T229 | L230 | I238 | L255 | V261 | I262 | K263 | E267 | D268 | S269 | | | | | | | | | | | | | |

• Molecule 3: DotF



| | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | MET | ALA | GLU | HIS | ASP | GLN | ASN | ASN | GLU | GLY | TYR | PHE | PHE | ALA | GLN | GLU | LEU | ASP | LEU | ASP | SER | TYR | GLN | GLN | GLY | VAL |
| VAL | PHE | ILE | LEU | MET | VAL | TYR | LYS | ILE | ILE | GLY | TRP | MET | PHE | PHE | GLN | SER | ASP | ASP | LEU | LEU | SER | SER | GLN | VAL | ALA | ASP |
| ASP | PRO | ASP | LEU | GLU | LYS | LYS | VAL | SER | ALA | ASP | ILE | GLY | TRP | GLU | THR | GLN | GLN | LEU | LEU | ARG | SER | GLU | VAL | VAL | ALA | GLN |
| SER | GLU | VAL | ILE | ASN | VAL | LEU | MET | ALA | ARG | THR | THR | PRO | LYS | LYS | VAL | VAL | VAL | LEU | LEU | VAL | SER | ARG | PRO | ILE | ALA | GLN |
| I208 | V211 | R219 | R233 | V244 | L255 | I266 | ASP | SER | | | | | | | | | | | | | | | | | | |

• Molecule 3: DotF



| | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | MET | ALA | GLU | HIS | ASP | GLN | ASN | ASN | GLU | GLY | TYR | PHE | PHE | ALA | GLN | GLU | LEU | ASP | LEU | ASP | SER | TYR | GLN | GLN | GLY | VAL |
| VAL | PHE | ILE | LEU | MET | VAL | TYR | LYS | ILE | ILE | GLY | TRP | MET | PHE | PHE | GLN | SER | ASP | ASP | LEU | LEU | SER | SER | GLN | VAL | ALA | ASP |
| ASP | PRO | ASP | LEU | GLU | LYS | LYS | VAL | SER | ALA | ASP | ILE | GLY | TRP | GLU | THR | GLN | GLN | LEU | LEU | ARG | SER | GLU | VAL | VAL | ALA | GLN |
| SER | GLU | VAL | ILE | ASN | VAL | LEU | MET | ALA | ARG | THR | THR | PRO | LYS | LYS | VAL | VAL | VAL | LEU | LEU | VAL | SER | ARG | PRO | ILE | ALA | GLN |
| R207 | V215 | T231 | K245 | L250 | L255 | V261 | I262 | K263 | D268 | S269 | | | | | | | | | | | | | | | | |

• Molecule 3: DotF



| | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | MET | ALA | GLU | HIS | ASP | GLN | ASN | ASN | GLU | GLY | TYR | PHE | PHE | ALA | GLN | GLU | LEU | ASP | LEU | ASP | SER | TYR | GLN | GLN | GLY | VAL |
| VAL | PHE | ILE | LEU | MET | VAL | TYR | LYS | ILE | ILE | GLY | TRP | MET | PHE | PHE | GLN | SER | ASP | ASP | LEU | LEU | SER | SER | GLN | VAL | ALA | ASP |
| ASP | PRO | ASP | LEU | GLU | LYS | LYS | VAL | SER | ALA | ASP | ILE | GLY | TRP | GLU | THR | GLN | GLN | LEU | LEU | ARG | SER | GLU | VAL | VAL | ALA | GLN |
| SER | GLU | VAL | ILE | ASN | VAL | LEU | MET | ALA | ARG | THR | THR | PRO | LYS | LYS | VAL | VAL | VAL | LEU | LEU | VAL | SER | ARG | PRO | ILE | ALA | GLN |
| R207 | V215 | T231 | K245 | L250 | L255 | V261 | I262 | K263 | D268 | S269 | | | | | | | | | | | | | | | | |

Chain Af:  20% 78%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | MET | ALA | GLU | HIS | ASP | GLN | ASN | ASN | SER | LEU | ASP | GLU | GLU | LEU | ASP | LEU | ASP | SER | TYR | MET | MET | GLN | ASP | GLN | GLY | ALA | GLY | GLU | VAL | |
| VAL | PHE | ILE | MET | VAL | MET | TYR | LYS | ILE | LYS | ILE | GLY | TRP | PHE | PHE | ALA | SER | ASP | LEU | SER | GLN | VAL | VAL | GLN | GLN | LEU | PRO | ALA | ILE | ASP | |
| ASP | PRO | ASP | LEU | VAL | LYS | LYS | VAL | SER | ALA | ALA | ILE | TRP | GLU | MET | THR | GLN | VAL | LEU | ARG | SER | GLU | VAL | VAL | ASN | LEU | SER | ALA | GLN | GLN | |
| SER | GLU | VAL | ILE | ASN | VAL | LEU | MET | ALA | ALA | THR | ARG | THR | PRO | THR | LYS | VAL | VAL | VAL | SER | ARG | GLU | PRO | ILE | ILE | GLN | ALA | ALA | GLU | GLN | |
| ILE | ASP | ASP | ASN | VAL | ASP | LEU | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP |
| I208 | I238 | R263 | I262 | K263 | F264 | S265 | Q266 | GLU | ASP | SER | | | | | | | | | | | | | | | | | | | | |

• Molecule 3: DotF

Chain BF:  20% 77%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | MET | ALA | GLU | HIS | ASP | GLN | ASN | ASN | SER | LEU | ASP | GLU | GLU | LEU | ASP | LEU | ASP | SER | TYR | MET | MET | GLN | ASP | GLN | GLY | ALA | GLY | GLU | VAL | |
| VAL | PHE | ILE | MET | VAL | MET | TYR | LYS | ILE | LYS | ILE | GLY | TRP | PHE | PHE | ALA | SER | ASP | LEU | SER | GLN | VAL | VAL | GLN | GLN | LEU | PRO | ALA | ILE | ASP | |
| ASP | PRO | ASP | LEU | VAL | LYS | LYS | VAL | SER | ALA | ALA | ILE | TRP | GLU | MET | THR | GLN | VAL | LEU | ARG | SER | GLU | VAL | VAL | ASN | LEU | SER | ALA | GLN | GLN | |
| SER | GLU | VAL | ILE | ASN | VAL | LEU | MET | ALA | ALA | THR | ARG | THR | PRO | THR | LYS | VAL | VAL | VAL | SER | ARG | GLU | PRO | ILE | ILE | GLN | ALA | ALA | GLU | GLN | |
| ILE | ASP | ASP | ASN | VAL | ASP | LEU | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP |
| R207 | I208 | V215 | G227 | L230 | I231 | I238 | K245 | L250 | F264 | E267 | D268 | S269 | | | | | | | | | | | | | | | | | | |

• Molecule 3: DotF

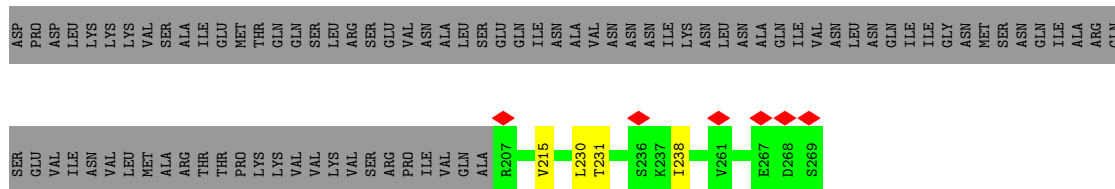
Chain Bf:  20% 78%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| MET | MET | ALA | GLU | HIS | ASP | GLN | ASN | ASN | SER | LEU | ASP | GLU | GLU | LEU | ASP | LEU | ASP | SER | TYR | MET | MET | GLN | ASP | GLN | GLY | ALA | GLY | GLU | VAL | |
| VAL | PHE | ILE | MET | VAL | MET | TYR | LYS | ILE | LYS | ILE | GLY | TRP | PHE | PHE | ALA | SER | ASP | LEU | SER | GLN | VAL | VAL | GLN | GLN | LEU | PRO | ALA | ILE | ASP | |
| ASP | PRO | ASP | LEU | VAL | LYS | LYS | VAL | SER | ALA | ALA | ILE | TRP | GLU | MET | THR | GLN | VAL | LEU | ARG | SER | GLU | VAL | VAL | ASN | LEU | SER | ALA | GLN | GLN | |
| SER | GLU | VAL | ILE | ASN | VAL | LEU | MET | ALA | ALA | THR | ARG | THR | PRO | THR | LYS | VAL | VAL | VAL | SER | ARG | GLU | PRO | ILE | ILE | GLN | ALA | ALA | GLU | GLN | |
| ILE | ASP | ASP | ASN | VAL | ASP | LEU | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP | ASP |
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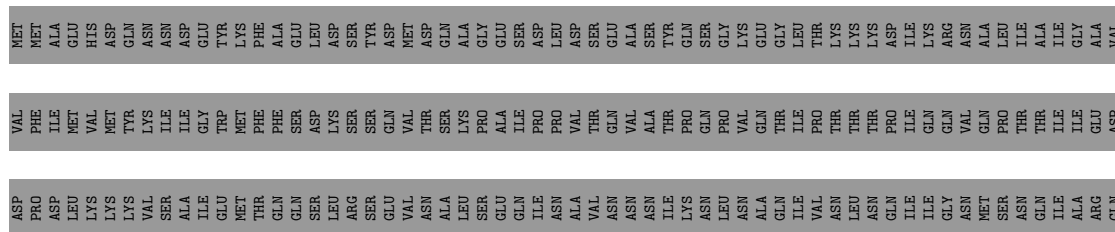
• Molecule 3: DotF

Chain Cf:  22% 77%

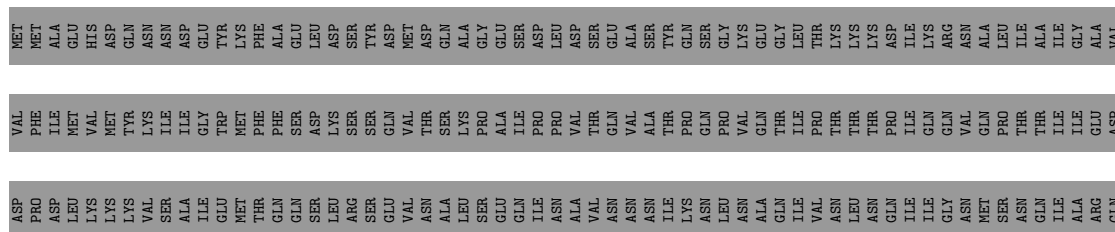
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | MET | ALA | GLU | HIS | ASP | GLN | ASN | ASN | SER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



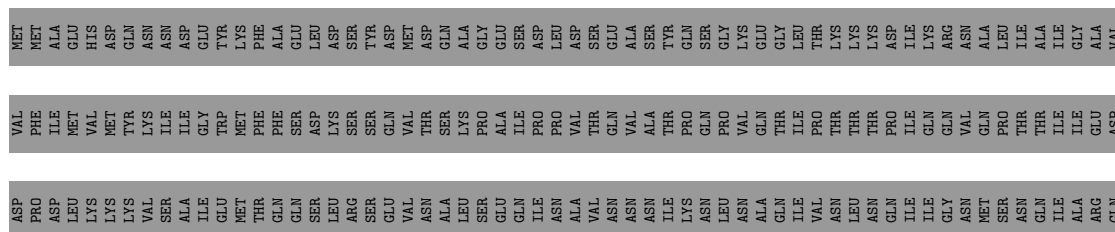
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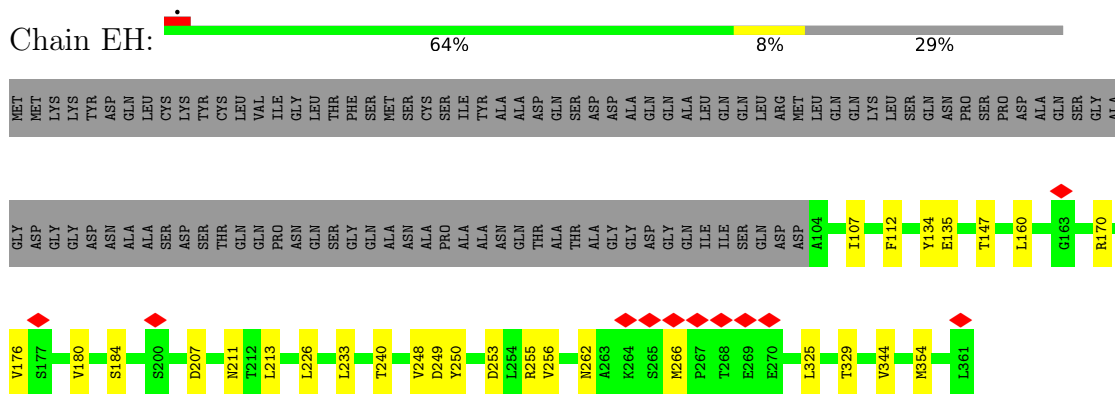
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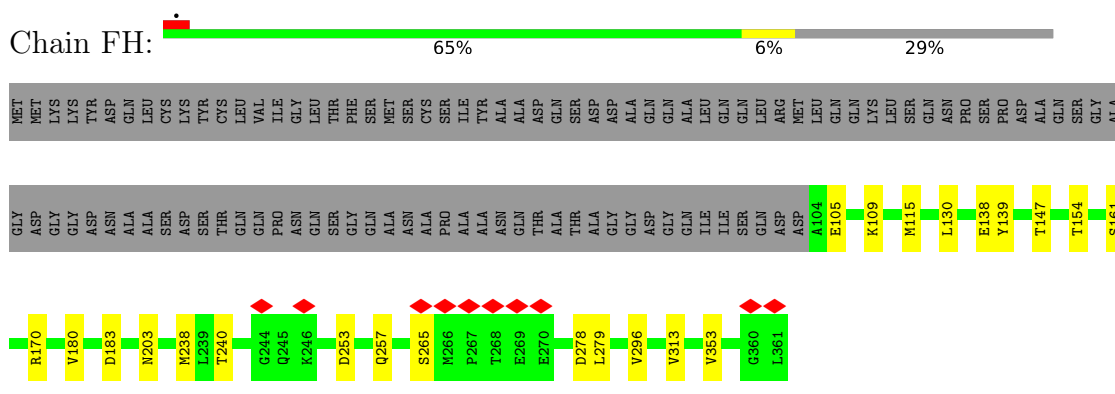
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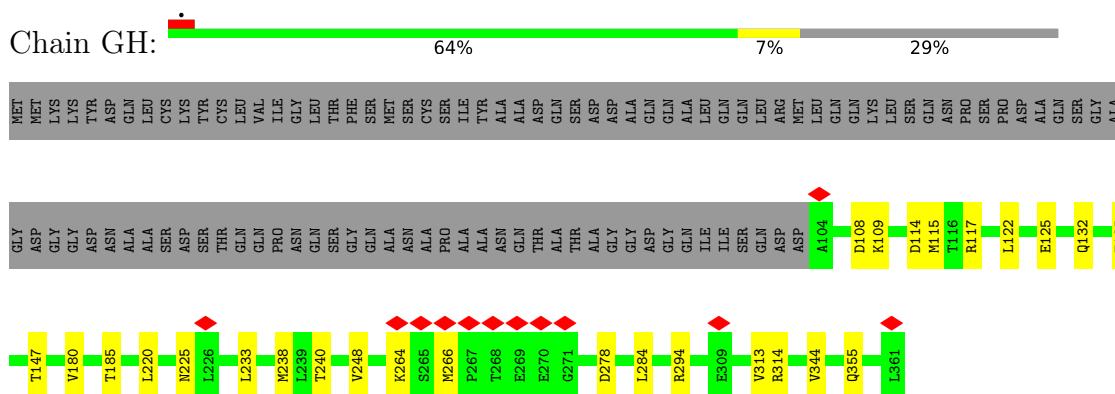
• Molecule 4: Type IV secretion protein IcmK



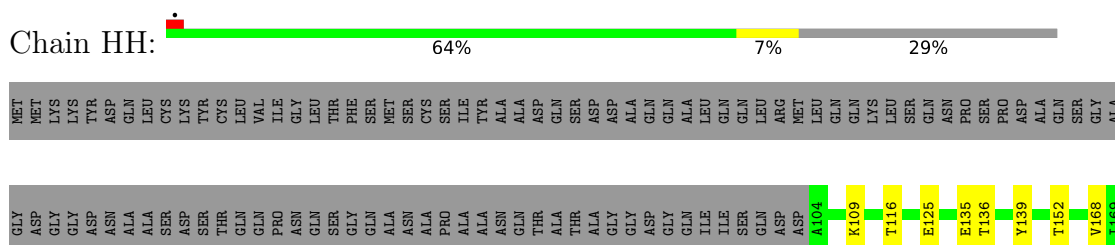
• Molecule 4: Type IV secretion protein IcmK

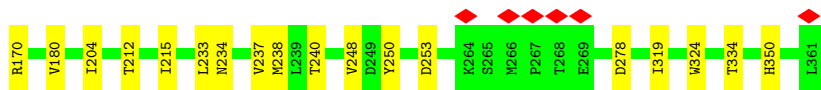


• Molecule 4: Type IV secretion protein IcmK

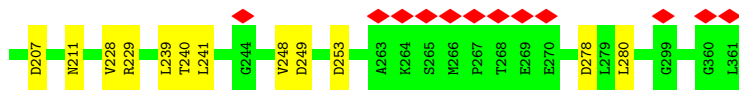
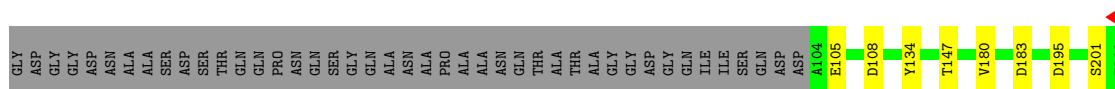
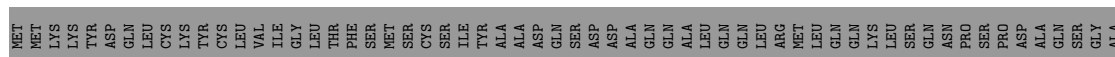


• Molecule 4: Type IV secretion protein IcmK

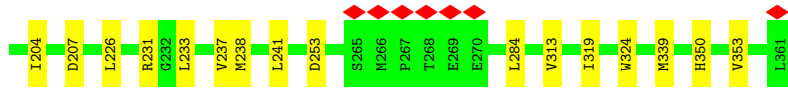
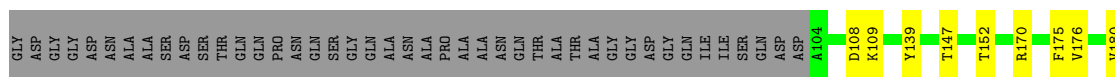




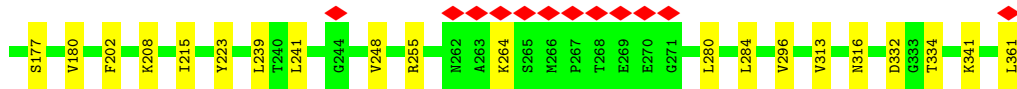
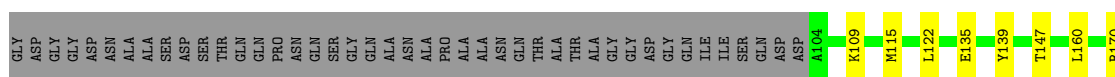
• Molecule 4: Type IV secretion protein IcmK



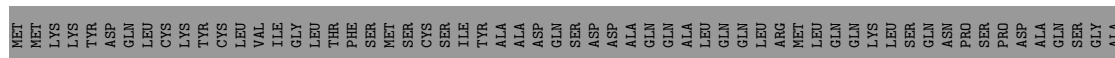
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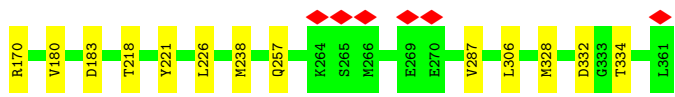
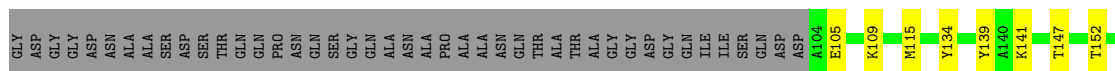


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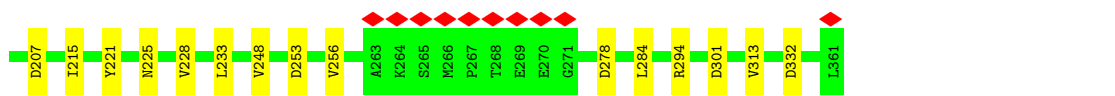
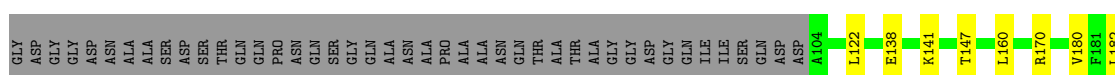
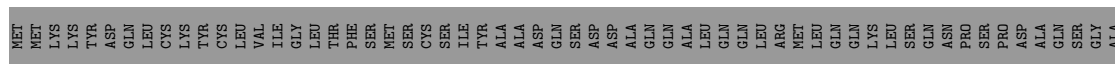


• Molecule 4: Type IV secretion protein IcmK

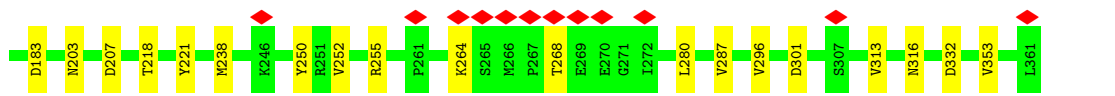
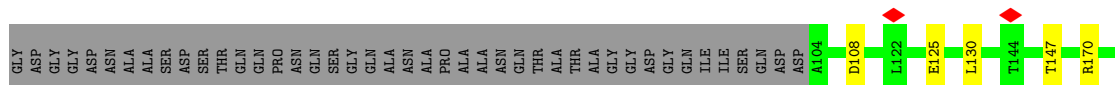
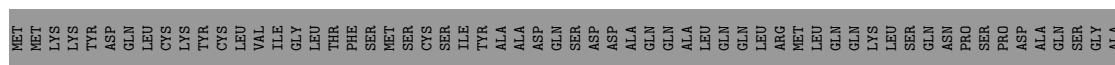




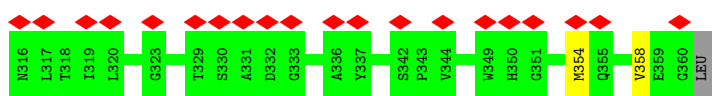
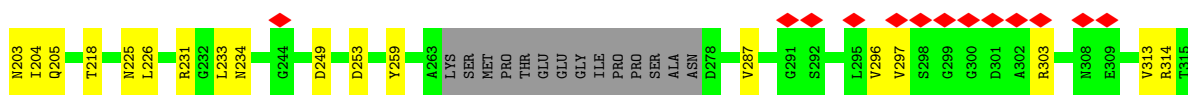
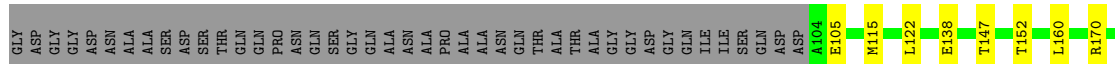
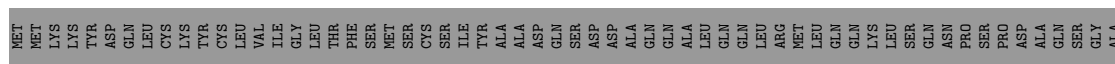
• Molecule 4: Type IV secretion protein IcmK



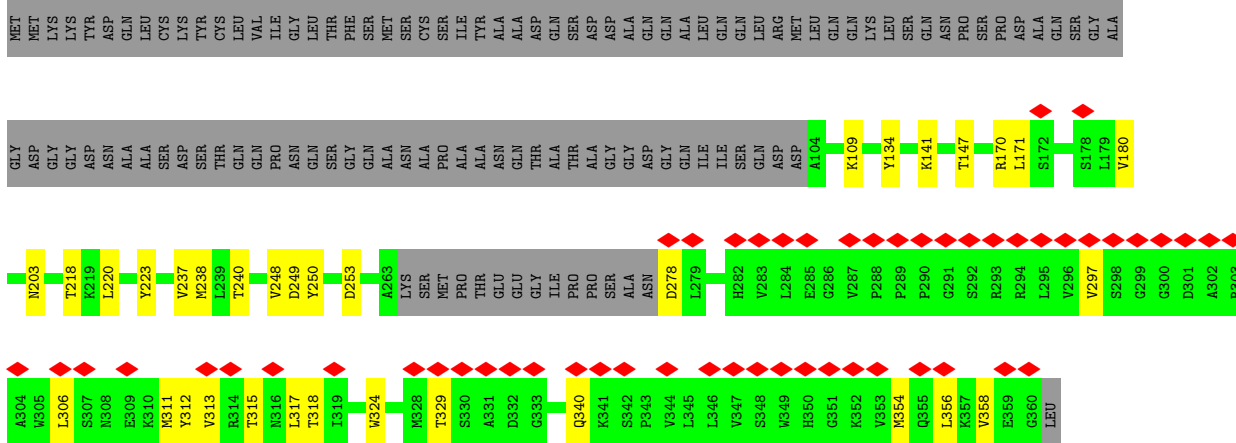
• Molecule 4: Type IV secretion protein IcmK



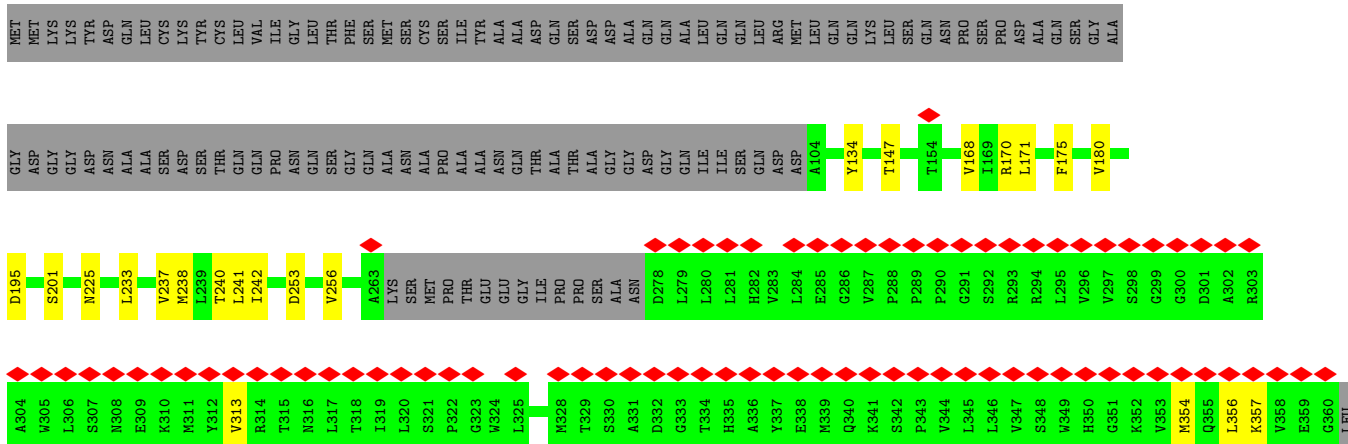
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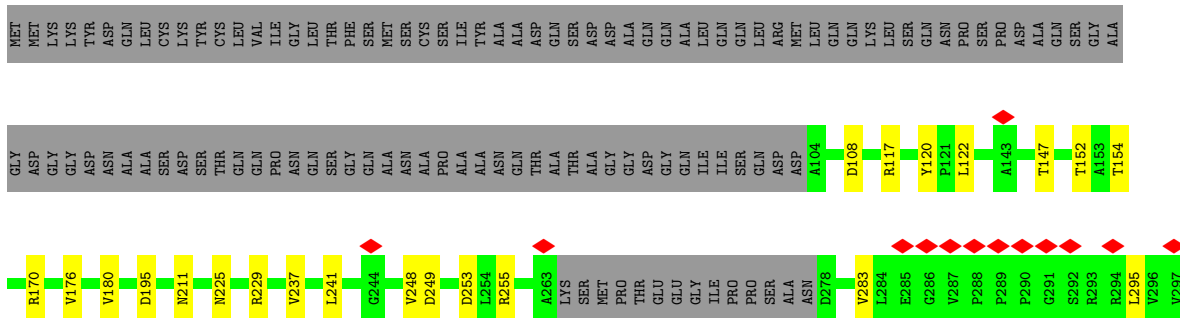
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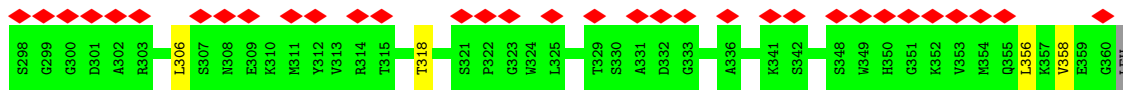


• Molecule 4: Type IV secretion protein IcmK

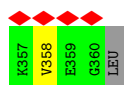
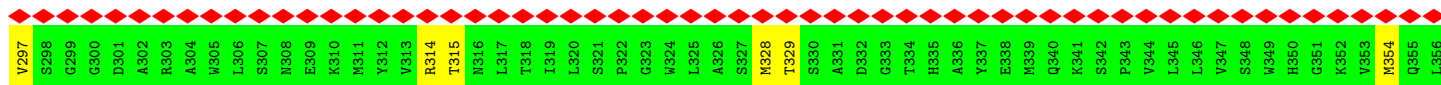
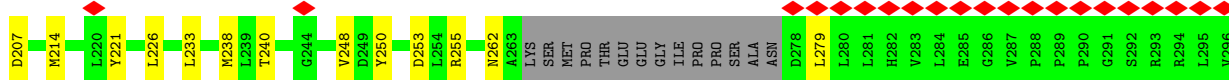
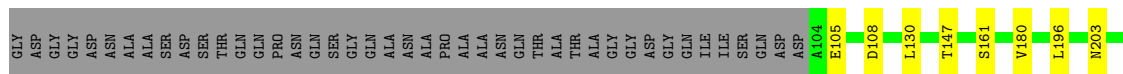
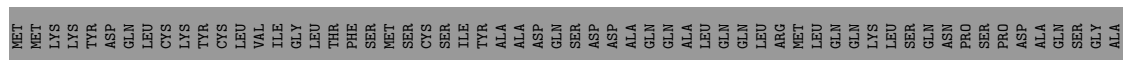


• Molecule 4: Type IV secretion protein IcmK

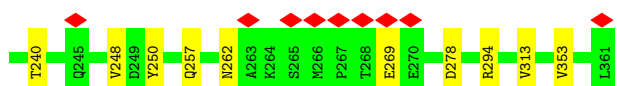
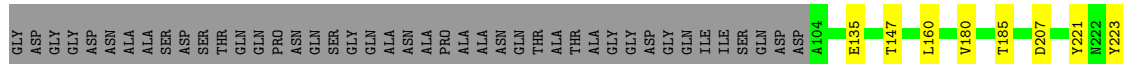
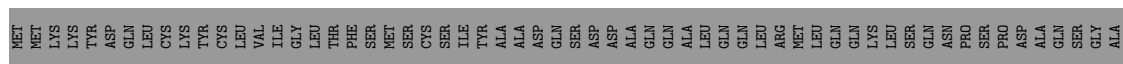




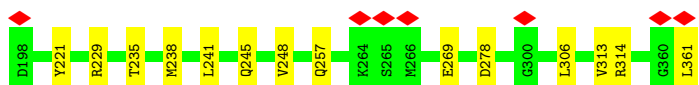
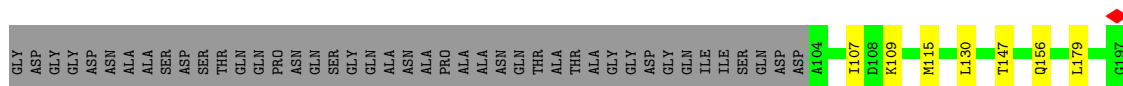
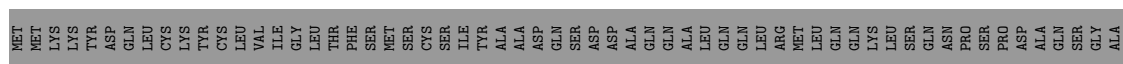
• Molecule 4: Type IV secretion protein IcmK



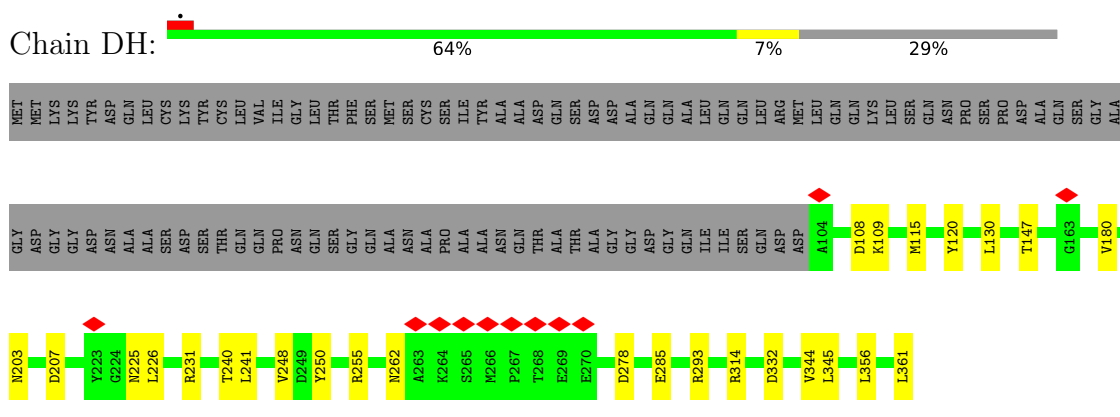
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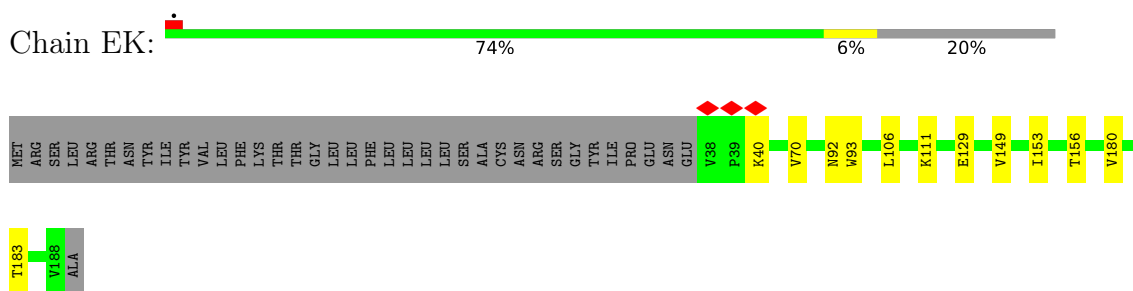
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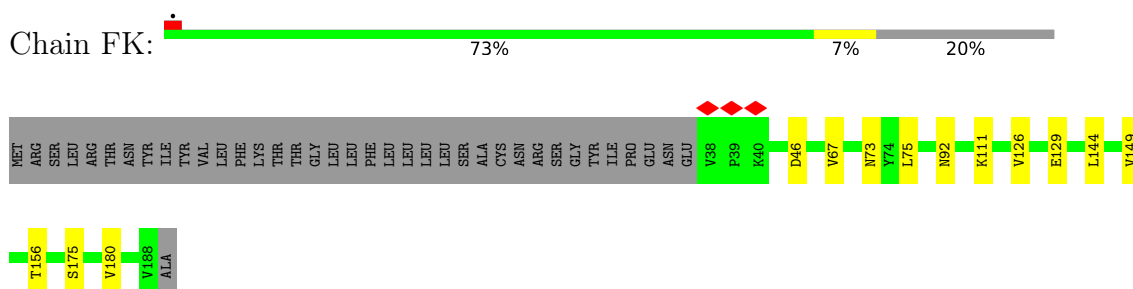
- Molecule 4: Type IV secretion protein IcmK



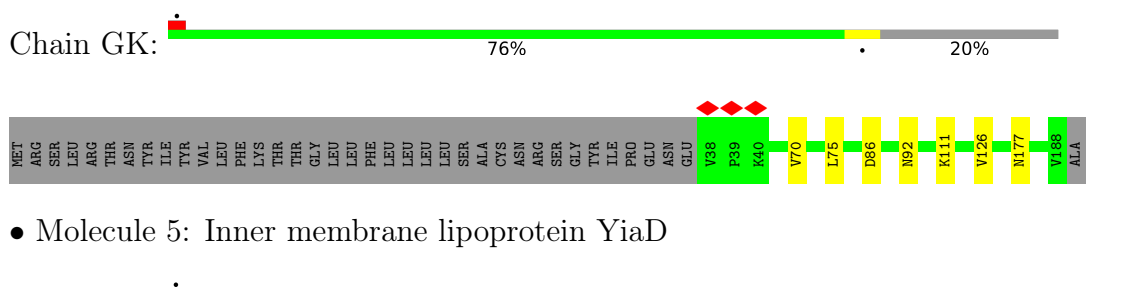
- Molecule 5: Inner membrane lipoprotein YiaD



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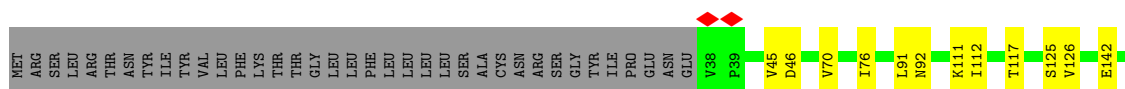
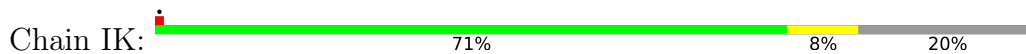


- Molecule 5: Inner membrane lipoprotein YiaD

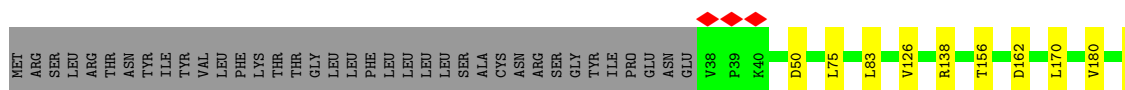
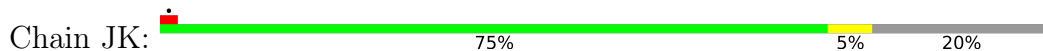




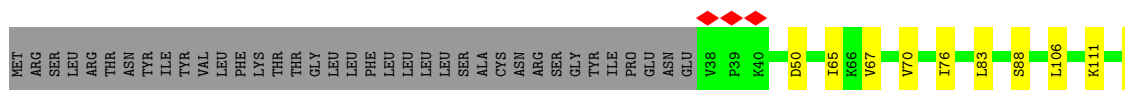
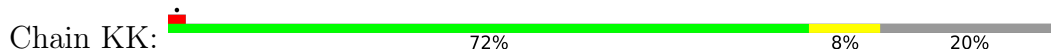
- Molecule 5: Inner membrane lipoprotein YiaD



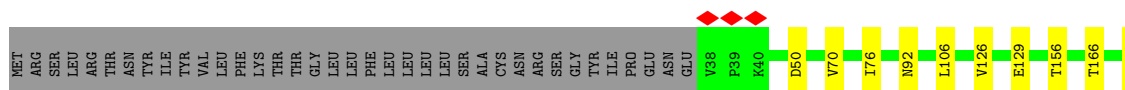
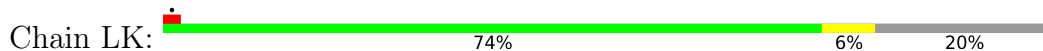
- Molecule 5: Inner membrane lipoprotein YiaD



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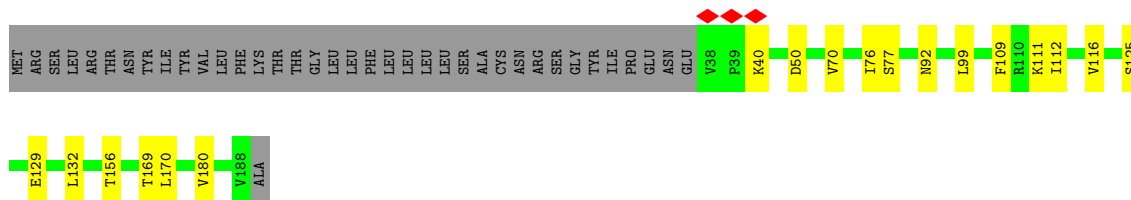


- Molecule 5: Inner membrane lipoprotein YiaD

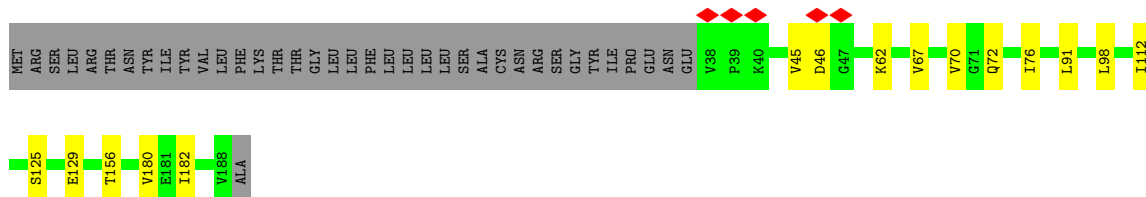
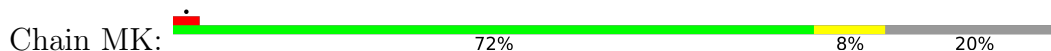


- Molecule 5: Inner membrane lipoprotein YiaD

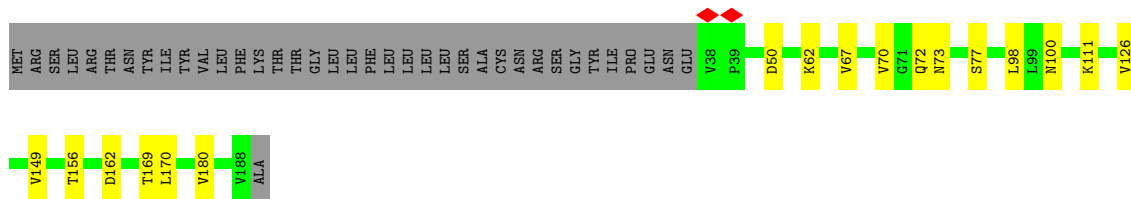




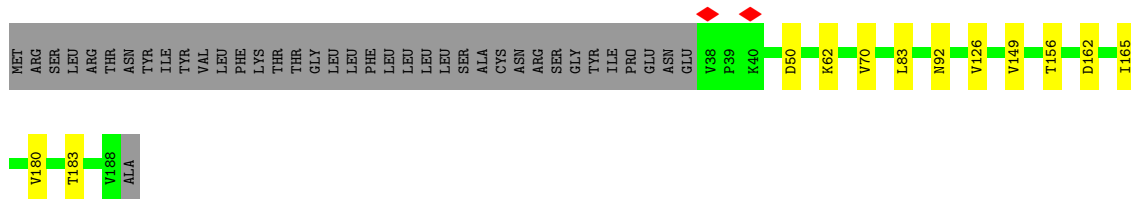
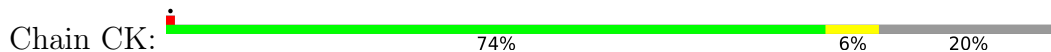
• Molecule 5: Inner membrane lipoprotein YiaD



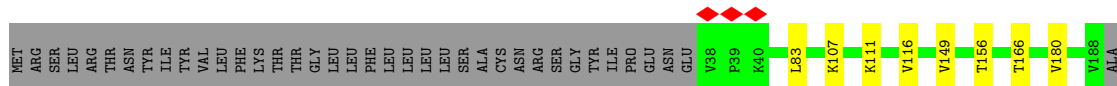
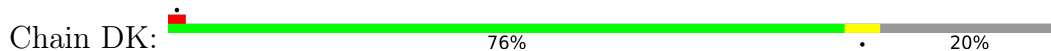
• Molecule 5: Inner membrane lipoprotein YiaD



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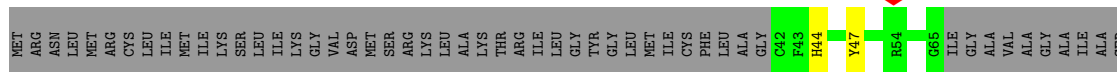


• Molecule 5: Inner membrane lipoprotein YiaD

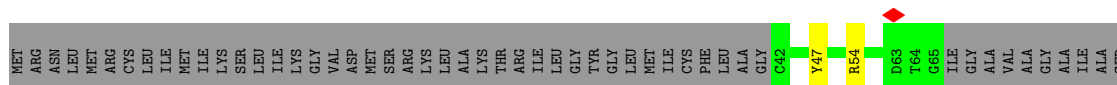


• Molecule 6: Outer membrane protein, OmpA family protein

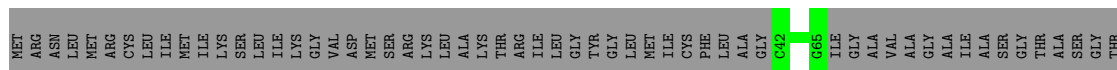




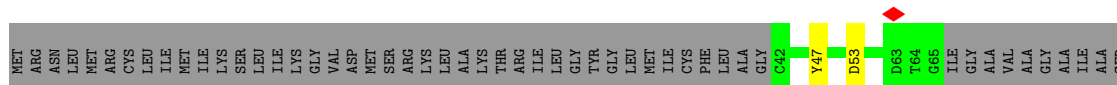
• Molecule 6: Outer membrane protein, OmpA family protein



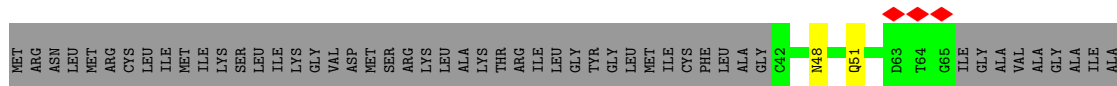
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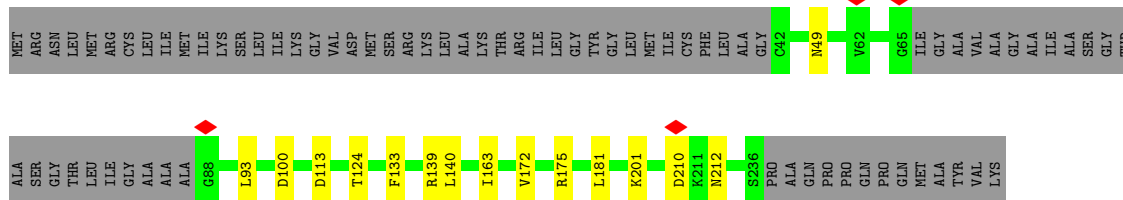
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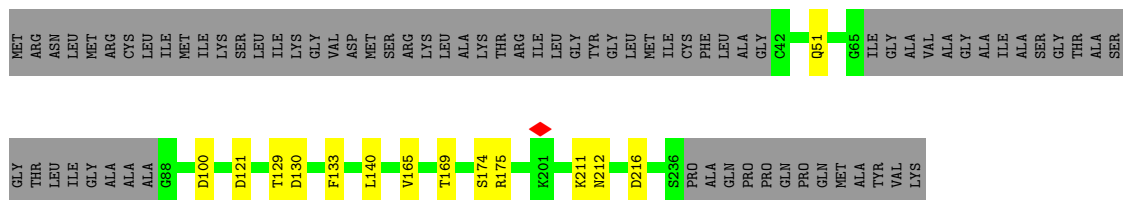
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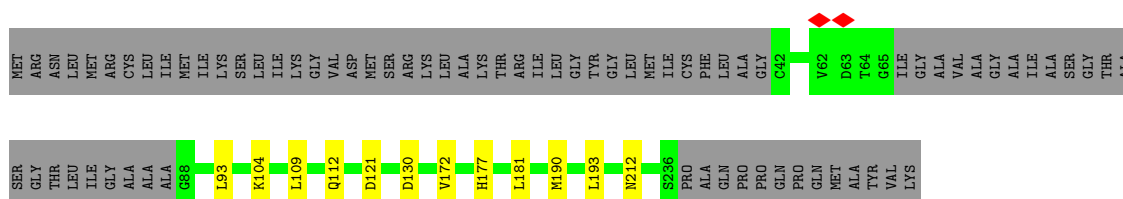
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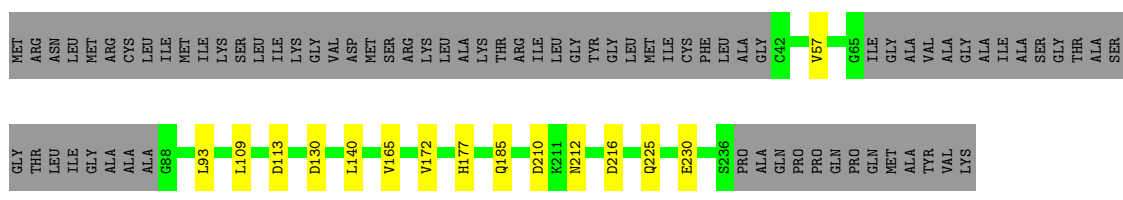
● Molecule 6: Outer membrane protein, OmpA family protein



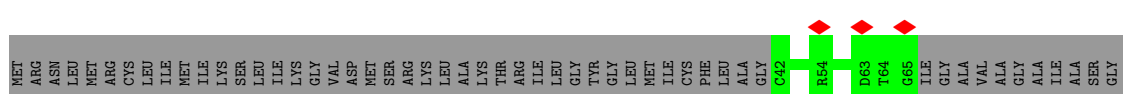
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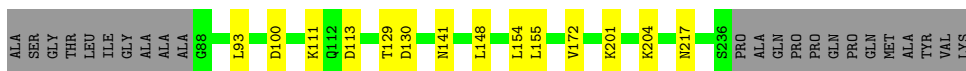


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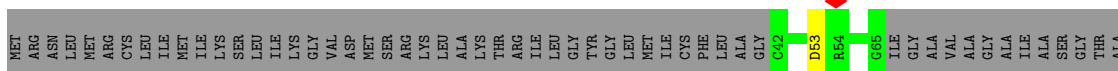


● Molecule 6: Outer membrane protein, OmpA family protein

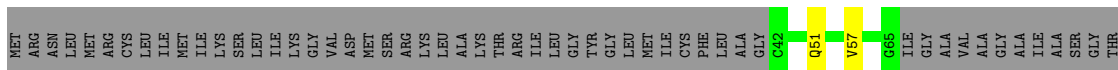




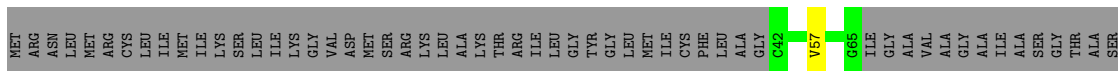
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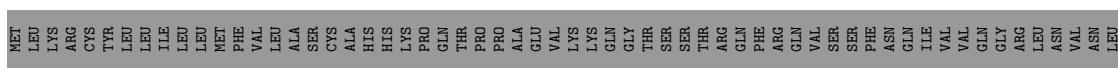
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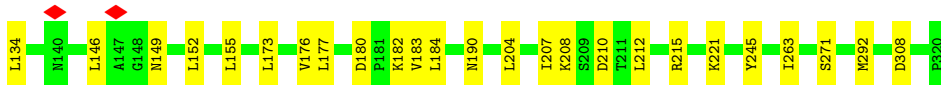
• Molecule 6: Outer membrane protein, OmpA family protein

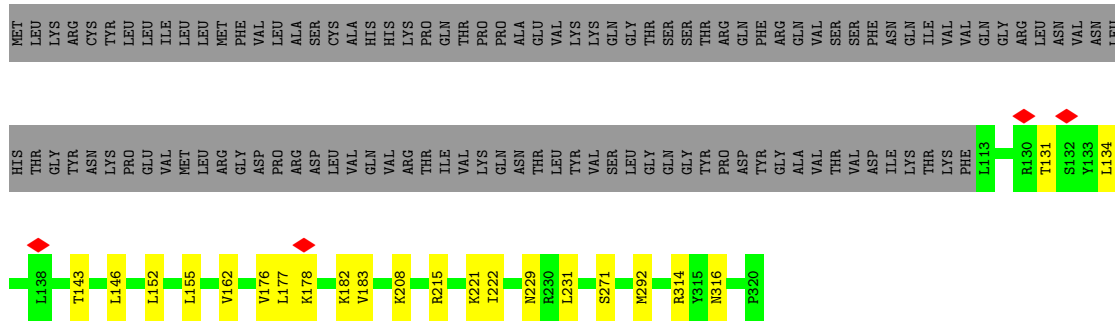


• Molecule 7: DUF2807 domain-containing protein

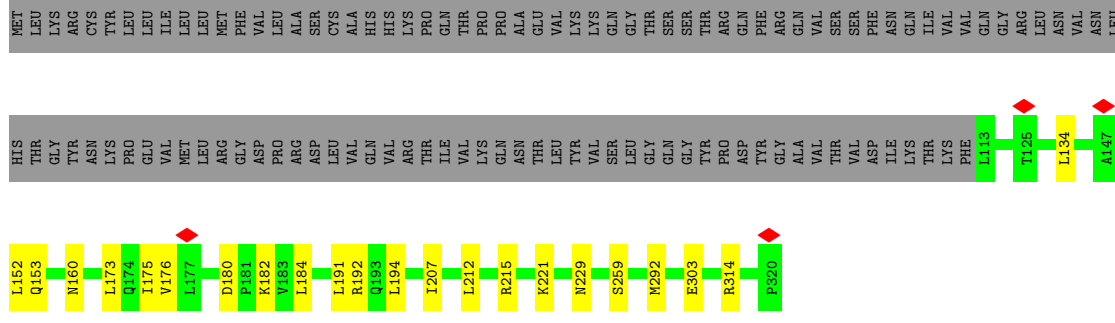


• Molecule 7: DUF2807 domain-containing protein

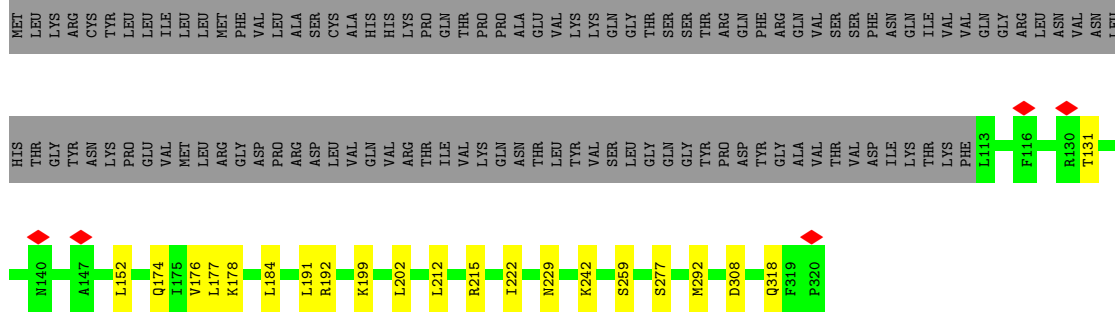




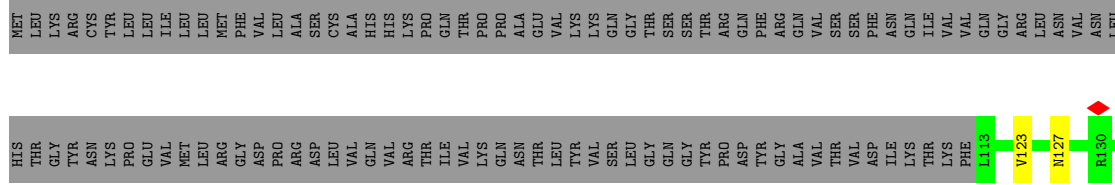
• Molecule 7: DUF2807 domain-containing protein



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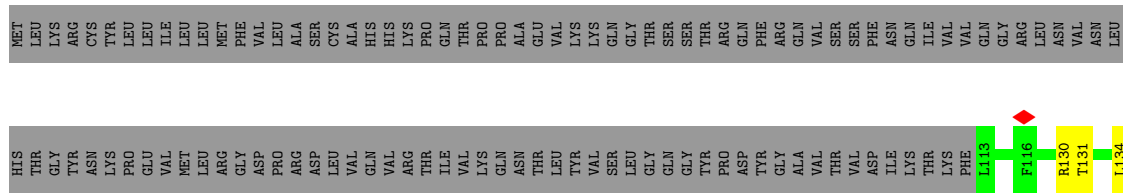


• Molecule 7: DUF2807 domain-containing protein

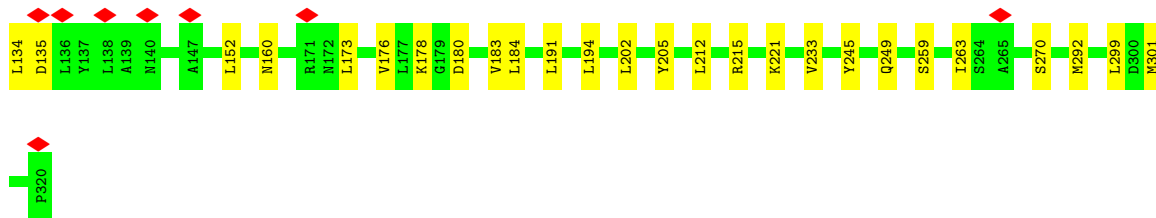
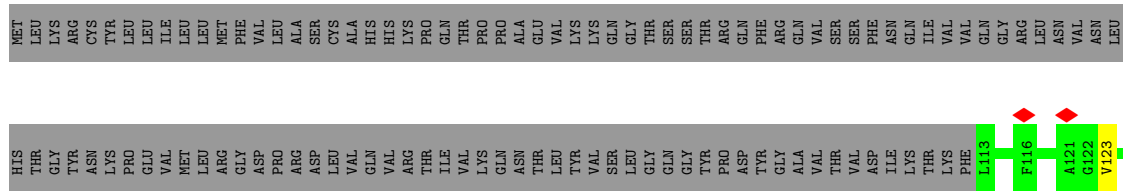




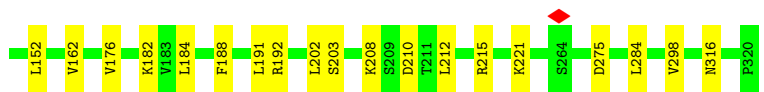
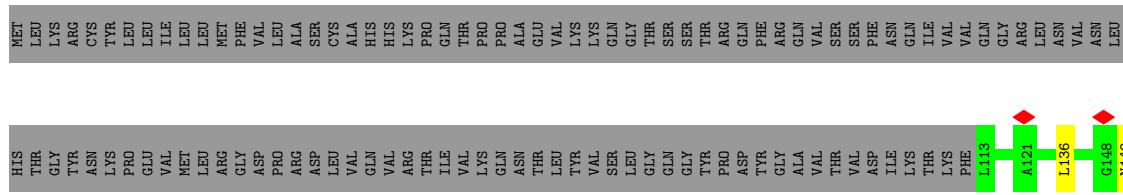
● Molecule 7: DUF2807 domain-containing protein



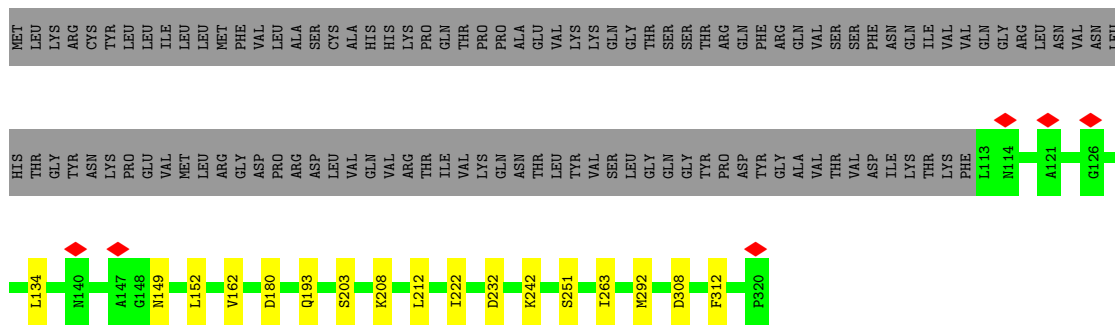
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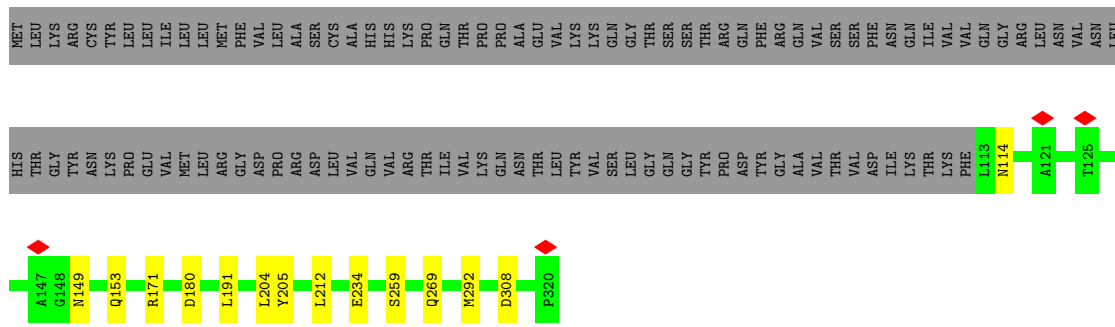
● Molecule 7: DUF2807 domain-containing protein



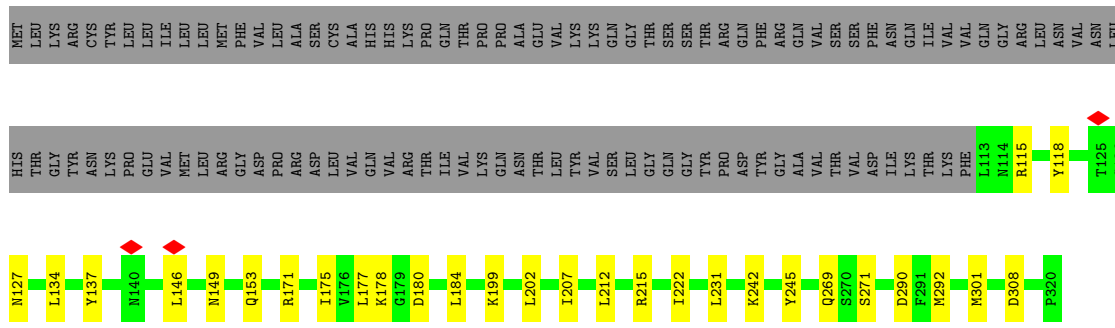
● Molecule 7: DUF2807 domain-containing protein



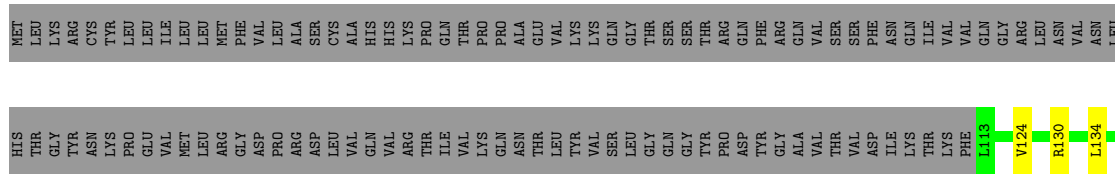
• Molecule 7: DUF2807 domain-containing protein



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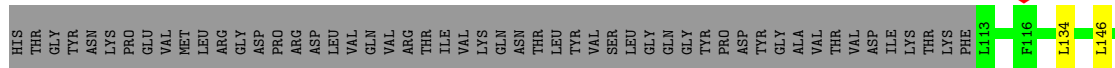
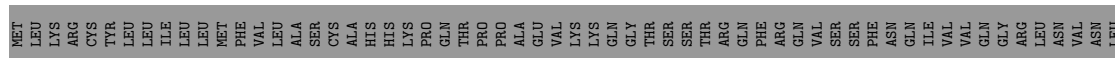


• Molecule 7: DUF2807 domain-containing protein

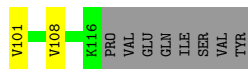
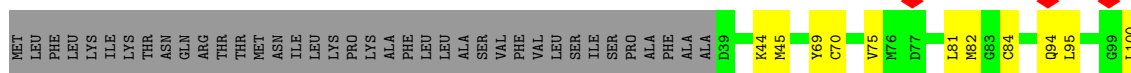




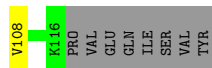
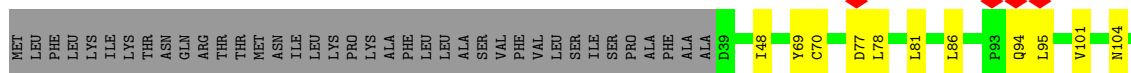
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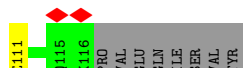
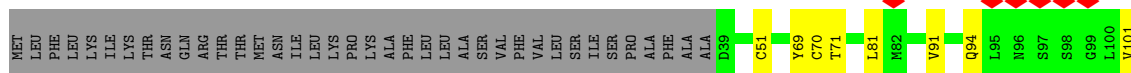
• Molecule 8: Neurogenic locus notch



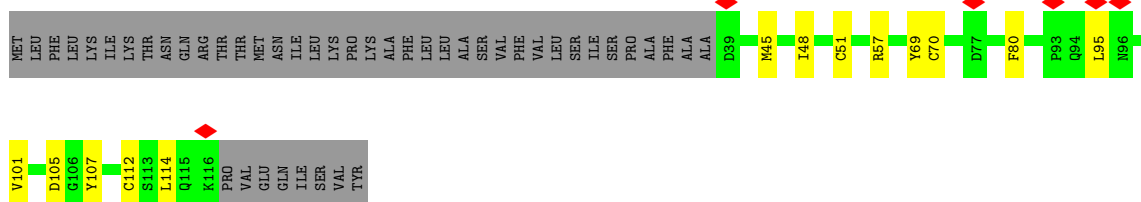
• Molecule 8: Neurogenic locus notch



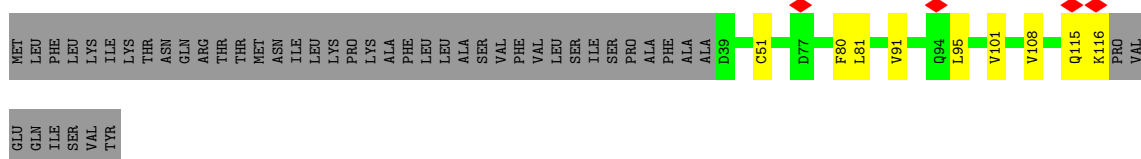
• Molecule 8: Neurogenic locus notch



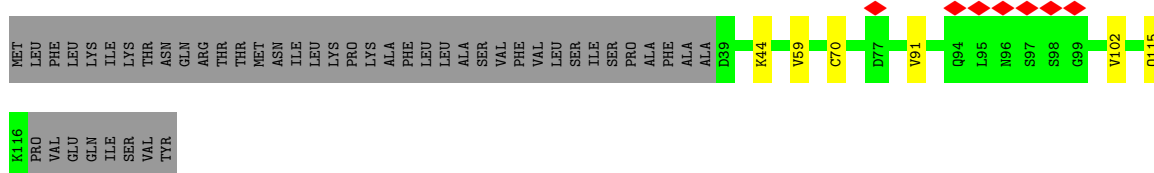
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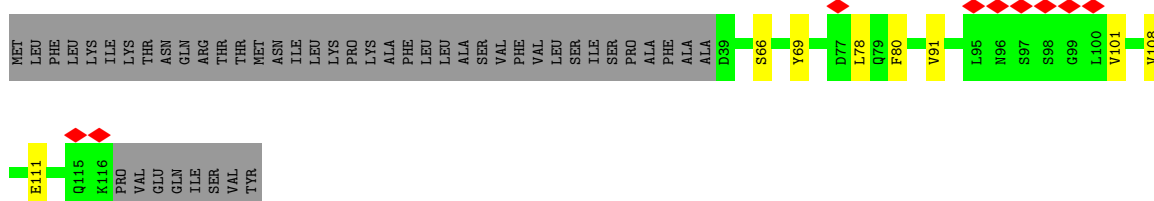
● Molecule 8: Neurogenic locus notch



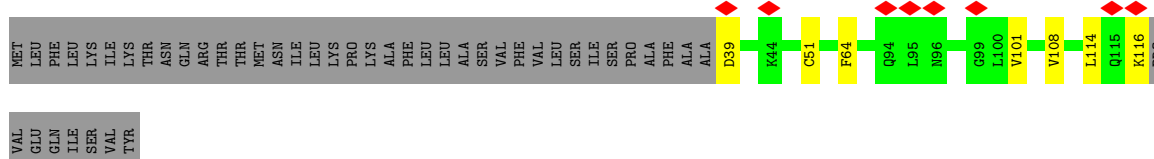
● Molecule 8: Neurogenic locus notch



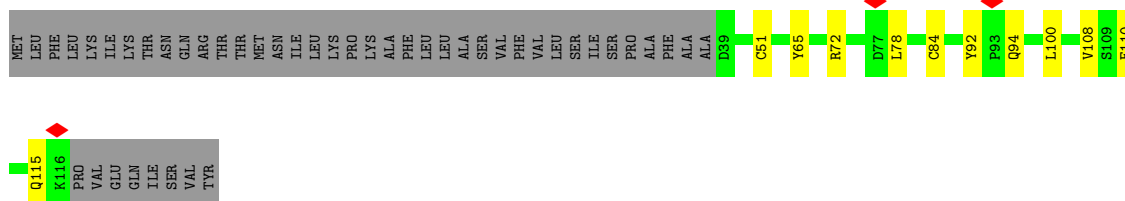
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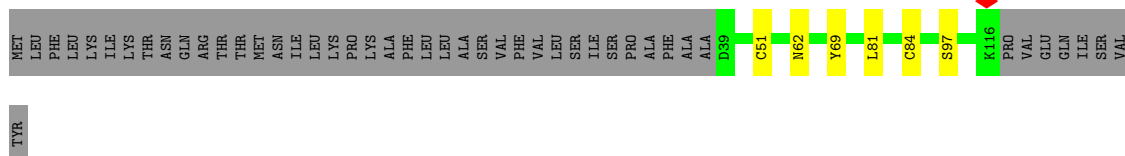
● Molecule 8: Neurogenic locus notch



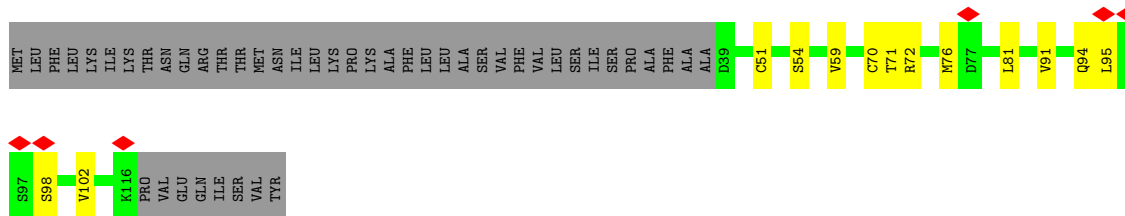
• Molecule 8: Neurogenic locus notch



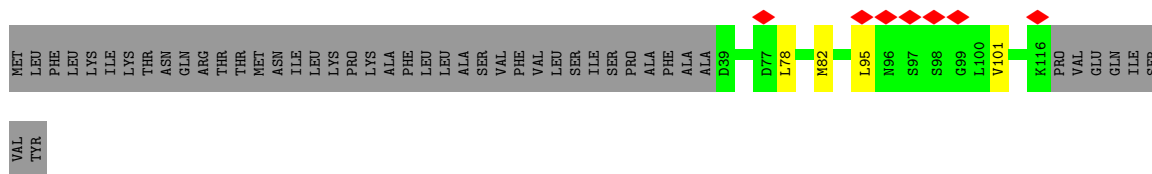
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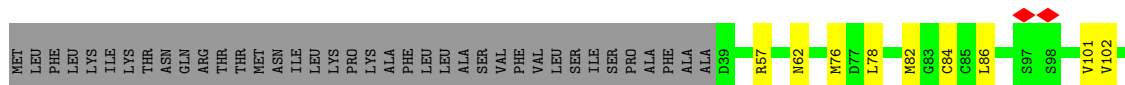
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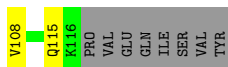


• Molecule 8: Neurogenic locus notch



• Molecule 8: Neurogenic locus notch





- Molecule 9: Unknown protein fragment

Chain EU:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown protein fragment

Chain FU:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown protein fragment

Chain GU:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown protein fragment

Chain HU:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown protein fragment

Chain IU:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown protein fragment

Chain JU:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown protein fragment

Chain KU:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown protein fragment

Chain LU:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown protein fragment

Chain MU:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown protein fragment

Chain AU:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown protein fragment

Chain BU:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown protein fragment

Chain CU:  100%

There are no outlier residues recorded for this chain.

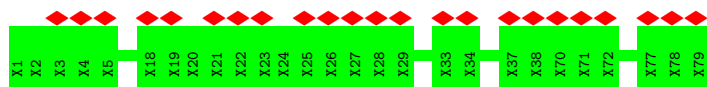
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Chain DU:  100%

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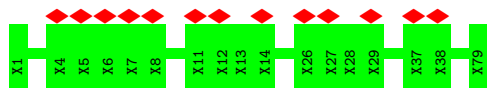
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Chain EX:  48% 100%



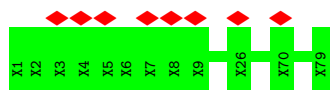
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Chain FX:  27% 100%

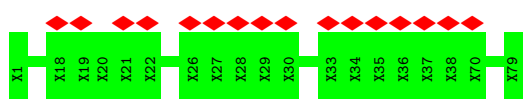


- Molecule 10: Unknown protein fragment

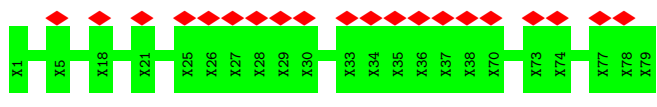
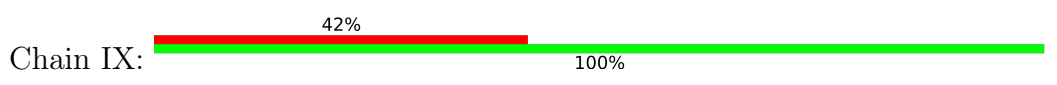
Chain GX:  17% 100%



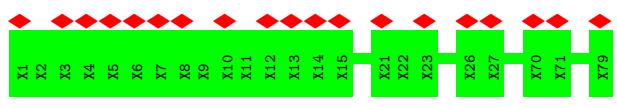
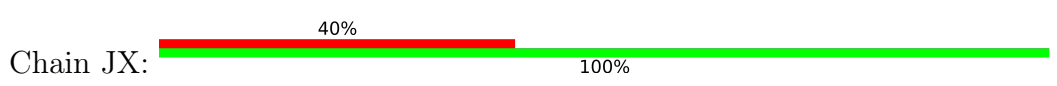
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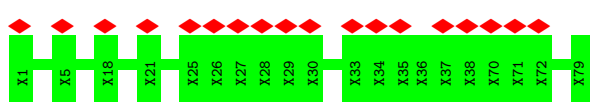
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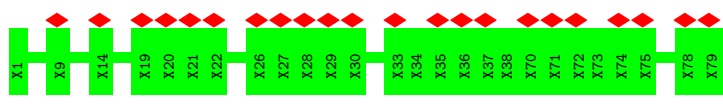
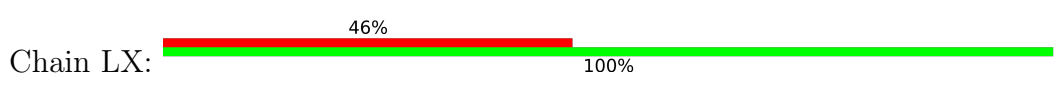
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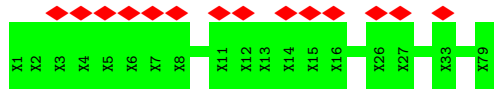
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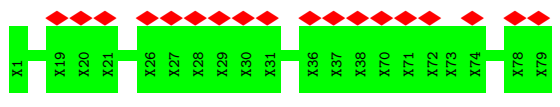
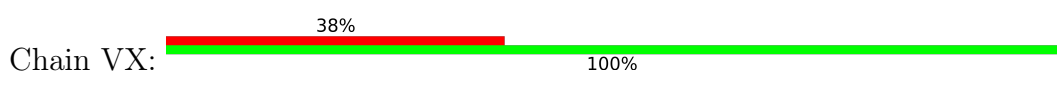
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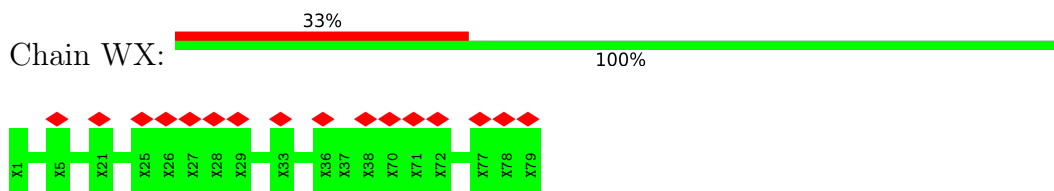
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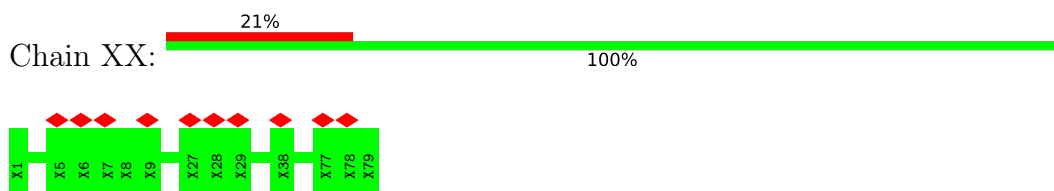
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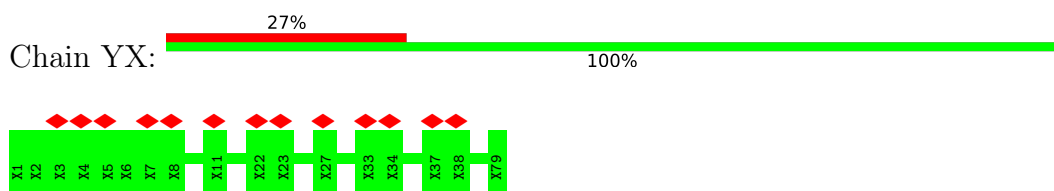
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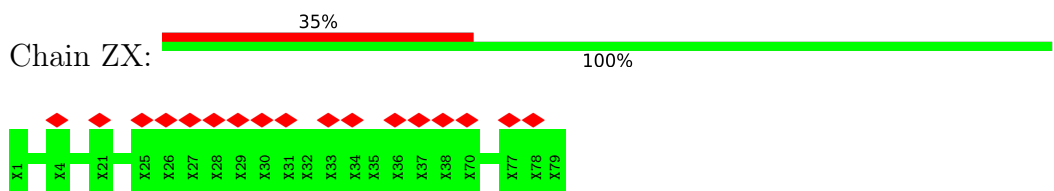
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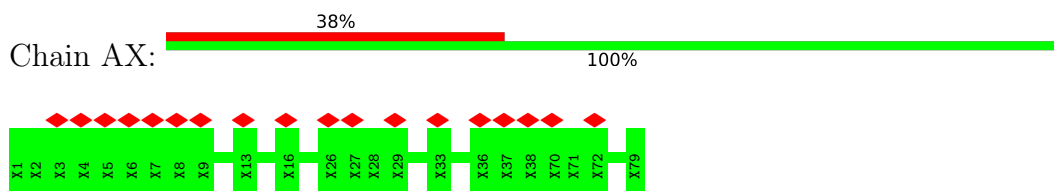
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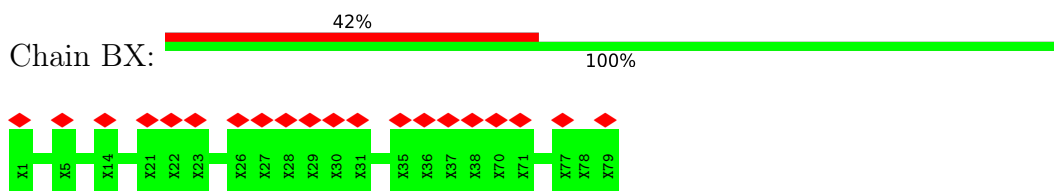
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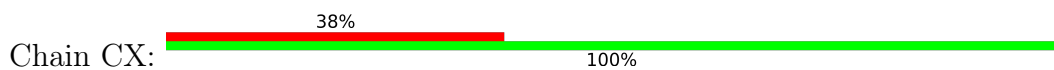
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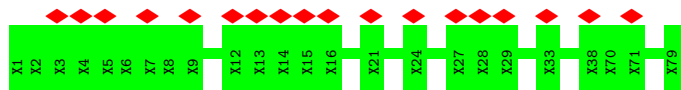


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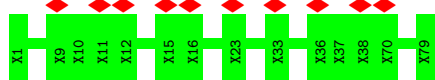


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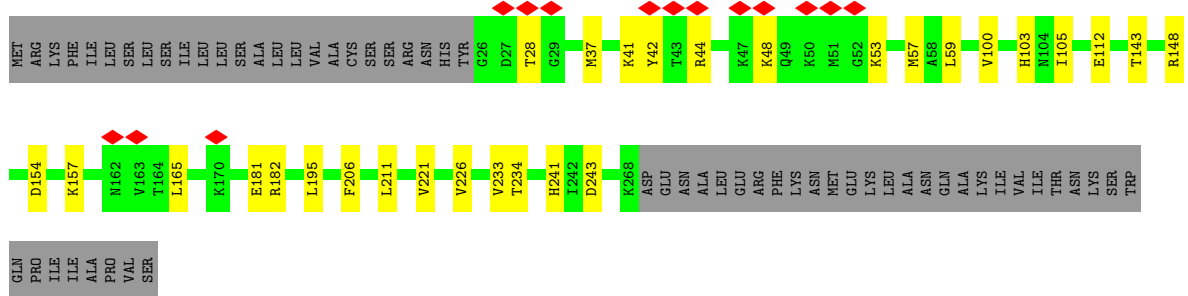




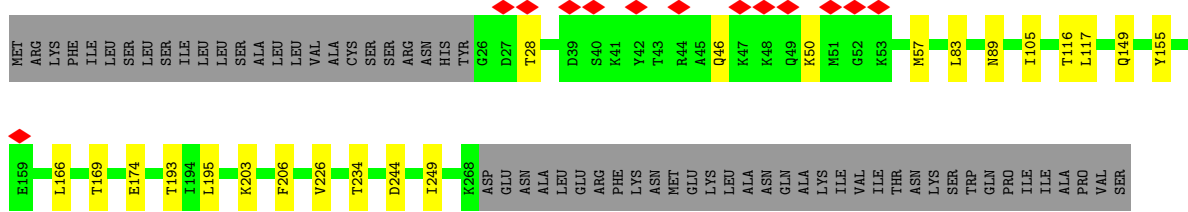
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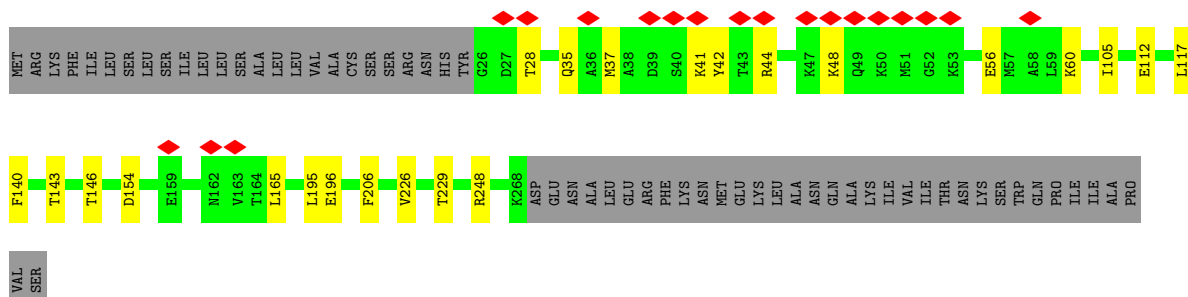
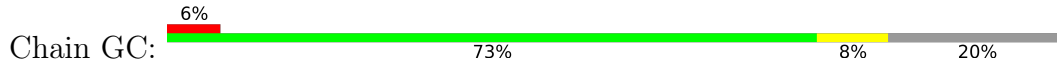
• Molecule 11: DotC



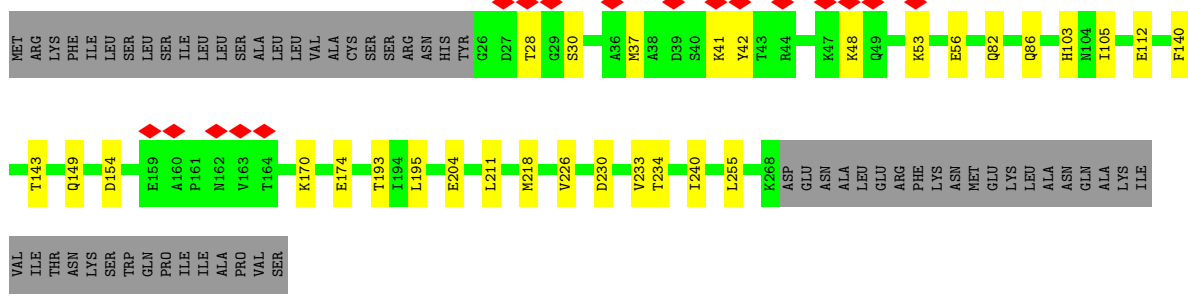
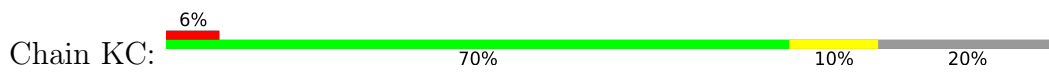
• Molecule 11: DotC



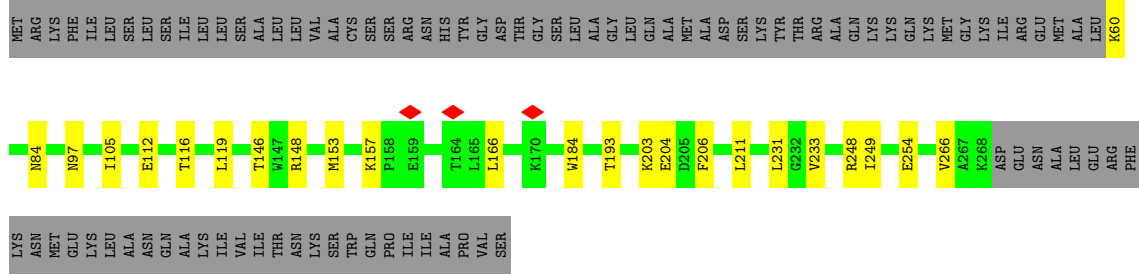
• Molecule 11: DotC



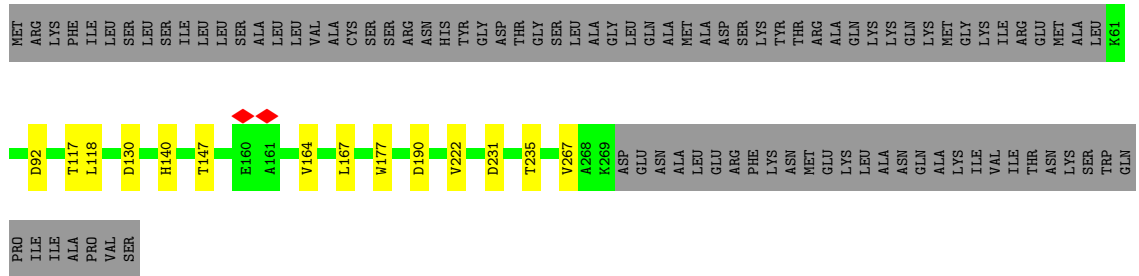
• Molecule 11: DotC



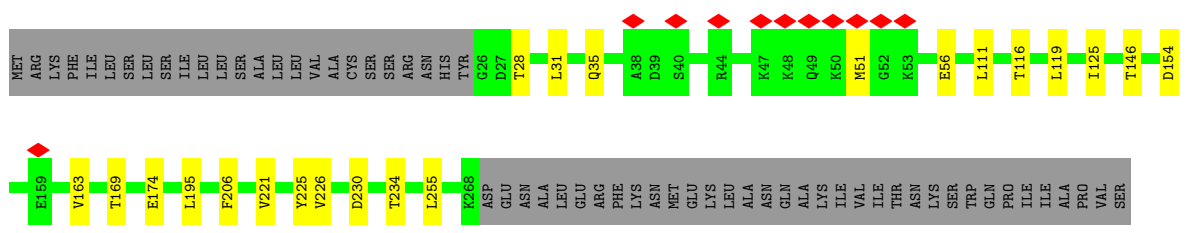
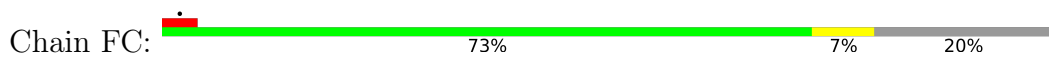
• Molecule 11: DotC



• Molecule 11: DotC

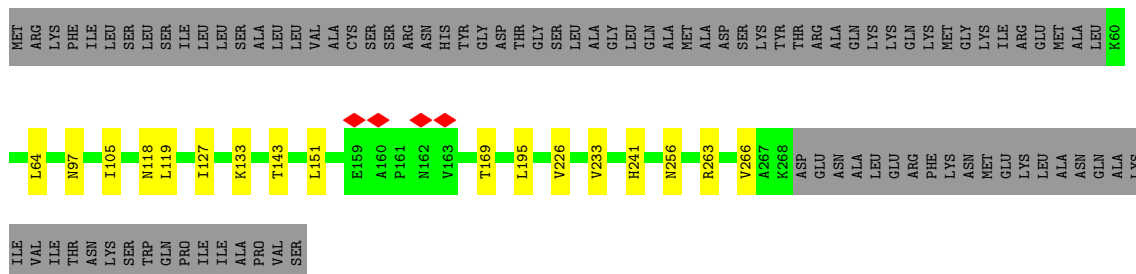


• Molecule 11: DotC

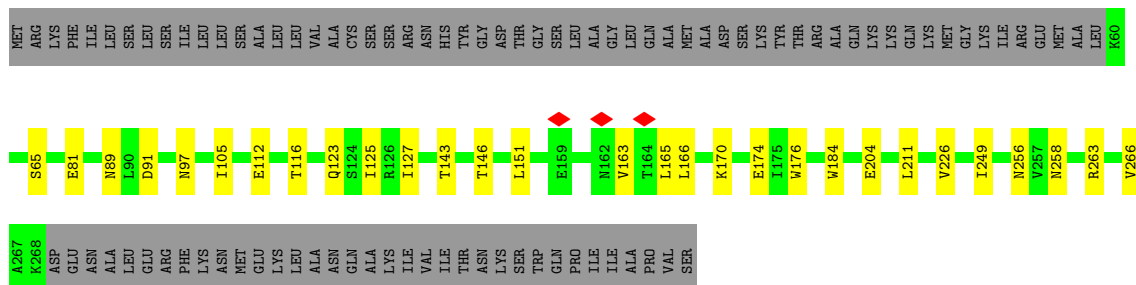


• Molecule 11: DotC

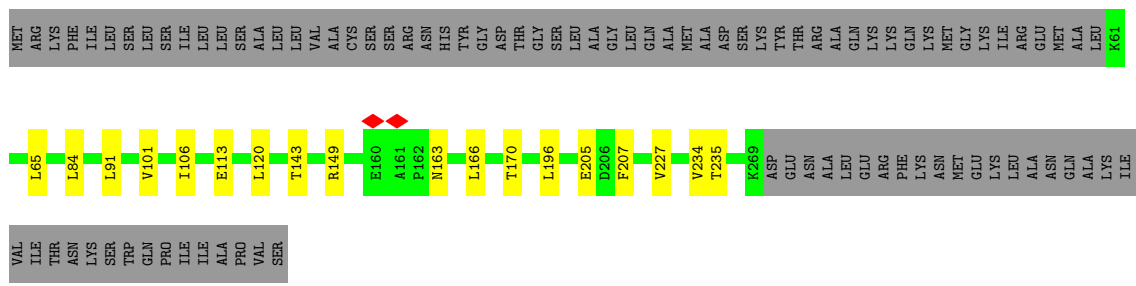




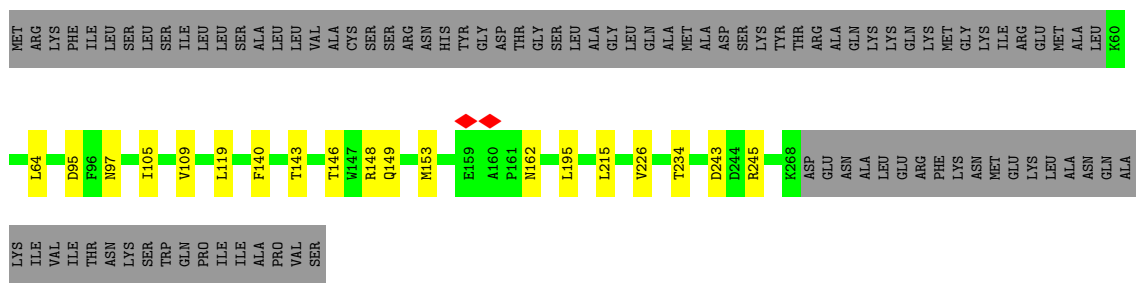
● Molecule 11: DotC



● Molecule 11: DotC

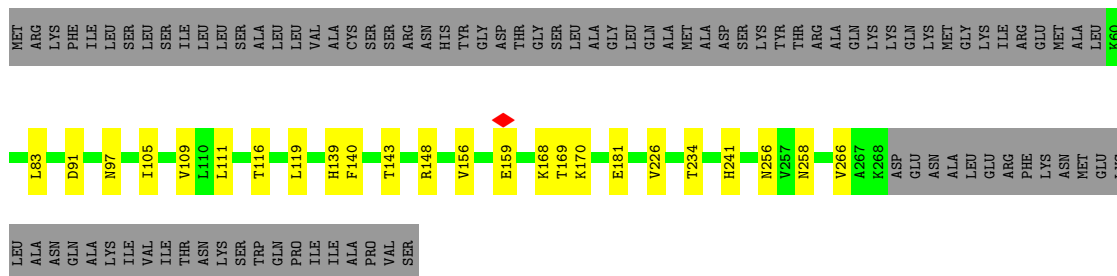


● Molecule 11: DotC

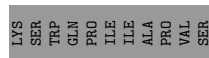
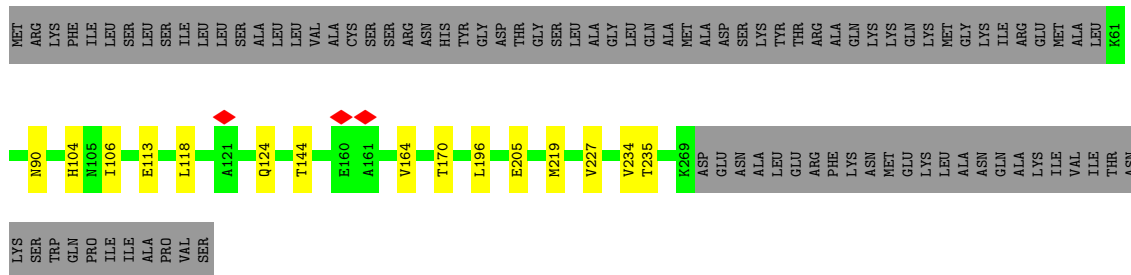


● Molecule 11: DotC





• Molecule 11: DotC



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 41057 | 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 ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 7.797 | Depositor |
| Minimum map value | -2.782 | Depositor |
| Average map value | 0.094 | Depositor |
| Map value standard deviation | 0.545 | Depositor |
| Recommended contour level | 2.25 | Depositor |
| Map size (Å) | 561.0, 561.0, 561.0 | wwPDB |
| Map dimensions | 250, 250, 250 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 2.244, 2.244, 2.244 | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 | AG | 0.29 | 0/1250 | 0.56 | 0/1699 |
| 1 | Ag | 0.26 | 0/278 | 0.46 | 0/377 |
| 1 | BG | 0.29 | 0/1250 | 0.57 | 0/1699 |
| 1 | Bg | 0.25 | 0/278 | 0.48 | 0/377 |
| 1 | CG | 0.29 | 0/1250 | 0.57 | 0/1699 |
| 1 | Cg | 0.27 | 0/278 | 0.51 | 0/377 |
| 1 | DG | 0.28 | 0/1250 | 0.57 | 0/1699 |
| 1 | Dg | 0.27 | 0/278 | 0.47 | 0/377 |
| 1 | EG | 0.28 | 0/1250 | 0.58 | 1/1699 (0.1%) |
| 1 | Eg | 0.26 | 0/278 | 0.48 | 0/377 |
| 1 | FG | 0.30 | 0/1250 | 0.57 | 0/1699 |
| 1 | Fg | 0.27 | 0/278 | 0.49 | 0/377 |
| 1 | GG | 0.29 | 0/1250 | 0.58 | 0/1699 |
| 1 | Gg | 0.26 | 0/278 | 0.48 | 0/377 |
| 1 | HG | 0.30 | 0/1250 | 0.58 | 0/1699 |
| 1 | Hg | 0.26 | 0/278 | 0.46 | 0/377 |
| 1 | IG | 0.29 | 0/1250 | 0.58 | 0/1699 |
| 1 | Ig | 0.26 | 0/278 | 0.48 | 0/377 |
| 1 | JG | 0.28 | 0/1250 | 0.57 | 0/1699 |
| 1 | Jg | 0.27 | 0/278 | 0.48 | 0/377 |
| 1 | KG | 0.29 | 0/1250 | 0.56 | 0/1699 |
| 1 | Kg | 0.25 | 0/278 | 0.48 | 0/377 |
| 1 | LG | 0.29 | 0/1250 | 0.57 | 1/1699 (0.1%) |
| 1 | Lg | 0.27 | 0/278 | 0.49 | 0/377 |
| 1 | MG | 0.29 | 0/1250 | 0.56 | 0/1699 |
| 1 | Mg | 0.28 | 0/278 | 0.46 | 0/377 |
| 1 | NG | 0.29 | 0/1250 | 0.55 | 0/1699 |
| 1 | OG | 0.29 | 0/1250 | 0.56 | 0/1699 |
| 1 | PG | 0.29 | 0/1250 | 0.56 | 0/1699 |
| 1 | VG | 0.28 | 0/278 | 0.59 | 0/377 |
| 1 | WG | 0.26 | 0/278 | 0.52 | 0/377 |
| 1 | XG | 0.26 | 0/278 | 0.51 | 0/377 |
| 1 | YG | 0.28 | 0/278 | 0.51 | 0/377 |
| 1 | ZG | 0.28 | 0/278 | 0.50 | 0/377 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | AD | 0.30 | 0/1107 | 0.52 | 0/1502 |
| 2 | Ad | 0.29 | 0/1078 | 0.51 | 0/1463 |
| 2 | BD | 0.31 | 0/1107 | 0.53 | 0/1502 |
| 2 | Bd | 0.28 | 0/1078 | 0.49 | 0/1463 |
| 2 | CD | 0.30 | 0/1107 | 0.53 | 0/1502 |
| 2 | Cd | 0.28 | 0/1078 | 0.51 | 0/1463 |
| 2 | DD | 0.30 | 0/1107 | 0.53 | 0/1502 |
| 2 | Dd | 0.30 | 0/1078 | 0.49 | 0/1463 |
| 2 | ED | 0.32 | 0/1107 | 0.53 | 0/1502 |
| 2 | Ed | 0.30 | 0/1078 | 0.50 | 0/1463 |
| 2 | FD | 0.31 | 0/1107 | 0.52 | 0/1502 |
| 2 | Fd | 0.29 | 0/1078 | 0.49 | 0/1463 |
| 2 | GD | 0.30 | 0/1107 | 0.53 | 0/1502 |
| 2 | Gd | 0.29 | 0/1078 | 0.51 | 0/1463 |
| 2 | HD | 0.30 | 0/1107 | 0.52 | 0/1502 |
| 2 | Hd | 0.29 | 0/1078 | 0.50 | 0/1463 |
| 2 | ID | 0.30 | 0/1107 | 0.53 | 0/1502 |
| 2 | Id | 0.29 | 0/1078 | 0.50 | 0/1463 |
| 2 | JD | 0.31 | 0/1107 | 0.53 | 0/1502 |
| 2 | Jd | 0.29 | 0/1078 | 0.49 | 0/1463 |
| 2 | KD | 0.30 | 0/1107 | 0.53 | 0/1502 |
| 2 | Kd | 0.29 | 0/1078 | 0.50 | 0/1463 |
| 2 | LD | 0.29 | 0/1107 | 0.52 | 0/1502 |
| 2 | Ld | 0.29 | 0/1078 | 0.50 | 0/1463 |
| 2 | MD | 0.30 | 0/1107 | 0.53 | 0/1502 |
| 2 | Md | 0.28 | 0/1078 | 0.49 | 0/1463 |
| 3 | AF | 0.26 | 0/490 | 0.55 | 0/660 |
| 3 | Af | 0.28 | 0/456 | 0.54 | 0/615 |
| 3 | BF | 0.27 | 0/490 | 0.52 | 0/660 |
| 3 | Bf | 0.27 | 0/456 | 0.55 | 0/615 |
| 3 | CF | 0.27 | 0/490 | 0.54 | 0/660 |
| 3 | Cf | 0.28 | 0/456 | 0.53 | 0/615 |
| 3 | DF | 0.27 | 0/490 | 0.55 | 0/660 |
| 3 | Df | 0.27 | 0/456 | 0.53 | 0/615 |
| 3 | EF | 0.27 | 0/490 | 0.54 | 0/660 |
| 3 | Ef | 0.28 | 0/456 | 0.52 | 0/615 |
| 3 | FF | 0.26 | 0/490 | 0.53 | 0/660 |
| 3 | Ff | 0.29 | 0/456 | 0.52 | 0/615 |
| 3 | GF | 0.26 | 0/490 | 0.54 | 0/660 |
| 3 | Gf | 0.28 | 0/456 | 0.51 | 0/615 |
| 3 | HF | 0.27 | 0/490 | 0.54 | 0/660 |
| 3 | Hf | 0.28 | 0/456 | 0.54 | 0/615 |
| 3 | IF | 0.27 | 0/490 | 0.53 | 0/660 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 3 | If | 0.26 | 0/456 | 0.55 | 0/615 |
| 3 | JF | 0.26 | 0/490 | 0.54 | 0/660 |
| 3 | Jf | 0.28 | 0/456 | 0.53 | 0/615 |
| 3 | KF | 0.26 | 0/490 | 0.54 | 0/660 |
| 3 | Kf | 0.27 | 0/456 | 0.54 | 0/615 |
| 3 | LF | 0.27 | 0/490 | 0.55 | 0/660 |
| 3 | Lf | 0.27 | 0/456 | 0.53 | 0/615 |
| 3 | MF | 0.27 | 0/490 | 0.54 | 0/660 |
| 3 | Mf | 0.28 | 0/456 | 0.52 | 0/615 |
| 3 | VF | 0.27 | 0/490 | 0.51 | 0/660 |
| 3 | WF | 0.27 | 0/490 | 0.55 | 0/660 |
| 3 | XF | 0.27 | 0/490 | 0.54 | 0/660 |
| 3 | YF | 0.25 | 0/490 | 0.55 | 0/660 |
| 3 | ZF | 0.27 | 0/490 | 0.53 | 0/660 |
| 4 | AH | 0.29 | 0/2033 | 0.52 | 0/2775 |
| 4 | BH | 0.30 | 0/2033 | 0.53 | 0/2775 |
| 4 | CH | 0.29 | 0/2033 | 0.51 | 0/2775 |
| 4 | DH | 0.29 | 0/2033 | 0.51 | 0/2775 |
| 4 | EH | 0.29 | 0/2033 | 0.51 | 0/2775 |
| 4 | FH | 0.29 | 0/2033 | 0.52 | 0/2775 |
| 4 | GH | 0.29 | 0/2033 | 0.51 | 0/2775 |
| 4 | HH | 0.30 | 0/2033 | 0.52 | 0/2775 |
| 4 | IH | 0.29 | 0/2033 | 0.52 | 0/2775 |
| 4 | JH | 0.29 | 0/2033 | 0.51 | 0/2775 |
| 4 | KH | 0.30 | 0/2033 | 0.53 | 0/2775 |
| 4 | LH | 0.29 | 0/2033 | 0.52 | 0/2775 |
| 4 | MH | 0.30 | 0/2033 | 0.53 | 0/2775 |
| 4 | VH | 0.27 | 0/1921 | 0.51 | 0/2620 |
| 4 | WH | 0.27 | 0/1921 | 0.54 | 0/2620 |
| 4 | XH | 0.27 | 0/1921 | 0.52 | 0/2620 |
| 4 | YH | 0.27 | 0/1921 | 0.53 | 0/2620 |
| 4 | ZH | 0.27 | 0/1921 | 0.52 | 0/2620 |
| 5 | AK | 0.30 | 0/1195 | 0.54 | 0/1616 |
| 5 | BK | 0.31 | 0/1195 | 0.55 | 0/1616 |
| 5 | CK | 0.30 | 0/1195 | 0.54 | 0/1616 |
| 5 | DK | 0.31 | 0/1195 | 0.54 | 0/1616 |
| 5 | EK | 0.29 | 0/1195 | 0.54 | 0/1616 |
| 5 | FK | 0.29 | 0/1195 | 0.55 | 0/1616 |
| 5 | GK | 0.30 | 0/1195 | 0.53 | 0/1616 |
| 5 | HK | 0.32 | 0/1195 | 0.55 | 0/1616 |
| 5 | IK | 0.29 | 0/1195 | 0.54 | 0/1616 |
| 5 | JK | 0.30 | 0/1195 | 0.53 | 0/1616 |
| 5 | KK | 0.30 | 0/1195 | 0.54 | 0/1616 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 5 | LK | 0.31 | 0/1195 | 0.54 | 0/1616 |
| 5 | MK | 0.30 | 0/1195 | 0.54 | 0/1616 |
| 6 | AL | 0.30 | 0/1417 | 0.54 | 0/1912 |
| 6 | BL | 0.30 | 0/1417 | 0.55 | 0/1912 |
| 6 | CL | 0.30 | 0/1417 | 0.54 | 0/1912 |
| 6 | DL | 0.30 | 0/1417 | 0.54 | 0/1912 |
| 6 | EL | 0.30 | 0/1417 | 0.54 | 0/1912 |
| 6 | FL | 0.30 | 0/1417 | 0.55 | 0/1912 |
| 6 | GL | 0.30 | 0/1417 | 0.55 | 0/1912 |
| 6 | HL | 0.30 | 0/1417 | 0.55 | 0/1912 |
| 6 | IL | 0.29 | 0/1417 | 0.56 | 0/1912 |
| 6 | JL | 0.30 | 0/1417 | 0.54 | 0/1912 |
| 6 | KL | 0.29 | 0/1417 | 0.56 | 0/1912 |
| 6 | LL | 0.31 | 0/1417 | 0.54 | 0/1912 |
| 6 | ML | 0.30 | 0/1417 | 0.55 | 0/1912 |
| 7 | AM | 0.29 | 0/1678 | 0.58 | 0/2262 |
| 7 | BM | 0.29 | 0/1678 | 0.58 | 0/2262 |
| 7 | CM | 0.29 | 0/1678 | 0.57 | 0/2262 |
| 7 | DM | 0.29 | 0/1678 | 0.57 | 0/2262 |
| 7 | EM | 0.28 | 0/1678 | 0.57 | 0/2262 |
| 7 | FM | 0.30 | 0/1678 | 0.58 | 0/2262 |
| 7 | GM | 0.29 | 0/1678 | 0.57 | 0/2262 |
| 7 | HM | 0.29 | 0/1678 | 0.58 | 0/2262 |
| 7 | IM | 0.29 | 0/1678 | 0.57 | 0/2262 |
| 7 | JM | 0.29 | 0/1678 | 0.57 | 0/2262 |
| 7 | KM | 0.28 | 0/1678 | 0.57 | 0/2262 |
| 7 | LM | 0.29 | 0/1678 | 0.58 | 0/2262 |
| 7 | MM | 0.28 | 0/1678 | 0.57 | 0/2262 |
| 8 | AN | 0.32 | 0/593 | 0.54 | 0/799 |
| 8 | BN | 0.31 | 0/593 | 0.56 | 0/799 |
| 8 | CN | 0.31 | 0/593 | 0.51 | 0/799 |
| 8 | DN | 0.31 | 0/593 | 0.53 | 0/799 |
| 8 | EN | 0.33 | 0/593 | 0.52 | 0/799 |
| 8 | FN | 0.33 | 0/593 | 0.52 | 0/799 |
| 8 | GN | 0.31 | 0/593 | 0.52 | 0/799 |
| 8 | HN | 0.31 | 0/593 | 0.53 | 0/799 |
| 8 | IN | 0.30 | 0/593 | 0.52 | 0/799 |
| 8 | JN | 0.31 | 0/593 | 0.53 | 0/799 |
| 8 | KN | 0.32 | 0/593 | 0.52 | 0/799 |
| 8 | LN | 0.32 | 0/593 | 0.51 | 0/799 |
| 8 | MN | 0.32 | 0/593 | 0.54 | 0/799 |
| 11 | AC | 0.30 | 0/1702 | 0.52 | 0/2315 |
| 11 | BC | 0.30 | 0/1957 | 0.52 | 0/2651 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 11 | CC | 0.29 | 0/1957 | 0.52 | 0/2651 |
| 11 | DC | 0.29 | 0/1702 | 0.51 | 0/2315 |
| 11 | EC | 0.30 | 0/1702 | 0.51 | 0/2315 |
| 11 | FC | 0.30 | 0/1957 | 0.50 | 0/2651 |
| 11 | GC | 0.29 | 0/1957 | 0.51 | 0/2651 |
| 11 | HC | 0.29 | 0/1702 | 0.50 | 0/2315 |
| 11 | IC | 0.29 | 0/1702 | 0.51 | 0/2315 |
| 11 | JC | 0.31 | 0/1702 | 0.52 | 0/2315 |
| 11 | KC | 0.29 | 0/1957 | 0.52 | 0/2651 |
| 11 | LC | 0.30 | 0/1702 | 0.55 | 0/2315 |
| 11 | MC | 0.30 | 0/1702 | 0.52 | 0/2315 |
| All | All | 0.29 | 0/191071 | 0.53 | 2/258997 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 1 | LG | 1040 | LEU | CA-CB-CG | 6.10 | 129.34 | 115.30 |
| 1 | EG | 965 | LEU | CA-CB-CG | 5.04 | 126.89 | 115.30 |

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 | AG | 161/1048 (15%) | 154 (96%) | 7 (4%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1 | Ag | 32/1048 (3%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| 1 | BG | 161/1048 (15%) | 155 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | Bg | 32/1048 (3%) | 30 (94%) | 2 (6%) | 0 | 100 | 100 |
| 1 | CG | 161/1048 (15%) | 152 (94%) | 9 (6%) | 0 | 100 | 100 |
| 1 | Cg | 32/1048 (3%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| 1 | DG | 161/1048 (15%) | 154 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | Dg | 32/1048 (3%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 1 | EG | 161/1048 (15%) | 156 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | Eg | 32/1048 (3%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| 1 | FG | 161/1048 (15%) | 153 (95%) | 8 (5%) | 0 | 100 | 100 |
| 1 | Fg | 32/1048 (3%) | 30 (94%) | 2 (6%) | 0 | 100 | 100 |
| 1 | GG | 161/1048 (15%) | 151 (94%) | 10 (6%) | 0 | 100 | 100 |
| 1 | Gg | 32/1048 (3%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 1 | HG | 161/1048 (15%) | 153 (95%) | 8 (5%) | 0 | 100 | 100 |
| 1 | Hg | 32/1048 (3%) | 30 (94%) | 2 (6%) | 0 | 100 | 100 |
| 1 | IG | 161/1048 (15%) | 153 (95%) | 8 (5%) | 0 | 100 | 100 |
| 1 | Ig | 32/1048 (3%) | 30 (94%) | 2 (6%) | 0 | 100 | 100 |
| 1 | JG | 161/1048 (15%) | 156 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | Jg | 32/1048 (3%) | 30 (94%) | 2 (6%) | 0 | 100 | 100 |
| 1 | KG | 161/1048 (15%) | 155 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | Kg | 32/1048 (3%) | 30 (94%) | 2 (6%) | 0 | 100 | 100 |
| 1 | LG | 161/1048 (15%) | 149 (92%) | 12 (8%) | 0 | 100 | 100 |
| 1 | Lg | 32/1048 (3%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| 1 | MG | 161/1048 (15%) | 154 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | Mg | 32/1048 (3%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| 1 | NG | 161/1048 (15%) | 153 (95%) | 8 (5%) | 0 | 100 | 100 |
| 1 | OG | 161/1048 (15%) | 157 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | PG | 161/1048 (15%) | 156 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | VG | 32/1048 (3%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| 1 | WG | 32/1048 (3%) | 30 (94%) | 2 (6%) | 0 | 100 | 100 |
| 1 | XG | 32/1048 (3%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | YG | 32/1048 (3%) | 30 (94%) | 2 (6%) | 0 | 100 | 100 |
| 1 | ZG | 32/1048 (3%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 2 | AD | 138/163 (85%) | 127 (92%) | 11 (8%) | 0 | 100 | 100 |
| 2 | Ad | 135/163 (83%) | 128 (95%) | 7 (5%) | 0 | 100 | 100 |
| 2 | BD | 138/163 (85%) | 133 (96%) | 5 (4%) | 0 | 100 | 100 |
| 2 | Bd | 135/163 (83%) | 127 (94%) | 8 (6%) | 0 | 100 | 100 |
| 2 | CD | 138/163 (85%) | 131 (95%) | 7 (5%) | 0 | 100 | 100 |
| 2 | Cd | 135/163 (83%) | 130 (96%) | 5 (4%) | 0 | 100 | 100 |
| 2 | DD | 138/163 (85%) | 133 (96%) | 5 (4%) | 0 | 100 | 100 |
| 2 | Dd | 135/163 (83%) | 130 (96%) | 5 (4%) | 0 | 100 | 100 |
| 2 | ED | 138/163 (85%) | 130 (94%) | 8 (6%) | 0 | 100 | 100 |
| 2 | Ed | 135/163 (83%) | 130 (96%) | 5 (4%) | 0 | 100 | 100 |
| 2 | FD | 138/163 (85%) | 130 (94%) | 8 (6%) | 0 | 100 | 100 |
| 2 | Fd | 135/163 (83%) | 127 (94%) | 8 (6%) | 0 | 100 | 100 |
| 2 | GD | 138/163 (85%) | 130 (94%) | 8 (6%) | 0 | 100 | 100 |
| 2 | Gd | 135/163 (83%) | 128 (95%) | 7 (5%) | 0 | 100 | 100 |
| 2 | HD | 138/163 (85%) | 130 (94%) | 8 (6%) | 0 | 100 | 100 |
| 2 | Hd | 135/163 (83%) | 130 (96%) | 5 (4%) | 0 | 100 | 100 |
| 2 | ID | 138/163 (85%) | 127 (92%) | 11 (8%) | 0 | 100 | 100 |
| 2 | Id | 135/163 (83%) | 131 (97%) | 4 (3%) | 0 | 100 | 100 |
| 2 | JD | 138/163 (85%) | 132 (96%) | 6 (4%) | 0 | 100 | 100 |
| 2 | Jd | 135/163 (83%) | 126 (93%) | 9 (7%) | 0 | 100 | 100 |
| 2 | KD | 138/163 (85%) | 126 (91%) | 12 (9%) | 0 | 100 | 100 |
| 2 | Kd | 135/163 (83%) | 131 (97%) | 4 (3%) | 0 | 100 | 100 |
| 2 | LD | 138/163 (85%) | 134 (97%) | 4 (3%) | 0 | 100 | 100 |
| 2 | Ld | 135/163 (83%) | 130 (96%) | 5 (4%) | 0 | 100 | 100 |
| 2 | MD | 138/163 (85%) | 130 (94%) | 8 (6%) | 0 | 100 | 100 |
| 2 | Md | 135/163 (83%) | 130 (96%) | 5 (4%) | 0 | 100 | 100 |
| 3 | AF | 61/269 (23%) | 58 (95%) | 3 (5%) | 0 | 100 | 100 |
| 3 | Af | 57/269 (21%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 3 | BF | 61/269 (23%) | 56 (92%) | 5 (8%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 3 | Bf | 57/269 (21%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 3 | CF | 61/269 (23%) | 56 (92%) | 5 (8%) | 0 | 100 | 100 |
| 3 | Cf | 57/269 (21%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 3 | DF | 61/269 (23%) | 59 (97%) | 2 (3%) | 0 | 100 | 100 |
| 3 | Df | 57/269 (21%) | 52 (91%) | 5 (9%) | 0 | 100 | 100 |
| 3 | EF | 61/269 (23%) | 57 (93%) | 4 (7%) | 0 | 100 | 100 |
| 3 | Ef | 57/269 (21%) | 52 (91%) | 5 (9%) | 0 | 100 | 100 |
| 3 | FF | 61/269 (23%) | 60 (98%) | 1 (2%) | 0 | 100 | 100 |
| 3 | Ff | 57/269 (21%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 3 | GF | 61/269 (23%) | 59 (97%) | 2 (3%) | 0 | 100 | 100 |
| 3 | Gf | 57/269 (21%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 3 | HF | 61/269 (23%) | 58 (95%) | 3 (5%) | 0 | 100 | 100 |
| 3 | Hf | 57/269 (21%) | 51 (90%) | 6 (10%) | 0 | 100 | 100 |
| 3 | IF | 61/269 (23%) | 56 (92%) | 5 (8%) | 0 | 100 | 100 |
| 3 | If | 57/269 (21%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 3 | JF | 61/269 (23%) | 58 (95%) | 3 (5%) | 0 | 100 | 100 |
| 3 | Jf | 57/269 (21%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 3 | KF | 61/269 (23%) | 55 (90%) | 6 (10%) | 0 | 100 | 100 |
| 3 | Kf | 57/269 (21%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 3 | LF | 61/269 (23%) | 59 (97%) | 2 (3%) | 0 | 100 | 100 |
| 3 | Lf | 57/269 (21%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 3 | MF | 61/269 (23%) | 60 (98%) | 1 (2%) | 0 | 100 | 100 |
| 3 | Mf | 57/269 (21%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 3 | VF | 61/269 (23%) | 61 (100%) | 0 | 0 | 100 | 100 |
| 3 | WF | 61/269 (23%) | 58 (95%) | 3 (5%) | 0 | 100 | 100 |
| 3 | XF | 61/269 (23%) | 60 (98%) | 1 (2%) | 0 | 100 | 100 |
| 3 | YF | 61/269 (23%) | 58 (95%) | 3 (5%) | 0 | 100 | 100 |
| 3 | ZF | 61/269 (23%) | 60 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | AH | 256/361 (71%) | 240 (94%) | 16 (6%) | 0 | 100 | 100 |
| 4 | BH | 256/361 (71%) | 244 (95%) | 12 (5%) | 0 | 100 | 100 |
| 4 | CH | 256/361 (71%) | 241 (94%) | 15 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 4 | DH | 256/361 (71%) | 241 (94%) | 15 (6%) | 0 | 100 | 100 |
| 4 | EH | 256/361 (71%) | 248 (97%) | 8 (3%) | 0 | 100 | 100 |
| 4 | FH | 256/361 (71%) | 246 (96%) | 10 (4%) | 0 | 100 | 100 |
| 4 | GH | 256/361 (71%) | 238 (93%) | 18 (7%) | 0 | 100 | 100 |
| 4 | HH | 256/361 (71%) | 244 (95%) | 12 (5%) | 0 | 100 | 100 |
| 4 | IH | 256/361 (71%) | 239 (93%) | 17 (7%) | 0 | 100 | 100 |
| 4 | JH | 256/361 (71%) | 245 (96%) | 11 (4%) | 0 | 100 | 100 |
| 4 | KH | 256/361 (71%) | 239 (93%) | 17 (7%) | 0 | 100 | 100 |
| 4 | LH | 256/361 (71%) | 239 (93%) | 17 (7%) | 0 | 100 | 100 |
| 4 | MH | 256/361 (71%) | 244 (95%) | 12 (5%) | 0 | 100 | 100 |
| 4 | VH | 239/361 (66%) | 229 (96%) | 10 (4%) | 0 | 100 | 100 |
| 4 | WH | 239/361 (66%) | 230 (96%) | 9 (4%) | 0 | 100 | 100 |
| 4 | XH | 239/361 (66%) | 232 (97%) | 7 (3%) | 0 | 100 | 100 |
| 4 | YH | 239/361 (66%) | 229 (96%) | 10 (4%) | 0 | 100 | 100 |
| 4 | ZH | 239/361 (66%) | 229 (96%) | 10 (4%) | 0 | 100 | 100 |
| 5 | AK | 149/189 (79%) | 145 (97%) | 4 (3%) | 0 | 100 | 100 |
| 5 | BK | 149/189 (79%) | 145 (97%) | 4 (3%) | 0 | 100 | 100 |
| 5 | CK | 149/189 (79%) | 141 (95%) | 8 (5%) | 0 | 100 | 100 |
| 5 | DK | 149/189 (79%) | 143 (96%) | 6 (4%) | 0 | 100 | 100 |
| 5 | EK | 149/189 (79%) | 146 (98%) | 3 (2%) | 0 | 100 | 100 |
| 5 | FK | 149/189 (79%) | 144 (97%) | 5 (3%) | 0 | 100 | 100 |
| 5 | GK | 149/189 (79%) | 142 (95%) | 7 (5%) | 0 | 100 | 100 |
| 5 | HK | 149/189 (79%) | 140 (94%) | 9 (6%) | 0 | 100 | 100 |
| 5 | IK | 149/189 (79%) | 141 (95%) | 8 (5%) | 0 | 100 | 100 |
| 5 | JK | 149/189 (79%) | 142 (95%) | 7 (5%) | 0 | 100 | 100 |
| 5 | KK | 149/189 (79%) | 142 (95%) | 7 (5%) | 0 | 100 | 100 |
| 5 | LK | 149/189 (79%) | 142 (95%) | 7 (5%) | 0 | 100 | 100 |
| 5 | MK | 149/189 (79%) | 142 (95%) | 7 (5%) | 0 | 100 | 100 |
| 6 | AL | 169/249 (68%) | 165 (98%) | 4 (2%) | 0 | 100 | 100 |
| 6 | BL | 169/249 (68%) | 162 (96%) | 7 (4%) | 0 | 100 | 100 |
| 6 | CL | 169/249 (68%) | 162 (96%) | 7 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 6 | DL | 169/249 (68%) | 158 (94%) | 11 (6%) | 0 | 100 | 100 |
| 6 | EL | 169/249 (68%) | 158 (94%) | 11 (6%) | 0 | 100 | 100 |
| 6 | FL | 169/249 (68%) | 162 (96%) | 7 (4%) | 0 | 100 | 100 |
| 6 | GL | 169/249 (68%) | 160 (95%) | 9 (5%) | 0 | 100 | 100 |
| 6 | HL | 169/249 (68%) | 158 (94%) | 11 (6%) | 0 | 100 | 100 |
| 6 | IL | 169/249 (68%) | 163 (96%) | 6 (4%) | 0 | 100 | 100 |
| 6 | JL | 169/249 (68%) | 159 (94%) | 10 (6%) | 0 | 100 | 100 |
| 6 | KL | 169/249 (68%) | 158 (94%) | 11 (6%) | 0 | 100 | 100 |
| 6 | LL | 169/249 (68%) | 160 (95%) | 9 (5%) | 0 | 100 | 100 |
| 6 | ML | 169/249 (68%) | 161 (95%) | 8 (5%) | 0 | 100 | 100 |
| 7 | AM | 206/320 (64%) | 190 (92%) | 16 (8%) | 0 | 100 | 100 |
| 7 | BM | 206/320 (64%) | 191 (93%) | 15 (7%) | 0 | 100 | 100 |
| 7 | CM | 206/320 (64%) | 194 (94%) | 12 (6%) | 0 | 100 | 100 |
| 7 | DM | 206/320 (64%) | 196 (95%) | 10 (5%) | 0 | 100 | 100 |
| 7 | EM | 206/320 (64%) | 193 (94%) | 13 (6%) | 0 | 100 | 100 |
| 7 | FM | 206/320 (64%) | 188 (91%) | 18 (9%) | 0 | 100 | 100 |
| 7 | GM | 206/320 (64%) | 193 (94%) | 13 (6%) | 0 | 100 | 100 |
| 7 | HM | 206/320 (64%) | 191 (93%) | 15 (7%) | 0 | 100 | 100 |
| 7 | IM | 206/320 (64%) | 188 (91%) | 18 (9%) | 0 | 100 | 100 |
| 7 | JM | 206/320 (64%) | 189 (92%) | 17 (8%) | 0 | 100 | 100 |
| 7 | KM | 206/320 (64%) | 189 (92%) | 17 (8%) | 0 | 100 | 100 |
| 7 | LM | 206/320 (64%) | 192 (93%) | 14 (7%) | 0 | 100 | 100 |
| 7 | MM | 206/320 (64%) | 191 (93%) | 15 (7%) | 0 | 100 | 100 |
| 8 | AN | 76/124 (61%) | 66 (87%) | 10 (13%) | 0 | 100 | 100 |
| 8 | BN | 76/124 (61%) | 68 (90%) | 8 (10%) | 0 | 100 | 100 |
| 8 | CN | 76/124 (61%) | 70 (92%) | 6 (8%) | 0 | 100 | 100 |
| 8 | DN | 76/124 (61%) | 71 (93%) | 5 (7%) | 0 | 100 | 100 |
| 8 | EN | 76/124 (61%) | 68 (90%) | 8 (10%) | 0 | 100 | 100 |
| 8 | FN | 76/124 (61%) | 68 (90%) | 8 (10%) | 0 | 100 | 100 |
| 8 | GN | 76/124 (61%) | 71 (93%) | 5 (7%) | 0 | 100 | 100 |
| 8 | HN | 76/124 (61%) | 70 (92%) | 6 (8%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 8 | IN | 76/124 (61%) | 71 (93%) | 5 (7%) | 0 | 100 | 100 |
| 8 | JN | 76/124 (61%) | 68 (90%) | 8 (10%) | 0 | 100 | 100 |
| 8 | KN | 76/124 (61%) | 70 (92%) | 6 (8%) | 0 | 100 | 100 |
| 8 | LN | 76/124 (61%) | 68 (90%) | 8 (10%) | 0 | 100 | 100 |
| 8 | MN | 76/124 (61%) | 70 (92%) | 6 (8%) | 0 | 100 | 100 |
| 11 | AC | 207/303 (68%) | 194 (94%) | 13 (6%) | 0 | 100 | 100 |
| 11 | BC | 241/303 (80%) | 231 (96%) | 10 (4%) | 0 | 100 | 100 |
| 11 | CC | 241/303 (80%) | 230 (95%) | 11 (5%) | 0 | 100 | 100 |
| 11 | DC | 207/303 (68%) | 194 (94%) | 13 (6%) | 0 | 100 | 100 |
| 11 | EC | 207/303 (68%) | 202 (98%) | 5 (2%) | 0 | 100 | 100 |
| 11 | FC | 241/303 (80%) | 230 (95%) | 11 (5%) | 0 | 100 | 100 |
| 11 | GC | 241/303 (80%) | 234 (97%) | 7 (3%) | 0 | 100 | 100 |
| 11 | HC | 207/303 (68%) | 193 (93%) | 14 (7%) | 0 | 100 | 100 |
| 11 | IC | 207/303 (68%) | 192 (93%) | 15 (7%) | 0 | 100 | 100 |
| 11 | JC | 207/303 (68%) | 198 (96%) | 9 (4%) | 0 | 100 | 100 |
| 11 | KC | 241/303 (80%) | 230 (95%) | 11 (5%) | 0 | 100 | 100 |
| 11 | LC | 207/303 (68%) | 190 (92%) | 17 (8%) | 0 | 100 | 100 |
| 11 | MC | 207/303 (68%) | 192 (93%) | 15 (7%) | 0 | 100 | 100 |
| All | All | 23724/70112 (34%) | 22457 (95%) | 1267 (5%) | 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 | AG | 135/765 (18%) | 120 (89%) | 15 (11%) | 6 | 25 |
| 1 | Ag | 31/765 (4%) | 23 (74%) | 8 (26%) | 0 | 4 |
| 1 | BG | 135/765 (18%) | 117 (87%) | 18 (13%) | 4 | 20 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | Bg | 31/765 (4%) | 28 (90%) | 3 (10%) | 8 | 29 |
| 1 | CG | 135/765 (18%) | 118 (87%) | 17 (13%) | 4 | 21 |
| 1 | Cg | 31/765 (4%) | 27 (87%) | 4 (13%) | 4 | 20 |
| 1 | DG | 135/765 (18%) | 118 (87%) | 17 (13%) | 4 | 21 |
| 1 | Dg | 31/765 (4%) | 25 (81%) | 6 (19%) | 1 | 9 |
| 1 | EG | 135/765 (18%) | 115 (85%) | 20 (15%) | 3 | 17 |
| 1 | Eg | 31/765 (4%) | 24 (77%) | 7 (23%) | 1 | 6 |
| 1 | FG | 135/765 (18%) | 120 (89%) | 15 (11%) | 6 | 25 |
| 1 | Fg | 31/765 (4%) | 24 (77%) | 7 (23%) | 1 | 6 |
| 1 | GG | 135/765 (18%) | 114 (84%) | 21 (16%) | 2 | 16 |
| 1 | Gg | 31/765 (4%) | 26 (84%) | 5 (16%) | 2 | 15 |
| 1 | HG | 135/765 (18%) | 117 (87%) | 18 (13%) | 4 | 20 |
| 1 | Hg | 31/765 (4%) | 26 (84%) | 5 (16%) | 2 | 15 |
| 1 | IG | 135/765 (18%) | 117 (87%) | 18 (13%) | 4 | 20 |
| 1 | Ig | 31/765 (4%) | 25 (81%) | 6 (19%) | 1 | 9 |
| 1 | JG | 135/765 (18%) | 118 (87%) | 17 (13%) | 4 | 21 |
| 1 | Jg | 31/765 (4%) | 23 (74%) | 8 (26%) | 0 | 4 |
| 1 | KG | 135/765 (18%) | 119 (88%) | 16 (12%) | 5 | 22 |
| 1 | Kg | 31/765 (4%) | 22 (71%) | 9 (29%) | 0 | 3 |
| 1 | LG | 135/765 (18%) | 116 (86%) | 19 (14%) | 3 | 18 |
| 1 | Lg | 31/765 (4%) | 24 (77%) | 7 (23%) | 1 | 6 |
| 1 | MG | 135/765 (18%) | 120 (89%) | 15 (11%) | 6 | 25 |
| 1 | Mg | 31/765 (4%) | 27 (87%) | 4 (13%) | 4 | 20 |
| 1 | NG | 135/765 (18%) | 124 (92%) | 11 (8%) | 11 | 37 |
| 1 | OG | 135/765 (18%) | 115 (85%) | 20 (15%) | 3 | 17 |
| 1 | PG | 135/765 (18%) | 116 (86%) | 19 (14%) | 3 | 18 |
| 1 | VG | 31/765 (4%) | 28 (90%) | 3 (10%) | 8 | 29 |
| 1 | WG | 31/765 (4%) | 24 (77%) | 7 (23%) | 1 | 6 |
| 1 | XG | 31/765 (4%) | 27 (87%) | 4 (13%) | 4 | 20 |
| 1 | YG | 31/765 (4%) | 24 (77%) | 7 (23%) | 1 | 6 |
| 1 | ZG | 31/765 (4%) | 27 (87%) | 4 (13%) | 4 | 20 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2 | AD | 121/139 (87%) | 107 (88%) | 14 (12%) | 5 | 23 |
| 2 | Ad | 118/139 (85%) | 106 (90%) | 12 (10%) | 7 | 27 |
| 2 | BD | 121/139 (87%) | 113 (93%) | 8 (7%) | 16 | 43 |
| 2 | Bd | 118/139 (85%) | 107 (91%) | 11 (9%) | 9 | 30 |
| 2 | CD | 121/139 (87%) | 105 (87%) | 16 (13%) | 4 | 20 |
| 2 | Cd | 118/139 (85%) | 104 (88%) | 14 (12%) | 5 | 22 |
| 2 | DD | 121/139 (87%) | 112 (93%) | 9 (7%) | 13 | 40 |
| 2 | Dd | 118/139 (85%) | 107 (91%) | 11 (9%) | 9 | 30 |
| 2 | ED | 121/139 (87%) | 114 (94%) | 7 (6%) | 20 | 47 |
| 2 | Ed | 118/139 (85%) | 106 (90%) | 12 (10%) | 7 | 27 |
| 2 | FD | 121/139 (87%) | 105 (87%) | 16 (13%) | 4 | 20 |
| 2 | Fd | 118/139 (85%) | 109 (92%) | 9 (8%) | 13 | 39 |
| 2 | GD | 121/139 (87%) | 110 (91%) | 11 (9%) | 9 | 31 |
| 2 | Gd | 118/139 (85%) | 106 (90%) | 12 (10%) | 7 | 27 |
| 2 | HD | 121/139 (87%) | 109 (90%) | 12 (10%) | 8 | 28 |
| 2 | Hd | 118/139 (85%) | 110 (93%) | 8 (7%) | 16 | 42 |
| 2 | ID | 121/139 (87%) | 112 (93%) | 9 (7%) | 13 | 40 |
| 2 | Id | 118/139 (85%) | 108 (92%) | 10 (8%) | 10 | 36 |
| 2 | JD | 121/139 (87%) | 111 (92%) | 10 (8%) | 11 | 36 |
| 2 | Jd | 118/139 (85%) | 110 (93%) | 8 (7%) | 16 | 42 |
| 2 | KD | 121/139 (87%) | 110 (91%) | 11 (9%) | 9 | 31 |
| 2 | Kd | 118/139 (85%) | 108 (92%) | 10 (8%) | 10 | 36 |
| 2 | LD | 121/139 (87%) | 106 (88%) | 15 (12%) | 4 | 21 |
| 2 | Ld | 118/139 (85%) | 108 (92%) | 10 (8%) | 10 | 36 |
| 2 | MD | 121/139 (87%) | 107 (88%) | 14 (12%) | 5 | 23 |
| 2 | Md | 118/139 (85%) | 106 (90%) | 12 (10%) | 7 | 27 |
| 3 | AF | 53/237 (22%) | 47 (89%) | 6 (11%) | 6 | 24 |
| 3 | Af | 49/237 (21%) | 43 (88%) | 6 (12%) | 5 | 22 |
| 3 | BF | 53/237 (22%) | 45 (85%) | 8 (15%) | 3 | 16 |
| 3 | Bf | 49/237 (21%) | 45 (92%) | 4 (8%) | 11 | 36 |
| 3 | CF | 53/237 (22%) | 49 (92%) | 4 (8%) | 13 | 40 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3 | Cf | 49/237 (21%) | 42 (86%) | 7 (14%) | 3 | 18 |
| 3 | DF | 53/237 (22%) | 45 (85%) | 8 (15%) | 3 | 16 |
| 3 | Df | 49/237 (21%) | 46 (94%) | 3 (6%) | 18 | 46 |
| 3 | EF | 53/237 (22%) | 46 (87%) | 7 (13%) | 4 | 20 |
| 3 | Ef | 49/237 (21%) | 48 (98%) | 1 (2%) | 55 | 73 |
| 3 | FF | 53/237 (22%) | 45 (85%) | 8 (15%) | 3 | 16 |
| 3 | Ff | 49/237 (21%) | 43 (88%) | 6 (12%) | 5 | 22 |
| 3 | GF | 53/237 (22%) | 46 (87%) | 7 (13%) | 4 | 20 |
| 3 | Gf | 49/237 (21%) | 43 (88%) | 6 (12%) | 5 | 22 |
| 3 | HF | 53/237 (22%) | 45 (85%) | 8 (15%) | 3 | 16 |
| 3 | Hf | 49/237 (21%) | 44 (90%) | 5 (10%) | 7 | 27 |
| 3 | IF | 53/237 (22%) | 47 (89%) | 6 (11%) | 6 | 24 |
| 3 | If | 49/237 (21%) | 43 (88%) | 6 (12%) | 5 | 22 |
| 3 | JF | 53/237 (22%) | 44 (83%) | 9 (17%) | 2 | 13 |
| 3 | Jf | 49/237 (21%) | 46 (94%) | 3 (6%) | 18 | 46 |
| 3 | KF | 53/237 (22%) | 48 (91%) | 5 (9%) | 8 | 30 |
| 3 | Kf | 49/237 (21%) | 46 (94%) | 3 (6%) | 18 | 46 |
| 3 | LF | 53/237 (22%) | 46 (87%) | 7 (13%) | 4 | 20 |
| 3 | Lf | 49/237 (21%) | 39 (80%) | 10 (20%) | 1 | 7 |
| 3 | MF | 53/237 (22%) | 45 (85%) | 8 (15%) | 3 | 16 |
| 3 | Mf | 49/237 (21%) | 44 (90%) | 5 (10%) | 7 | 27 |
| 3 | VF | 53/237 (22%) | 48 (91%) | 5 (9%) | 8 | 30 |
| 3 | WF | 53/237 (22%) | 47 (89%) | 6 (11%) | 6 | 24 |
| 3 | XF | 53/237 (22%) | 49 (92%) | 4 (8%) | 13 | 40 |
| 3 | YF | 53/237 (22%) | 47 (89%) | 6 (11%) | 6 | 24 |
| 3 | ZF | 53/237 (22%) | 49 (92%) | 4 (8%) | 13 | 40 |
| 4 | AH | 220/300 (73%) | 192 (87%) | 28 (13%) | 4 | 21 |
| 4 | BH | 220/300 (73%) | 202 (92%) | 18 (8%) | 11 | 36 |
| 4 | CH | 220/300 (73%) | 199 (90%) | 21 (10%) | 8 | 29 |
| 4 | DH | 220/300 (73%) | 193 (88%) | 27 (12%) | 4 | 22 |
| 4 | EH | 220/300 (73%) | 192 (87%) | 28 (13%) | 4 | 21 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 4 | FH | 220/300 (73%) | 197 (90%) | 23 (10%) | 7 | 26 |
| 4 | GH | 220/300 (73%) | 193 (88%) | 27 (12%) | 4 | 22 |
| 4 | HH | 220/300 (73%) | 194 (88%) | 26 (12%) | 5 | 23 |
| 4 | IH | 220/300 (73%) | 200 (91%) | 20 (9%) | 9 | 31 |
| 4 | JH | 220/300 (73%) | 195 (89%) | 25 (11%) | 5 | 24 |
| 4 | KH | 220/300 (73%) | 199 (90%) | 21 (10%) | 8 | 29 |
| 4 | LH | 220/300 (73%) | 197 (90%) | 23 (10%) | 7 | 26 |
| 4 | MH | 220/300 (73%) | 195 (89%) | 25 (11%) | 5 | 24 |
| 4 | VH | 207/300 (69%) | 179 (86%) | 28 (14%) | 4 | 19 |
| 4 | WH | 207/300 (69%) | 174 (84%) | 33 (16%) | 2 | 15 |
| 4 | XH | 207/300 (69%) | 185 (89%) | 22 (11%) | 6 | 26 |
| 4 | YH | 207/300 (69%) | 181 (87%) | 26 (13%) | 4 | 21 |
| 4 | ZH | 207/300 (69%) | 179 (86%) | 28 (14%) | 4 | 19 |
| 5 | AK | 129/163 (79%) | 111 (86%) | 18 (14%) | 3 | 19 |
| 5 | BK | 129/163 (79%) | 112 (87%) | 17 (13%) | 4 | 20 |
| 5 | CK | 129/163 (79%) | 117 (91%) | 12 (9%) | 9 | 30 |
| 5 | DK | 129/163 (79%) | 121 (94%) | 8 (6%) | 18 | 45 |
| 5 | EK | 129/163 (79%) | 117 (91%) | 12 (9%) | 9 | 30 |
| 5 | FK | 129/163 (79%) | 116 (90%) | 13 (10%) | 7 | 27 |
| 5 | GK | 129/163 (79%) | 122 (95%) | 7 (5%) | 22 | 49 |
| 5 | HK | 129/163 (79%) | 119 (92%) | 10 (8%) | 12 | 38 |
| 5 | IK | 129/163 (79%) | 113 (88%) | 16 (12%) | 4 | 21 |
| 5 | JK | 129/163 (79%) | 119 (92%) | 10 (8%) | 12 | 38 |
| 5 | KK | 129/163 (79%) | 114 (88%) | 15 (12%) | 5 | 23 |
| 5 | LK | 129/163 (79%) | 117 (91%) | 12 (9%) | 9 | 30 |
| 5 | MK | 129/163 (79%) | 114 (88%) | 15 (12%) | 5 | 23 |
| 6 | AL | 148/203 (73%) | 134 (90%) | 14 (10%) | 8 | 29 |
| 6 | BL | 148/203 (73%) | 130 (88%) | 18 (12%) | 5 | 22 |
| 6 | CL | 148/203 (73%) | 133 (90%) | 15 (10%) | 7 | 27 |
| 6 | DL | 148/203 (73%) | 137 (93%) | 11 (7%) | 13 | 40 |
| 6 | EL | 148/203 (73%) | 131 (88%) | 17 (12%) | 5 | 23 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 6 | FL | 148/203 (73%) | 133 (90%) | 15 (10%) | 7 | 27 |
| 6 | GL | 148/203 (73%) | 132 (89%) | 16 (11%) | 6 | 26 |
| 6 | HL | 148/203 (73%) | 132 (89%) | 16 (11%) | 6 | 26 |
| 6 | IL | 148/203 (73%) | 134 (90%) | 14 (10%) | 8 | 29 |
| 6 | JL | 148/203 (73%) | 133 (90%) | 15 (10%) | 7 | 27 |
| 6 | KL | 148/203 (73%) | 134 (90%) | 14 (10%) | 8 | 29 |
| 6 | LL | 148/203 (73%) | 136 (92%) | 12 (8%) | 11 | 37 |
| 6 | ML | 148/203 (73%) | 133 (90%) | 15 (10%) | 7 | 27 |
| 7 | AM | 175/276 (63%) | 160 (91%) | 15 (9%) | 10 | 35 |
| 7 | BM | 175/276 (63%) | 146 (83%) | 29 (17%) | 2 | 14 |
| 7 | CM | 175/276 (63%) | 148 (85%) | 27 (15%) | 2 | 16 |
| 7 | DM | 175/276 (63%) | 154 (88%) | 21 (12%) | 5 | 22 |
| 7 | EM | 175/276 (63%) | 148 (85%) | 27 (15%) | 2 | 16 |
| 7 | FM | 175/276 (63%) | 153 (87%) | 22 (13%) | 4 | 21 |
| 7 | GM | 175/276 (63%) | 153 (87%) | 22 (13%) | 4 | 21 |
| 7 | HM | 175/276 (63%) | 153 (87%) | 22 (13%) | 4 | 21 |
| 7 | IM | 175/276 (63%) | 148 (85%) | 27 (15%) | 2 | 16 |
| 7 | JM | 175/276 (63%) | 151 (86%) | 24 (14%) | 3 | 19 |
| 7 | KM | 175/276 (63%) | 148 (85%) | 27 (15%) | 2 | 16 |
| 7 | LM | 175/276 (63%) | 154 (88%) | 21 (12%) | 5 | 22 |
| 7 | MM | 175/276 (63%) | 158 (90%) | 17 (10%) | 8 | 29 |
| 8 | AN | 66/107 (62%) | 60 (91%) | 6 (9%) | 9 | 31 |
| 8 | BN | 66/107 (62%) | 53 (80%) | 13 (20%) | 1 | 9 |
| 8 | CN | 66/107 (62%) | 62 (94%) | 4 (6%) | 18 | 46 |
| 8 | DN | 66/107 (62%) | 55 (83%) | 11 (17%) | 2 | 14 |
| 8 | EN | 66/107 (62%) | 53 (80%) | 13 (20%) | 1 | 9 |
| 8 | FN | 66/107 (62%) | 54 (82%) | 12 (18%) | 1 | 11 |
| 8 | GN | 66/107 (62%) | 57 (86%) | 9 (14%) | 3 | 19 |
| 8 | HN | 66/107 (62%) | 53 (80%) | 13 (20%) | 1 | 9 |
| 8 | IN | 66/107 (62%) | 57 (86%) | 9 (14%) | 3 | 19 |
| 8 | JN | 66/107 (62%) | 60 (91%) | 6 (9%) | 9 | 31 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|-------------|----|
| 8 | KN | 66/107 (62%) | 58 (88%) | 8 (12%) | 5 | 22 |
| 8 | LN | 66/107 (62%) | 59 (89%) | 7 (11%) | 6 | 26 |
| 8 | MN | 66/107 (62%) | 55 (83%) | 11 (17%) | 2 | 14 |
| 11 | AC | 178/257 (69%) | 163 (92%) | 15 (8%) | 11 | 36 |
| 11 | BC | 203/257 (79%) | 181 (89%) | 22 (11%) | 6 | 26 |
| 11 | CC | 203/257 (79%) | 174 (86%) | 29 (14%) | 3 | 18 |
| 11 | DC | 178/257 (69%) | 154 (86%) | 24 (14%) | 4 | 19 |
| 11 | EC | 178/257 (69%) | 164 (92%) | 14 (8%) | 12 | 38 |
| 11 | FC | 203/257 (79%) | 181 (89%) | 22 (11%) | 6 | 26 |
| 11 | GC | 203/257 (79%) | 180 (89%) | 23 (11%) | 6 | 24 |
| 11 | HC | 178/257 (69%) | 161 (90%) | 17 (10%) | 8 | 29 |
| 11 | IC | 178/257 (69%) | 149 (84%) | 29 (16%) | 2 | 14 |
| 11 | JC | 178/257 (69%) | 160 (90%) | 18 (10%) | 7 | 27 |
| 11 | KC | 203/257 (79%) | 173 (85%) | 30 (15%) | 3 | 17 |
| 11 | LC | 178/257 (69%) | 159 (89%) | 19 (11%) | 6 | 26 |
| 11 | MC | 178/257 (69%) | 154 (86%) | 24 (14%) | 4 | 19 |
| All | All | 20484/55449 (37%) | 18117 (88%) | 2367 (12%) | 9 | 23 |

All (2367) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AG | 873 | LEU |
| 1 | AG | 898 | LYS |
| 1 | AG | 900 | ILE |
| 1 | AG | 911 | LYS |
| 1 | AG | 916 | PHE |
| 1 | AG | 930 | ILE |
| 1 | AG | 933 | TYR |
| 1 | AG | 944 | LEU |
| 1 | AG | 947 | ARG |
| 1 | AG | 956 | TYR |
| 1 | AG | 962 | SER |
| 1 | AG | 965 | LEU |
| 1 | AG | 972 | PHE |
| 1 | AG | 1010 | THR |
| 1 | AG | 1028 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | ED | 51 | SER |
| 2 | ED | 53 | LEU |
| 2 | ED | 85 | VAL |
| 2 | ED | 86 | ASP |
| 2 | ED | 108 | VAL |
| 2 | ED | 115 | VAL |
| 2 | ED | 150 | ASN |
| 3 | EF | 208 | ILE |
| 3 | EF | 215 | VAL |
| 3 | EF | 230 | LEU |
| 3 | EF | 231 | THR |
| 3 | EF | 238 | ILE |
| 3 | EF | 250 | LEU |
| 3 | EF | 263 | LYS |
| 1 | Eg | 797 | ARG |
| 1 | Eg | 801 | MET |
| 1 | Eg | 802 | LEU |
| 1 | Eg | 810 | GLN |
| 1 | Eg | 814 | GLN |
| 1 | Eg | 815 | VAL |
| 1 | Eg | 819 | VAL |
| 4 | EH | 107 | ILE |
| 4 | EH | 112 | PHE |
| 4 | EH | 134 | TYR |
| 4 | EH | 135 | GLU |
| 4 | EH | 147 | THR |
| 4 | EH | 160 | LEU |
| 4 | EH | 170 | ARG |
| 4 | EH | 176 | VAL |
| 4 | EH | 180 | VAL |
| 4 | EH | 184 | SER |
| 4 | EH | 207 | ASP |
| 4 | EH | 211 | ASN |
| 4 | EH | 213 | LEU |
| 4 | EH | 226 | LEU |
| 4 | EH | 233 | LEU |
| 4 | EH | 240 | THR |
| 4 | EH | 248 | VAL |
| 4 | EH | 249 | ASP |
| 4 | EH | 250 | TYR |
| 4 | EH | 253 | ASP |
| 4 | EH | 255 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | EH | 256 | VAL |
| 4 | EH | 262 | ASN |
| 4 | EH | 266 | MET |
| 4 | EH | 325 | LEU |
| 4 | EH | 329 | THR |
| 4 | EH | 344 | VAL |
| 4 | EH | 354 | MET |
| 5 | EK | 40 | LYS |
| 5 | EK | 70 | VAL |
| 5 | EK | 92 | ASN |
| 5 | EK | 93 | TRP |
| 5 | EK | 106 | LEU |
| 5 | EK | 111 | LYS |
| 5 | EK | 129 | GLU |
| 5 | EK | 149 | VAL |
| 5 | EK | 153 | ILE |
| 5 | EK | 156 | THR |
| 5 | EK | 180 | VAL |
| 5 | EK | 183 | THR |
| 6 | EL | 44 | HIS |
| 6 | EL | 47 | TYR |
| 6 | EL | 93 | LEU |
| 6 | EL | 109 | LEU |
| 6 | EL | 113 | ASP |
| 6 | EL | 115 | GLN |
| 6 | EL | 119 | TYR |
| 6 | EL | 130 | ASP |
| 6 | EL | 133 | PHE |
| 6 | EL | 154 | LEU |
| 6 | EL | 155 | LEU |
| 6 | EL | 163 | ILE |
| 6 | EL | 172 | VAL |
| 6 | EL | 174 | SER |
| 6 | EL | 212 | ASN |
| 6 | EL | 216 | ASP |
| 6 | EL | 219 | ILE |
| 7 | EM | 123 | VAL |
| 7 | EM | 131 | THR |
| 7 | EM | 134 | LEU |
| 7 | EM | 146 | LEU |
| 7 | EM | 149 | ASN |
| 7 | EM | 152 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | EM | 155 | LEU |
| 7 | EM | 173 | LEU |
| 7 | EM | 176 | VAL |
| 7 | EM | 177 | LEU |
| 7 | EM | 180 | ASP |
| 7 | EM | 182 | LYS |
| 7 | EM | 183 | VAL |
| 7 | EM | 184 | LEU |
| 7 | EM | 190 | ASN |
| 7 | EM | 204 | LEU |
| 7 | EM | 207 | ILE |
| 7 | EM | 208 | LYS |
| 7 | EM | 210 | ASP |
| 7 | EM | 212 | LEU |
| 7 | EM | 215 | ARG |
| 7 | EM | 221 | LYS |
| 7 | EM | 245 | TYR |
| 7 | EM | 263 | ILE |
| 7 | EM | 271 | SER |
| 7 | EM | 292 | MET |
| 7 | EM | 308 | ASP |
| 8 | EN | 44 | LYS |
| 8 | EN | 45 | MET |
| 8 | EN | 69 | TYR |
| 8 | EN | 70 | CYS |
| 8 | EN | 75 | VAL |
| 8 | EN | 81 | LEU |
| 8 | EN | 82 | MET |
| 8 | EN | 84 | CYS |
| 8 | EN | 94 | GLN |
| 8 | EN | 95 | LEU |
| 8 | EN | 100 | LEU |
| 8 | EN | 101 | VAL |
| 8 | EN | 108 | VAL |
| 2 | Ed | 41 | LEU |
| 2 | Ed | 53 | LEU |
| 2 | Ed | 61 | VAL |
| 2 | Ed | 70 | THR |
| 2 | Ed | 80 | GLN |
| 2 | Ed | 91 | ILE |
| 2 | Ed | 93 | GLU |
| 2 | Ed | 108 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | Ed | 115 | VAL |
| 2 | Ed | 126 | GLU |
| 2 | Ed | 154 | VAL |
| 2 | Ed | 156 | LEU |
| 3 | Ef | 255 | LEU |
| 2 | FD | 30 | ILE |
| 2 | FD | 47 | SER |
| 2 | FD | 63 | THR |
| 2 | FD | 70 | THR |
| 2 | FD | 73 | ILE |
| 2 | FD | 80 | GLN |
| 2 | FD | 85 | VAL |
| 2 | FD | 91 | ILE |
| 2 | FD | 108 | VAL |
| 2 | FD | 123 | THR |
| 2 | FD | 126 | GLU |
| 2 | FD | 136 | ASP |
| 2 | FD | 137 | TYR |
| 2 | FD | 155 | GLU |
| 2 | FD | 156 | LEU |
| 2 | FD | 160 | LYS |
| 3 | FF | 208 | ILE |
| 3 | FF | 215 | VAL |
| 3 | FF | 230 | LEU |
| 3 | FF | 231 | THR |
| 3 | FF | 238 | ILE |
| 3 | FF | 243 | MET |
| 3 | FF | 245 | LYS |
| 3 | FF | 261 | VAL |
| 1 | Fg | 796 | GLN |
| 1 | Fg | 802 | LEU |
| 1 | Fg | 807 | GLN |
| 1 | Fg | 808 | LEU |
| 1 | Fg | 809 | VAL |
| 1 | Fg | 815 | VAL |
| 1 | Fg | 819 | VAL |
| 11 | CC | 28 | THR |
| 11 | CC | 37 | MET |
| 11 | CC | 41 | LYS |
| 11 | CC | 42 | TYR |
| 11 | CC | 44 | ARG |
| 11 | CC | 48 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | CC | 53 | LYS |
| 11 | CC | 57 | MET |
| 11 | CC | 59 | LEU |
| 11 | CC | 100 | VAL |
| 11 | CC | 103 | HIS |
| 11 | CC | 105 | ILE |
| 11 | CC | 112 | GLU |
| 11 | CC | 143 | THR |
| 11 | CC | 148 | ARG |
| 11 | CC | 154 | ASP |
| 11 | CC | 157 | LYS |
| 11 | CC | 165 | LEU |
| 11 | CC | 181 | GLU |
| 11 | CC | 182 | ARG |
| 11 | CC | 195 | LEU |
| 11 | CC | 206 | PHE |
| 11 | CC | 211 | LEU |
| 11 | CC | 221 | VAL |
| 11 | CC | 226 | VAL |
| 11 | CC | 233 | VAL |
| 11 | CC | 234 | THR |
| 11 | CC | 241 | HIS |
| 11 | CC | 243 | ASP |
| 4 | FH | 105 | GLU |
| 4 | FH | 109 | LYS |
| 4 | FH | 115 | MET |
| 4 | FH | 130 | LEU |
| 4 | FH | 138 | GLU |
| 4 | FH | 139 | TYR |
| 4 | FH | 147 | THR |
| 4 | FH | 154 | THR |
| 4 | FH | 161 | SER |
| 4 | FH | 170 | ARG |
| 4 | FH | 180 | VAL |
| 4 | FH | 183 | ASP |
| 4 | FH | 203 | ASN |
| 4 | FH | 238 | MET |
| 4 | FH | 240 | THR |
| 4 | FH | 253 | ASP |
| 4 | FH | 257 | GLN |
| 4 | FH | 265 | SER |
| 4 | FH | 278 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | FH | 279 | LEU |
| 4 | FH | 296 | VAL |
| 4 | FH | 313 | VAL |
| 4 | FH | 353 | VAL |
| 5 | FK | 46 | ASP |
| 5 | FK | 67 | VAL |
| 5 | FK | 73 | ASN |
| 5 | FK | 75 | LEU |
| 5 | FK | 92 | ASN |
| 5 | FK | 111 | LYS |
| 5 | FK | 126 | VAL |
| 5 | FK | 129 | GLU |
| 5 | FK | 144 | LEU |
| 5 | FK | 149 | VAL |
| 5 | FK | 156 | THR |
| 5 | FK | 175 | SER |
| 5 | FK | 180 | VAL |
| 6 | FL | 47 | TYR |
| 6 | FL | 54 | ARG |
| 6 | FL | 93 | LEU |
| 6 | FL | 109 | LEU |
| 6 | FL | 113 | ASP |
| 6 | FL | 121 | ASP |
| 6 | FL | 125 | LEU |
| 6 | FL | 143 | ILE |
| 6 | FL | 165 | VAL |
| 6 | FL | 169 | THR |
| 6 | FL | 172 | VAL |
| 6 | FL | 177 | HIS |
| 6 | FL | 212 | ASN |
| 6 | FL | 225 | GLN |
| 6 | FL | 227 | ARG |
| 7 | FM | 131 | THR |
| 7 | FM | 134 | LEU |
| 7 | FM | 143 | THR |
| 7 | FM | 146 | LEU |
| 7 | FM | 152 | LEU |
| 7 | FM | 155 | LEU |
| 7 | FM | 162 | VAL |
| 7 | FM | 176 | VAL |
| 7 | FM | 177 | LEU |
| 7 | FM | 178 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | FM | 182 | LYS |
| 7 | FM | 183 | VAL |
| 7 | FM | 208 | LYS |
| 7 | FM | 215 | ARG |
| 7 | FM | 221 | LYS |
| 7 | FM | 222 | ILE |
| 7 | FM | 229 | ASN |
| 7 | FM | 231 | LEU |
| 7 | FM | 271 | SER |
| 7 | FM | 292 | MET |
| 7 | FM | 314 | ARG |
| 7 | FM | 316 | ASN |
| 8 | FN | 48 | ILE |
| 8 | FN | 69 | TYR |
| 8 | FN | 70 | CYS |
| 8 | FN | 77 | ASP |
| 8 | FN | 78 | LEU |
| 8 | FN | 81 | LEU |
| 8 | FN | 86 | LEU |
| 8 | FN | 94 | GLN |
| 8 | FN | 95 | LEU |
| 8 | FN | 101 | VAL |
| 8 | FN | 104 | ASN |
| 8 | FN | 108 | VAL |
| 2 | Fd | 41 | LEU |
| 2 | Fd | 53 | LEU |
| 2 | Fd | 63 | THR |
| 2 | Fd | 82 | ARG |
| 2 | Fd | 85 | VAL |
| 2 | Fd | 92 | GLU |
| 2 | Fd | 93 | GLU |
| 2 | Fd | 108 | VAL |
| 2 | Fd | 115 | VAL |
| 3 | Ff | 210 | TYR |
| 3 | Ff | 215 | VAL |
| 3 | Ff | 222 | LEU |
| 3 | Ff | 230 | LEU |
| 3 | Ff | 232 | VAL |
| 3 | Ff | 255 | LEU |
| 11 | BC | 28 | THR |
| 11 | BC | 46 | GLN |
| 11 | BC | 50 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | BC | 57 | MET |
| 11 | BC | 83 | LEU |
| 11 | BC | 89 | ASN |
| 11 | BC | 105 | ILE |
| 11 | BC | 116 | THR |
| 11 | BC | 117 | LEU |
| 11 | BC | 149 | GLN |
| 11 | BC | 155 | TYR |
| 11 | BC | 166 | LEU |
| 11 | BC | 169 | THR |
| 11 | BC | 174 | GLU |
| 11 | BC | 193 | THR |
| 11 | BC | 195 | LEU |
| 11 | BC | 203 | LYS |
| 11 | BC | 206 | PHE |
| 11 | BC | 226 | VAL |
| 11 | BC | 234 | THR |
| 11 | BC | 244 | ASP |
| 11 | BC | 249 | ILE |
| 1 | BG | 869 | MET |
| 1 | BG | 873 | LEU |
| 1 | BG | 911 | LYS |
| 1 | BG | 912 | MET |
| 1 | BG | 913 | VAL |
| 1 | BG | 915 | THR |
| 1 | BG | 916 | PHE |
| 1 | BG | 930 | ILE |
| 1 | BG | 938 | ASN |
| 1 | BG | 944 | LEU |
| 1 | BG | 949 | ASN |
| 1 | BG | 962 | SER |
| 1 | BG | 963 | SER |
| 1 | BG | 965 | LEU |
| 1 | BG | 972 | PHE |
| 1 | BG | 1001 | LEU |
| 1 | BG | 1010 | THR |
| 1 | BG | 1024 | ASN |
| 3 | AF | 215 | VAL |
| 3 | AF | 223 | ILE |
| 3 | AF | 230 | LEU |
| 3 | AF | 231 | THR |
| 3 | AF | 263 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | AF | 266 | GLN |
| 2 | GD | 30 | ILE |
| 2 | GD | 50 | ASP |
| 2 | GD | 53 | LEU |
| 2 | GD | 55 | MET |
| 2 | GD | 85 | VAL |
| 2 | GD | 86 | ASP |
| 2 | GD | 115 | VAL |
| 2 | GD | 119 | ILE |
| 2 | GD | 155 | GLU |
| 2 | GD | 156 | LEU |
| 2 | GD | 162 | TYR |
| 3 | GF | 223 | ILE |
| 3 | GF | 230 | LEU |
| 3 | GF | 231 | THR |
| 3 | GF | 233 | ARG |
| 3 | GF | 238 | ILE |
| 3 | GF | 250 | LEU |
| 3 | GF | 261 | VAL |
| 1 | Gg | 793 | GLU |
| 1 | Gg | 802 | LEU |
| 1 | Gg | 803 | THR |
| 1 | Gg | 815 | VAL |
| 1 | Gg | 819 | VAL |
| 4 | GH | 108 | ASP |
| 4 | GH | 109 | LYS |
| 4 | GH | 114 | ASP |
| 4 | GH | 115 | MET |
| 4 | GH | 117 | ARG |
| 4 | GH | 122 | LEU |
| 4 | GH | 125 | GLU |
| 4 | GH | 132 | GLN |
| 4 | GH | 135 | GLU |
| 4 | GH | 147 | THR |
| 4 | GH | 180 | VAL |
| 4 | GH | 185 | THR |
| 4 | GH | 220 | LEU |
| 4 | GH | 225 | ASN |
| 4 | GH | 233 | LEU |
| 4 | GH | 238 | MET |
| 4 | GH | 240 | THR |
| 4 | GH | 248 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | GH | 264 | LYS |
| 4 | GH | 266 | MET |
| 4 | GH | 278 | ASP |
| 4 | GH | 284 | LEU |
| 4 | GH | 294 | ARG |
| 4 | GH | 313 | VAL |
| 4 | GH | 314 | ARG |
| 4 | GH | 344 | VAL |
| 4 | GH | 355 | GLN |
| 5 | GK | 70 | VAL |
| 5 | GK | 75 | LEU |
| 5 | GK | 86 | ASP |
| 5 | GK | 92 | ASN |
| 5 | GK | 111 | LYS |
| 5 | GK | 126 | VAL |
| 5 | GK | 177 | ASN |
| 6 | GL | 99 | ARG |
| 6 | GL | 109 | LEU |
| 6 | GL | 110 | GLN |
| 6 | GL | 121 | ASP |
| 6 | GL | 129 | THR |
| 6 | GL | 130 | ASP |
| 6 | GL | 172 | VAL |
| 6 | GL | 174 | SER |
| 6 | GL | 177 | HIS |
| 6 | GL | 183 | GLN |
| 6 | GL | 198 | ILE |
| 6 | GL | 216 | ASP |
| 6 | GL | 227 | ARG |
| 6 | GL | 233 | TRP |
| 6 | GL | 234 | PHE |
| 6 | GL | 235 | THR |
| 7 | GM | 134 | LEU |
| 7 | GM | 152 | LEU |
| 7 | GM | 153 | GLN |
| 7 | GM | 160 | ASN |
| 7 | GM | 173 | LEU |
| 7 | GM | 175 | ILE |
| 7 | GM | 176 | VAL |
| 7 | GM | 180 | ASP |
| 7 | GM | 182 | LYS |
| 7 | GM | 184 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | GM | 191 | LEU |
| 7 | GM | 192 | ARG |
| 7 | GM | 194 | LEU |
| 7 | GM | 207 | ILE |
| 7 | GM | 212 | LEU |
| 7 | GM | 215 | ARG |
| 7 | GM | 221 | LYS |
| 7 | GM | 229 | ASN |
| 7 | GM | 259 | SER |
| 7 | GM | 292 | MET |
| 7 | GM | 303 | GLU |
| 7 | GM | 314 | ARG |
| 8 | GN | 51 | CYS |
| 8 | GN | 69 | TYR |
| 8 | GN | 70 | CYS |
| 8 | GN | 71 | THR |
| 8 | GN | 81 | LEU |
| 8 | GN | 91 | VAL |
| 8 | GN | 94 | GLN |
| 8 | GN | 101 | VAL |
| 8 | GN | 111 | GLU |
| 2 | Gd | 30 | ILE |
| 2 | Gd | 31 | ASN |
| 2 | Gd | 53 | LEU |
| 2 | Gd | 61 | VAL |
| 2 | Gd | 63 | THR |
| 2 | Gd | 94 | LEU |
| 2 | Gd | 108 | VAL |
| 2 | Gd | 119 | ILE |
| 2 | Gd | 128 | LEU |
| 2 | Gd | 145 | ILE |
| 2 | Gd | 147 | VAL |
| 2 | Gd | 150 | ASN |
| 3 | Gf | 215 | VAL |
| 3 | Gf | 221 | TRP |
| 3 | Gf | 229 | THR |
| 3 | Gf | 244 | VAL |
| 3 | Gf | 255 | LEU |
| 3 | Gf | 263 | LYS |
| 2 | HD | 38 | THR |
| 2 | HD | 50 | ASP |
| 2 | HD | 51 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | HD | 52 | MET |
| 2 | HD | 55 | MET |
| 2 | HD | 91 | ILE |
| 2 | HD | 108 | VAL |
| 2 | HD | 115 | VAL |
| 2 | HD | 127 | SER |
| 2 | HD | 152 | GLN |
| 2 | HD | 154 | VAL |
| 2 | HD | 156 | LEU |
| 11 | GC | 28 | THR |
| 11 | GC | 35 | GLN |
| 11 | GC | 37 | MET |
| 11 | GC | 41 | LYS |
| 11 | GC | 42 | TYR |
| 11 | GC | 44 | ARG |
| 11 | GC | 48 | LYS |
| 11 | GC | 56 | GLU |
| 11 | GC | 60 | LYS |
| 11 | GC | 105 | ILE |
| 11 | GC | 112 | GLU |
| 11 | GC | 117 | LEU |
| 11 | GC | 140 | PHE |
| 11 | GC | 143 | THR |
| 11 | GC | 146 | THR |
| 11 | GC | 154 | ASP |
| 11 | GC | 165 | LEU |
| 11 | GC | 195 | LEU |
| 11 | GC | 196 | GLU |
| 11 | GC | 206 | PHE |
| 11 | GC | 226 | VAL |
| 11 | GC | 229 | THR |
| 11 | GC | 248 | ARG |
| 3 | HF | 215 | VAL |
| 3 | HF | 229 | THR |
| 3 | HF | 230 | LEU |
| 3 | HF | 238 | ILE |
| 3 | HF | 255 | LEU |
| 3 | HF | 261 | VAL |
| 3 | HF | 263 | LYS |
| 3 | HF | 267 | GLU |
| 1 | Hg | 793 | GLU |
| 1 | Hg | 801 | MET |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | Hg | 808 | LEU |
| 1 | Hg | 815 | VAL |
| 1 | Hg | 819 | VAL |
| 4 | HH | 109 | LYS |
| 4 | HH | 116 | THR |
| 4 | HH | 125 | GLU |
| 4 | HH | 135 | GLU |
| 4 | HH | 136 | THR |
| 4 | HH | 139 | TYR |
| 4 | HH | 152 | THR |
| 4 | HH | 168 | VAL |
| 4 | HH | 170 | ARG |
| 4 | HH | 180 | VAL |
| 4 | HH | 204 | ILE |
| 4 | HH | 212 | THR |
| 4 | HH | 215 | ILE |
| 4 | HH | 233 | LEU |
| 4 | HH | 234 | ASN |
| 4 | HH | 237 | VAL |
| 4 | HH | 238 | MET |
| 4 | HH | 240 | THR |
| 4 | HH | 248 | VAL |
| 4 | HH | 250 | TYR |
| 4 | HH | 253 | ASP |
| 4 | HH | 278 | ASP |
| 4 | HH | 319 | ILE |
| 4 | HH | 324 | TRP |
| 4 | HH | 334 | THR |
| 4 | HH | 350 | HIS |
| 5 | HK | 40 | LYS |
| 5 | HK | 62 | LYS |
| 5 | HK | 70 | VAL |
| 5 | HK | 75 | LEU |
| 5 | HK | 106 | LEU |
| 5 | HK | 111 | LYS |
| 5 | HK | 156 | THR |
| 5 | HK | 166 | THR |
| 5 | HK | 180 | VAL |
| 5 | HK | 182 | ILE |
| 6 | HL | 47 | TYR |
| 6 | HL | 53 | ASP |
| 6 | HL | 100 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 6 | HL | 108 | ASP |
| 6 | HL | 109 | LEU |
| 6 | HL | 122 | THR |
| 6 | HL | 130 | ASP |
| 6 | HL | 148 | LEU |
| 6 | HL | 160 | GLN |
| 6 | HL | 174 | SER |
| 6 | HL | 181 | LEU |
| 6 | HL | 193 | LEU |
| 6 | HL | 206 | GLU |
| 6 | HL | 210 | ASP |
| 6 | HL | 211 | LYS |
| 6 | HL | 212 | ASN |
| 7 | HM | 131 | THR |
| 7 | HM | 134 | LEU |
| 7 | HM | 152 | LEU |
| 7 | HM | 174 | GLN |
| 7 | HM | 176 | VAL |
| 7 | HM | 177 | LEU |
| 7 | HM | 178 | LYS |
| 7 | HM | 184 | LEU |
| 7 | HM | 191 | LEU |
| 7 | HM | 192 | ARG |
| 7 | HM | 199 | LYS |
| 7 | HM | 202 | LEU |
| 7 | HM | 212 | LEU |
| 7 | HM | 215 | ARG |
| 7 | HM | 222 | ILE |
| 7 | HM | 229 | ASN |
| 7 | HM | 242 | LYS |
| 7 | HM | 259 | SER |
| 7 | HM | 277 | SER |
| 7 | HM | 292 | MET |
| 7 | HM | 308 | ASP |
| 7 | HM | 318 | GLN |
| 8 | HN | 45 | MET |
| 8 | HN | 48 | ILE |
| 8 | HN | 51 | CYS |
| 8 | HN | 57 | ARG |
| 8 | HN | 69 | TYR |
| 8 | HN | 70 | CYS |
| 8 | HN | 80 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 8 | HN | 95 | LEU |
| 8 | HN | 101 | VAL |
| 8 | HN | 105 | ASP |
| 8 | HN | 107 | TYR |
| 8 | HN | 112 | CYS |
| 8 | HN | 114 | LEU |
| 2 | Hd | 41 | LEU |
| 2 | Hd | 51 | SER |
| 2 | Hd | 61 | VAL |
| 2 | Hd | 93 | GLU |
| 2 | Hd | 115 | VAL |
| 2 | Hd | 123 | THR |
| 2 | Hd | 147 | VAL |
| 2 | Hd | 150 | ASN |
| 3 | Hf | 211 | TYR |
| 3 | Hf | 219 | ARG |
| 3 | Hf | 233 | ARG |
| 3 | Hf | 244 | VAL |
| 3 | Hf | 255 | LEU |
| 1 | CG | 869 | MET |
| 1 | CG | 886 | LEU |
| 1 | CG | 889 | ILE |
| 1 | CG | 895 | LYS |
| 1 | CG | 898 | LYS |
| 1 | CG | 911 | LYS |
| 1 | CG | 913 | VAL |
| 1 | CG | 916 | PHE |
| 1 | CG | 930 | ILE |
| 1 | CG | 944 | LEU |
| 1 | CG | 956 | TYR |
| 1 | CG | 962 | SER |
| 1 | CG | 965 | LEU |
| 1 | CG | 972 | PHE |
| 1 | CG | 1010 | THR |
| 1 | CG | 1017 | GLN |
| 1 | CG | 1044 | ASP |
| 1 | Bg | 795 | GLN |
| 1 | Bg | 815 | VAL |
| 1 | Bg | 819 | VAL |
| 2 | ID | 25 | PHE |
| 2 | ID | 52 | MET |
| 2 | ID | 73 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | ID | 86 | ASP |
| 2 | ID | 106 | PHE |
| 2 | ID | 115 | VAL |
| 2 | ID | 127 | SER |
| 2 | ID | 137 | TYR |
| 2 | ID | 160 | LYS |
| 3 | IF | 207 | ARG |
| 3 | IF | 215 | VAL |
| 3 | IF | 231 | THR |
| 3 | IF | 250 | LEU |
| 3 | IF | 255 | LEU |
| 3 | IF | 263 | LYS |
| 1 | Ig | 794 | ILE |
| 1 | Ig | 807 | GLN |
| 1 | Ig | 810 | GLN |
| 1 | Ig | 815 | VAL |
| 1 | Ig | 816 | GLU |
| 1 | Ig | 817 | THR |
| 4 | IH | 105 | GLU |
| 4 | IH | 108 | ASP |
| 4 | IH | 134 | TYR |
| 4 | IH | 147 | THR |
| 4 | IH | 180 | VAL |
| 4 | IH | 183 | ASP |
| 4 | IH | 195 | ASP |
| 4 | IH | 201 | SER |
| 4 | IH | 207 | ASP |
| 4 | IH | 211 | ASN |
| 4 | IH | 228 | VAL |
| 4 | IH | 229 | ARG |
| 4 | IH | 239 | LEU |
| 4 | IH | 240 | THR |
| 4 | IH | 241 | LEU |
| 4 | IH | 248 | VAL |
| 4 | IH | 249 | ASP |
| 4 | IH | 253 | ASP |
| 4 | IH | 278 | ASP |
| 4 | IH | 280 | LEU |
| 5 | IK | 45 | VAL |
| 5 | IK | 46 | ASP |
| 5 | IK | 70 | VAL |
| 5 | IK | 76 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | IK | 91 | LEU |
| 5 | IK | 92 | ASN |
| 5 | IK | 111 | LYS |
| 5 | IK | 112 | ILE |
| 5 | IK | 117 | THR |
| 5 | IK | 125 | SER |
| 5 | IK | 126 | VAL |
| 5 | IK | 142 | GLU |
| 5 | IK | 156 | THR |
| 5 | IK | 162 | ASP |
| 5 | IK | 177 | ASN |
| 5 | IK | 180 | VAL |
| 6 | IL | 48 | ASN |
| 6 | IL | 51 | GLN |
| 6 | IL | 93 | LEU |
| 6 | IL | 109 | LEU |
| 6 | IL | 123 | ARG |
| 6 | IL | 130 | ASP |
| 6 | IL | 154 | LEU |
| 6 | IL | 155 | LEU |
| 6 | IL | 163 | ILE |
| 6 | IL | 172 | VAL |
| 6 | IL | 174 | SER |
| 6 | IL | 185 | GLN |
| 6 | IL | 193 | LEU |
| 6 | IL | 203 | LEU |
| 7 | IM | 123 | VAL |
| 7 | IM | 127 | ASN |
| 7 | IM | 134 | LEU |
| 7 | IM | 136 | LEU |
| 7 | IM | 149 | ASN |
| 7 | IM | 152 | LEU |
| 7 | IM | 155 | LEU |
| 7 | IM | 170 | SER |
| 7 | IM | 171 | ARG |
| 7 | IM | 176 | VAL |
| 7 | IM | 184 | LEU |
| 7 | IM | 192 | ARG |
| 7 | IM | 194 | LEU |
| 7 | IM | 201 | THR |
| 7 | IM | 207 | ILE |
| 7 | IM | 212 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | IM | 221 | LYS |
| 7 | IM | 222 | ILE |
| 7 | IM | 232 | ASP |
| 7 | IM | 246 | LEU |
| 7 | IM | 251 | SER |
| 7 | IM | 255 | THR |
| 7 | IM | 263 | ILE |
| 7 | IM | 274 | THR |
| 7 | IM | 280 | TYR |
| 7 | IM | 292 | MET |
| 7 | IM | 301 | MET |
| 8 | IN | 51 | CYS |
| 8 | IN | 80 | PHE |
| 8 | IN | 81 | LEU |
| 8 | IN | 91 | VAL |
| 8 | IN | 95 | LEU |
| 8 | IN | 101 | VAL |
| 8 | IN | 108 | VAL |
| 8 | IN | 115 | GLN |
| 8 | IN | 116 | LYS |
| 2 | Id | 41 | LEU |
| 2 | Id | 53 | LEU |
| 2 | Id | 61 | VAL |
| 2 | Id | 63 | THR |
| 2 | Id | 78 | ASN |
| 2 | Id | 111 | LYS |
| 2 | Id | 115 | VAL |
| 2 | Id | 145 | ILE |
| 2 | Id | 147 | VAL |
| 2 | Id | 154 | VAL |
| 11 | KC | 28 | THR |
| 11 | KC | 30 | SER |
| 11 | KC | 37 | MET |
| 11 | KC | 41 | LYS |
| 11 | KC | 42 | TYR |
| 11 | KC | 48 | LYS |
| 11 | KC | 53 | LYS |
| 11 | KC | 56 | GLU |
| 11 | KC | 82 | GLN |
| 11 | KC | 86 | GLN |
| 11 | KC | 103 | HIS |
| 11 | KC | 105 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | KC | 112 | GLU |
| 11 | KC | 140 | PHE |
| 11 | KC | 143 | THR |
| 11 | KC | 149 | GLN |
| 11 | KC | 154 | ASP |
| 11 | KC | 170 | LYS |
| 11 | KC | 174 | GLU |
| 11 | KC | 193 | THR |
| 11 | KC | 195 | LEU |
| 11 | KC | 204 | GLU |
| 11 | KC | 211 | LEU |
| 11 | KC | 218 | MET |
| 11 | KC | 226 | VAL |
| 11 | KC | 230 | ASP |
| 11 | KC | 233 | VAL |
| 11 | KC | 234 | THR |
| 11 | KC | 240 | ILE |
| 11 | KC | 255 | LEU |
| 3 | If | 215 | VAL |
| 3 | If | 230 | LEU |
| 3 | If | 238 | ILE |
| 3 | If | 244 | VAL |
| 3 | If | 255 | LEU |
| 3 | If | 261 | VAL |
| 2 | JD | 23 | MET |
| 2 | JD | 35 | ASP |
| 2 | JD | 50 | ASP |
| 2 | JD | 51 | SER |
| 2 | JD | 55 | MET |
| 2 | JD | 63 | THR |
| 2 | JD | 71 | LEU |
| 2 | JD | 91 | ILE |
| 2 | JD | 115 | VAL |
| 2 | JD | 127 | SER |
| 3 | JF | 208 | ILE |
| 3 | JF | 215 | VAL |
| 3 | JF | 230 | LEU |
| 3 | JF | 231 | THR |
| 3 | JF | 233 | ARG |
| 3 | JF | 238 | ILE |
| 3 | JF | 246 | LEU |
| 3 | JF | 250 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | JF | 253 | ARG |
| 1 | Jg | 793 | GLU |
| 1 | Jg | 795 | GLN |
| 1 | Jg | 808 | LEU |
| 1 | Jg | 814 | GLN |
| 1 | Jg | 815 | VAL |
| 1 | Jg | 816 | GLU |
| 1 | Jg | 817 | THR |
| 1 | Jg | 819 | VAL |
| 4 | JH | 108 | ASP |
| 4 | JH | 109 | LYS |
| 4 | JH | 139 | TYR |
| 4 | JH | 147 | THR |
| 4 | JH | 152 | THR |
| 4 | JH | 170 | ARG |
| 4 | JH | 175 | PHE |
| 4 | JH | 176 | VAL |
| 4 | JH | 180 | VAL |
| 4 | JH | 204 | ILE |
| 4 | JH | 207 | ASP |
| 4 | JH | 226 | LEU |
| 4 | JH | 231 | ARG |
| 4 | JH | 233 | LEU |
| 4 | JH | 237 | VAL |
| 4 | JH | 238 | MET |
| 4 | JH | 241 | LEU |
| 4 | JH | 253 | ASP |
| 4 | JH | 284 | LEU |
| 4 | JH | 313 | VAL |
| 4 | JH | 319 | ILE |
| 4 | JH | 324 | TRP |
| 4 | JH | 339 | MET |
| 4 | JH | 350 | HIS |
| 4 | JH | 353 | VAL |
| 5 | JK | 50 | ASP |
| 5 | JK | 75 | LEU |
| 5 | JK | 83 | LEU |
| 5 | JK | 126 | VAL |
| 5 | JK | 138 | ARG |
| 5 | JK | 156 | THR |
| 5 | JK | 162 | ASP |
| 5 | JK | 170 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | JK | 180 | VAL |
| 5 | JK | 183 | THR |
| 6 | JL | 49 | ASN |
| 6 | JL | 93 | LEU |
| 6 | JL | 100 | ASP |
| 6 | JL | 113 | ASP |
| 6 | JL | 124 | THR |
| 6 | JL | 133 | PHE |
| 6 | JL | 139 | ARG |
| 6 | JL | 140 | LEU |
| 6 | JL | 163 | ILE |
| 6 | JL | 172 | VAL |
| 6 | JL | 175 | ARG |
| 6 | JL | 181 | LEU |
| 6 | JL | 201 | LYS |
| 6 | JL | 210 | ASP |
| 6 | JL | 212 | ASN |
| 7 | JM | 130 | ARG |
| 7 | JM | 131 | THR |
| 7 | JM | 134 | LEU |
| 7 | JM | 144 | THR |
| 7 | JM | 162 | VAL |
| 7 | JM | 173 | LEU |
| 7 | JM | 174 | GLN |
| 7 | JM | 175 | ILE |
| 7 | JM | 176 | VAL |
| 7 | JM | 180 | ASP |
| 7 | JM | 184 | LEU |
| 7 | JM | 191 | LEU |
| 7 | JM | 202 | LEU |
| 7 | JM | 208 | LYS |
| 7 | JM | 212 | LEU |
| 7 | JM | 221 | LYS |
| 7 | JM | 229 | ASN |
| 7 | JM | 275 | ASP |
| 7 | JM | 277 | SER |
| 7 | JM | 284 | LEU |
| 7 | JM | 292 | MET |
| 7 | JM | 310 | LYS |
| 7 | JM | 313 | ASP |
| 7 | JM | 316 | ASN |
| 8 | JN | 44 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 8 | JN | 59 | VAL |
| 8 | JN | 70 | CYS |
| 8 | JN | 91 | VAL |
| 8 | JN | 102 | VAL |
| 8 | JN | 115 | GLN |
| 2 | Jd | 36 | ASP |
| 2 | Jd | 61 | VAL |
| 2 | Jd | 63 | THR |
| 2 | Jd | 72 | THR |
| 2 | Jd | 93 | GLU |
| 2 | Jd | 108 | VAL |
| 2 | Jd | 115 | VAL |
| 2 | Jd | 119 | ILE |
| 3 | Jf | 221 | TRP |
| 3 | Jf | 230 | LEU |
| 3 | Jf | 261 | VAL |
| 1 | DG | 873 | LEU |
| 1 | DG | 880 | ASP |
| 1 | DG | 910 | ASP |
| 1 | DG | 913 | VAL |
| 1 | DG | 916 | PHE |
| 1 | DG | 930 | ILE |
| 1 | DG | 935 | ILE |
| 1 | DG | 944 | LEU |
| 1 | DG | 962 | SER |
| 1 | DG | 963 | SER |
| 1 | DG | 965 | LEU |
| 1 | DG | 968 | PHE |
| 1 | DG | 972 | PHE |
| 1 | DG | 1010 | THR |
| 1 | DG | 1017 | GLN |
| 1 | DG | 1028 | THR |
| 1 | DG | 1040 | LEU |
| 4 | AH | 109 | LYS |
| 4 | AH | 115 | MET |
| 4 | AH | 122 | LEU |
| 4 | AH | 135 | GLU |
| 4 | AH | 139 | TYR |
| 4 | AH | 147 | THR |
| 4 | AH | 160 | LEU |
| 4 | AH | 170 | ARG |
| 4 | AH | 177 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | AH | 180 | VAL |
| 4 | AH | 202 | PHE |
| 4 | AH | 208 | LYS |
| 4 | AH | 215 | ILE |
| 4 | AH | 223 | TYR |
| 4 | AH | 239 | LEU |
| 4 | AH | 241 | LEU |
| 4 | AH | 248 | VAL |
| 4 | AH | 255 | ARG |
| 4 | AH | 264 | LYS |
| 4 | AH | 280 | LEU |
| 4 | AH | 284 | LEU |
| 4 | AH | 296 | VAL |
| 4 | AH | 313 | VAL |
| 4 | AH | 316 | ASN |
| 4 | AH | 332 | ASP |
| 4 | AH | 334 | THR |
| 4 | AH | 341 | LYS |
| 4 | AH | 361 | LEU |
| 2 | KD | 35 | ASP |
| 2 | KD | 43 | GLU |
| 2 | KD | 50 | ASP |
| 2 | KD | 51 | SER |
| 2 | KD | 55 | MET |
| 2 | KD | 91 | ILE |
| 2 | KD | 111 | LYS |
| 2 | KD | 136 | ASP |
| 2 | KD | 138 | GLN |
| 2 | KD | 150 | ASN |
| 2 | KD | 154 | VAL |
| 3 | KF | 215 | VAL |
| 3 | KF | 230 | LEU |
| 3 | KF | 231 | THR |
| 3 | KF | 238 | ILE |
| 3 | KF | 261 | VAL |
| 1 | Kg | 793 | GLU |
| 1 | Kg | 794 | ILE |
| 1 | Kg | 801 | MET |
| 1 | Kg | 810 | GLN |
| 1 | Kg | 814 | GLN |
| 1 | Kg | 815 | VAL |
| 1 | Kg | 816 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | Kg | 819 | VAL |
| 1 | Kg | 821 | THR |
| 4 | KH | 105 | GLU |
| 4 | KH | 109 | LYS |
| 4 | KH | 115 | MET |
| 4 | KH | 134 | TYR |
| 4 | KH | 139 | TYR |
| 4 | KH | 141 | LYS |
| 4 | KH | 147 | THR |
| 4 | KH | 152 | THR |
| 4 | KH | 170 | ARG |
| 4 | KH | 180 | VAL |
| 4 | KH | 183 | ASP |
| 4 | KH | 218 | THR |
| 4 | KH | 221 | TYR |
| 4 | KH | 226 | LEU |
| 4 | KH | 238 | MET |
| 4 | KH | 257 | GLN |
| 4 | KH | 287 | VAL |
| 4 | KH | 306 | LEU |
| 4 | KH | 328 | MET |
| 4 | KH | 332 | ASP |
| 4 | KH | 334 | THR |
| 5 | KK | 50 | ASP |
| 5 | KK | 65 | ILE |
| 5 | KK | 67 | VAL |
| 5 | KK | 70 | VAL |
| 5 | KK | 76 | ILE |
| 5 | KK | 83 | LEU |
| 5 | KK | 88 | SER |
| 5 | KK | 106 | LEU |
| 5 | KK | 111 | LYS |
| 5 | KK | 126 | VAL |
| 5 | KK | 156 | THR |
| 5 | KK | 162 | ASP |
| 5 | KK | 170 | LEU |
| 5 | KK | 181 | GLU |
| 5 | KK | 183 | THR |
| 6 | KL | 51 | GLN |
| 6 | KL | 100 | ASP |
| 6 | KL | 121 | ASP |
| 6 | KL | 129 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 6 | KL | 130 | ASP |
| 6 | KL | 133 | PHE |
| 6 | KL | 140 | LEU |
| 6 | KL | 165 | VAL |
| 6 | KL | 169 | THR |
| 6 | KL | 174 | SER |
| 6 | KL | 175 | ARG |
| 6 | KL | 211 | LYS |
| 6 | KL | 212 | ASN |
| 6 | KL | 216 | ASP |
| 7 | KM | 123 | VAL |
| 7 | KM | 134 | LEU |
| 7 | KM | 135 | ASP |
| 7 | KM | 152 | LEU |
| 7 | KM | 160 | ASN |
| 7 | KM | 173 | LEU |
| 7 | KM | 176 | VAL |
| 7 | KM | 178 | LYS |
| 7 | KM | 180 | ASP |
| 7 | KM | 183 | VAL |
| 7 | KM | 184 | LEU |
| 7 | KM | 191 | LEU |
| 7 | KM | 194 | LEU |
| 7 | KM | 202 | LEU |
| 7 | KM | 205 | TYR |
| 7 | KM | 212 | LEU |
| 7 | KM | 215 | ARG |
| 7 | KM | 221 | LYS |
| 7 | KM | 233 | VAL |
| 7 | KM | 245 | TYR |
| 7 | KM | 249 | GLN |
| 7 | KM | 259 | SER |
| 7 | KM | 263 | ILE |
| 7 | KM | 270 | SER |
| 7 | KM | 292 | MET |
| 7 | KM | 299 | LEU |
| 7 | KM | 301 | MET |
| 8 | KN | 66 | SER |
| 8 | KN | 69 | TYR |
| 8 | KN | 78 | LEU |
| 8 | KN | 80 | PHE |
| 8 | KN | 91 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 8 | KN | 101 | VAL |
| 8 | KN | 108 | VAL |
| 8 | KN | 111 | GLU |
| 2 | Kd | 36 | ASP |
| 2 | Kd | 53 | LEU |
| 2 | Kd | 59 | GLU |
| 2 | Kd | 61 | VAL |
| 2 | Kd | 63 | THR |
| 2 | Kd | 73 | ILE |
| 2 | Kd | 78 | ASN |
| 2 | Kd | 93 | GLU |
| 2 | Kd | 111 | LYS |
| 2 | Kd | 128 | LEU |
| 3 | Kf | 250 | LEU |
| 3 | Kf | 260 | GLN |
| 3 | Kf | 261 | VAL |
| 2 | LD | 23 | MET |
| 2 | LD | 32 | ASN |
| 2 | LD | 35 | ASP |
| 2 | LD | 51 | SER |
| 2 | LD | 52 | MET |
| 2 | LD | 55 | MET |
| 2 | LD | 70 | THR |
| 2 | LD | 71 | LEU |
| 2 | LD | 85 | VAL |
| 2 | LD | 91 | ILE |
| 2 | LD | 115 | VAL |
| 2 | LD | 126 | GLU |
| 2 | LD | 141 | LYS |
| 2 | LD | 147 | VAL |
| 2 | LD | 156 | LEU |
| 3 | LF | 215 | VAL |
| 3 | LF | 223 | ILE |
| 3 | LF | 230 | LEU |
| 3 | LF | 231 | THR |
| 3 | LF | 238 | ILE |
| 3 | LF | 256 | THR |
| 3 | LF | 263 | LYS |
| 1 | Lg | 798 | THR |
| 1 | Lg | 806 | THR |
| 1 | Lg | 808 | LEU |
| 1 | Lg | 809 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | Lg | 814 | GLN |
| 1 | Lg | 815 | VAL |
| 1 | Lg | 821 | THR |
| 4 | LH | 122 | LEU |
| 4 | LH | 138 | GLU |
| 4 | LH | 141 | LYS |
| 4 | LH | 147 | THR |
| 4 | LH | 160 | LEU |
| 4 | LH | 170 | ARG |
| 4 | LH | 180 | VAL |
| 4 | LH | 182 | LEU |
| 4 | LH | 207 | ASP |
| 4 | LH | 215 | ILE |
| 4 | LH | 221 | TYR |
| 4 | LH | 225 | ASN |
| 4 | LH | 228 | VAL |
| 4 | LH | 233 | LEU |
| 4 | LH | 248 | VAL |
| 4 | LH | 253 | ASP |
| 4 | LH | 256 | VAL |
| 4 | LH | 278 | ASP |
| 4 | LH | 284 | LEU |
| 4 | LH | 294 | ARG |
| 4 | LH | 301 | ASP |
| 4 | LH | 313 | VAL |
| 4 | LH | 332 | ASP |
| 5 | LK | 50 | ASP |
| 5 | LK | 70 | VAL |
| 5 | LK | 76 | ILE |
| 5 | LK | 92 | ASN |
| 5 | LK | 106 | LEU |
| 5 | LK | 126 | VAL |
| 5 | LK | 129 | GLU |
| 5 | LK | 156 | THR |
| 5 | LK | 166 | THR |
| 5 | LK | 180 | VAL |
| 5 | LK | 182 | ILE |
| 5 | LK | 183 | THR |
| 6 | LL | 93 | LEU |
| 6 | LL | 104 | LYS |
| 6 | LL | 109 | LEU |
| 6 | LL | 112 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 6 | LL | 121 | ASP |
| 6 | LL | 130 | ASP |
| 6 | LL | 172 | VAL |
| 6 | LL | 177 | HIS |
| 6 | LL | 181 | LEU |
| 6 | LL | 190 | MET |
| 6 | LL | 193 | LEU |
| 6 | LL | 212 | ASN |
| 7 | LM | 136 | LEU |
| 7 | LM | 149 | ASN |
| 7 | LM | 152 | LEU |
| 7 | LM | 162 | VAL |
| 7 | LM | 176 | VAL |
| 7 | LM | 182 | LYS |
| 7 | LM | 184 | LEU |
| 7 | LM | 188 | PHE |
| 7 | LM | 191 | LEU |
| 7 | LM | 192 | ARG |
| 7 | LM | 202 | LEU |
| 7 | LM | 203 | SER |
| 7 | LM | 208 | LYS |
| 7 | LM | 210 | ASP |
| 7 | LM | 212 | LEU |
| 7 | LM | 215 | ARG |
| 7 | LM | 221 | LYS |
| 7 | LM | 275 | ASP |
| 7 | LM | 284 | LEU |
| 7 | LM | 298 | VAL |
| 7 | LM | 316 | ASN |
| 8 | LN | 39 | ASP |
| 8 | LN | 51 | CYS |
| 8 | LN | 64 | PHE |
| 8 | LN | 101 | VAL |
| 8 | LN | 108 | VAL |
| 8 | LN | 114 | LEU |
| 8 | LN | 116 | LYS |
| 2 | Ld | 41 | LEU |
| 2 | Ld | 53 | LEU |
| 2 | Ld | 61 | VAL |
| 2 | Ld | 63 | THR |
| 2 | Ld | 68 | ASP |
| 2 | Ld | 78 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | Ld | 93 | GLU |
| 2 | Ld | 115 | VAL |
| 2 | Ld | 124 | LYS |
| 2 | Ld | 147 | VAL |
| 3 | Lf | 212 | ILE |
| 3 | Lf | 215 | VAL |
| 3 | Lf | 222 | LEU |
| 3 | Lf | 223 | ILE |
| 3 | Lf | 238 | ILE |
| 3 | Lf | 250 | LEU |
| 3 | Lf | 253 | ARG |
| 3 | Lf | 260 | GLN |
| 3 | Lf | 261 | VAL |
| 3 | Lf | 262 | ILE |
| 5 | AK | 40 | LYS |
| 5 | AK | 50 | ASP |
| 5 | AK | 70 | VAL |
| 5 | AK | 76 | ILE |
| 5 | AK | 77 | SER |
| 5 | AK | 92 | ASN |
| 5 | AK | 99 | LEU |
| 5 | AK | 109 | PHE |
| 5 | AK | 111 | LYS |
| 5 | AK | 112 | ILE |
| 5 | AK | 116 | VAL |
| 5 | AK | 125 | SER |
| 5 | AK | 129 | GLU |
| 5 | AK | 132 | LEU |
| 5 | AK | 156 | THR |
| 5 | AK | 169 | THR |
| 5 | AK | 170 | LEU |
| 5 | AK | 180 | VAL |
| 1 | EG | 865 | THR |
| 1 | EG | 869 | MET |
| 1 | EG | 874 | ASP |
| 1 | EG | 890 | VAL |
| 1 | EG | 895 | LYS |
| 1 | EG | 898 | LYS |
| 1 | EG | 910 | ASP |
| 1 | EG | 911 | LYS |
| 1 | EG | 916 | PHE |
| 1 | EG | 930 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | EG | 944 | LEU |
| 1 | EG | 954 | MET |
| 1 | EG | 962 | SER |
| 1 | EG | 963 | SER |
| 1 | EG | 965 | LEU |
| 1 | EG | 972 | PHE |
| 1 | EG | 1010 | THR |
| 1 | EG | 1017 | GLN |
| 1 | EG | 1028 | THR |
| 1 | EG | 1037 | LEU |
| 2 | MD | 23 | MET |
| 2 | MD | 32 | ASN |
| 2 | MD | 38 | THR |
| 2 | MD | 41 | LEU |
| 2 | MD | 50 | ASP |
| 2 | MD | 61 | VAL |
| 2 | MD | 86 | ASP |
| 2 | MD | 91 | ILE |
| 2 | MD | 92 | GLU |
| 2 | MD | 108 | VAL |
| 2 | MD | 115 | VAL |
| 2 | MD | 128 | LEU |
| 2 | MD | 138 | GLN |
| 2 | MD | 154 | VAL |
| 3 | MF | 211 | TYR |
| 3 | MF | 215 | VAL |
| 3 | MF | 223 | ILE |
| 3 | MF | 231 | THR |
| 3 | MF | 233 | ARG |
| 3 | MF | 238 | ILE |
| 3 | MF | 250 | LEU |
| 3 | MF | 256 | THR |
| 1 | Mg | 795 | GLN |
| 1 | Mg | 809 | VAL |
| 1 | Mg | 810 | GLN |
| 1 | Mg | 815 | VAL |
| 4 | MH | 108 | ASP |
| 4 | MH | 125 | GLU |
| 4 | MH | 130 | LEU |
| 4 | MH | 147 | THR |
| 4 | MH | 170 | ARG |
| 4 | MH | 175 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | MH | 183 | ASP |
| 4 | MH | 203 | ASN |
| 4 | MH | 207 | ASP |
| 4 | MH | 218 | THR |
| 4 | MH | 221 | TYR |
| 4 | MH | 238 | MET |
| 4 | MH | 250 | TYR |
| 4 | MH | 252 | VAL |
| 4 | MH | 255 | ARG |
| 4 | MH | 264 | LYS |
| 4 | MH | 268 | THR |
| 4 | MH | 280 | LEU |
| 4 | MH | 287 | VAL |
| 4 | MH | 296 | VAL |
| 4 | MH | 301 | ASP |
| 4 | MH | 313 | VAL |
| 4 | MH | 316 | ASN |
| 4 | MH | 332 | ASP |
| 4 | MH | 353 | VAL |
| 5 | MK | 45 | VAL |
| 5 | MK | 46 | ASP |
| 5 | MK | 62 | LYS |
| 5 | MK | 67 | VAL |
| 5 | MK | 70 | VAL |
| 5 | MK | 72 | GLN |
| 5 | MK | 76 | ILE |
| 5 | MK | 91 | LEU |
| 5 | MK | 98 | LEU |
| 5 | MK | 112 | ILE |
| 5 | MK | 125 | SER |
| 5 | MK | 129 | GLU |
| 5 | MK | 156 | THR |
| 5 | MK | 180 | VAL |
| 5 | MK | 182 | ILE |
| 6 | ML | 57 | VAL |
| 6 | ML | 93 | LEU |
| 6 | ML | 109 | LEU |
| 6 | ML | 113 | ASP |
| 6 | ML | 130 | ASP |
| 6 | ML | 140 | LEU |
| 6 | ML | 165 | VAL |
| 6 | ML | 172 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 6 | ML | 177 | HIS |
| 6 | ML | 185 | GLN |
| 6 | ML | 210 | ASP |
| 6 | ML | 212 | ASN |
| 6 | ML | 216 | ASP |
| 6 | ML | 225 | GLN |
| 6 | ML | 230 | GLU |
| 7 | MM | 134 | LEU |
| 7 | MM | 149 | ASN |
| 7 | MM | 152 | LEU |
| 7 | MM | 162 | VAL |
| 7 | MM | 180 | ASP |
| 7 | MM | 193 | GLN |
| 7 | MM | 203 | SER |
| 7 | MM | 208 | LYS |
| 7 | MM | 212 | LEU |
| 7 | MM | 222 | ILE |
| 7 | MM | 232 | ASP |
| 7 | MM | 242 | LYS |
| 7 | MM | 251 | SER |
| 7 | MM | 263 | ILE |
| 7 | MM | 292 | MET |
| 7 | MM | 308 | ASP |
| 7 | MM | 312 | PHE |
| 8 | MN | 51 | CYS |
| 8 | MN | 65 | TYR |
| 8 | MN | 72 | ARG |
| 8 | MN | 78 | LEU |
| 8 | MN | 84 | CYS |
| 8 | MN | 92 | TYR |
| 8 | MN | 94 | GLN |
| 8 | MN | 100 | LEU |
| 8 | MN | 108 | VAL |
| 8 | MN | 110 | GLU |
| 8 | MN | 115 | GLN |
| 2 | Md | 25 | PHE |
| 2 | Md | 41 | LEU |
| 2 | Md | 51 | SER |
| 2 | Md | 61 | VAL |
| 2 | Md | 63 | THR |
| 2 | Md | 67 | LYS |
| 2 | Md | 92 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | Md | 97 | ARG |
| 2 | Md | 108 | VAL |
| 2 | Md | 115 | VAL |
| 2 | Md | 147 | VAL |
| 2 | Md | 155 | GLU |
| 3 | Mf | 212 | ILE |
| 3 | Mf | 219 | ARG |
| 3 | Mf | 255 | LEU |
| 3 | Mf | 260 | GLN |
| 3 | Mf | 261 | VAL |
| 3 | VF | 215 | VAL |
| 3 | VF | 230 | LEU |
| 3 | VF | 231 | THR |
| 3 | VF | 238 | ILE |
| 3 | VF | 256 | THR |
| 1 | VG | 793 | GLU |
| 1 | VG | 800 | ASP |
| 1 | VG | 815 | VAL |
| 4 | VH | 105 | GLU |
| 4 | VH | 115 | MET |
| 4 | VH | 122 | LEU |
| 4 | VH | 138 | GLU |
| 4 | VH | 147 | THR |
| 4 | VH | 152 | THR |
| 4 | VH | 160 | LEU |
| 4 | VH | 170 | ARG |
| 4 | VH | 203 | ASN |
| 4 | VH | 204 | ILE |
| 4 | VH | 205 | GLN |
| 4 | VH | 218 | THR |
| 4 | VH | 225 | ASN |
| 4 | VH | 226 | LEU |
| 4 | VH | 231 | ARG |
| 4 | VH | 233 | LEU |
| 4 | VH | 234 | ASN |
| 4 | VH | 249 | ASP |
| 4 | VH | 253 | ASP |
| 4 | VH | 259 | TYR |
| 4 | VH | 287 | VAL |
| 4 | VH | 296 | VAL |
| 4 | VH | 297 | VAL |
| 4 | VH | 303 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | VH | 313 | VAL |
| 4 | VH | 314 | ARG |
| 4 | VH | 354 | MET |
| 4 | VH | 358 | VAL |
| 3 | WF | 215 | VAL |
| 3 | WF | 223 | ILE |
| 3 | WF | 230 | LEU |
| 3 | WF | 232 | VAL |
| 3 | WF | 238 | ILE |
| 3 | WF | 261 | VAL |
| 1 | WG | 795 | GLN |
| 1 | WG | 797 | ARG |
| 1 | WG | 800 | ASP |
| 1 | WG | 815 | VAL |
| 1 | WG | 816 | GLU |
| 1 | WG | 817 | THR |
| 1 | WG | 821 | THR |
| 4 | WH | 109 | LYS |
| 4 | WH | 134 | TYR |
| 4 | WH | 141 | LYS |
| 4 | WH | 147 | THR |
| 4 | WH | 170 | ARG |
| 4 | WH | 171 | LEU |
| 4 | WH | 180 | VAL |
| 4 | WH | 203 | ASN |
| 4 | WH | 218 | THR |
| 4 | WH | 220 | LEU |
| 4 | WH | 223 | TYR |
| 4 | WH | 237 | VAL |
| 4 | WH | 238 | MET |
| 4 | WH | 240 | THR |
| 4 | WH | 248 | VAL |
| 4 | WH | 249 | ASP |
| 4 | WH | 250 | TYR |
| 4 | WH | 253 | ASP |
| 4 | WH | 278 | ASP |
| 4 | WH | 297 | VAL |
| 4 | WH | 306 | LEU |
| 4 | WH | 311 | MET |
| 4 | WH | 312 | TYR |
| 4 | WH | 313 | VAL |
| 4 | WH | 315 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | WH | 317 | LEU |
| 4 | WH | 318 | THR |
| 4 | WH | 324 | TRP |
| 4 | WH | 329 | THR |
| 4 | WH | 340 | GLN |
| 4 | WH | 354 | MET |
| 4 | WH | 356 | LEU |
| 4 | WH | 358 | VAL |
| 3 | XF | 215 | VAL |
| 3 | XF | 223 | ILE |
| 3 | XF | 230 | LEU |
| 3 | XF | 232 | VAL |
| 1 | XG | 794 | ILE |
| 1 | XG | 796 | GLN |
| 1 | XG | 815 | VAL |
| 1 | XG | 816 | GLU |
| 4 | XH | 134 | TYR |
| 4 | XH | 147 | THR |
| 4 | XH | 168 | VAL |
| 4 | XH | 170 | ARG |
| 4 | XH | 171 | LEU |
| 4 | XH | 175 | PHE |
| 4 | XH | 180 | VAL |
| 4 | XH | 195 | ASP |
| 4 | XH | 201 | SER |
| 4 | XH | 225 | ASN |
| 4 | XH | 233 | LEU |
| 4 | XH | 237 | VAL |
| 4 | XH | 238 | MET |
| 4 | XH | 240 | THR |
| 4 | XH | 241 | LEU |
| 4 | XH | 242 | ILE |
| 4 | XH | 253 | ASP |
| 4 | XH | 256 | VAL |
| 4 | XH | 313 | VAL |
| 4 | XH | 354 | MET |
| 4 | XH | 356 | LEU |
| 4 | XH | 357 | LYS |
| 3 | YF | 211 | TYR |
| 3 | YF | 230 | LEU |
| 3 | YF | 231 | THR |
| 3 | YF | 238 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | YF | 264 | PHE |
| 3 | YF | 267 | GLU |
| 6 | AL | 93 | LEU |
| 6 | AL | 100 | ASP |
| 6 | AL | 111 | LYS |
| 6 | AL | 113 | ASP |
| 6 | AL | 129 | THR |
| 6 | AL | 130 | ASP |
| 6 | AL | 141 | ASN |
| 6 | AL | 148 | LEU |
| 6 | AL | 154 | LEU |
| 6 | AL | 155 | LEU |
| 6 | AL | 172 | VAL |
| 6 | AL | 201 | LYS |
| 6 | AL | 204 | LYS |
| 6 | AL | 217 | ASN |
| 1 | FG | 867 | ASP |
| 1 | FG | 873 | LEU |
| 1 | FG | 885 | ILE |
| 1 | FG | 900 | ILE |
| 1 | FG | 913 | VAL |
| 1 | FG | 916 | PHE |
| 1 | FG | 930 | ILE |
| 1 | FG | 946 | SER |
| 1 | FG | 949 | ASN |
| 1 | FG | 962 | SER |
| 1 | FG | 965 | LEU |
| 1 | FG | 968 | PHE |
| 1 | FG | 972 | PHE |
| 1 | FG | 1010 | THR |
| 1 | FG | 1037 | LEU |
| 1 | YG | 795 | GLN |
| 1 | YG | 802 | LEU |
| 1 | YG | 808 | LEU |
| 1 | YG | 812 | TRP |
| 1 | YG | 814 | GLN |
| 1 | YG | 817 | THR |
| 1 | YG | 819 | VAL |
| 4 | YH | 108 | ASP |
| 4 | YH | 117 | ARG |
| 4 | YH | 120 | TYR |
| 4 | YH | 122 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | YH | 147 | THR |
| 4 | YH | 152 | THR |
| 4 | YH | 154 | THR |
| 4 | YH | 170 | ARG |
| 4 | YH | 176 | VAL |
| 4 | YH | 180 | VAL |
| 4 | YH | 195 | ASP |
| 4 | YH | 211 | ASN |
| 4 | YH | 225 | ASN |
| 4 | YH | 229 | ARG |
| 4 | YH | 237 | VAL |
| 4 | YH | 241 | LEU |
| 4 | YH | 248 | VAL |
| 4 | YH | 249 | ASP |
| 4 | YH | 253 | ASP |
| 4 | YH | 255 | ARG |
| 4 | YH | 283 | VAL |
| 4 | YH | 295 | LEU |
| 4 | YH | 306 | LEU |
| 4 | YH | 318 | THR |
| 4 | YH | 356 | LEU |
| 4 | YH | 358 | VAL |
| 11 | DC | 60 | LYS |
| 11 | DC | 84 | ASN |
| 11 | DC | 97 | ASN |
| 11 | DC | 105 | ILE |
| 11 | DC | 112 | GLU |
| 11 | DC | 116 | THR |
| 11 | DC | 119 | LEU |
| 11 | DC | 146 | THR |
| 11 | DC | 148 | ARG |
| 11 | DC | 153 | MET |
| 11 | DC | 157 | LYS |
| 11 | DC | 166 | LEU |
| 11 | DC | 184 | TRP |
| 11 | DC | 193 | THR |
| 11 | DC | 203 | LYS |
| 11 | DC | 204 | GLU |
| 11 | DC | 206 | PHE |
| 11 | DC | 211 | LEU |
| 11 | DC | 231 | LEU |
| 11 | DC | 233 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | DC | 248 | ARG |
| 11 | DC | 249 | ILE |
| 11 | DC | 254 | GLU |
| 11 | DC | 266 | VAL |
| 3 | ZF | 211 | TYR |
| 3 | ZF | 230 | LEU |
| 3 | ZF | 231 | THR |
| 3 | ZF | 264 | PHE |
| 1 | ZG | 792 | GLN |
| 1 | ZG | 815 | VAL |
| 1 | ZG | 819 | VAL |
| 1 | ZG | 821 | THR |
| 4 | ZH | 105 | GLU |
| 4 | ZH | 108 | ASP |
| 4 | ZH | 130 | LEU |
| 4 | ZH | 147 | THR |
| 4 | ZH | 161 | SER |
| 4 | ZH | 180 | VAL |
| 4 | ZH | 196 | LEU |
| 4 | ZH | 203 | ASN |
| 4 | ZH | 207 | ASP |
| 4 | ZH | 214 | MET |
| 4 | ZH | 221 | TYR |
| 4 | ZH | 226 | LEU |
| 4 | ZH | 233 | LEU |
| 4 | ZH | 238 | MET |
| 4 | ZH | 240 | THR |
| 4 | ZH | 248 | VAL |
| 4 | ZH | 250 | TYR |
| 4 | ZH | 253 | ASP |
| 4 | ZH | 255 | ARG |
| 4 | ZH | 262 | ASN |
| 4 | ZH | 279 | LEU |
| 4 | ZH | 297 | VAL |
| 4 | ZH | 314 | ARG |
| 4 | ZH | 315 | THR |
| 4 | ZH | 328 | MET |
| 4 | ZH | 329 | THR |
| 4 | ZH | 354 | MET |
| 4 | ZH | 358 | VAL |
| 7 | AM | 114 | ASN |
| 7 | AM | 134 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | AM | 149 | ASN |
| 7 | AM | 153 | GLN |
| 7 | AM | 171 | ARG |
| 7 | AM | 180 | ASP |
| 7 | AM | 191 | LEU |
| 7 | AM | 204 | LEU |
| 7 | AM | 205 | TYR |
| 7 | AM | 212 | LEU |
| 7 | AM | 234 | GLU |
| 7 | AM | 259 | SER |
| 7 | AM | 269 | GLN |
| 7 | AM | 292 | MET |
| 7 | AM | 308 | ASP |
| 8 | AN | 51 | CYS |
| 8 | AN | 62 | ASN |
| 8 | AN | 69 | TYR |
| 8 | AN | 81 | LEU |
| 8 | AN | 84 | CYS |
| 8 | AN | 97 | SER |
| 2 | Ad | 41 | LEU |
| 2 | Ad | 53 | LEU |
| 2 | Ad | 61 | VAL |
| 2 | Ad | 63 | THR |
| 2 | Ad | 68 | ASP |
| 2 | Ad | 73 | ILE |
| 2 | Ad | 85 | VAL |
| 2 | Ad | 94 | LEU |
| 2 | Ad | 115 | VAL |
| 2 | Ad | 123 | THR |
| 2 | Ad | 128 | LEU |
| 2 | Ad | 150 | ASN |
| 3 | Af | 238 | ILE |
| 3 | Af | 253 | ARG |
| 3 | Af | 261 | VAL |
| 3 | Af | 263 | LYS |
| 3 | Af | 264 | PHE |
| 3 | Af | 266 | GLN |
| 2 | BD | 35 | ASP |
| 2 | BD | 51 | SER |
| 2 | BD | 63 | THR |
| 2 | BD | 71 | LEU |
| 2 | BD | 84 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | BD | 85 | VAL |
| 2 | BD | 97 | ARG |
| 2 | BD | 115 | VAL |
| 3 | BF | 207 | ARG |
| 3 | BF | 208 | ILE |
| 3 | BF | 215 | VAL |
| 3 | BF | 230 | LEU |
| 3 | BF | 231 | THR |
| 3 | BF | 238 | ILE |
| 3 | BF | 250 | LEU |
| 3 | BF | 264 | PHE |
| 4 | BH | 135 | GLU |
| 4 | BH | 147 | THR |
| 4 | BH | 160 | LEU |
| 4 | BH | 180 | VAL |
| 4 | BH | 185 | THR |
| 4 | BH | 207 | ASP |
| 4 | BH | 221 | TYR |
| 4 | BH | 223 | TYR |
| 4 | BH | 240 | THR |
| 4 | BH | 248 | VAL |
| 4 | BH | 250 | TYR |
| 4 | BH | 257 | GLN |
| 4 | BH | 262 | ASN |
| 4 | BH | 269 | GLU |
| 4 | BH | 278 | ASP |
| 4 | BH | 294 | ARG |
| 4 | BH | 313 | VAL |
| 4 | BH | 353 | VAL |
| 5 | BK | 50 | ASP |
| 5 | BK | 62 | LYS |
| 5 | BK | 67 | VAL |
| 5 | BK | 70 | VAL |
| 5 | BK | 72 | GLN |
| 5 | BK | 73 | ASN |
| 5 | BK | 77 | SER |
| 5 | BK | 98 | LEU |
| 5 | BK | 100 | ASN |
| 5 | BK | 111 | LYS |
| 5 | BK | 126 | VAL |
| 5 | BK | 149 | VAL |
| 5 | BK | 156 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | BK | 162 | ASP |
| 5 | BK | 169 | THR |
| 5 | BK | 170 | LEU |
| 5 | BK | 180 | VAL |
| 6 | BL | 53 | ASP |
| 6 | BL | 93 | LEU |
| 6 | BL | 109 | LEU |
| 6 | BL | 113 | ASP |
| 6 | BL | 121 | ASP |
| 6 | BL | 123 | ARG |
| 6 | BL | 129 | THR |
| 6 | BL | 130 | ASP |
| 6 | BL | 134 | MET |
| 6 | BL | 165 | VAL |
| 6 | BL | 172 | VAL |
| 6 | BL | 177 | HIS |
| 6 | BL | 183 | GLN |
| 6 | BL | 190 | MET |
| 6 | BL | 206 | GLU |
| 6 | BL | 210 | ASP |
| 6 | BL | 212 | ASN |
| 6 | BL | 216 | ASP |
| 7 | BM | 115 | ARG |
| 7 | BM | 118 | TYR |
| 7 | BM | 127 | ASN |
| 7 | BM | 134 | LEU |
| 7 | BM | 137 | TYR |
| 7 | BM | 146 | LEU |
| 7 | BM | 149 | ASN |
| 7 | BM | 153 | GLN |
| 7 | BM | 171 | ARG |
| 7 | BM | 175 | ILE |
| 7 | BM | 177 | LEU |
| 7 | BM | 178 | LYS |
| 7 | BM | 180 | ASP |
| 7 | BM | 184 | LEU |
| 7 | BM | 199 | LYS |
| 7 | BM | 202 | LEU |
| 7 | BM | 207 | ILE |
| 7 | BM | 212 | LEU |
| 7 | BM | 215 | ARG |
| 7 | BM | 222 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | BM | 231 | LEU |
| 7 | BM | 242 | LYS |
| 7 | BM | 245 | TYR |
| 7 | BM | 269 | GLN |
| 7 | BM | 271 | SER |
| 7 | BM | 290 | ASP |
| 7 | BM | 292 | MET |
| 7 | BM | 301 | MET |
| 7 | BM | 308 | ASP |
| 8 | BN | 51 | CYS |
| 8 | BN | 54 | SER |
| 8 | BN | 59 | VAL |
| 8 | BN | 70 | CYS |
| 8 | BN | 71 | THR |
| 8 | BN | 72 | ARG |
| 8 | BN | 76 | MET |
| 8 | BN | 81 | LEU |
| 8 | BN | 91 | VAL |
| 8 | BN | 94 | GLN |
| 8 | BN | 95 | LEU |
| 8 | BN | 98 | SER |
| 8 | BN | 102 | VAL |
| 2 | Bd | 26 | LYS |
| 2 | Bd | 41 | LEU |
| 2 | Bd | 51 | SER |
| 2 | Bd | 52 | MET |
| 2 | Bd | 61 | VAL |
| 2 | Bd | 63 | THR |
| 2 | Bd | 78 | ASN |
| 2 | Bd | 115 | VAL |
| 2 | Bd | 145 | ILE |
| 2 | Bd | 146 | HIS |
| 2 | Bd | 150 | ASN |
| 3 | Bf | 232 | VAL |
| 3 | Bf | 247 | ILE |
| 3 | Bf | 250 | LEU |
| 3 | Bf | 253 | ARG |
| 11 | EC | 92 | ASP |
| 11 | EC | 117 | THR |
| 11 | EC | 118 | LEU |
| 11 | EC | 130 | ASP |
| 11 | EC | 140 | HIS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | EC | 147 | THR |
| 11 | EC | 164 | VAL |
| 11 | EC | 167 | LEU |
| 11 | EC | 177 | TRP |
| 11 | EC | 190 | ASP |
| 11 | EC | 222 | VAL |
| 11 | EC | 231 | ASP |
| 11 | EC | 235 | THR |
| 11 | EC | 267 | VAL |
| 1 | GG | 865 | THR |
| 1 | GG | 869 | MET |
| 1 | GG | 885 | ILE |
| 1 | GG | 895 | LYS |
| 1 | GG | 900 | ILE |
| 1 | GG | 910 | ASP |
| 1 | GG | 913 | VAL |
| 1 | GG | 918 | THR |
| 1 | GG | 930 | ILE |
| 1 | GG | 944 | LEU |
| 1 | GG | 956 | TYR |
| 1 | GG | 962 | SER |
| 1 | GG | 963 | SER |
| 1 | GG | 965 | LEU |
| 1 | GG | 966 | GLN |
| 1 | GG | 972 | PHE |
| 1 | GG | 1010 | THR |
| 1 | GG | 1017 | GLN |
| 1 | GG | 1028 | THR |
| 1 | GG | 1037 | LEU |
| 1 | GG | 1044 | ASP |
| 11 | FC | 28 | THR |
| 11 | FC | 31 | LEU |
| 11 | FC | 35 | GLN |
| 11 | FC | 51 | MET |
| 11 | FC | 56 | GLU |
| 11 | FC | 111 | LEU |
| 11 | FC | 116 | THR |
| 11 | FC | 119 | LEU |
| 11 | FC | 125 | ILE |
| 11 | FC | 146 | THR |
| 11 | FC | 154 | ASP |
| 11 | FC | 163 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | FC | 169 | THR |
| 11 | FC | 174 | GLU |
| 11 | FC | 195 | LEU |
| 11 | FC | 206 | PHE |
| 11 | FC | 221 | VAL |
| 11 | FC | 225 | TYR |
| 11 | FC | 226 | VAL |
| 11 | FC | 230 | ASP |
| 11 | FC | 234 | THR |
| 11 | FC | 255 | LEU |
| 11 | HC | 64 | LEU |
| 11 | HC | 97 | ASN |
| 11 | HC | 105 | ILE |
| 11 | HC | 118 | ASN |
| 11 | HC | 119 | LEU |
| 11 | HC | 127 | ILE |
| 11 | HC | 133 | LYS |
| 11 | HC | 143 | THR |
| 11 | HC | 151 | LEU |
| 11 | HC | 169 | THR |
| 11 | HC | 195 | LEU |
| 11 | HC | 226 | VAL |
| 11 | HC | 233 | VAL |
| 11 | HC | 241 | HIS |
| 11 | HC | 256 | ASN |
| 11 | HC | 263 | ARG |
| 11 | HC | 266 | VAL |
| 11 | IC | 65 | SER |
| 11 | IC | 81 | GLU |
| 11 | IC | 89 | ASN |
| 11 | IC | 91 | ASP |
| 11 | IC | 97 | ASN |
| 11 | IC | 105 | ILE |
| 11 | IC | 112 | GLU |
| 11 | IC | 116 | THR |
| 11 | IC | 123 | GLN |
| 11 | IC | 125 | ILE |
| 11 | IC | 127 | ILE |
| 11 | IC | 143 | THR |
| 11 | IC | 146 | THR |
| 11 | IC | 151 | LEU |
| 11 | IC | 163 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | IC | 165 | LEU |
| 11 | IC | 166 | LEU |
| 11 | IC | 170 | LYS |
| 11 | IC | 174 | GLU |
| 11 | IC | 176 | TRP |
| 11 | IC | 184 | TRP |
| 11 | IC | 204 | GLU |
| 11 | IC | 211 | LEU |
| 11 | IC | 226 | VAL |
| 11 | IC | 249 | ILE |
| 11 | IC | 256 | ASN |
| 11 | IC | 258 | ASN |
| 11 | IC | 263 | ARG |
| 11 | IC | 266 | VAL |
| 11 | JC | 65 | LEU |
| 11 | JC | 84 | LEU |
| 11 | JC | 91 | LEU |
| 11 | JC | 101 | VAL |
| 11 | JC | 106 | ILE |
| 11 | JC | 113 | GLU |
| 11 | JC | 120 | LEU |
| 11 | JC | 143 | THR |
| 11 | JC | 149 | ARG |
| 11 | JC | 163 | ASN |
| 11 | JC | 166 | LEU |
| 11 | JC | 170 | THR |
| 11 | JC | 196 | LEU |
| 11 | JC | 205 | GLU |
| 11 | JC | 207 | PHE |
| 11 | JC | 227 | VAL |
| 11 | JC | 234 | VAL |
| 11 | JC | 235 | THR |
| 11 | LC | 64 | LEU |
| 11 | LC | 95 | ASP |
| 11 | LC | 97 | ASN |
| 11 | LC | 105 | ILE |
| 11 | LC | 109 | VAL |
| 11 | LC | 119 | LEU |
| 11 | LC | 140 | PHE |
| 11 | LC | 143 | THR |
| 11 | LC | 146 | THR |
| 11 | LC | 148 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | LC | 149 | GLN |
| 11 | LC | 153 | MET |
| 11 | LC | 162 | ASN |
| 11 | LC | 195 | LEU |
| 11 | LC | 215 | LEU |
| 11 | LC | 226 | VAL |
| 11 | LC | 234 | THR |
| 11 | LC | 243 | ASP |
| 11 | LC | 245 | ARG |
| 11 | MC | 83 | LEU |
| 11 | MC | 91 | ASP |
| 11 | MC | 97 | ASN |
| 11 | MC | 105 | ILE |
| 11 | MC | 109 | VAL |
| 11 | MC | 111 | LEU |
| 11 | MC | 116 | THR |
| 11 | MC | 119 | LEU |
| 11 | MC | 139 | HIS |
| 11 | MC | 140 | PHE |
| 11 | MC | 143 | THR |
| 11 | MC | 148 | ARG |
| 11 | MC | 156 | VAL |
| 11 | MC | 159 | GLU |
| 11 | MC | 168 | LYS |
| 11 | MC | 169 | THR |
| 11 | MC | 170 | LYS |
| 11 | MC | 181 | GLU |
| 11 | MC | 226 | VAL |
| 11 | MC | 234 | THR |
| 11 | MC | 241 | HIS |
| 11 | MC | 256 | ASN |
| 11 | MC | 258 | ASN |
| 11 | MC | 266 | VAL |
| 2 | CD | 26 | LYS |
| 2 | CD | 30 | ILE |
| 2 | CD | 35 | ASP |
| 2 | CD | 50 | ASP |
| 2 | CD | 55 | MET |
| 2 | CD | 78 | ASN |
| 2 | CD | 84 | SER |
| 2 | CD | 85 | VAL |
| 2 | CD | 92 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | CD | 108 | VAL |
| 2 | CD | 111 | LYS |
| 2 | CD | 115 | VAL |
| 2 | CD | 123 | THR |
| 2 | CD | 154 | VAL |
| 2 | CD | 156 | LEU |
| 2 | CD | 161 | ILE |
| 3 | CF | 215 | VAL |
| 3 | CF | 230 | LEU |
| 3 | CF | 231 | THR |
| 3 | CF | 238 | ILE |
| 1 | Cg | 810 | GLN |
| 1 | Cg | 811 | ASP |
| 1 | Cg | 812 | TRP |
| 1 | Cg | 815 | VAL |
| 4 | CH | 107 | ILE |
| 4 | CH | 109 | LYS |
| 4 | CH | 115 | MET |
| 4 | CH | 130 | LEU |
| 4 | CH | 147 | THR |
| 4 | CH | 156 | GLN |
| 4 | CH | 179 | LEU |
| 4 | CH | 221 | TYR |
| 4 | CH | 229 | ARG |
| 4 | CH | 235 | THR |
| 4 | CH | 238 | MET |
| 4 | CH | 241 | LEU |
| 4 | CH | 245 | GLN |
| 4 | CH | 248 | VAL |
| 4 | CH | 257 | GLN |
| 4 | CH | 269 | GLU |
| 4 | CH | 278 | ASP |
| 4 | CH | 306 | LEU |
| 4 | CH | 313 | VAL |
| 4 | CH | 314 | ARG |
| 4 | CH | 361 | LEU |
| 5 | CK | 50 | ASP |
| 5 | CK | 62 | LYS |
| 5 | CK | 70 | VAL |
| 5 | CK | 83 | LEU |
| 5 | CK | 92 | ASN |
| 5 | CK | 126 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | CK | 149 | VAL |
| 5 | CK | 156 | THR |
| 5 | CK | 162 | ASP |
| 5 | CK | 165 | ILE |
| 5 | CK | 180 | VAL |
| 5 | CK | 183 | THR |
| 6 | CL | 51 | GLN |
| 6 | CL | 57 | VAL |
| 6 | CL | 93 | LEU |
| 6 | CL | 109 | LEU |
| 6 | CL | 121 | ASP |
| 6 | CL | 123 | ARG |
| 6 | CL | 129 | THR |
| 6 | CL | 163 | ILE |
| 6 | CL | 172 | VAL |
| 6 | CL | 174 | SER |
| 6 | CL | 177 | HIS |
| 6 | CL | 212 | ASN |
| 6 | CL | 216 | ASP |
| 6 | CL | 217 | ASN |
| 6 | CL | 225 | GLN |
| 7 | CM | 124 | VAL |
| 7 | CM | 130 | ARG |
| 7 | CM | 134 | LEU |
| 7 | CM | 152 | LEU |
| 7 | CM | 155 | LEU |
| 7 | CM | 175 | ILE |
| 7 | CM | 176 | VAL |
| 7 | CM | 180 | ASP |
| 7 | CM | 182 | LYS |
| 7 | CM | 184 | LEU |
| 7 | CM | 191 | LEU |
| 7 | CM | 192 | ARG |
| 7 | CM | 212 | LEU |
| 7 | CM | 215 | ARG |
| 7 | CM | 233 | VAL |
| 7 | CM | 245 | TYR |
| 7 | CM | 257 | ASP |
| 7 | CM | 263 | ILE |
| 7 | CM | 271 | SER |
| 7 | CM | 275 | ASP |
| 7 | CM | 290 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | CM | 292 | MET |
| 7 | CM | 301 | MET |
| 7 | CM | 308 | ASP |
| 7 | CM | 310 | LYS |
| 7 | CM | 312 | PHE |
| 7 | CM | 316 | ASN |
| 8 | CN | 78 | LEU |
| 8 | CN | 82 | MET |
| 8 | CN | 95 | LEU |
| 8 | CN | 101 | VAL |
| 2 | Cd | 30 | ILE |
| 2 | Cd | 41 | LEU |
| 2 | Cd | 51 | SER |
| 2 | Cd | 59 | GLU |
| 2 | Cd | 61 | VAL |
| 2 | Cd | 62 | ILE |
| 2 | Cd | 91 | ILE |
| 2 | Cd | 108 | VAL |
| 2 | Cd | 115 | VAL |
| 2 | Cd | 126 | GLU |
| 2 | Cd | 128 | LEU |
| 2 | Cd | 131 | ILE |
| 2 | Cd | 147 | VAL |
| 2 | Cd | 150 | ASN |
| 3 | Cf | 209 | ILE |
| 3 | Cf | 212 | ILE |
| 3 | Cf | 230 | LEU |
| 3 | Cf | 233 | ARG |
| 3 | Cf | 236 | SER |
| 3 | Cf | 250 | LEU |
| 3 | Cf | 263 | LYS |
| 2 | DD | 30 | ILE |
| 2 | DD | 41 | LEU |
| 2 | DD | 43 | GLU |
| 2 | DD | 51 | SER |
| 2 | DD | 63 | THR |
| 2 | DD | 108 | VAL |
| 2 | DD | 115 | VAL |
| 2 | DD | 154 | VAL |
| 2 | DD | 161 | ILE |
| 3 | DF | 209 | ILE |
| 3 | DF | 215 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | DF | 223 | ILE |
| 3 | DF | 230 | LEU |
| 3 | DF | 238 | ILE |
| 3 | DF | 250 | LEU |
| 3 | DF | 256 | THR |
| 3 | DF | 263 | LYS |
| 1 | Dg | 793 | GLU |
| 1 | Dg | 808 | LEU |
| 1 | Dg | 814 | GLN |
| 1 | Dg | 815 | VAL |
| 1 | Dg | 816 | GLU |
| 1 | Dg | 819 | VAL |
| 4 | DH | 108 | ASP |
| 4 | DH | 109 | LYS |
| 4 | DH | 115 | MET |
| 4 | DH | 120 | TYR |
| 4 | DH | 130 | LEU |
| 4 | DH | 147 | THR |
| 4 | DH | 180 | VAL |
| 4 | DH | 203 | ASN |
| 4 | DH | 207 | ASP |
| 4 | DH | 225 | ASN |
| 4 | DH | 226 | LEU |
| 4 | DH | 231 | ARG |
| 4 | DH | 240 | THR |
| 4 | DH | 241 | LEU |
| 4 | DH | 248 | VAL |
| 4 | DH | 250 | TYR |
| 4 | DH | 255 | ARG |
| 4 | DH | 262 | ASN |
| 4 | DH | 278 | ASP |
| 4 | DH | 285 | GLU |
| 4 | DH | 293 | ARG |
| 4 | DH | 314 | ARG |
| 4 | DH | 332 | ASP |
| 4 | DH | 344 | VAL |
| 4 | DH | 345 | LEU |
| 4 | DH | 356 | LEU |
| 4 | DH | 361 | LEU |
| 5 | DK | 83 | LEU |
| 5 | DK | 107 | LYS |
| 5 | DK | 111 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | DK | 116 | VAL |
| 5 | DK | 149 | VAL |
| 5 | DK | 156 | THR |
| 5 | DK | 166 | THR |
| 5 | DK | 180 | VAL |
| 1 | HG | 865 | THR |
| 1 | HG | 898 | LYS |
| 1 | HG | 910 | ASP |
| 1 | HG | 912 | MET |
| 1 | HG | 913 | VAL |
| 1 | HG | 916 | PHE |
| 1 | HG | 930 | ILE |
| 1 | HG | 939 | THR |
| 1 | HG | 944 | LEU |
| 1 | HG | 947 | ARG |
| 1 | HG | 962 | SER |
| 1 | HG | 963 | SER |
| 1 | HG | 965 | LEU |
| 1 | HG | 968 | PHE |
| 1 | HG | 972 | PHE |
| 1 | HG | 1010 | THR |
| 1 | HG | 1017 | GLN |
| 1 | HG | 1044 | ASP |
| 1 | IG | 865 | THR |
| 1 | IG | 869 | MET |
| 1 | IG | 886 | LEU |
| 1 | IG | 898 | LYS |
| 1 | IG | 913 | VAL |
| 1 | IG | 916 | PHE |
| 1 | IG | 933 | TYR |
| 1 | IG | 939 | THR |
| 1 | IG | 944 | LEU |
| 1 | IG | 947 | ARG |
| 1 | IG | 962 | SER |
| 1 | IG | 963 | SER |
| 1 | IG | 965 | LEU |
| 1 | IG | 966 | GLN |
| 1 | IG | 972 | PHE |
| 1 | IG | 1010 | THR |
| 1 | IG | 1037 | LEU |
| 1 | IG | 1044 | ASP |
| 1 | JG | 865 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | JG | 867 | ASP |
| 1 | JG | 880 | ASP |
| 1 | JG | 885 | ILE |
| 1 | JG | 895 | LYS |
| 1 | JG | 898 | LYS |
| 1 | JG | 913 | VAL |
| 1 | JG | 916 | PHE |
| 1 | JG | 917 | ASN |
| 1 | JG | 930 | ILE |
| 1 | JG | 944 | LEU |
| 1 | JG | 962 | SER |
| 1 | JG | 968 | PHE |
| 1 | JG | 972 | PHE |
| 1 | JG | 1010 | THR |
| 1 | JG | 1028 | THR |
| 1 | JG | 1037 | LEU |
| 1 | KG | 864 | LYS |
| 1 | KG | 874 | ASP |
| 1 | KG | 885 | ILE |
| 1 | KG | 886 | LEU |
| 1 | KG | 913 | VAL |
| 1 | KG | 930 | ILE |
| 1 | KG | 944 | LEU |
| 1 | KG | 956 | TYR |
| 1 | KG | 962 | SER |
| 1 | KG | 963 | SER |
| 1 | KG | 965 | LEU |
| 1 | KG | 966 | GLN |
| 1 | KG | 972 | PHE |
| 1 | KG | 1010 | THR |
| 1 | KG | 1037 | LEU |
| 1 | KG | 1045 | VAL |
| 1 | LG | 867 | ASP |
| 1 | LG | 869 | MET |
| 1 | LG | 881 | GLU |
| 1 | LG | 886 | LEU |
| 1 | LG | 898 | LYS |
| 1 | LG | 911 | LYS |
| 1 | LG | 913 | VAL |
| 1 | LG | 916 | PHE |
| 1 | LG | 930 | ILE |
| 1 | LG | 944 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | LG | 956 | TYR |
| 1 | LG | 962 | SER |
| 1 | LG | 963 | SER |
| 1 | LG | 968 | PHE |
| 1 | LG | 972 | PHE |
| 1 | LG | 1010 | THR |
| 1 | LG | 1017 | GLN |
| 1 | LG | 1037 | LEU |
| 1 | LG | 1044 | ASP |
| 1 | MG | 869 | MET |
| 1 | MG | 886 | LEU |
| 1 | MG | 898 | LYS |
| 1 | MG | 911 | LYS |
| 1 | MG | 913 | VAL |
| 1 | MG | 916 | PHE |
| 1 | MG | 930 | ILE |
| 1 | MG | 944 | LEU |
| 1 | MG | 956 | TYR |
| 1 | MG | 962 | SER |
| 1 | MG | 963 | SER |
| 1 | MG | 965 | LEU |
| 1 | MG | 1010 | THR |
| 1 | MG | 1017 | GLN |
| 1 | MG | 1037 | LEU |
| 1 | NG | 869 | MET |
| 1 | NG | 898 | LYS |
| 1 | NG | 911 | LYS |
| 1 | NG | 916 | PHE |
| 1 | NG | 930 | ILE |
| 1 | NG | 944 | LEU |
| 1 | NG | 962 | SER |
| 1 | NG | 965 | LEU |
| 1 | NG | 972 | PHE |
| 1 | NG | 1010 | THR |
| 1 | NG | 1017 | GLN |
| 1 | OG | 867 | ASP |
| 1 | OG | 869 | MET |
| 1 | OG | 873 | LEU |
| 1 | OG | 886 | LEU |
| 1 | OG | 898 | LYS |
| 1 | OG | 912 | MET |
| 1 | OG | 916 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | OG | 930 | ILE |
| 1 | OG | 933 | TYR |
| 1 | OG | 944 | LEU |
| 1 | OG | 947 | ARG |
| 1 | OG | 956 | TYR |
| 1 | OG | 962 | SER |
| 1 | OG | 963 | SER |
| 1 | OG | 965 | LEU |
| 1 | OG | 966 | GLN |
| 1 | OG | 1010 | THR |
| 1 | OG | 1017 | GLN |
| 1 | OG | 1040 | LEU |
| 1 | OG | 1045 | VAL |
| 1 | PG | 867 | ASP |
| 1 | PG | 869 | MET |
| 1 | PG | 886 | LEU |
| 1 | PG | 898 | LYS |
| 1 | PG | 910 | ASP |
| 1 | PG | 911 | LYS |
| 1 | PG | 913 | VAL |
| 1 | PG | 916 | PHE |
| 1 | PG | 930 | ILE |
| 1 | PG | 944 | LEU |
| 1 | PG | 947 | ARG |
| 1 | PG | 956 | TYR |
| 1 | PG | 962 | SER |
| 1 | PG | 965 | LEU |
| 1 | PG | 972 | PHE |
| 1 | PG | 1010 | THR |
| 1 | PG | 1017 | GLN |
| 1 | PG | 1037 | LEU |
| 1 | PG | 1044 | ASP |
| 11 | AC | 90 | ASN |
| 11 | AC | 104 | HIS |
| 11 | AC | 106 | ILE |
| 11 | AC | 113 | GLU |
| 11 | AC | 118 | LEU |
| 11 | AC | 124 | GLN |
| 11 | AC | 144 | THR |
| 11 | AC | 164 | VAL |
| 11 | AC | 170 | THR |
| 11 | AC | 196 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | AC | 205 | GLU |
| 11 | AC | 219 | MET |
| 11 | AC | 227 | VAL |
| 11 | AC | 234 | VAL |
| 11 | AC | 235 | THR |
| 6 | DL | 57 | VAL |
| 6 | DL | 98 | TYR |
| 6 | DL | 104 | LYS |
| 6 | DL | 109 | LEU |
| 6 | DL | 113 | ASP |
| 6 | DL | 130 | ASP |
| 6 | DL | 133 | PHE |
| 6 | DL | 135 | PHE |
| 6 | DL | 172 | VAL |
| 6 | DL | 212 | ASN |
| 6 | DL | 217 | ASN |
| 7 | DM | 134 | LEU |
| 7 | DM | 146 | LEU |
| 7 | DM | 149 | ASN |
| 7 | DM | 152 | LEU |
| 7 | DM | 171 | ARG |
| 7 | DM | 178 | LYS |
| 7 | DM | 180 | ASP |
| 7 | DM | 183 | VAL |
| 7 | DM | 184 | LEU |
| 7 | DM | 192 | ARG |
| 7 | DM | 194 | LEU |
| 7 | DM | 201 | THR |
| 7 | DM | 205 | TYR |
| 7 | DM | 215 | ARG |
| 7 | DM | 245 | TYR |
| 7 | DM | 246 | LEU |
| 7 | DM | 255 | THR |
| 7 | DM | 274 | THR |
| 7 | DM | 292 | MET |
| 7 | DM | 310 | LYS |
| 7 | DM | 317 | LYS |
| 8 | DN | 57 | ARG |
| 8 | DN | 62 | ASN |
| 8 | DN | 76 | MET |
| 8 | DN | 78 | LEU |
| 8 | DN | 82 | MET |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 8 | DN | 84 | CYS |
| 8 | DN | 86 | LEU |
| 8 | DN | 101 | VAL |
| 8 | DN | 102 | VAL |
| 8 | DN | 108 | VAL |
| 8 | DN | 115 | GLN |
| 2 | Dd | 30 | ILE |
| 2 | Dd | 41 | LEU |
| 2 | Dd | 52 | MET |
| 2 | Dd | 54 | GLU |
| 2 | Dd | 61 | VAL |
| 2 | Dd | 78 | ASN |
| 2 | Dd | 108 | VAL |
| 2 | Dd | 115 | VAL |
| 2 | Dd | 126 | GLU |
| 2 | Dd | 147 | VAL |
| 2 | Dd | 154 | VAL |
| 1 | Ag | 793 | GLU |
| 1 | Ag | 794 | ILE |
| 1 | Ag | 801 | MET |
| 1 | Ag | 808 | LEU |
| 1 | Ag | 811 | ASP |
| 1 | Ag | 814 | GLN |
| 1 | Ag | 815 | VAL |
| 1 | Ag | 819 | VAL |
| 3 | Df | 230 | LEU |
| 3 | Df | 232 | VAL |
| 3 | Df | 246 | LEU |
| 2 | AD | 24 | LYS |
| 2 | AD | 32 | ASN |
| 2 | AD | 51 | SER |
| 2 | AD | 54 | GLU |
| 2 | AD | 70 | THR |
| 2 | AD | 71 | LEU |
| 2 | AD | 85 | VAL |
| 2 | AD | 115 | VAL |
| 2 | AD | 117 | VAL |
| 2 | AD | 138 | GLN |
| 2 | AD | 147 | VAL |
| 2 | AD | 154 | VAL |
| 2 | AD | 155 | GLU |
| 2 | AD | 156 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AG | 1017 | GLN |
| 2 | Ed | 32 | ASN |
| 11 | BC | 69 | GLN |
| 1 | BG | 1020 | GLN |
| 1 | Gg | 810 | GLN |
| 1 | Gg | 818 | GLN |
| 7 | GM | 153 | GLN |
| 11 | GC | 149 | GLN |
| 6 | HL | 160 | GLN |
| 6 | HL | 196 | ASN |
| 7 | HM | 306 | GLN |
| 1 | Bg | 810 | GLN |
| 1 | Ig | 810 | GLN |
| 7 | IM | 269 | GLN |
| 8 | IN | 94 | GLN |
| 6 | JL | 196 | ASN |
| 7 | JM | 249 | GLN |
| 7 | JM | 267 | ASN |
| 1 | DG | 1017 | GLN |
| 1 | DG | 1020 | GLN |
| 2 | KD | 138 | GLN |
| 2 | Kd | 32 | ASN |
| 7 | LM | 153 | GLN |
| 2 | Ld | 32 | ASN |
| 1 | EG | 1020 | GLN |
| 1 | Mg | 795 | GLN |
| 7 | MM | 249 | GLN |
| 4 | WH | 205 | GLN |
| 4 | WH | 355 | GLN |
| 4 | YH | 205 | GLN |
| 11 | DC | 69 | GLN |
| 11 | DC | 84 | ASN |
| 4 | ZH | 205 | GLN |
| 4 | ZH | 225 | ASN |
| 8 | AN | 94 | GLN |
| 2 | Ad | 32 | ASN |
| 6 | BL | 196 | ASN |
| 6 | BL | 226 | ASN |
| 6 | BL | 232 | GLN |
| 7 | BM | 267 | ASN |
| 6 | CL | 225 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | CM | 306 | GLN |
| 3 | Cf | 251 | GLN |
| 1 | HG | 1020 | GLN |
| 1 | IG | 1017 | GLN |
| 1 | JG | 1020 | GLN |
| 1 | KG | 1017 | GLN |
| 1 | OG | 1017 | GLN |
| 1 | PG | 1020 | GLN |
| 1 | Ag | 818 | GLN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 10 | JX | 1 |
| 10 | WX | 1 |
| 10 | YX | 1 |

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| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 10 | XX | 1 |
| 10 | GX | 1 |
| 10 | CX | 1 |
| 10 | MX | 1 |
| 10 | ZX | 1 |
| 10 | KX | 1 |
| 10 | HX | 1 |
| 10 | FX | 1 |
| 10 | EX | 1 |
| 10 | IX | 1 |
| 10 | DX | 1 |
| 10 | BX | 1 |
| 10 | AX | 1 |
| 10 | VX | 1 |
| 10 | LX | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | JX | 38:UNK | C | 70:UNK | N | 25.78 |
| 1 | WX | 38:UNK | C | 70:UNK | N | 25.34 |
| 1 | YX | 38:UNK | C | 70:UNK | N | 25.23 |
| 1 | XX | 38:UNK | C | 70:UNK | N | 25.08 |
| 1 | GX | 38:UNK | C | 70:UNK | N | 24.81 |
| 1 | CX | 38:UNK | C | 70:UNK | N | 24.61 |
| 1 | MX | 38:UNK | C | 70:UNK | N | 24.45 |
| 1 | ZX | 38:UNK | C | 70:UNK | N | 24.28 |
| 1 | KX | 38:UNK | C | 70:UNK | N | 23.87 |
| 1 | HX | 38:UNK | C | 70:UNK | N | 23.68 |
| 1 | FX | 38:UNK | C | 70:UNK | N | 23.65 |
| 1 | EX | 38:UNK | C | 70:UNK | N | 23.35 |
| 1 | IX | 38:UNK | C | 70:UNK | N | 23.30 |
| 1 | DX | 38:UNK | C | 70:UNK | N | 23.06 |
| 1 | BX | 38:UNK | C | 70:UNK | N | 22.80 |
| 1 | AX | 38:UNK | C | 70:UNK | N | 22.26 |
| 1 | VX | 38:UNK | C | 70:UNK | N | 22.09 |
| 1 | LX | 38:UNK | C | 70:UNK | N | 21.21 |

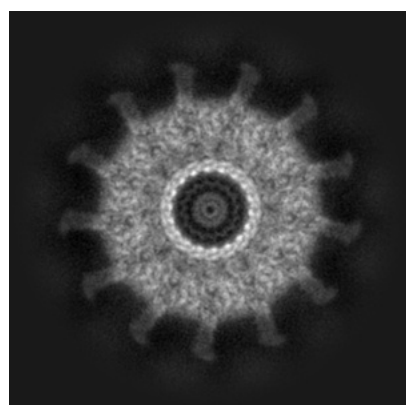
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24026. These allow visual inspection of the internal detail of the map and identification of artifacts.

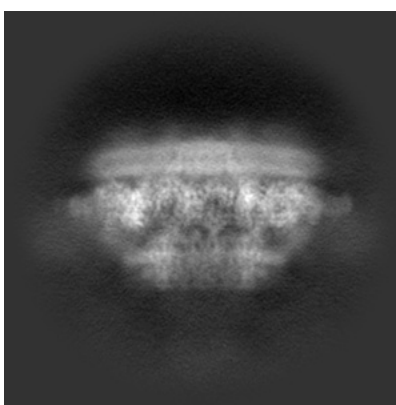
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

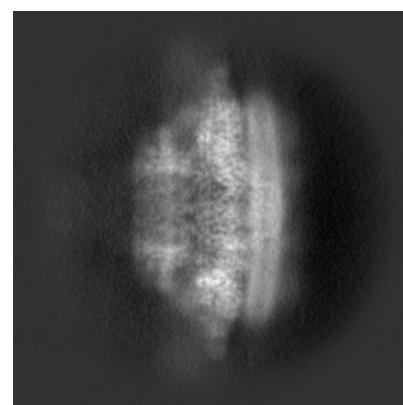
6.1.1 Primary map



X



Y

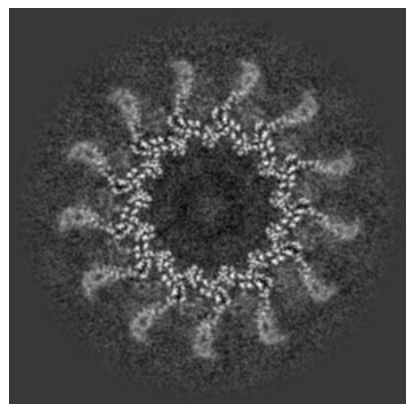


Z

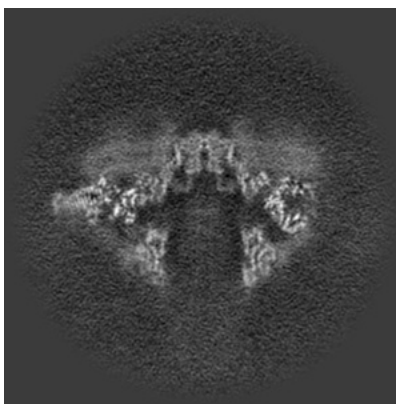
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

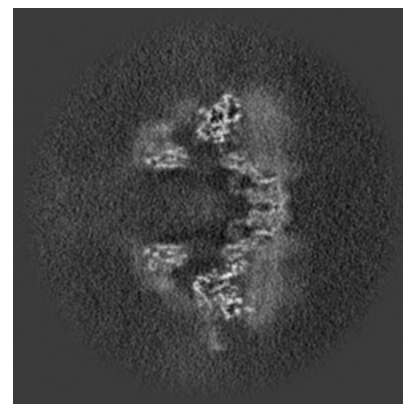
6.2.1 Primary map



X Index: 125



Y Index: 125

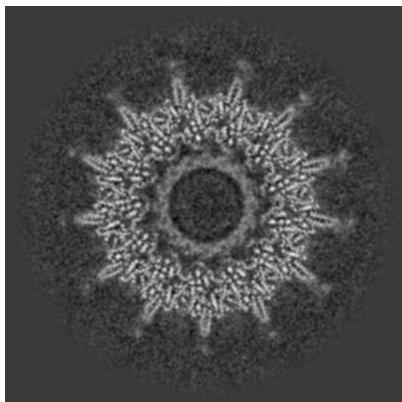


Z Index: 125

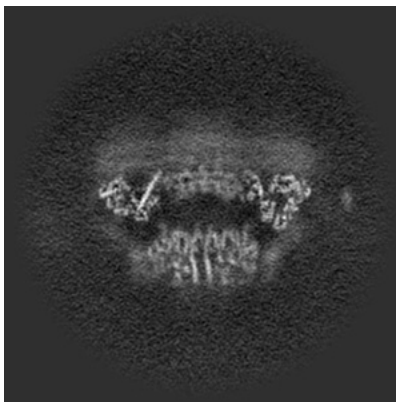
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

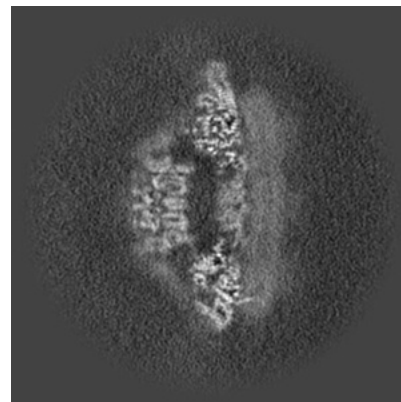
6.3.1 Primary map



X Index: 134



Y Index: 101

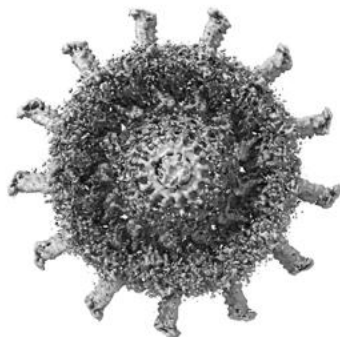


Z Index: 152

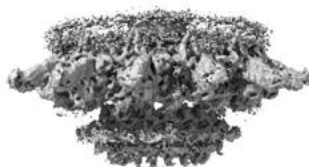
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

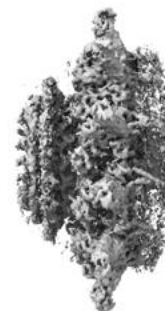
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

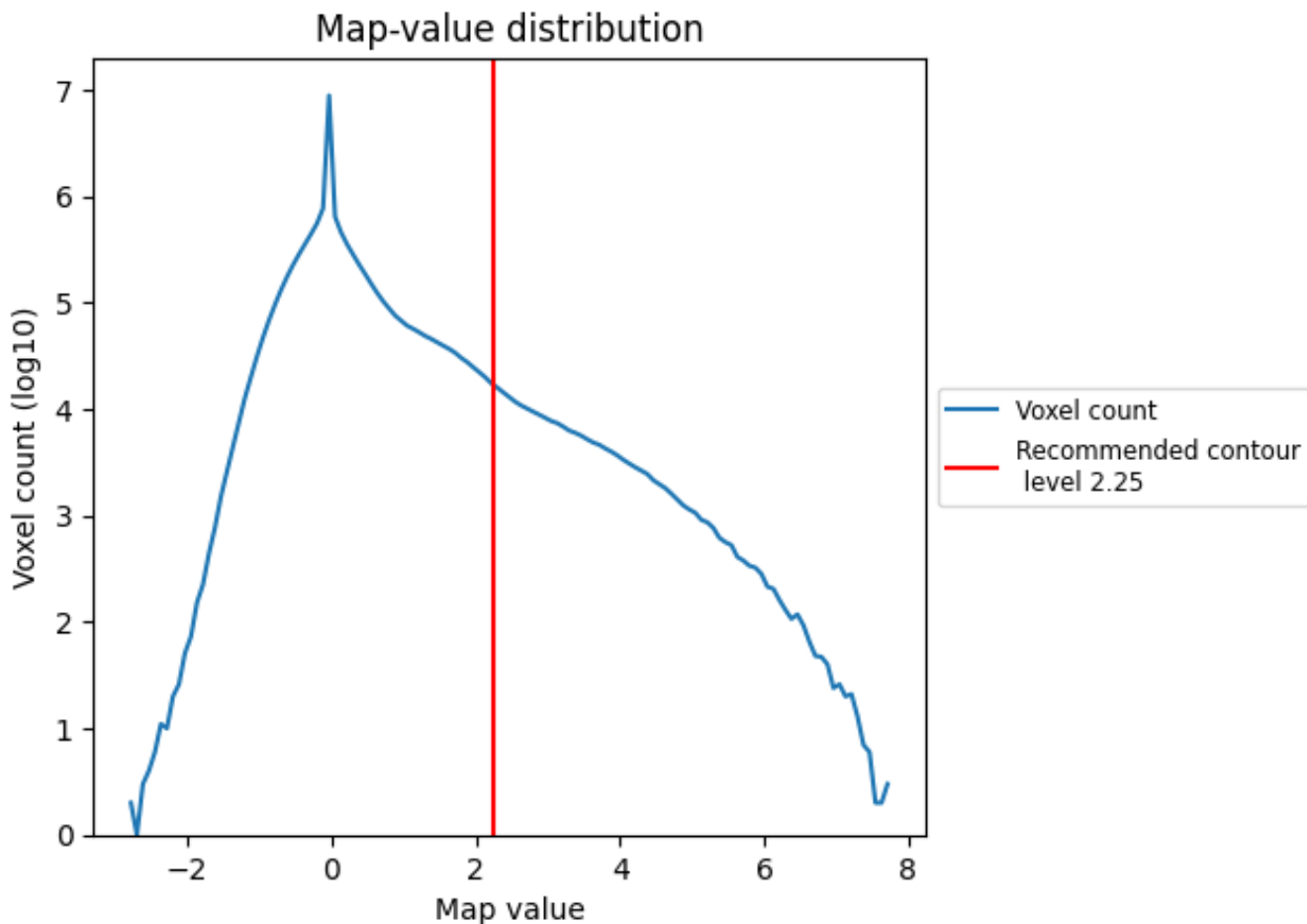
6.5 Mask visualisation

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

7 Map analysis [i](#)

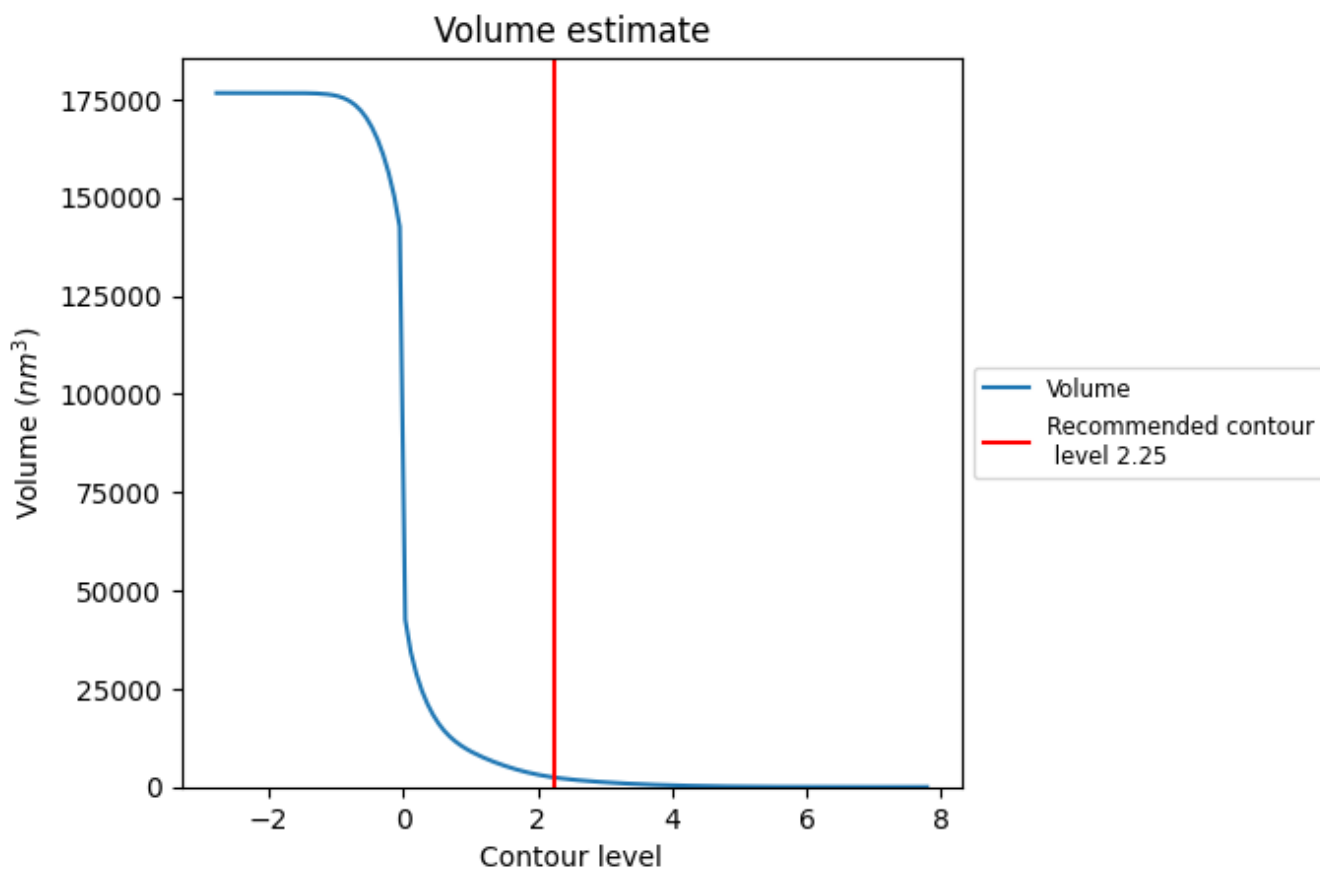
This section contains the results of statistical analysis of the map.

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.

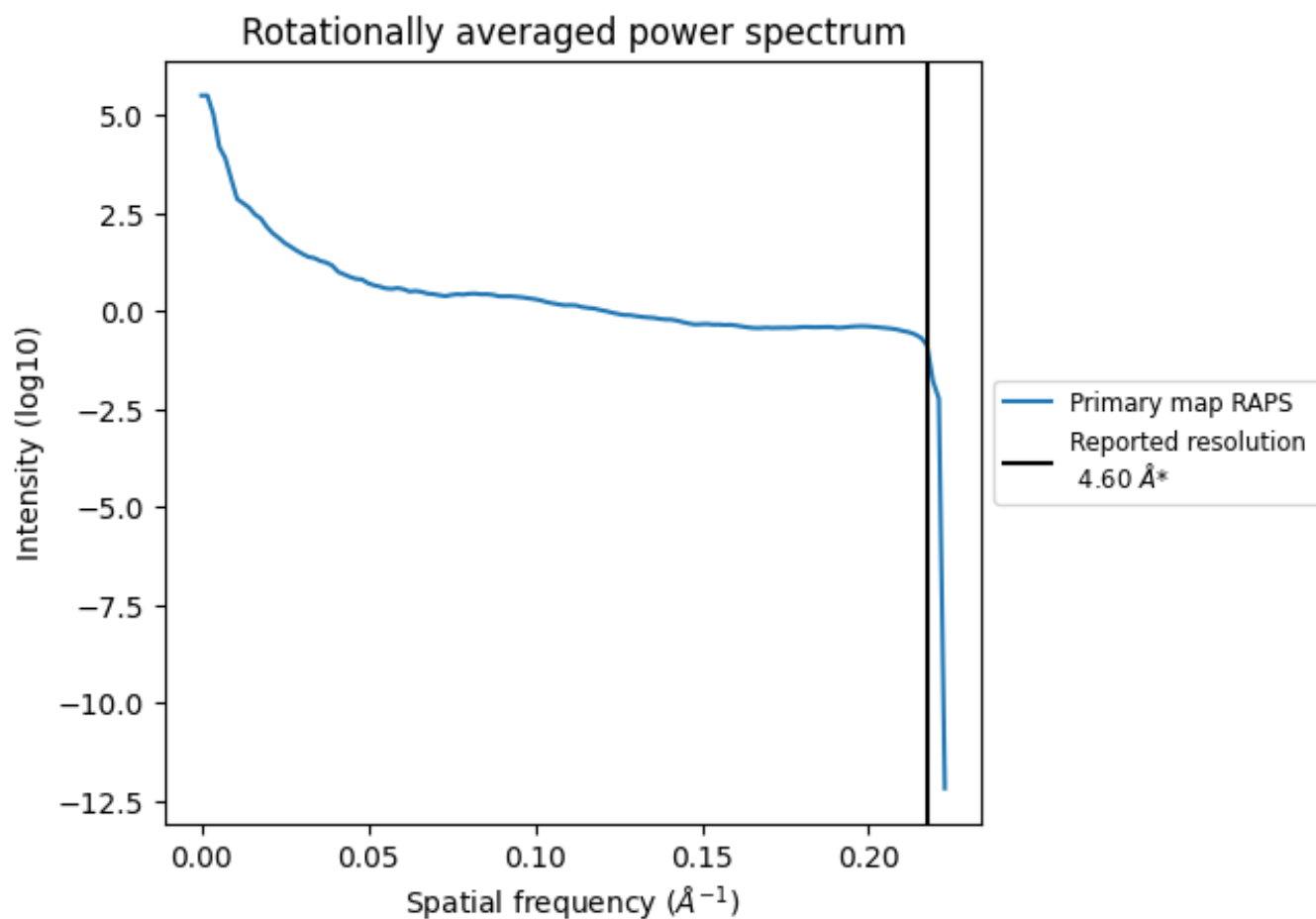
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2412 nm³; this corresponds to an approximate mass of 2179 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 0.217 Å⁻¹

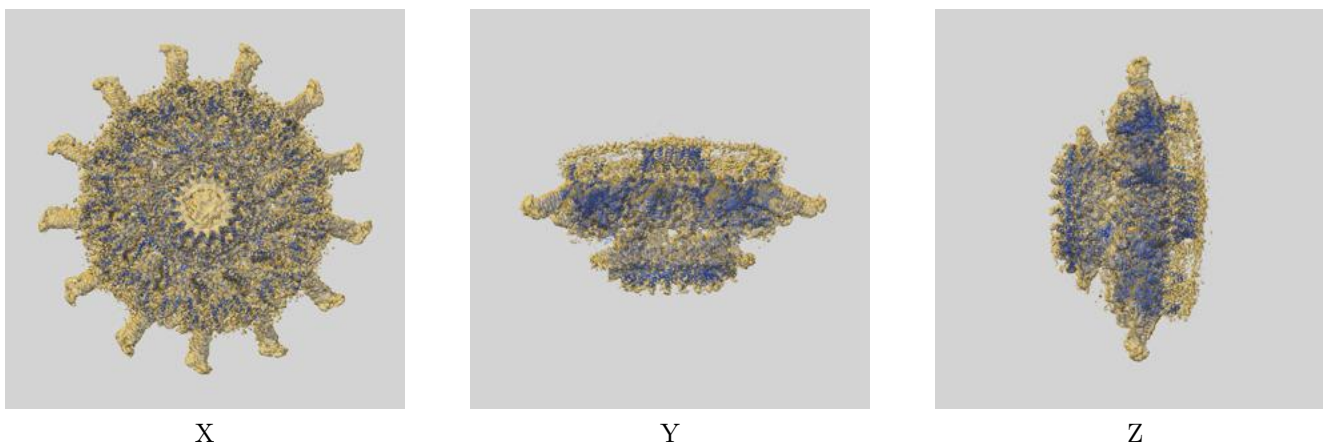
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

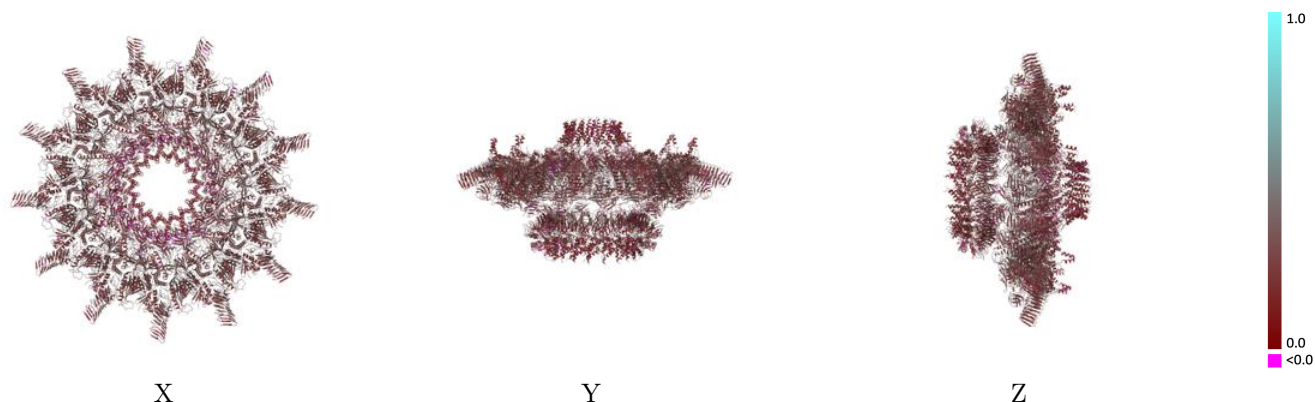
This section contains information regarding the fit between EMDB map EMD-24026 and PDB model 7MUU. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



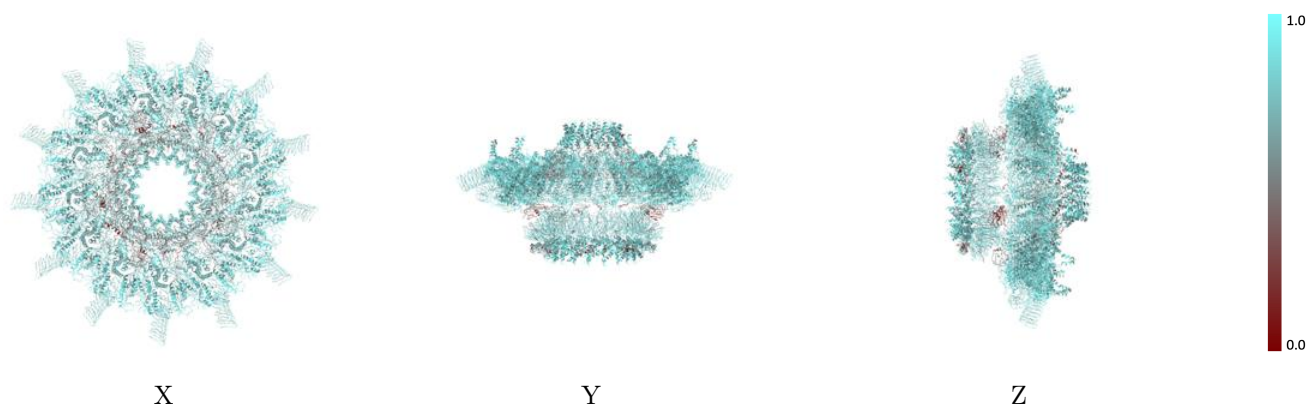
The images above show the 3D surface view of the map at the recommended contour level 2.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



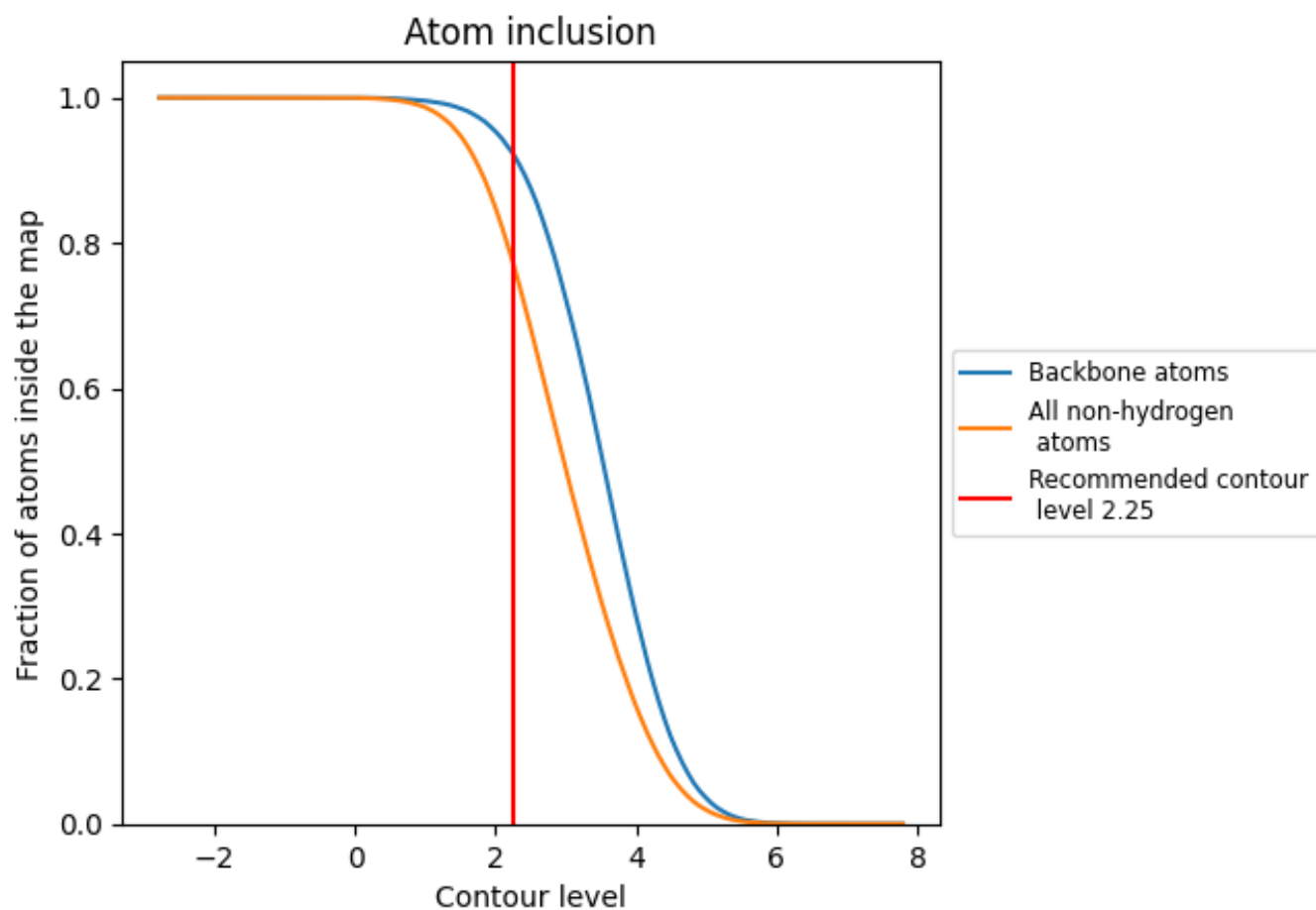
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.25).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 77% 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 (2.25) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.7728 |  0.2760 |
| AC |  0.8092 |  0.3010 |
| AD |  0.8296 |  0.3070 |
| AF |  0.8068 |  0.2390 |
| AG |  0.6782 |  0.1990 |
| AH |  0.7931 |  0.2780 |
| AK |  0.8241 |  0.3060 |
| AL |  0.8317 |  0.2870 |
| AM |  0.8113 |  0.2930 |
| AN |  0.8059 |  0.3290 |
| AU |  0.9778 |  0.4800 |
| AX |  0.5625 |  0.1910 |
| Ad |  0.8357 |  0.3050 |
| Af |  0.8405 |  0.2840 |
| Ag |  0.8676 |  0.2400 |
| BC |  0.7685 |  0.3000 |
| BD |  0.8109 |  0.3100 |
| BF |  0.8004 |  0.2210 |
| BG |  0.5764 |  0.1780 |
| BH |  0.8039 |  0.2840 |
| BK |  0.8443 |  0.3160 |
| BL |  0.8480 |  0.2920 |
| BM |  0.8367 |  0.2960 |
| BN |  0.7727 |  0.3370 |
| BU |  1.0000 |  0.4440 |
| BX |  0.5167 |  0.1940 |
| Bd |  0.8271 |  0.3040 |
| Bf |  0.7950 |  0.2670 |
| Bg |  0.8419 |  0.2520 |
| CC |  0.7445 |  0.2840 |
| CD |  0.8221 |  0.3190 |
| CF |  0.7367 |  0.2400 |
| CG |  0.5846 |  0.1750 |
| CH |  0.8054 |  0.2760 |
| CK |  0.8268 |  0.3190 |























































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| CL |  0.8288 |  0.2950 |
| CM |  0.8101 |  0.2900 |
| CN |  0.7413 |  0.3380 |
| CU |  0.9778 |  0.4570 |
| CX |  0.6042 |  0.2160 |
| Cd |  0.8280 |  0.2950 |
| Cf |  0.8018 |  0.2600 |
| Cg |  0.8603 |  0.2560 |
| DC |  0.8215 |  0.2960 |
| DD |  0.8006 |  0.3120 |
| DF |  0.8004 |  0.2370 |
| DG |  0.5665 |  0.1720 |
| DH |  0.7900 |  0.2790 |
| DK |  0.8101 |  0.3170 |
| DL |  0.8221 |  0.2850 |
| DM |  0.8225 |  0.2840 |
| DN |  0.8112 |  0.3340 |
| DU |  0.8667 |  0.4170 |
| DX |  0.6917 |  0.2460 |
| Dd |  0.8108 |  0.3070 |
| Df |  0.7677 |  0.2910 |
| Dg |  0.8419 |  0.2580 |
| EC |  0.8135 |  0.3010 |
| ED |  0.8034 |  0.3060 |
| EF |  0.7665 |  0.2310 |
| EG |  0.5673 |  0.1690 |
| EH |  0.7834 |  0.2780 |
| EK |  0.8364 |  0.3140 |
| EL |  0.8288 |  0.2990 |
| EM |  0.8355 |  0.2900 |
| EN |  0.8077 |  0.3250 |
| EU |  1.0000 |  0.4630 |
| EX |  0.5000 |  0.2210 |
| Ed |  0.8309 |  0.3090 |
| Ef |  0.8064 |  0.2840 |
| Eg |  0.8088 |  0.2370 |
| FC |  0.7653 |  0.2860 |
| FD |  0.8062 |  0.3090 |
| FF |  0.7792 |  0.2250 |
| FG |  0.5722 |  0.1640 |
| FH |  0.7885 |  0.2810 |
| FK |  0.8233 |  0.3110 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| FL |  0.8184 |  0.2830 |
| FM |  0.8107 |  0.2900 |
| FN |  0.7920 |  0.3320 |
| FU |  0.8889 |  0.4460 |
| FX |  0.6833 |  0.2640 |
| Fd |  0.8223 |  0.3010 |
| Ff |  0.7631 |  0.2770 |
| Fg |  0.8199 |  0.2510 |
| GC |  0.7541 |  0.2760 |
| GD |  0.8071 |  0.3110 |
| GF |  0.7941 |  0.2330 |
| GG |  0.5493 |  0.1540 |
| GH |  0.7895 |  0.2720 |
| GK |  0.8285 |  0.3170 |
| GL |  0.8458 |  0.2970 |
| GM |  0.8063 |  0.2900 |
| GN |  0.7605 |  0.3230 |
| GU |  0.9778 |  0.4930 |
| GX |  0.7542 |  0.2280 |
| Gd |  0.8156 |  0.3040 |
| Gf |  0.7813 |  0.2770 |
| Gg |  0.8125 |  0.2400 |
| HC |  0.8190 |  0.2860 |
| HD |  0.7987 |  0.3110 |
| HF |  0.7558 |  0.2290 |
| HG |  0.5739 |  0.1470 |
| HH |  0.7900 |  0.2830 |
| HK |  0.8128 |  0.3070 |
| HL |  0.8354 |  0.2900 |
| HM |  0.8268 |  0.2810 |
| HN |  0.7430 |  0.3150 |
| HU |  0.9778 |  0.4660 |
| HX |  0.6333 |  0.2130 |
| Hd |  0.8338 |  0.3130 |
| Hf |  0.8087 |  0.2770 |
| Hg |  0.8235 |  0.2530 |
| IC |  0.8117 |  0.3000 |
| ID |  0.8127 |  0.3190 |
| IF |  0.7919 |  0.2090 |
| IG |  0.5887 |  0.1470 |
| IH |  0.7772 |  0.2780 |
| IK |  0.8198 |  0.3100 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| IL |  0.8191 |  0.2860 |
| IM |  0.8038 |  0.2980 |
| IN |  0.8199 |  0.3340 |
| IU |  0.9333 |  0.4130 |
| IX |  0.5333 |  0.2020 |
| Id |  0.8357 |  0.3110 |
| If |  0.7768 |  0.2870 |
| Ig |  0.8382 |  0.2560 |
| JC |  0.8135 |  0.3040 |
| JD |  0.8006 |  0.3240 |
| JF |  0.7919 |  0.2260 |
| JG |  0.5468 |  0.1340 |
| JH |  0.7972 |  0.2810 |
| JK |  0.8023 |  0.3110 |
| JL |  0.8258 |  0.2990 |
| JM |  0.8156 |  0.2980 |
| JN |  0.7762 |  0.3380 |
| JU |  0.9556 |  0.4960 |
| JX |  0.5917 |  0.1790 |
| Jd |  0.8252 |  0.3120 |
| Jf |  0.7859 |  0.2530 |
| Jg |  0.8382 |  0.2630 |
| KC |  0.7722 |  0.2850 |
| KD |  0.8221 |  0.3120 |
| KF |  0.7558 |  0.2180 |
| KG |  0.5583 |  0.1490 |
| KH |  0.8070 |  0.2800 |
| KK |  0.8136 |  0.3140 |
| KL |  0.8073 |  0.2920 |
| KM |  0.8057 |  0.2860 |
| KN |  0.7500 |  0.3350 |
| KU |  0.9556 |  0.4320 |
| KX |  0.6000 |  0.2380 |
| Kd |  0.8396 |  0.3020 |
| Kf |  0.8223 |  0.2720 |
| Kg |  0.8419 |  0.2560 |
| LC |  0.8153 |  0.2930 |
| LD |  0.8184 |  0.3060 |
| LF |  0.8089 |  0.2360 |
| LG |  0.6232 |  0.1850 |
| LH |  0.7906 |  0.2780 |
| LK |  0.8285 |  0.3050 |







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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| LL |  0.8362 |  0.2980 |
| LM |  0.8293 |  0.2920 |
| LN |  0.7920 |  0.3200 |
| LU |  0.9778 |  0.4390 |
| LX |  0.5708 |  0.2220 |
| Ld |  0.8136 |  0.2990 |
| Lf |  0.8178 |  0.2670 |
| Lg |  0.8382 |  0.2540 |
| MC |  0.8258 |  0.3020 |
| MD |  0.8240 |  0.3130 |
| MF |  0.7622 |  0.2100 |
| MG |  0.6429 |  0.2100 |
| MH |  0.7803 |  0.2660 |
| MK |  0.8154 |  0.3140 |
| ML |  0.8480 |  0.2960 |
| MM |  0.8181 |  0.2790 |
| MN |  0.8042 |  0.3250 |
| MU |  0.9556 |  0.4300 |
| MX |  0.7208 |  0.2410 |
| Md |  0.8453 |  0.3040 |
| Mf |  0.7517 |  0.2790 |
| Mg |  0.8088 |  0.2370 |
| NG |  0.6149 |  0.1880 |
| OG |  0.6429 |  0.2060 |
| PG |  0.6461 |  0.1920 |
| VF |  0.7877 |  0.2260 |
| VG |  0.8272 |  0.2320 |
| VH |  0.6908 |  0.2720 |
| VX |  0.5583 |  0.2250 |
| WF |  0.7580 |  0.2210 |
| WG |  0.7941 |  0.2310 |
| WH |  0.6337 |  0.2520 |
| WX |  0.6042 |  0.2630 |
| XF |  0.7325 |  0.2210 |
| XG |  0.8382 |  0.2520 |
| XH |  0.5364 |  0.2570 |
| XX |  0.7583 |  0.2450 |
| YF |  0.7877 |  0.2220 |
| YG |  0.8125 |  0.2310 |
| YH |  0.6783 |  0.2530 |
| YX |  0.6875 |  0.2570 |
| ZF |  0.7452 |  0.2220 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| ZG |  0.8309 |  0.2490 |
| ZH |  0.5511 |  0.2250 |
| ZX |  0.6000 |  0.2180 |