



## Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 02:40 AM EST

PDB ID : 6X65  
EMDB ID : EMD-22070  
Title : Legionella pneumophila Dot/Icm T4SS  
Authors : Durie, C.L.; Sheedlo, M.J.; Chung, J.M.; Byrne, B.G.; Su, M.; Knight, T.; Swanson, M.S.; Lacy, D.B.; Ohi, M.D.  
Deposited on : 2020-05-27  
Resolution : 3.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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 : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

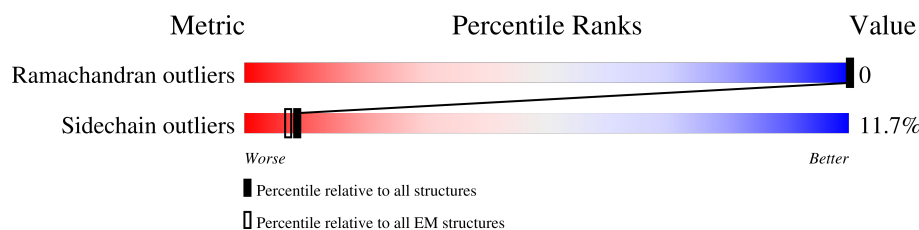
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 Å.

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





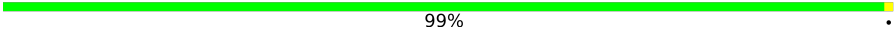




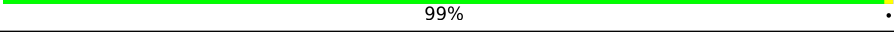




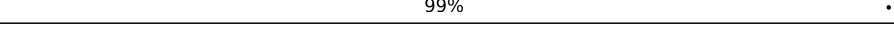




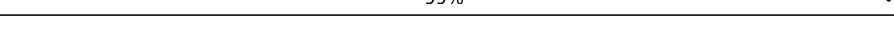

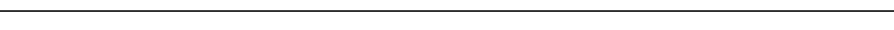

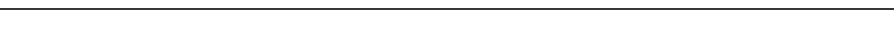
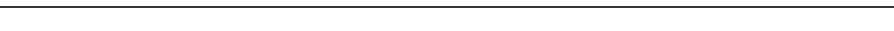


| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 154571                      | 4023                        |
| Sidechain outliers    | 154315                      | 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  $\geq 3$ , 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  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | AV    | 228    | 63% 37%          |
| 1   | AW    | 228    | 14% 86%          |
| 1   | AX    | 228    | 99% .            |
| 1   | AY    | 228    | 23% 77%          |
| 1   | AZ    | 228    | 30% . 69%        |
| 1   | BV    | 228    | 62% . 37%        |
| 1   | BW    | 228    | 14% 86%          |
| 1   | BX    | 228    | 99% .            |
| 1   | BY    | 228    | 23% 77%          |
| 1   | BZ    | 228    | 30% . 69%        |



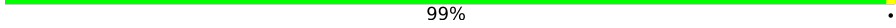

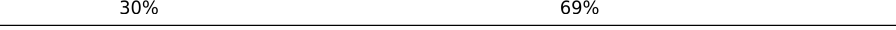
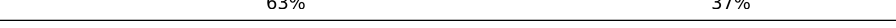

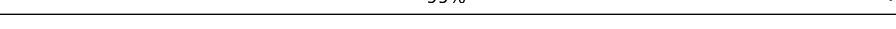
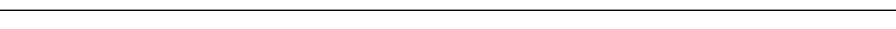
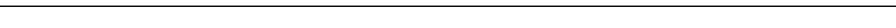






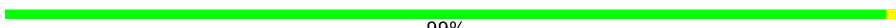




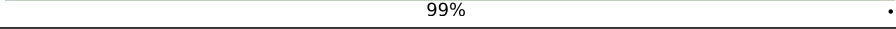



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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | CV    | 228    |    |
| 1   | CW    | 228    |    |
| 1   | CX    | 228    |    |
| 1   | CY    | 228    |    |
| 1   | CZ    | 228    |    |
| 1   | DV    | 228    |    |
| 1   | DW    | 228    |    |
| 1   | DX    | 228    |    |
| 1   | DY    | 228    |    |
| 1   | DZ    | 228    |    |
| 1   | EV    | 228    |   |
| 1   | EW    | 228    |  |
| 1   | EX    | 228    |  |
| 1   | EY    | 228    |  |
| 1   | EZ    | 228    |  |
| 1   | FV    | 228    |  |
| 1   | FW    | 228    |  |
| 1   | FX    | 228    |  |
| 1   | FY    | 228    |  |
| 1   | FZ    | 228    |  |
| 1   | GV    | 228    |  |
| 1   | GW    | 228    |  |
| 1   | GX    | 228    |  |
| 1   | GY    | 228    |  |
| 1   | GZ    | 228    |  |



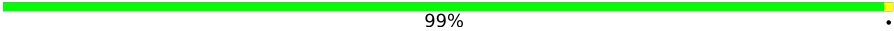








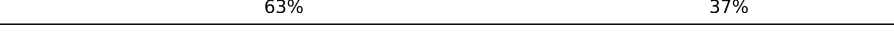







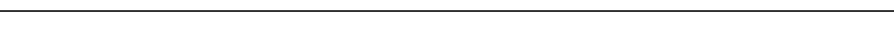

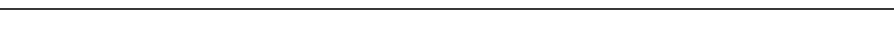
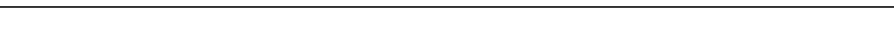


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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | HV    | 228    |  63% 37%     |
| 1   | HW    | 228    |  14% 86%     |
| 1   | HX    | 228    |  99% .       |
| 1   | HY    | 228    |  23% 77%     |
| 1   | HZ    | 228    |  30% 69%     |
| 1   | IV    | 228    |  63% 37%     |
| 1   | IW    | 228    |  14% 86%     |
| 1   | IX    | 228    |  99% .       |
| 1   | IY    | 228    |  23% 77%     |
| 1   | IZ    | 228    |  30% 69%     |
| 1   | JV    | 228    |  63% 37%     |
| 1   | JW    | 228    |  14% 86%   |
| 1   | JX    | 228    |  99% .     |
| 1   | JY    | 228    |  23% 77%   |
| 1   | JZ    | 228    |  30% 69%   |
| 1   | KV    | 228    |  63% 37%   |
| 1   | KW    | 228    |  14% 86%   |
| 1   | KX    | 228    |  99% .     |
| 1   | KY    | 228    |  23% 77%   |
| 1   | KZ    | 228    |  30% 69%   |
| 1   | LV    | 228    |  63% 37%   |
| 1   | LW    | 228    |  14% 86%   |
| 1   | LX    | 228    |  99% .     |
| 1   | LY    | 228    |  23% 77%   |
| 1   | LZ    | 228    |  30% . 69% |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | MV    | 228    |  63% 37%      |
| 1   | MW    | 228    |  14% 86%      |
| 1   | MX    | 228    |  99% .        |
| 1   | MY    | 228    |  23% 77%      |
| 1   | MZ    | 228    |  30% 69%      |
| 1   | NV    | 228    |  63% 37%      |
| 1   | NW    | 228    |  14% 86%      |
| 1   | OV    | 228    |  62% . 37%    |
| 1   | OW    | 228    |  14% 86%      |
| 1   | PV    | 228    |  63% 37%      |
| 1   | PW    | 228    |  14% 86%      |
| 1   | QV    | 228    |  63% 37%     |
| 1   | QW    | 228    |  14% 86%    |
| 1   | RV    | 228    |  63% 37%    |
| 1   | RW    | 228    |  14% 86%    |
| 2   | AC    | 303    |  62% . 34%  |
| 2   | BC    | 303    |  60% 6% 34% |
| 2   | CC    | 303    |  60% 6% 34% |
| 2   | DC    | 303    |  59% 7% 34% |
| 2   | EC    | 303    |  60% 6% 34% |
| 2   | FC    | 303    |  61% 5% 34% |
| 2   | GC    | 303    |  60% 6% 34% |
| 2   | HC    | 303    |  61% 5% 34% |
| 2   | IC    | 303    |  60% 6% 34% |
| 2   | JC    | 303    |  61% . 34%  |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | KC    | 303    |                  |
| 2   | LC    | 303    |                  |
| 2   | MC    | 303    |                  |
| 3   | AD    | 163    |                  |
| 3   | Ad    | 163    |                  |
| 3   | BD    | 163    |                  |
| 3   | Bd    | 163    |                  |
| 3   | CD    | 163    |                  |
| 3   | Cd    | 163    |                  |
| 3   | DD    | 163    |                  |
| 3   | Dd    | 163    |                  |
| 3   | ED    | 163    |                  |
| 3   | Ed    | 163    |                  |
| 3   | FD    | 163    |                  |
| 3   | Fd    | 163    |                  |
| 3   | GD    | 163    |                  |
| 3   | Gd    | 163    |                  |
| 3   | HD    | 163    |                  |
| 3   | Hd    | 163    |                  |
| 3   | ID    | 163    |                  |
| 3   | Id    | 163    |                  |
| 3   | JD    | 163    |                  |
| 3   | Jd    | 163    |                  |
| 3   | KD    | 163    |                  |
| 3   | Kd    | 163    |                  |







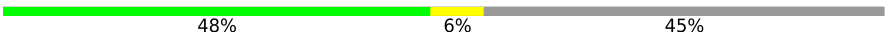

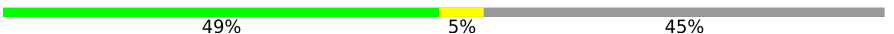

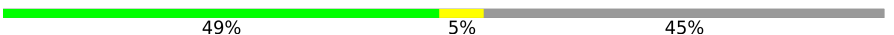
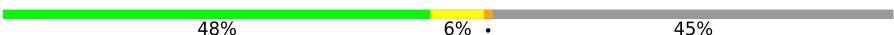
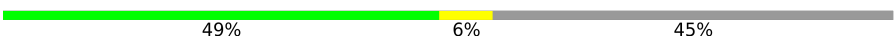





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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 3   | LD    | 163    |    |
| 3   | Ld    | 163    |    |
| 3   | MD    | 163    |    |
| 3   | Md    | 163    |    |
| 4   | AH    | 361    |    |
| 4   | BH    | 361    |    |
| 4   | CH    | 361    |    |
| 4   | DH    | 361    |    |
| 4   | EH    | 361    |    |
| 4   | FH    | 361    |    |
| 4   | GH    | 361    |    |
| 4   | HH    | 361    |   |
| 4   | IH    | 361    |  |
| 4   | JH    | 361    |  |
| 4   | KH    | 361    |  |
| 4   | LH    | 361    |  |
| 4   | MH    | 361    |  |
| 5   | AK    | 189    |  |
| 5   | BK    | 189    |  |
| 5   | CK    | 189    |  |
| 5   | DK    | 189    |  |
| 5   | EK    | 189    |  |
| 5   | FK    | 189    |  |
| 5   | GK    | 189    |  |
| 5   | HK    | 189    |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 5   | IK    | 189    |  71%7%22%    |
| 5   | JK    | 189    |  69%9%22%    |
| 5   | KK    | 189    |  70%8%22%    |
| 5   | LK    | 189    |  70%8%22%    |
| 5   | MK    | 189    |  71%7%22%    |
| 6   | N     | 249    |  50%. .45%   |
| 6   | O     | 249    |  48%6%45%    |
| 6   | P     | 249    |  51%.45%     |
| 6   | Q     | 249    |  49%5%45%    |
| 6   | R     | 249    |  51%.45%     |
| 6   | S     | 249    |  49%5%45%    |
| 6   | T     | 249    |  48%6%.45%  |
| 6   | U     | 249    |  49%6%45%  |
| 6   | V     | 249    |  50%.45%   |
| 6   | W     | 249    |  50%.45%   |
| 6   | X     | 249    |  50%.45%   |
| 6   | Y     | 249    |  51%. .45% |
| 6   | Z     | 249    |  49%5%45%  |



## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 124910 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 Type IV secretion system unknown protein fragment.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 1   | AV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | AW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | BV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | BW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | CV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | CW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | DV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | DW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | EV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | EW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | FV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | FW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | GV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | GW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | HV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | HW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | IV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 1   | IW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | JV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | JW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | KV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | KW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | LV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | LW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | MV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | MW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | NV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | NW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | OV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | OW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | PV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | PW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | QV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | QW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | RV    | 144      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 720   | 432 | 144 | 144 |         |       |
| 1   | RW    | 32       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 160   | 96  | 32  | 32  |         |       |
| 1   | AX    | 228      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1140  | 684 | 228 | 228 |         |       |
| 1   | AY    | 52       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 260   | 156 | 52  | 52  |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 1   | AZ    | 70       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 350   | 210 | 70  | 70  |         |       |
| 1   | BX    | 228      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1140  | 684 | 228 | 228 |         |       |
| 1   | BY    | 52       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 260   | 156 | 52  | 52  |         |       |
| 1   | BZ    | 70       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 350   | 210 | 70  | 70  |         |       |
| 1   | CX    | 228      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1140  | 684 | 228 | 228 |         |       |
| 1   | CY    | 52       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 260   | 156 | 52  | 52  |         |       |
| 1   | CZ    | 70       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 350   | 210 | 70  | 70  |         |       |
| 1   | DX    | 228      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1140  | 684 | 228 | 228 |         |       |
| 1   | DY    | 52       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 260   | 156 | 52  | 52  |         |       |
| 1   | DZ    | 70       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 350   | 210 | 70  | 70  |         |       |
| 1   | EX    | 228      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1140  | 684 | 228 | 228 |         |       |
| 1   | EY    | 52       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 260   | 156 | 52  | 52  |         |       |
| 1   | EZ    | 70       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 350   | 210 | 70  | 70  |         |       |
| 1   | FX    | 228      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1140  | 684 | 228 | 228 |         |       |
| 1   | FY    | 52       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 260   | 156 | 52  | 52  |         |       |
| 1   | FZ    | 70       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 350   | 210 | 70  | 70  |         |       |
| 1   | GX    | 228      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1140  | 684 | 228 | 228 |         |       |
| 1   | GY    | 52       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 260   | 156 | 52  | 52  |         |       |
| 1   | GZ    | 70       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 350   | 210 | 70  | 70  |         |       |
| 1   | HX    | 228      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1140  | 684 | 228 | 228 |         |       |
| 1   | HY    | 52       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 260   | 156 | 52  | 52  |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 1   | HZ    | 70       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 350   | 210 | 70  | 70  |         |       |
| 1   | IX    | 228      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1140  | 684 | 228 | 228 |         |       |
| 1   | IY    | 52       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 260   | 156 | 52  | 52  |         |       |
| 1   | IZ    | 70       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 350   | 210 | 70  | 70  |         |       |
| 1   | JX    | 228      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1140  | 684 | 228 | 228 |         |       |
| 1   | JY    | 52       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 260   | 156 | 52  | 52  |         |       |
| 1   | JZ    | 70       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 350   | 210 | 70  | 70  |         |       |
| 1   | KX    | 228      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1140  | 684 | 228 | 228 |         |       |
| 1   | KY    | 52       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 260   | 156 | 52  | 52  |         |       |
| 1   | KZ    | 70       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 350   | 210 | 70  | 70  |         |       |
| 1   | LX    | 228      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1140  | 684 | 228 | 228 |         |       |
| 1   | LY    | 52       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 260   | 156 | 52  | 52  |         |       |
| 1   | LZ    | 70       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 350   | 210 | 70  | 70  |         |       |
| 1   | MX    | 228      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1140  | 684 | 228 | 228 |         |       |
| 1   | MY    | 52       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 260   | 156 | 52  | 52  |         |       |
| 1   | MZ    | 70       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 350   | 210 | 70  | 70  |         |       |

- Molecule 2 is a protein called DotC.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | AC    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1016 | 280 | 295 | 5 |         |       |
| 2   | BC    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1016 | 280 | 295 | 5 |         |       |
| 2   | CC    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1016 | 280 | 295 | 5 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | DC    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1016 | 280 | 295 | 5 |         |       |
| 2   | EC    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1016 | 280 | 295 | 5 |         |       |
| 2   | FC    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1016 | 280 | 295 | 5 |         |       |
| 2   | GC    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1016 | 280 | 295 | 5 |         |       |
| 2   | HC    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1016 | 280 | 295 | 5 |         |       |
| 2   | IC    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1016 | 280 | 295 | 5 |         |       |
| 2   | JC    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1016 | 280 | 295 | 5 |         |       |
| 2   | KC    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1016 | 280 | 295 | 5 |         |       |
| 2   | LC    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1016 | 280 | 295 | 5 |         |       |
| 2   | MC    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1596  | 1016 | 280 | 295 | 5 |         |       |

- Molecule 3 is a protein called DotD.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | AD    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 660 | 178 | 200 | 2 |         |       |
| 3   | Ad    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 678 | 183 | 203 | 2 |         |       |
| 3   | BD    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 660 | 178 | 200 | 2 |         |       |
| 3   | Bd    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 678 | 183 | 203 | 2 |         |       |
| 3   | CD    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 660 | 178 | 200 | 2 |         |       |
| 3   | Cd    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 678 | 183 | 203 | 2 |         |       |
| 3   | DD    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 660 | 178 | 200 | 2 |         |       |
| 3   | Dd    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 678 | 183 | 203 | 2 |         |       |
| 3   | ED    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 660 | 178 | 200 | 2 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | Ed    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 678 | 183 | 203 | 2 |         |       |
| 3   | FD    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 660 | 178 | 200 | 2 |         |       |
| 3   | Fd    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 678 | 183 | 203 | 2 |         |       |
| 3   | GD    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 660 | 178 | 200 | 2 |         |       |
| 3   | Gd    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 678 | 183 | 203 | 2 |         |       |
| 3   | HD    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 660 | 178 | 200 | 2 |         |       |
| 3   | Hd    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 678 | 183 | 203 | 2 |         |       |
| 3   | ID    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 660 | 178 | 200 | 2 |         |       |
| 3   | Id    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 678 | 183 | 203 | 2 |         |       |
| 3   | JD    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 660 | 178 | 200 | 2 |         |       |
| 3   | Jd    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 678 | 183 | 203 | 2 |         |       |
| 3   | KD    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 660 | 178 | 200 | 2 |         |       |
| 3   | Kd    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 678 | 183 | 203 | 2 |         |       |
| 3   | LD    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 660 | 178 | 200 | 2 |         |       |
| 3   | Ld    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 678 | 183 | 203 | 2 |         |       |
| 3   | MD    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 660 | 178 | 200 | 2 |         |       |
| 3   | Md    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 678 | 183 | 203 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | AH    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 678   | 432 | 119 | 123 | 4 |         |       |
| 4   | BH    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 678   | 432 | 119 | 123 | 4 |         |       |

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| Mol | Chain | Residues | Atoms        |          |          |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 4   | CH    | 89       | Total<br>678 | C<br>432 | N<br>119 | O<br>123 | S<br>4 | 0       | 0     |
| 4   | DH    | 89       | Total<br>678 | C<br>432 | N<br>119 | O<br>123 | S<br>4 | 0       | 0     |
| 4   | EH    | 89       | Total<br>678 | C<br>432 | N<br>119 | O<br>123 | S<br>4 | 0       | 0     |
| 4   | FH    | 89       | Total<br>678 | C<br>432 | N<br>119 | O<br>123 | S<br>4 | 0       | 0     |
| 4   | GH    | 89       | Total<br>678 | C<br>432 | N<br>119 | O<br>123 | S<br>4 | 0       | 0     |
| 4   | HH    | 89       | Total<br>678 | C<br>432 | N<br>119 | O<br>123 | S<br>4 | 0       | 0     |
| 4   | IH    | 89       | Total<br>678 | C<br>432 | N<br>119 | O<br>123 | S<br>4 | 0       | 0     |
| 4   | JH    | 89       | Total<br>678 | C<br>432 | N<br>119 | O<br>123 | S<br>4 | 0       | 0     |
| 4   | KH    | 89       | Total<br>678 | C<br>432 | N<br>119 | O<br>123 | S<br>4 | 0       | 0     |
| 4   | LH    | 89       | Total<br>678 | C<br>432 | N<br>119 | O<br>123 | S<br>4 | 0       | 0     |
| 4   | MH    | 89       | Total<br>678 | C<br>432 | N<br>119 | O<br>123 | S<br>4 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms         |          |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| 5   | AK    | 148      | Total<br>1152 | C<br>731 | N<br>205 | O<br>212 | S<br>4 | 0       | 0     |
| 5   | BK    | 148      | Total<br>1152 | C<br>731 | N<br>205 | O<br>212 | S<br>4 | 0       | 0     |
| 5   | CK    | 148      | Total<br>1152 | C<br>731 | N<br>205 | O<br>212 | S<br>4 | 0       | 0     |
| 5   | DK    | 148      | Total<br>1152 | C<br>731 | N<br>205 | O<br>212 | S<br>4 | 0       | 0     |
| 5   | EK    | 148      | Total<br>1152 | C<br>731 | N<br>205 | O<br>212 | S<br>4 | 0       | 0     |
| 5   | FK    | 148      | Total<br>1152 | C<br>731 | N<br>205 | O<br>212 | S<br>4 | 0       | 0     |
| 5   | GK    | 148      | Total<br>1152 | C<br>731 | N<br>205 | O<br>212 | S<br>4 | 0       | 0     |
| 5   | HK    | 148      | Total<br>1152 | C<br>731 | N<br>205 | O<br>212 | S<br>4 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | IK    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 731 | 205 | 212 | 4 |         |       |
| 5   | JK    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 731 | 205 | 212 | 4 |         |       |
| 5   | KK    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 731 | 205 | 212 | 4 |         |       |
| 5   | LK    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 731 | 205 | 212 | 4 |         |       |
| 5   | MK    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 731 | 205 | 212 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | N     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 201 | 202 | 4 |         |       |
| 6   | O     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 201 | 202 | 4 |         |       |
| 6   | P     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 201 | 202 | 4 |         |       |
| 6   | Q     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 201 | 202 | 4 |         |       |
| 6   | R     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 201 | 202 | 4 |         |       |
| 6   | S     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 201 | 202 | 4 |         |       |
| 6   | T     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 201 | 202 | 4 |         |       |
| 6   | U     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 201 | 202 | 4 |         |       |
| 6   | V     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 201 | 202 | 4 |         |       |
| 6   | W     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 201 | 202 | 4 |         |       |
| 6   | X     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 201 | 202 | 4 |         |       |
| 6   | Y     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 201 | 202 | 4 |         |       |
| 6   | Z     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 701 | 201 | 202 | 4 |         |       |



### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

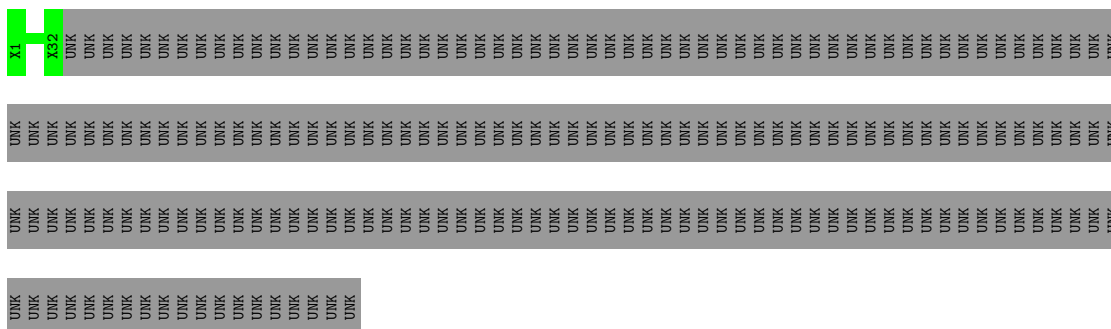
- Molecule 1: Type IV secretion system unknown protein fragment

Chain AV:  63% 37%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain AW:  14% 86%



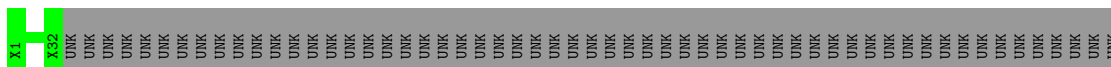
- Molecule 1: Type IV secretion system unknown protein fragment

Chain BV:  62% 37%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain BW:  14% 86%



UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

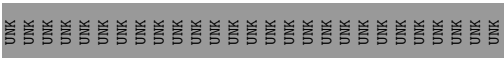
[illegible][illegible]

UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

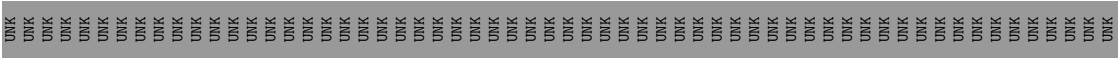
[illegible][illegible]



● Molecule 1: Type IV secretion system unknown protein fragment



● Molecule 1: Type IV secretion system unknown protein fragment



● Molecule 1: Type IV secretion system unknown protein fragment



● Molecule 1: Type IV secretion system unknown protein fragment





- Molecule 1: Type IV secretion system unknown protein fragment

Chain IV:  63% 37%



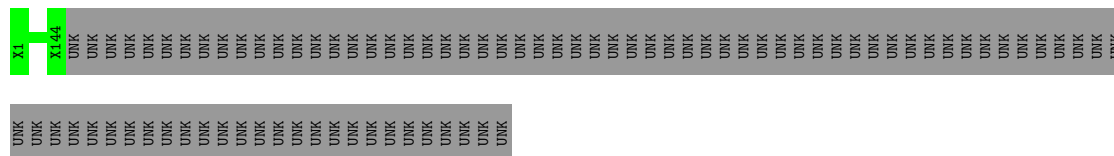
- Molecule 1: Type IV secretion system unknown protein fragment

Chain IW:  14% 86%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain JV:  63% 37%

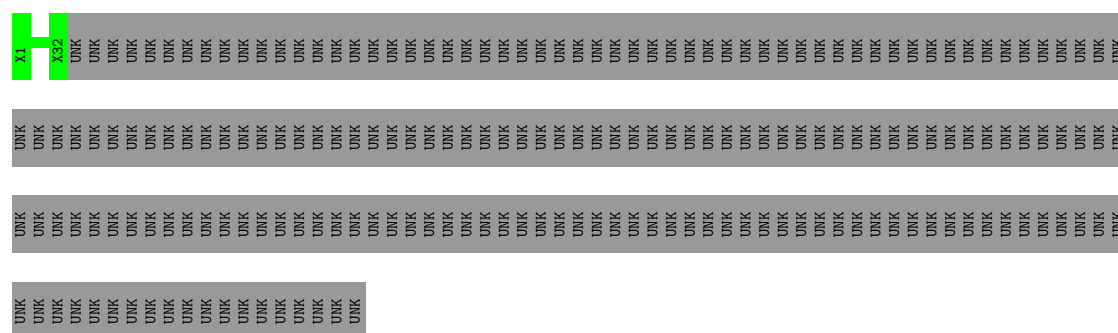
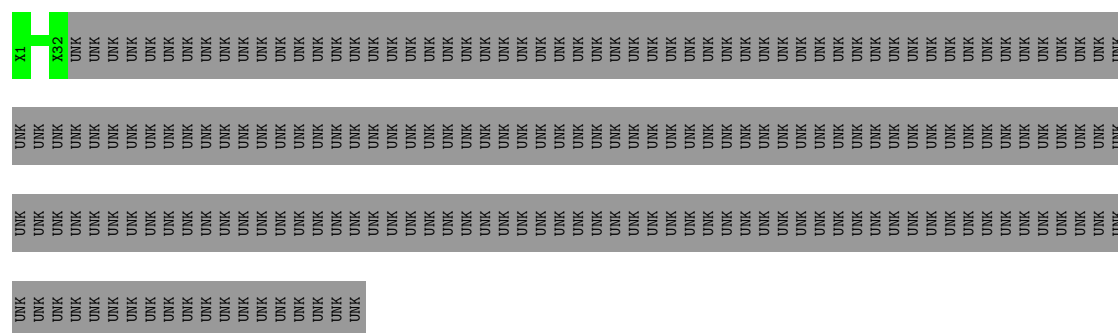


- Molecule 1: Type IV secretion system unknown protein fragment

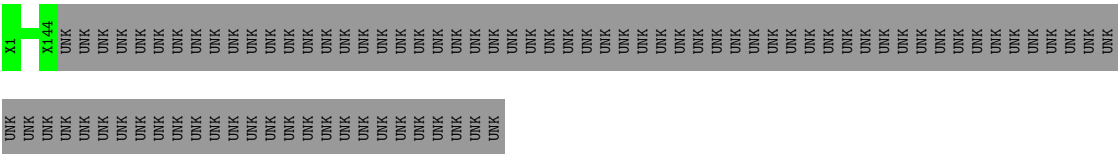
Chain JW:  14% 86%



- Molecule 1: Type IV secretion system unknown protein fragment



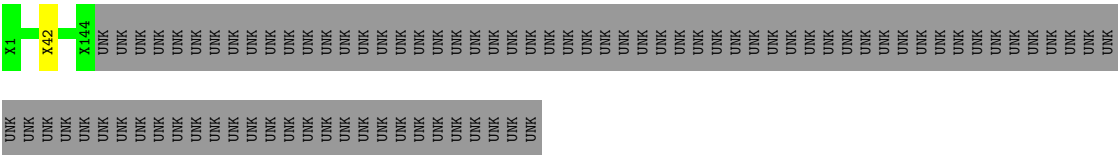
Chain MV:  63% 37%



• Molecule 1: Type IV secretion system unknown protein fragment



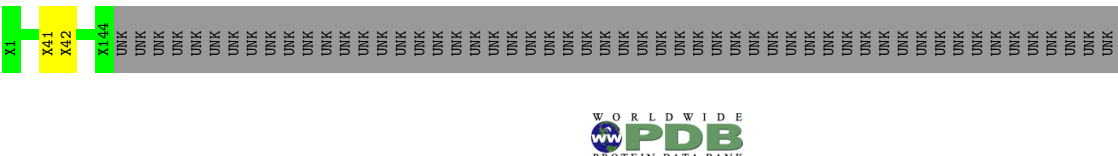
• Molecule 1: Type IV secretion system unknown protein fragment

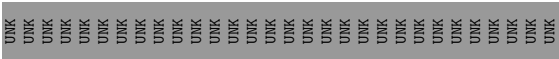


• Molecule 1: Type IV secretion system unknown protein fragment

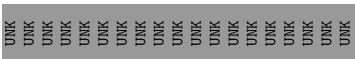
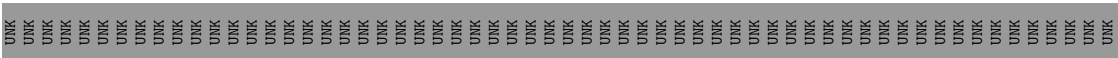
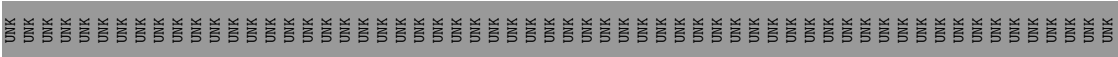


• Molecule 1: Type IV secretion system unknown protein fragment





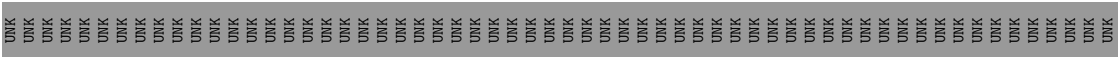
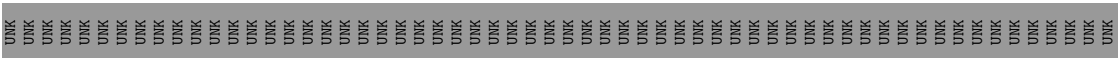
• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment



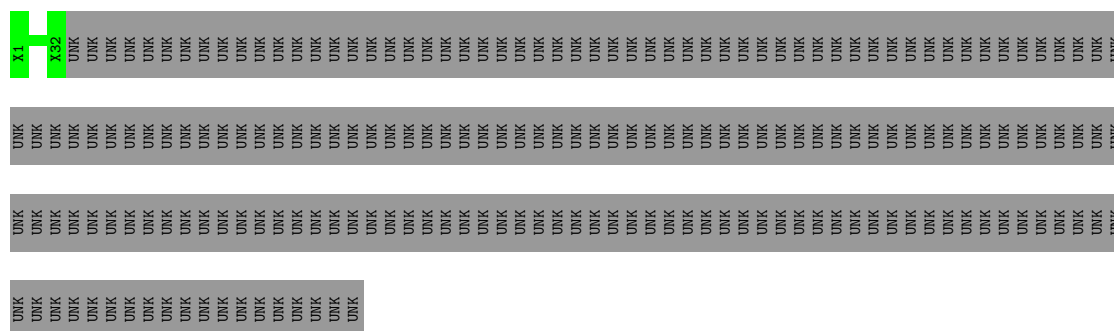
• Molecule 1: Type IV secretion system unknown protein fragment





- Molecule 1: Type IV secretion system unknown protein fragment

Chain QW:  14% 86%



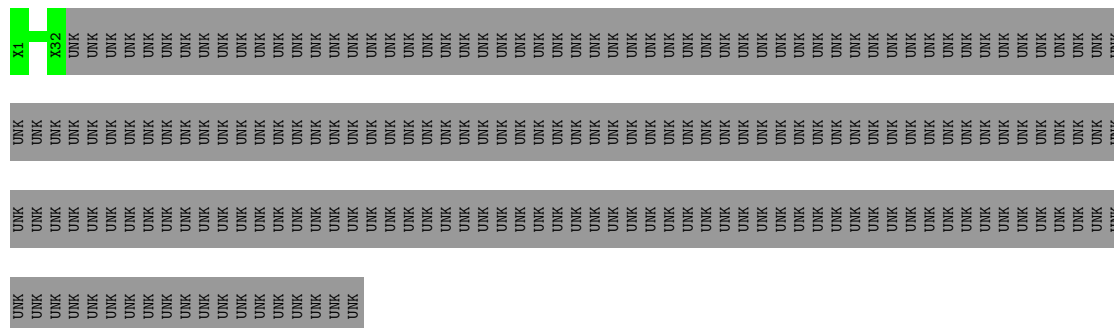
- Molecule 1: Type IV secretion system unknown protein fragment

Chain RV:  63% 37%



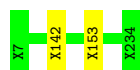
- Molecule 1: Type IV secretion system unknown protein fragment

Chain RW:  14% 86%



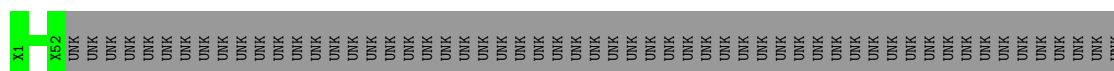
- Molecule 1: Type IV secretion system unknown protein fragment

Chain AX:  99%



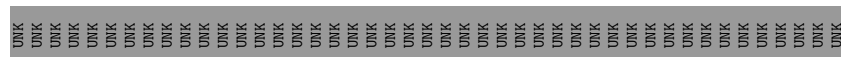
- Molecule 1: Type IV secretion system unknown protein fragment

Chain AY:  23% 77%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain AZ:  30% 69%



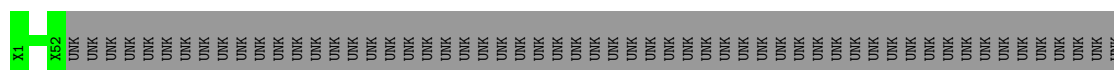
- Molecule 1: Type IV secretion system unknown protein fragment

Chain BX:  99%



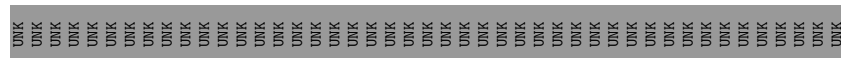
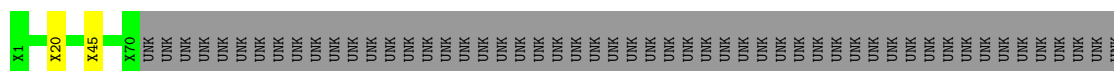
- Molecule 1: Type IV secretion system unknown protein fragment

Chain BY:  23% 77%



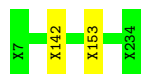
- Molecule 1: Type IV secretion system unknown protein fragment

Chain BZ:  30% 69%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain CX:  99%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain CY:  23%  77%



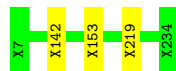
- Molecule 1: Type IV secretion system unknown protein fragment

Chain CZ:  30%  69%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain DX:  99%



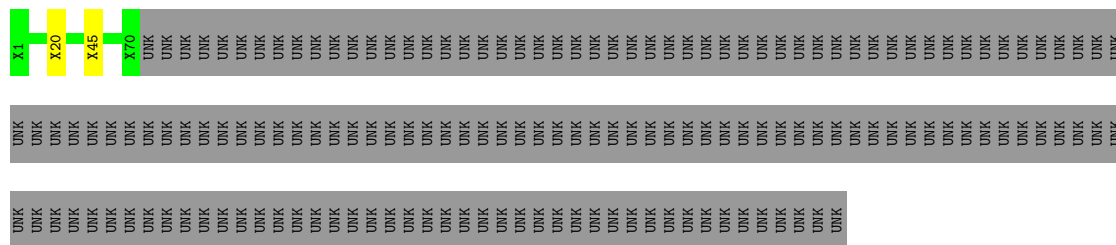
- Molecule 1: Type IV secretion system unknown protein fragment

Chain DY:  23%  77%



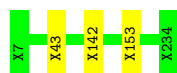
- Molecule 1: Type IV secretion system unknown protein fragment

Chain DZ:  30% 69%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain EX:  99%



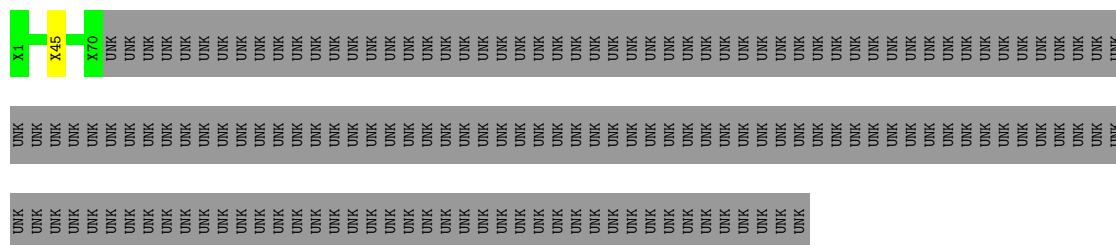
- Molecule 1: Type IV secretion system unknown protein fragment

Chain EY:  23% 77%



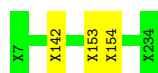
- Molecule 1: Type IV secretion system unknown protein fragment

Chain EZ:  30% 69%



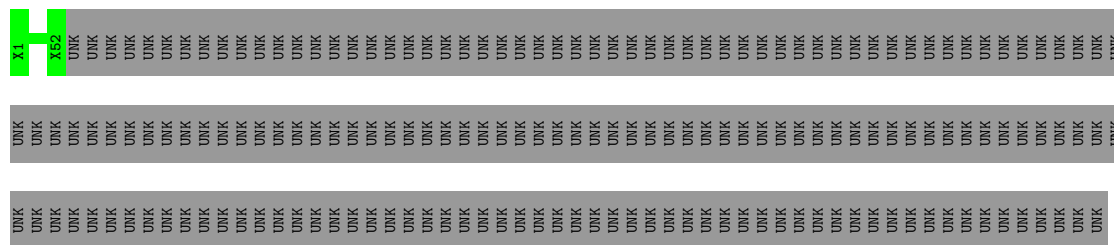
- Molecule 1: Type IV secretion system unknown protein fragment

Chain FX:  99%



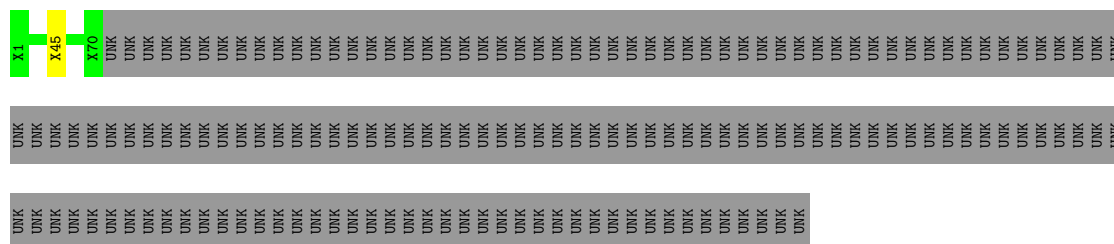
- Molecule 1: Type IV secretion system unknown protein fragment

Chain FY:  23% 77%



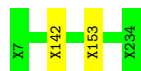
- Molecule 1: Type IV secretion system unknown protein fragment

Chain FZ:  30% 69%



- Molecule 1: Type IV secretion system unknown protein fragment

Chain GX:  99%



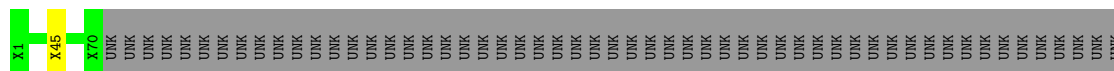
- Molecule 1: Type IV secretion system unknown protein fragment

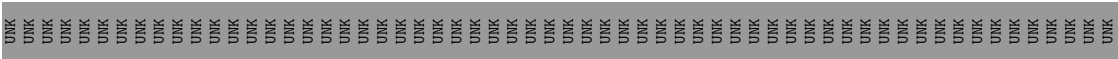
Chain GY:  23% 77%



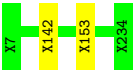
- Molecule 1: Type IV secretion system unknown protein fragment

Chain GZ:  30% 69%

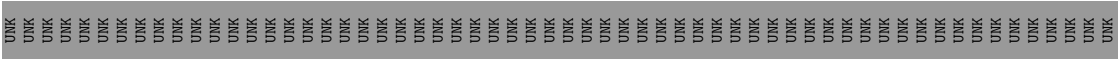




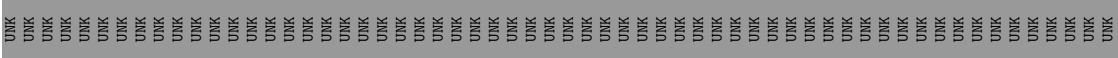
• Molecule 1: Type IV secretion system unknown protein fragment



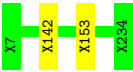
• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment



• Molecule 1: Type IV secretion system unknown protein fragment



**UNK**

- Chain IZ:  30% 69%

**UNK**

[illegible]

- Chain JX: 

- Molecule 1: Type IV secretion system unknown protein fragment

Chain JY:  23% 77%

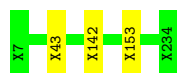
[illegible][illegible]

- Chain JZ:  30% 69%

[illegible][illegible]

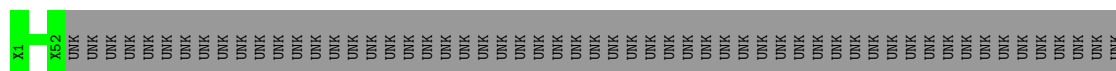
- Molecule 1: Type IV secretion system unknown protein fragment

Chain KX:  99% .



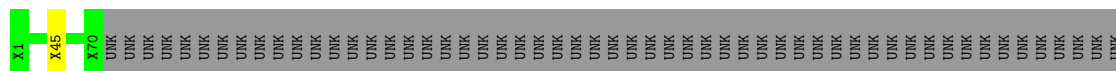
- Molecule 1: Type IV secretion system unknown protein fragment

Chain KY:  23%  77%



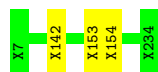
- Molecule 1: Type IV secretion system unknown protein fragment

Chain KZ:  30%  69%



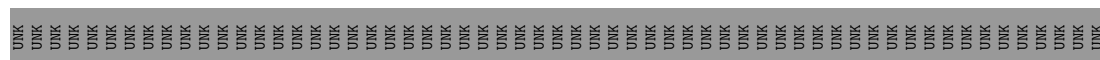
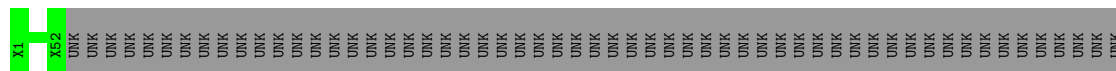
- Molecule 1: Type IV secretion system unknown protein fragment

Chain LX:  99% .



- Molecule 1: Type IV secretion system unknown protein fragment

Chain LY:  23%  77%



- Molecule 1: Type IV secretion system unknown protein fragment



[illegible]

- Chain MX:  99%

A diagram showing a sequence of five nodes: X7, X43, X142, X153, and X234. X7 and X234 are green, while X43, X142, and X153 are yellow. They are connected by horizontal lines.

- Chain MY:  23% 77%

[illegible]

- Chain MZ:  30% 69%

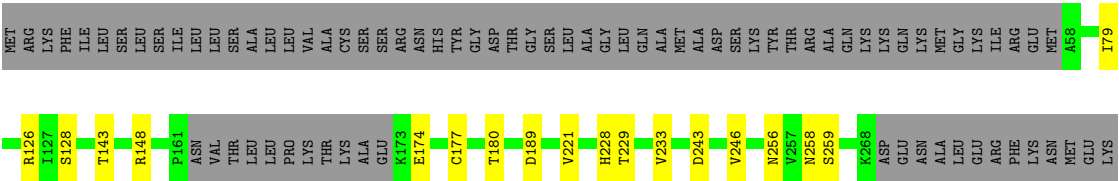
[illegible]

- Chain AC: 

[illegible]

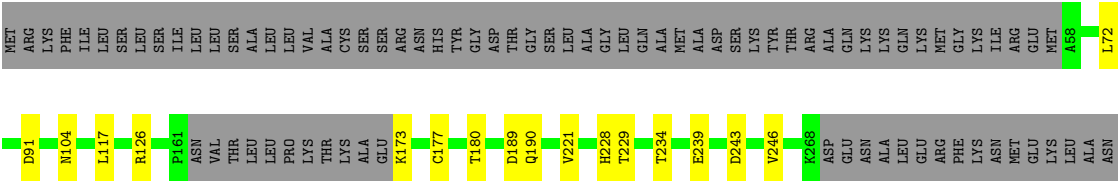
SER  
TRP  
GLN  
PRO  
ILE  
ALA  
PRO  
VAL  
SER

• Molecule 2: DotC



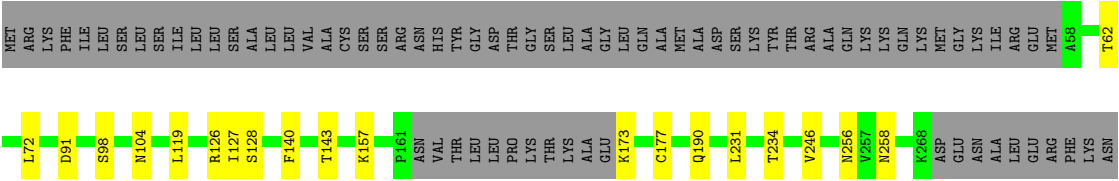
LEU  
ALA  
ASN  
GLN  
ALA  
LYS  
ILE  
VAL  
ILE  
ILE  
THR  
ASN  
SER  
TRP  
GLN  
PRO  
ILE  
ILE  
ALA  
PRO  
VAL  
SER

• Molecule 2: DotC



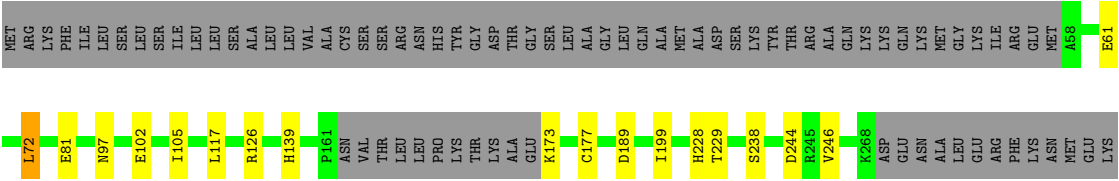
GLN  
ALA  
LYS  
ILE  
VAL  
ILE  
THR  
ASN  
SER  
TRP  
GLN  
PRO  
ILE  
ILE  
ALA  
PRO  
VAL  
SER

• Molecule 2: DotC



MET  
GLU  
LYS  
LEU  
ALA  
ASN  
GLN  
ALA  
LYS  
ILE  
ILE  
VAL  
THR  
ASN  
LYS  
TRP  
GLN  
PRO  
ILE  
ILE  
ALA  
PRO  
VAL  
SER

• Molecule 2: DotC





LEU  
ALA  
ASN  
GLN  
ALA  
LYS  
ILE  
ILE  
VAL  
THR  
ASN  
LEU  
LYS  
SER  
TRP  
GLN  
LEU  
ILE  
ILE  
ALA  
PRO  
VAL  
SER

• Molecule 2: DotC



MET ARG LYS PHE ILE LEU SER LEU LEU ILE ILE THR ASN LEU LEU SER ALA LEU LEU VAL ALA CYS SER SER ARG ASN HIS TYR GLY ASP THR GLY SER LEU ALA LEU LEU GLN MET ALA ASP SER LYS TYR THR ARG ALA GLN LYS LYS MET GLN LYS MET GLY LYS ILE ARG MET A58 E61

L90 T143 Q149 P161 VAL THR LEU LEU PRO LYS THR LYS ALA CYS K173 C177 T180 E181 D189 L211 H228 T229 V246 N258 K268 ASP GLU ASN ALA LEU ARG PHE LYS ASN MET GLU LYS LEU ALA ASN GLN ALA LYS ILE VAL ILE

THR ASN LYS SER TRP PRO ILE ILE ALA PRO VAL SER

• Molecule 2: DotC



MET ARG LYS PHE ILE SER LEU SER LEU ILE ILE THR ASN LEU LEU SER ALA LEU LEU VAL ALA CYS SER SER ARG ASN HIS TYR GLY ASP THR GLY SER LEU ALA LEU GLN MET ALA ASP SER LYS TYR THR ARG ALA GLN LYS LYS MET GLU LYS MET GLY LYS ILE ARG MET A58 E61

L64 K85 R130 H139 K157 P161 ASN VAL THR LEU LEU PRO LYS THR LYS ALA CYS K173 C177 T180 Q190 H228 E239 D243 V246 N256 V257 N258 V266 K267 K268 ASP GLU ASN ALA LEU ARG PHE LYS ASN MET GLU LYS ILE VAL ILE

ALA ASN GLN ALA LYS ILE VAL THR ASN LYS SER TRP GLN PRO ILE ILE ALA PRO VAL SER

• Molecule 2: DotC



MET ARG LYS PHE ILE LEU SER LEU SER LEU ILE ILE THR ASN LEU LEU SER ALA LEU LEU VAL ALA CYS SER SER ARG ASN HIS TYR GLY ASP THR GLY SER LEU ALA LEU GLN MET ALA ASP SER LYS TYR THR ARG ALA GLN LYS LYS MET GLU LYS MET GLY LYS ILE ARG MET A58 E81

N104 T116 V134 M153 P161 ASN VAL THR LEU LEU PRO LYS THR LYS ALA CYS K173 C177 T180 D189 V221 H228 T229 D243 D244 R245 V246 N256 K268 ASP GLU ASN ALA LEU ARG PHE LYS ASN MET GLU LYS LEU ALA ASN GLN ALA


LYS ILE VAL ILE THR ASN LYS SER TRP GLN PRO ILE ILE ALA PRO VAL SER

• Molecule 2: DotC



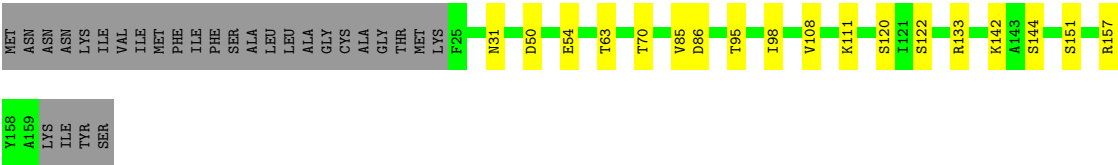
MET ARG LYS PHE ILE LEU SER LEU SER LEU ILE ILE THR ASN LEU LEU SER ALA LEU LEU VAL ALA CYS SER SER ARG ASN HIS TYR GLY ASP THR GLY SER LEU ALA LEU GLN MET ALA ASP SER LYS TYR THR ARG ALA GLN LYS LYS MET GLU LYS MET GLY LYS ILE ARG MET A58 L72

D91 R126 V134 T143 P161 ASN VAL THR LEU LEU PRO LYS THR LYS ALA CYS K173 C177 L211 H228 T229 D243 V246 L255 N258 K268 ASP GLU ASN ALA LEU ARG PHE LYS LYS MET GLU LYS LEU ALA ASN GLN ALA LYS ILE VAL

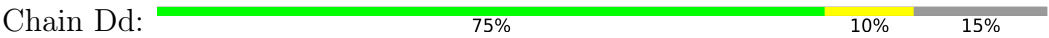
Chain Cd: 



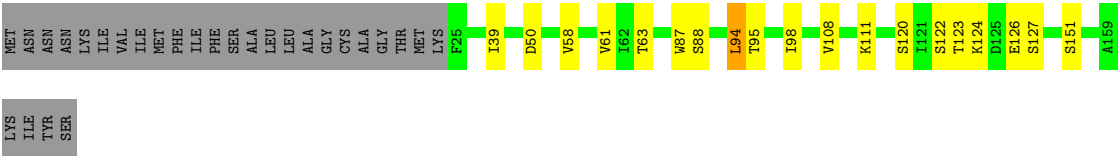
• Molecule 3: DotD



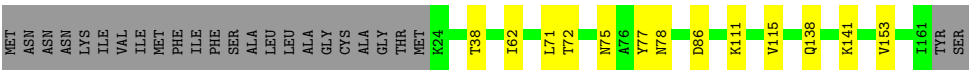
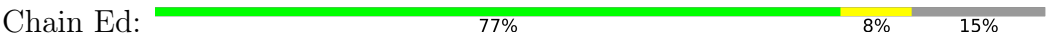
• Molecule 3: DotD



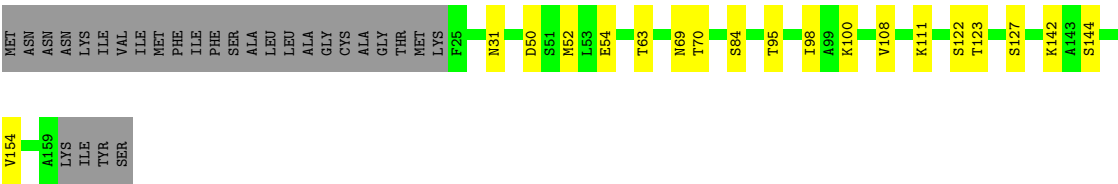
• Molecule 3: DotD



• Molecule 3: DotD

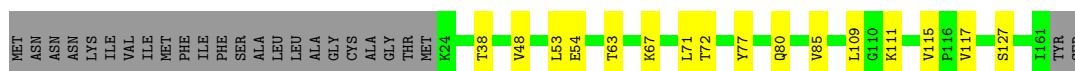


• Molecule 3: DotD

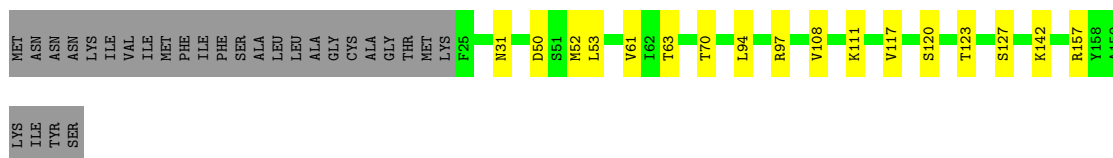
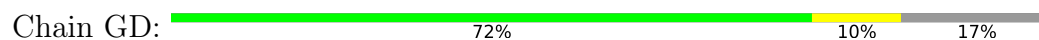


• Molecule 3: DotD

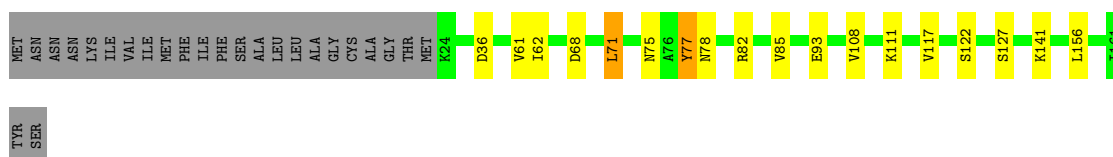
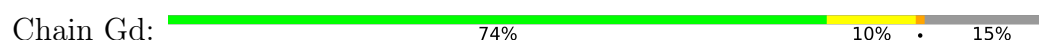




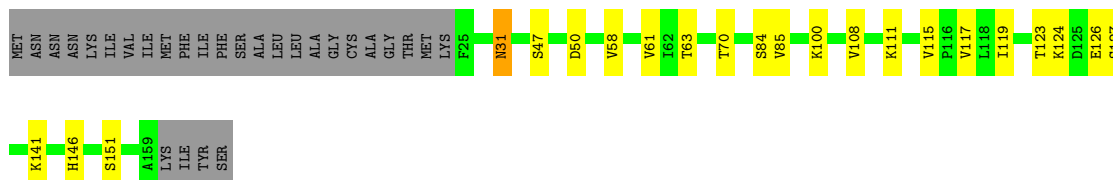
• Molecule 3: DotD



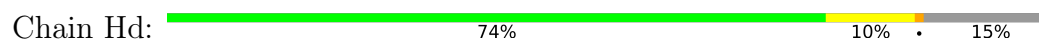
• Molecule 3: DotD



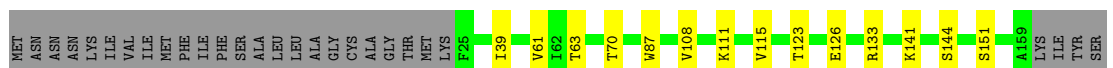
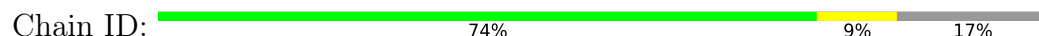
• Molecule 3: DotD



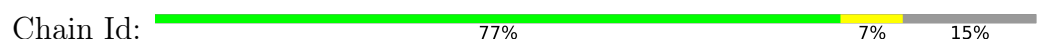
• Molecule 3: DotD



• Molecule 3: DotD

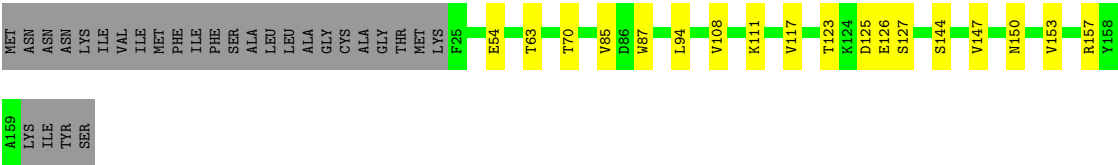


• Molecule 3: DotD





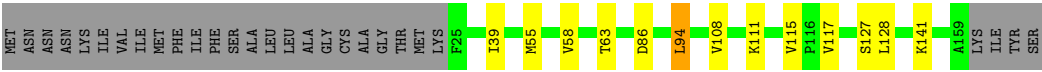
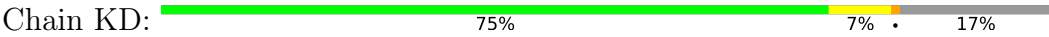
• Molecule 3: DotD



• Molecule 3: DotD



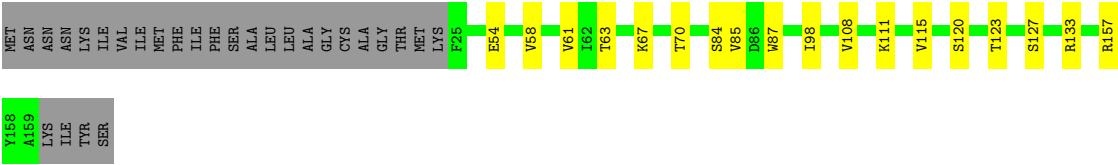
• Molecule 3: DotD



• Molecule 3: DotD



• Molecule 3: DotD



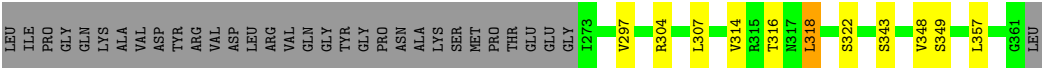
• Molecule 3: DotD



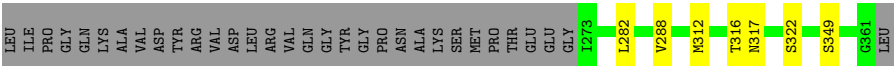
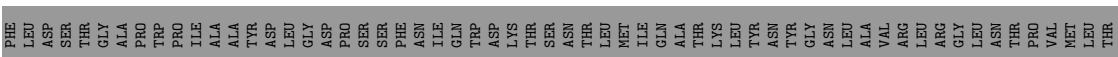
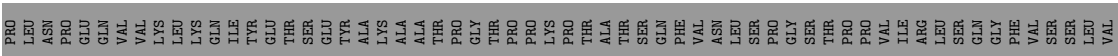
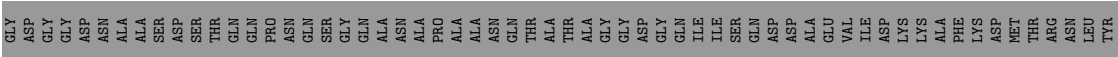
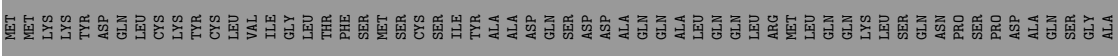




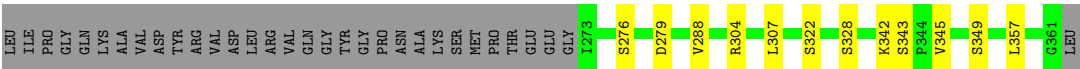
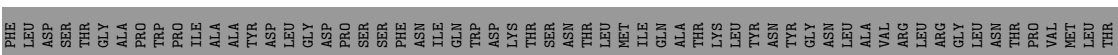
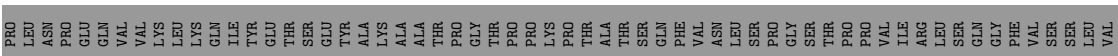
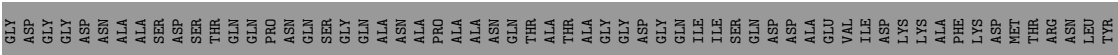
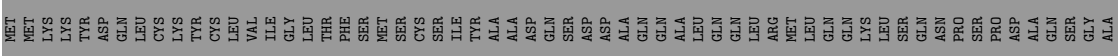




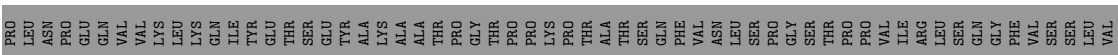
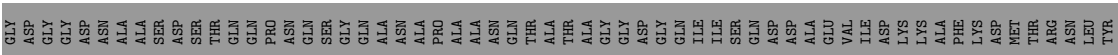
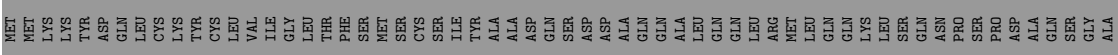
• Molecule 4: Type IV secretion protein IcmK



• Molecule 4: Type IV secretion protein IcmK

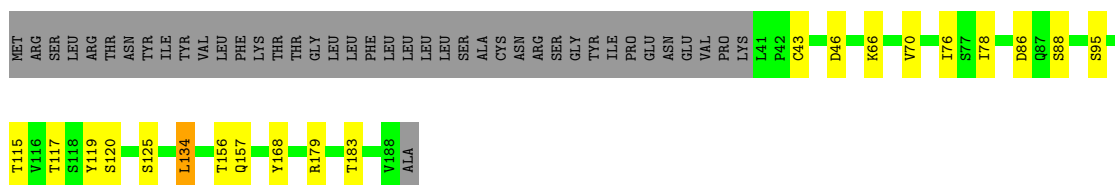


• Molecule 4: Type IV secretion protein IcmK



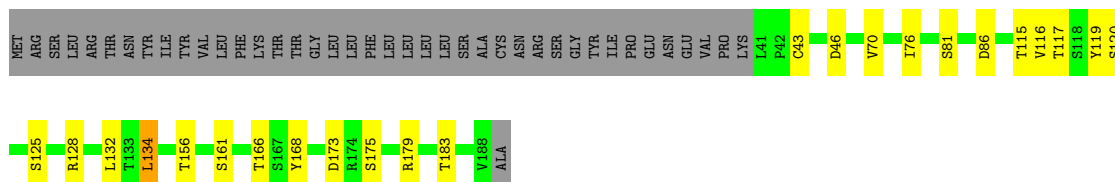






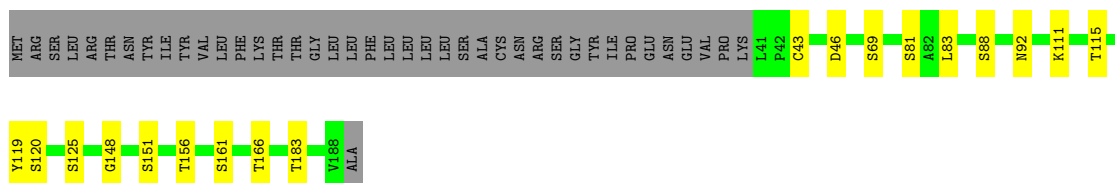
- Molecule 5: Inner membrane lipoprotein YiaD

Chain CK: 66% 12% 22%



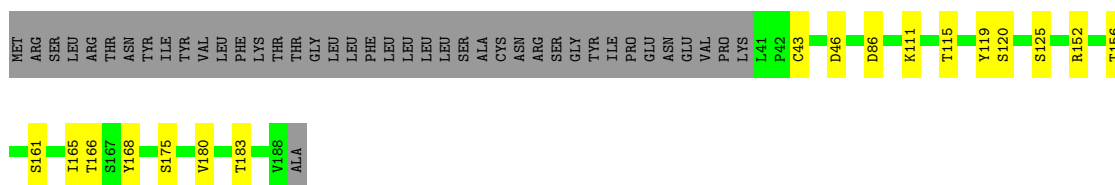
- Molecule 5: Inner membrane lipoprotein YiaD

Chain DK: 69% 10% 22%



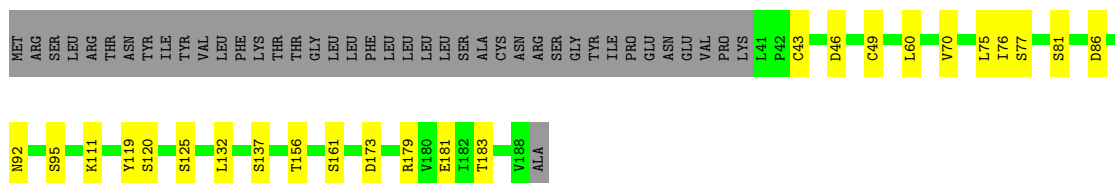
- Molecule 5: Inner membrane lipoprotein YiaD

Chain EK: 69% 9% 22%



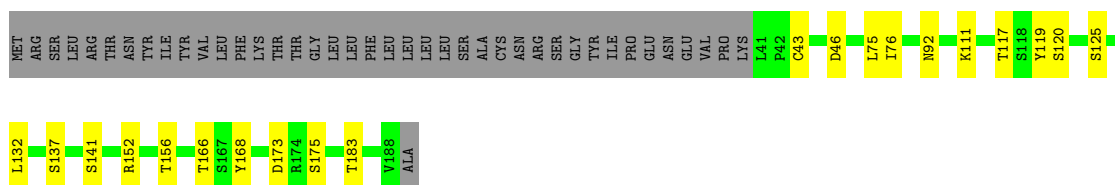
- Molecule 5: Inner membrane lipoprotein YiaD

Chain FK: 66% 13% 22%



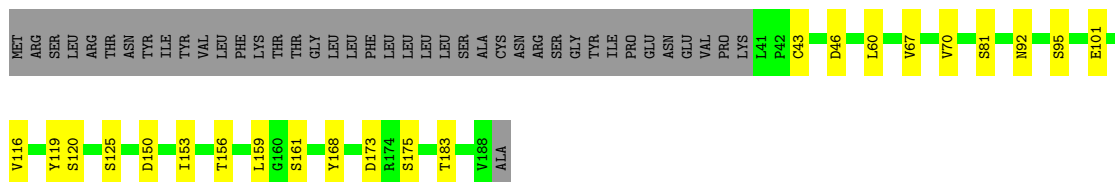
- Molecule 5: Inner membrane lipoprotein YiaD

Chain GK: 68% 11% 22%



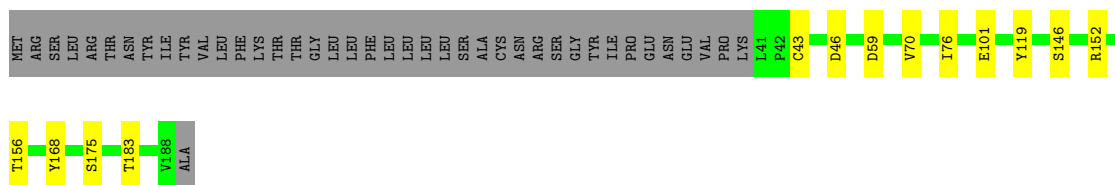
- Molecule 5: Inner membrane lipoprotein YiaD

Chain HK: 67% 12% 22%



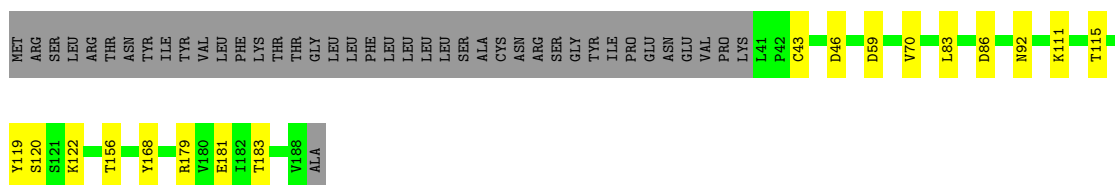
- Molecule 5: Inner membrane lipoprotein YiaD

Chain IK: 71% 7% 22%



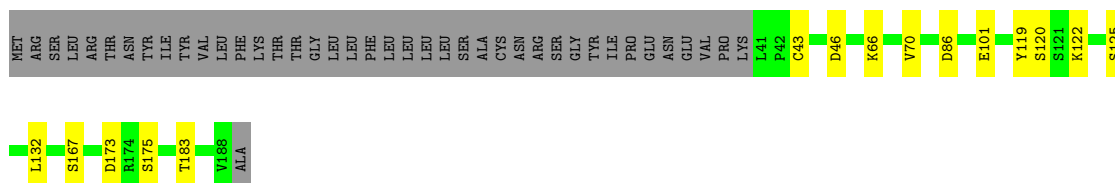
- Molecule 5: Inner membrane lipoprotein YiaD

Chain JK: 69% 9% 22%



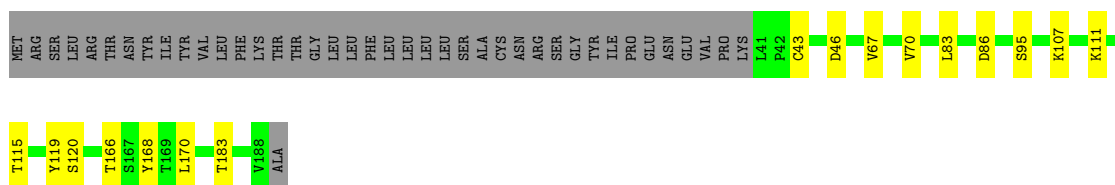
- Molecule 5: Inner membrane lipoprotein YiaD

Chain KK: 70% 8% 22%



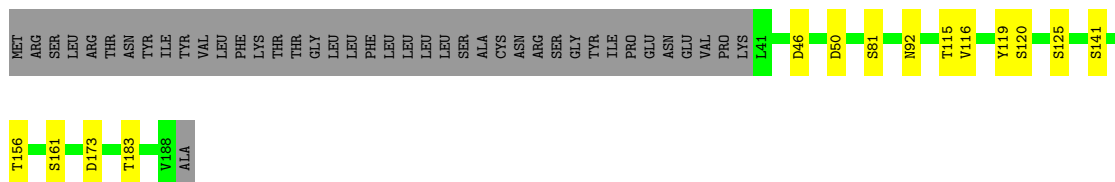
- Molecule 5: Inner membrane lipoprotein YiaD

Chain LK: 70% 8% 22%



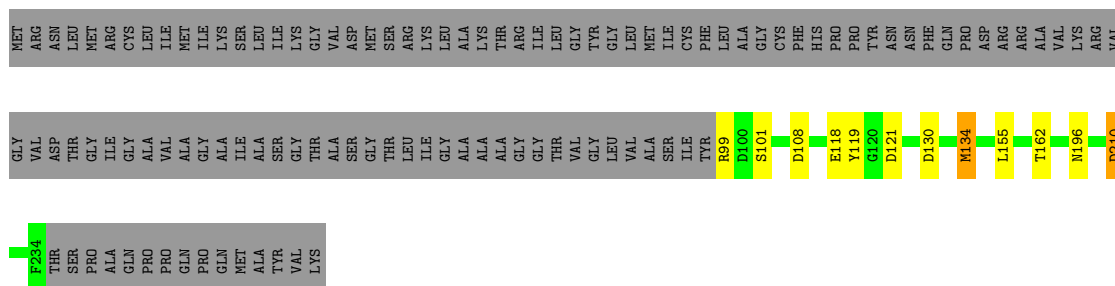
- Molecule 5: Inner membrane lipoprotein YiaD

Chain MK: 71% 7% 22%



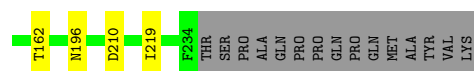
- Molecule 6: Outer membrane protein, OmpA family protein

Chain N: 50% 45%



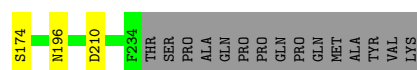
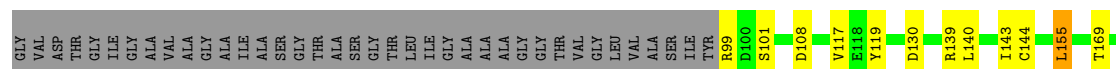
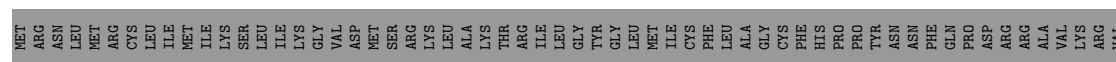






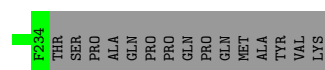
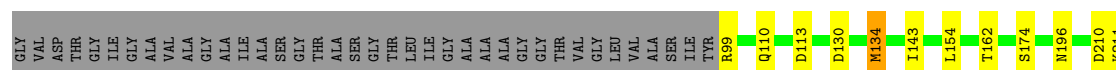
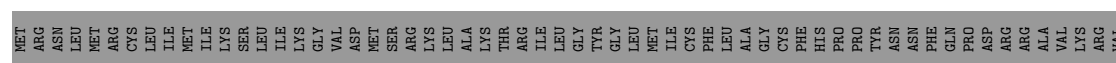
- Molecule 6: Outer membrane protein, OmpA family protein

Chain U: 49% 6% 45%



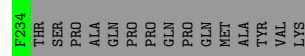
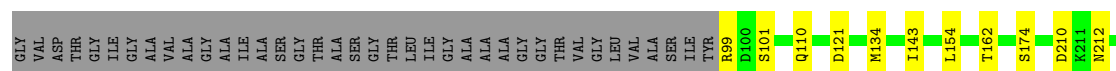
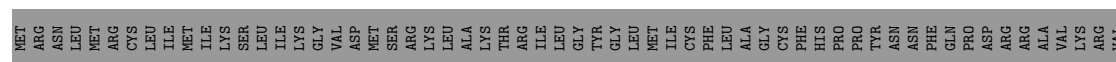
- Molecule 6: Outer membrane protein, OmpA family protein

Chain V: 50% . 45%



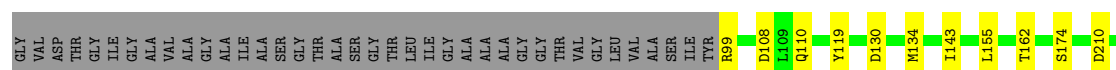
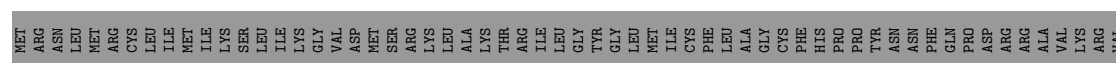
- Molecule 6: Outer membrane protein, OmpA family protein

Chain W: 50% . 45%



- Molecule 6: Outer membrane protein, OmpA family protein

Chain X: 50% . 45%



F234

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- Molecule 6: Outer membrane protein, OmpA family protein



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D100  
S101  
D108  
T124  
T129  
D130  
L155  
T169  
S174  
D210  
F234  
THR  
SER

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- Molecule 6: Outer membrane protein, OmpA family protein



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D100  
S101  
D108  
E118  
D130  
R139  
L140  
I143  
T162  
Y165  
S174  
L181

M196

THR  
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PRO  
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PRO  
GLN  
MET  
ALA  
TYR  
VAL  
LYS

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 12200                                   | 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 ( $e^-/\text{\AA}^2$ ) | 58.1                                    | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 2   | AC    | 0.51         | 0/1629        | 0.67        | 0/2214        |
| 2   | BC    | 0.51         | 0/1629        | 0.70        | 1/2214 (0.0%) |
| 2   | CC    | 0.52         | 0/1629        | 0.73        | 2/2214 (0.1%) |
| 2   | DC    | 0.49         | 0/1629        | 0.67        | 0/2214        |
| 2   | EC    | 0.53         | 0/1629        | 0.74        | 2/2214 (0.1%) |
| 2   | FC    | 0.52         | 0/1629        | 0.71        | 2/2214 (0.1%) |
| 2   | GC    | 0.52         | 0/1629        | 0.78        | 3/2214 (0.1%) |
| 2   | HC    | 0.52         | 0/1629        | 0.79        | 3/2214 (0.1%) |
| 2   | IC    | 0.52         | 0/1629        | 0.74        | 2/2214 (0.1%) |
| 2   | JC    | 0.51         | 0/1629        | 0.74        | 2/2214 (0.1%) |
| 2   | KC    | 0.53         | 0/1629        | 0.75        | 1/2214 (0.0%) |
| 2   | LC    | 0.53         | 0/1629        | 0.71        | 1/2214 (0.0%) |
| 2   | MC    | 0.53         | 0/1629        | 0.73        | 3/2214 (0.1%) |
| 3   | AD    | 0.49         | 0/1060        | 0.76        | 3/1441 (0.2%) |
| 3   | Ad    | 0.50         | 0/1086        | 0.81        | 2/1474 (0.1%) |
| 3   | BD    | 0.50         | 0/1060        | 0.80        | 3/1441 (0.2%) |
| 3   | Bd    | 0.52         | 0/1086        | 0.78        | 1/1474 (0.1%) |
| 3   | CD    | 0.50         | 0/1060        | 0.80        | 1/1441 (0.1%) |
| 3   | Cd    | 0.53         | 1/1086 (0.1%) | 0.82        | 2/1474 (0.1%) |
| 3   | DD    | 0.50         | 0/1060        | 0.78        | 2/1441 (0.1%) |
| 3   | Dd    | 0.53         | 0/1086        | 0.80        | 1/1474 (0.1%) |
| 3   | ED    | 0.52         | 0/1060        | 0.77        | 2/1441 (0.1%) |
| 3   | Ed    | 0.51         | 0/1086        | 0.77        | 1/1474 (0.1%) |
| 3   | FD    | 0.52         | 0/1060        | 0.75        | 1/1441 (0.1%) |
| 3   | Fd    | 0.55         | 0/1086        | 0.78        | 2/1474 (0.1%) |
| 3   | GD    | 0.50         | 0/1060        | 0.79        | 2/1441 (0.1%) |
| 3   | Gd    | 0.49         | 0/1086        | 0.78        | 2/1474 (0.1%) |
| 3   | HD    | 0.56         | 1/1060 (0.1%) | 0.78        | 1/1441 (0.1%) |
| 3   | Hd    | 0.53         | 0/1086        | 0.82        | 2/1474 (0.1%) |
| 3   | ID    | 0.49         | 0/1060        | 0.76        | 0/1441        |
| 3   | Id    | 0.52         | 0/1086        | 0.82        | 2/1474 (0.1%) |
| 3   | JD    | 0.49         | 0/1060        | 0.75        | 2/1441 (0.1%) |
| 3   | Jd    | 0.54         | 0/1086        | 0.82        | 2/1474 (0.1%) |
| 3   | KD    | 0.51         | 0/1060        | 0.77        | 3/1441 (0.2%) |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 3   | Kd    | 0.52         | 0/1086  | 0.77        | 1/1474 (0.1%) |
| 3   | LD    | 0.55         | 0/1060  | 0.80        | 1/1441 (0.1%) |
| 3   | Ld    | 0.51         | 0/1086  | 0.77        | 2/1474 (0.1%) |
| 3   | MD    | 0.51         | 0/1060  | 0.76        | 2/1441 (0.1%) |
| 3   | Md    | 0.53         | 0/1086  | 0.77        | 1/1474 (0.1%) |
| 4   | AH    | 0.61         | 0/695   | 0.79        | 0/947         |
| 4   | BH    | 0.59         | 0/695   | 0.82        | 0/947         |
| 4   | CH    | 0.59         | 0/695   | 0.78        | 0/947         |
| 4   | DH    | 0.57         | 0/695   | 0.77        | 0/947         |
| 4   | EH    | 0.61         | 0/695   | 0.79        | 1/947 (0.1%)  |
| 4   | FH    | 0.59         | 0/695   | 0.76        | 0/947         |
| 4   | GH    | 0.58         | 0/695   | 0.77        | 2/947 (0.2%)  |
| 4   | HH    | 0.55         | 0/695   | 0.72        | 0/947         |
| 4   | IH    | 0.57         | 0/695   | 0.76        | 1/947 (0.1%)  |
| 4   | JH    | 0.64         | 0/695   | 0.79        | 1/947 (0.1%)  |
| 4   | KH    | 0.59         | 0/695   | 0.81        | 1/947 (0.1%)  |
| 4   | LH    | 0.62         | 0/695   | 0.80        | 1/947 (0.1%)  |
| 4   | MH    | 0.59         | 0/695   | 0.78        | 0/947         |
| 5   | AK    | 0.54         | 0/1171  | 0.70        | 0/1583        |
| 5   | BK    | 0.52         | 0/1171  | 0.73        | 1/1583 (0.1%) |
| 5   | CK    | 0.52         | 0/1171  | 0.75        | 3/1583 (0.2%) |
| 5   | DK    | 0.53         | 0/1171  | 0.70        | 1/1583 (0.1%) |
| 5   | EK    | 0.53         | 0/1171  | 0.71        | 0/1583        |
| 5   | FK    | 0.51         | 0/1171  | 0.73        | 1/1583 (0.1%) |
| 5   | GK    | 0.54         | 0/1171  | 0.74        | 1/1583 (0.1%) |
| 5   | HK    | 0.52         | 0/1171  | 0.70        | 0/1583        |
| 5   | IK    | 0.53         | 0/1171  | 0.71        | 1/1583 (0.1%) |
| 5   | JK    | 0.53         | 0/1171  | 0.76        | 1/1583 (0.1%) |
| 5   | KK    | 0.53         | 0/1171  | 0.71        | 1/1583 (0.1%) |
| 5   | LK    | 0.53         | 0/1171  | 0.68        | 1/1583 (0.1%) |
| 5   | MK    | 0.50         | 0/1171  | 0.69        | 0/1583        |
| 6   | N     | 0.52         | 0/1130  | 0.75        | 2/1522 (0.1%) |
| 6   | O     | 0.52         | 0/1130  | 0.71        | 0/1522        |
| 6   | P     | 0.52         | 0/1130  | 0.74        | 0/1522        |
| 6   | Q     | 0.49         | 0/1130  | 0.69        | 0/1522        |
| 6   | R     | 0.50         | 0/1130  | 0.77        | 1/1522 (0.1%) |
| 6   | S     | 0.51         | 0/1130  | 0.71        | 0/1522        |
| 6   | T     | 0.54         | 0/1130  | 0.74        | 1/1522 (0.1%) |
| 6   | U     | 0.49         | 0/1130  | 0.74        | 2/1522 (0.1%) |
| 6   | V     | 0.51         | 0/1130  | 0.77        | 1/1522 (0.1%) |
| 6   | W     | 0.52         | 0/1130  | 0.71        | 0/1522        |
| 6   | X     | 0.53         | 0/1130  | 0.75        | 1/1522 (0.1%) |
| 6   | Y     | 0.54         | 0/1130  | 0.74        | 2/1522 (0.1%) |

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 6   | Z     | 0.50         | 0/1130         | 0.69        | 0/1522           |
| All | All   | 0.53         | 2/88023 (0.0%) | 0.75        | 94/119353 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | AX    | 0                   | 2                   |
| 1   | AZ    | 0                   | 2                   |
| 1   | BV    | 0                   | 2                   |
| 1   | BX    | 0                   | 2                   |
| 1   | BZ    | 0                   | 2                   |
| 1   | CV    | 0                   | 1                   |
| 1   | CX    | 0                   | 2                   |
| 1   | CZ    | 0                   | 1                   |
| 1   | DX    | 0                   | 3                   |
| 1   | DZ    | 0                   | 2                   |
| 1   | EX    | 0                   | 3                   |
| 1   | EZ    | 0                   | 1                   |
| 1   | FV    | 0                   | 1                   |
| 1   | FX    | 0                   | 3                   |
| 1   | FZ    | 0                   | 1                   |
| 1   | GV    | 0                   | 1                   |
| 1   | GX    | 0                   | 2                   |
| 1   | GZ    | 0                   | 1                   |
| 1   | HV    | 0                   | 1                   |
| 1   | HX    | 0                   | 2                   |
| 1   | HZ    | 0                   | 1                   |
| 1   | IV    | 0                   | 1                   |
| 1   | IX    | 0                   | 2                   |
| 1   | IZ    | 0                   | 1                   |
| 1   | JX    | 0                   | 3                   |
| 1   | JZ    | 0                   | 1                   |
| 1   | KV    | 0                   | 1                   |
| 1   | KX    | 0                   | 3                   |
| 1   | KZ    | 0                   | 1                   |
| 1   | LX    | 0                   | 3                   |
| 1   | LZ    | 0                   | 2                   |
| 1   | MX    | 0                   | 3                   |
| 1   | MZ    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | NV    | 0                   | 1                   |
| 1   | OV    | 0                   | 2                   |
| 1   | PV    | 0                   | 1                   |
| 1   | RV    | 0                   | 1                   |
| 2   | BC    | 0                   | 1                   |
| 3   | Bd    | 0                   | 1                   |
| 3   | Ed    | 0                   | 1                   |
| 3   | Fd    | 0                   | 1                   |
| 3   | Id    | 0                   | 1                   |
| 3   | Jd    | 0                   | 1                   |
| 3   | Kd    | 0                   | 1                   |
| 3   | Md    | 0                   | 1                   |
| 4   | AH    | 0                   | 1                   |
| 4   | BH    | 0                   | 1                   |
| 4   | DH    | 0                   | 2                   |
| 4   | EH    | 0                   | 1                   |
| 4   | FH    | 0                   | 1                   |
| 4   | GH    | 0                   | 1                   |
| 4   | HH    | 0                   | 1                   |
| 4   | IH    | 0                   | 1                   |
| 4   | JH    | 0                   | 1                   |
| 4   | KH    | 0                   | 1                   |
| 4   | LH    | 0                   | 1                   |
| 5   | DK    | 0                   | 1                   |
| 6   | N     | 0                   | 2                   |
| 6   | O     | 0                   | 2                   |
| 6   | Q     | 0                   | 2                   |
| 6   | T     | 0                   | 1                   |
| 6   | V     | 0                   | 2                   |
| 6   | W     | 0                   | 1                   |
| 6   | X     | 0                   | 1                   |
| 6   | Z     | 0                   | 1                   |
| All | All   | 0                   | 96                  |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | Cd    | 58  | VAL  | CB-CG1 | -5.97 | 1.40        | 1.52     |
| 3   | HD    | 31  | ASN  | C-N    | -5.41 | 1.21        | 1.34     |

All (94) bond angle outliers are listed below:



| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 5   | JK    | 59  | ASP  | CB-CG-OD2 | 10.30 | 127.58      | 118.30   |
| 2   | HC    | 117 | LEU  | CA-CB-CG  | 10.27 | 138.92      | 115.30   |
| 6   | X     | 155 | LEU  | CA-CB-CG  | 9.98  | 138.26      | 115.30   |
| 6   | V     | 113 | ASP  | CB-CG-OD1 | 9.90  | 127.21      | 118.30   |
| 2   | GC    | 117 | LEU  | CA-CB-CG  | 9.13  | 136.30      | 115.30   |
| 2   | GC    | 119 | LEU  | CA-CB-CG  | 8.36  | 134.54      | 115.30   |
| 2   | KC    | 64  | LEU  | CA-CB-CG  | 8.35  | 134.50      | 115.30   |
| 6   | R     | 155 | LEU  | CA-CB-CG  | 8.31  | 134.41      | 115.30   |
| 6   | T     | 155 | LEU  | CA-CB-CG  | 7.86  | 133.38      | 115.30   |
| 3   | HD    | 50  | ASP  | CB-CG-OD1 | 7.82  | 125.34      | 118.30   |
| 3   | Jd    | 53  | LEU  | CB-CG-CD1 | -7.56 | 98.14       | 111.00   |
| 3   | Gd    | 71  | LEU  | CA-CB-CG  | 7.47  | 132.49      | 115.30   |
| 3   | ED    | 50  | ASP  | CB-CG-OD1 | 7.42  | 124.98      | 118.30   |
| 2   | IC    | 64  | LEU  | CA-CB-CG  | 7.39  | 132.29      | 115.30   |
| 3   | AD    | 128 | LEU  | CA-CB-CG  | 7.35  | 132.21      | 115.30   |
| 2   | MC    | 211 | LEU  | CA-CB-CG  | 7.23  | 131.94      | 115.30   |
| 2   | IC    | 99  | LEU  | CA-CB-CG  | 7.17  | 131.79      | 115.30   |
| 2   | JC    | 211 | LEU  | CA-CB-CG  | 7.05  | 131.53      | 115.30   |
| 3   | MD    | 50  | ASP  | CB-CG-OD2 | 7.02  | 124.62      | 118.30   |
| 3   | DD    | 50  | ASP  | CB-CG-OD2 | 6.84  | 124.46      | 118.30   |
| 2   | BC    | 243 | ASP  | CB-CG-OD1 | 6.65  | 124.28      | 118.30   |
| 3   | JD    | 94  | LEU  | CB-CG-CD2 | 6.58  | 122.19      | 111.00   |
| 6   | U     | 108 | ASP  | CB-CG-OD2 | 6.52  | 124.17      | 118.30   |
| 5   | LK    | 83  | LEU  | CA-CB-CG  | 6.51  | 130.27      | 115.30   |
| 3   | GD    | 50  | ASP  | CB-CG-OD2 | 6.41  | 124.07      | 118.30   |
| 2   | GC    | 243 | ASP  | CB-CG-OD1 | 6.39  | 124.05      | 118.30   |
| 5   | CK    | 134 | LEU  | CA-CB-CG  | 6.30  | 129.79      | 115.30   |
| 5   | IK    | 59  | ASP  | CB-CG-OD1 | 6.27  | 123.94      | 118.30   |
| 2   | EC    | 72  | LEU  | CA-CB-CG  | 6.23  | 129.62      | 115.30   |
| 5   | CK    | 132 | LEU  | CA-CB-CG  | 6.21  | 129.59      | 115.30   |
| 3   | Fd    | 109 | LEU  | CA-CB-CG  | 6.21  | 129.58      | 115.30   |
| 4   | KH    | 318 | LEU  | CA-CB-CG  | 6.20  | 129.56      | 115.30   |
| 3   | ED    | 94  | LEU  | CA-CB-CG  | 6.17  | 129.48      | 115.30   |
| 3   | AD    | 50  | ASP  | CB-CG-OD2 | 6.08  | 123.78      | 118.30   |
| 3   | Hd    | 77  | TYR  | C-N-CA    | 6.03  | 136.78      | 121.70   |
| 3   | Ld    | 77  | TYR  | C-N-CA    | 6.02  | 136.76      | 121.70   |
| 5   | GK    | 132 | LEU  | CA-CB-CG  | 6.01  | 129.12      | 115.30   |
| 3   | BD    | 94  | LEU  | CB-CG-CD2 | 6.01  | 121.21      | 111.00   |
| 2   | CC    | 243 | ASP  | CB-CG-OD2 | 5.92  | 123.62      | 118.30   |
| 3   | CD    | 59  | GLU  | CA-CB-CG  | 5.92  | 126.42      | 113.40   |
| 5   | FK    | 132 | LEU  | CA-CB-CG  | 5.90  | 128.87      | 115.30   |
| 3   | Ad    | 77  | TYR  | C-N-CA    | 5.88  | 136.41      | 121.70   |
| 5   | BK    | 134 | LEU  | CA-CB-CG  | 5.86  | 128.78      | 115.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | KD    | 128 | LEU  | CA-CB-CG   | 5.84  | 128.74      | 115.30   |
| 3   | Gd    | 77  | TYR  | C-N-CA     | 5.78  | 136.14      | 121.70   |
| 3   | Ad    | 131 | ILE  | CG1-CB-CG2 | -5.77 | 98.70       | 111.40   |
| 4   | JH    | 357 | LEU  | CA-CB-CG   | 5.75  | 128.52      | 115.30   |
| 3   | BD    | 98  | ILE  | CG1-CB-CG2 | -5.71 | 98.84       | 111.40   |
| 2   | MC    | 72  | LEU  | CA-CB-CG   | 5.71  | 128.43      | 115.30   |
| 3   | Cd    | 58  | VAL  | CG1-CB-CG2 | -5.69 | 101.79      | 110.90   |
| 3   | Id    | 117 | VAL  | CG1-CB-CG2 | -5.69 | 101.80      | 110.90   |
| 3   | Hd    | 50  | ASP  | CB-CG-OD2  | 5.67  | 123.40      | 118.30   |
| 6   | Y     | 155 | LEU  | CA-CB-CG   | 5.65  | 128.31      | 115.30   |
| 3   | Dd    | 77  | TYR  | C-N-CA     | 5.64  | 135.79      | 121.70   |
| 5   | DK    | 83  | LEU  | CA-CB-CG   | 5.62  | 128.22      | 115.30   |
| 3   | BD    | 50  | ASP  | CB-CG-OD2  | 5.59  | 123.33      | 118.30   |
| 3   | Cd    | 77  | TYR  | C-N-CA     | 5.58  | 135.66      | 121.70   |
| 2   | HC    | 189 | ASP  | CB-CG-OD1  | 5.58  | 123.32      | 118.30   |
| 3   | Id    | 77  | TYR  | C-N-CA     | 5.57  | 135.63      | 121.70   |
| 2   | LC    | 243 | ASP  | CB-CG-OD1  | 5.52  | 123.27      | 118.30   |
| 6   | N     | 121 | ASP  | CB-CG-OD1  | 5.49  | 123.24      | 118.30   |
| 3   | Fd    | 53  | LEU  | CA-CB-CG   | 5.47  | 127.89      | 115.30   |
| 2   | JC    | 90  | LEU  | CA-CB-CG   | -5.46 | 102.73      | 115.30   |
| 3   | Md    | 77  | TYR  | C-N-CA     | 5.43  | 135.27      | 121.70   |
| 3   | LD    | 67  | LYS  | CA-CB-CG   | 5.42  | 125.33      | 113.40   |
| 3   | Ed    | 71  | LEU  | CA-CB-CG   | 5.42  | 127.75      | 115.30   |
| 3   | JD    | 125 | ASP  | CB-CG-OD2  | 5.36  | 123.13      | 118.30   |
| 2   | FC    | 199 | ILE  | CG1-CB-CG2 | -5.35 | 99.64       | 111.40   |
| 3   | Bd    | 77  | TYR  | C-N-CA     | 5.34  | 135.05      | 121.70   |
| 3   | Ld    | 58  | VAL  | CG1-CB-CG2 | -5.34 | 102.36      | 110.90   |
| 3   | DD    | 86  | ASP  | CB-CG-OD1  | 5.31  | 123.08      | 118.30   |
| 4   | IH    | 318 | LEU  | CA-CB-CG   | 5.30  | 127.50      | 115.30   |
| 2   | FC    | 64  | LEU  | CA-CB-CG   | 5.29  | 127.46      | 115.30   |
| 4   | GH    | 357 | LEU  | CA-CB-CG   | 5.29  | 127.46      | 115.30   |
| 6   | Y     | 210 | ASP  | CB-CG-OD1  | 5.27  | 123.05      | 118.30   |
| 3   | AD    | 94  | LEU  | CB-CG-CD2  | 5.23  | 119.89      | 111.00   |
| 3   | Kd    | 77  | TYR  | C-N-CA     | 5.23  | 134.77      | 121.70   |
| 6   | N     | 210 | ASP  | CB-CG-OD1  | 5.20  | 122.98      | 118.30   |
| 4   | GH    | 279 | ASP  | CB-CG-OD2  | 5.20  | 122.98      | 118.30   |
| 6   | U     | 155 | LEU  | CA-CB-CG   | 5.19  | 127.23      | 115.30   |
| 2   | CC    | 117 | LEU  | CA-CB-CG   | 5.19  | 127.23      | 115.30   |
| 3   | MD    | 86  | ASP  | CB-CG-OD1  | 5.19  | 122.97      | 118.30   |
| 2   | MC    | 243 | ASP  | CB-CG-OD1  | 5.18  | 122.96      | 118.30   |
| 5   | KK    | 70  | VAL  | CG1-CB-CG2 | -5.16 | 102.64      | 110.90   |
| 4   | LH    | 357 | LEU  | CA-CB-CG   | 5.16  | 127.17      | 115.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | KD    | 86  | ASP  | CB-CG-OD1  | 5.16  | 122.94      | 118.30   |
| 3   | GD    | 94  | LEU  | CB-CG-CD2  | 5.15  | 119.75      | 111.00   |
| 3   | KD    | 94  | LEU  | CA-CB-CG   | 5.12  | 127.07      | 115.30   |
| 3   | FD    | 50  | ASP  | CB-CG-OD2  | 5.10  | 122.89      | 118.30   |
| 2   | EC    | 117 | LEU  | CA-CB-CG   | 5.07  | 126.97      | 115.30   |
| 5   | CK    | 70  | VAL  | CG1-CB-CG2 | -5.05 | 102.81      | 110.90   |
| 2   | HC    | 90  | LEU  | CA-CB-CG   | -5.03 | 103.72      | 115.30   |
| 3   | Jd    | 77  | TYR  | C-N-CA     | 5.03  | 134.27      | 121.70   |
| 4   | EH    | 318 | LEU  | CA-CB-CG   | 5.02  | 126.86      | 115.30   |

There are no chirality outliers.

All (96) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 4   | AH    | 322 | SER  | Peptide |
| 1   | AX    | 142 | UNK  | Peptide |
| 1   | AX    | 153 | UNK  | Peptide |
| 1   | AZ    | 20  | UNK  | Peptide |
| 1   | AZ    | 45  | UNK  | Peptide |
| 2   | BC    | 233 | VAL  | Peptide |
| 4   | BH    | 277 | ALA  | Peptide |
| 1   | BV    | 42  | UNK  | Peptide |
| 1   | BV    | 46  | UNK  | Peptide |
| 1   | BX    | 142 | UNK  | Peptide |
| 1   | BX    | 153 | UNK  | Peptide |
| 1   | BZ    | 20  | UNK  | Peptide |
| 1   | BZ    | 45  | UNK  | Peptide |
| 3   | Bd    | 27  | LYS  | Peptide |
| 1   | CV    | 77  | UNK  | Peptide |
| 1   | CX    | 142 | UNK  | Peptide |
| 1   | CX    | 153 | UNK  | Peptide |
| 1   | CZ    | 45  | UNK  | Peptide |
| 4   | DH    | 277 | ALA  | Peptide |
| 4   | DH    | 322 | SER  | Peptide |
| 5   | DK    | 148 | GLY  | Peptide |
| 1   | DX    | 142 | UNK  | Peptide |
| 1   | DX    | 153 | UNK  | Peptide |
| 1   | DX    | 219 | UNK  | Peptide |
| 1   | DZ    | 20  | UNK  | Peptide |
| 1   | DZ    | 45  | UNK  | Peptide |
| 4   | EH    | 322 | SER  | Peptide |
| 1   | EX    | 142 | UNK  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | EX    | 153 | UNK  | Peptide |
| 1   | EX    | 43  | UNK  | Peptide |
| 1   | EZ    | 45  | UNK  | Peptide |
| 3   | Ed    | 78  | ASN  | Peptide |
| 4   | FH    | 322 | SER  | Peptide |
| 1   | FV    | 42  | UNK  | Peptide |
| 1   | FX    | 142 | UNK  | Peptide |
| 1   | FX    | 153 | UNK  | Peptide |
| 1   | FX    | 154 | UNK  | Peptide |
| 1   | FZ    | 45  | UNK  | Peptide |
| 3   | Fd    | 85  | VAL  | Peptide |
| 4   | GH    | 322 | SER  | Peptide |
| 1   | GV    | 77  | UNK  | Peptide |
| 1   | GX    | 142 | UNK  | Peptide |
| 1   | GX    | 153 | UNK  | Peptide |
| 1   | GZ    | 45  | UNK  | Peptide |
| 4   | HH    | 322 | SER  | Peptide |
| 1   | HV    | 77  | UNK  | Peptide |
| 1   | HX    | 142 | UNK  | Peptide |
| 1   | HX    | 153 | UNK  | Peptide |
| 1   | HZ    | 45  | UNK  | Peptide |
| 4   | IH    | 322 | SER  | Peptide |
| 1   | IV    | 77  | UNK  | Peptide |
| 1   | IX    | 142 | UNK  | Peptide |
| 1   | IX    | 153 | UNK  | Peptide |
| 1   | IZ    | 45  | UNK  | Peptide |
| 3   | Id    | 85  | VAL  | Peptide |
| 4   | JH    | 322 | SER  | Peptide |
| 1   | JX    | 142 | UNK  | Peptide |
| 1   | JX    | 153 | UNK  | Peptide |
| 1   | JX    | 43  | UNK  | Peptide |
| 1   | JZ    | 45  | UNK  | Peptide |
| 3   | Jd    | 85  | VAL  | Peptide |
| 4   | KH    | 322 | SER  | Peptide |
| 1   | KV    | 42  | UNK  | Peptide |
| 1   | KX    | 142 | UNK  | Peptide |
| 1   | KX    | 153 | UNK  | Peptide |
| 1   | KX    | 43  | UNK  | Peptide |
| 1   | KZ    | 45  | UNK  | Peptide |
| 3   | Kd    | 78  | ASN  | Peptide |
| 4   | LH    | 277 | ALA  | Peptide |
| 1   | LX    | 142 | UNK  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | LX    | 153 | UNK  | Peptide |
| 1   | LX    | 154 | UNK  | Peptide |
| 1   | LZ    | 20  | UNK  | Peptide |
| 1   | LZ    | 45  | UNK  | Peptide |
| 1   | MX    | 142 | UNK  | Peptide |
| 1   | MX    | 153 | UNK  | Peptide |
| 1   | MX    | 43  | UNK  | Peptide |
| 1   | MZ    | 45  | UNK  | Peptide |
| 3   | Md    | 85  | VAL  | Peptide |
| 6   | N     | 134 | MET  | Peptide |
| 6   | N     | 196 | ASN  | Peptide |
| 1   | NV    | 42  | UNK  | Peptide |
| 6   | O     | 112 | GLN  | Peptide |
| 6   | O     | 155 | LEU  | Peptide |
| 1   | OV    | 41  | UNK  | Peptide |
| 1   | OV    | 42  | UNK  | Peptide |
| 1   | PV    | 77  | UNK  | Peptide |
| 6   | Q     | 134 | MET  | Peptide |
| 6   | Q     | 212 | ASN  | Peptide |
| 1   | RV    | 77  | UNK  | Peptide |
| 6   | T     | 134 | MET  | Peptide |
| 6   | V     | 134 | MET  | Peptide |
| 6   | V     | 196 | ASN  | Peptide |
| 6   | W     | 134 | MET  | Peptide |
| 6   | X     | 134 | MET  | Peptide |
| 6   | Z     | 196 | ASN  | Peptide |

## 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 |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | AC    | 196/303 (65%) | 190 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 2   | BC    | 196/303 (65%) | 189 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 2   | CC    | 196/303 (65%) | 189 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 2   | DC    | 196/303 (65%) | 187 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 2   | EC    | 196/303 (65%) | 187 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 2   | FC    | 196/303 (65%) | 187 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 2   | GC    | 196/303 (65%) | 189 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 2   | HC    | 196/303 (65%) | 190 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 2   | IC    | 196/303 (65%) | 191 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 2   | JC    | 196/303 (65%) | 187 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 2   | KC    | 196/303 (65%) | 189 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 2   | LC    | 196/303 (65%) | 188 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 2   | MC    | 196/303 (65%) | 191 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 3   | AD    | 133/163 (82%) | 127 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 3   | Ad    | 136/163 (83%) | 126 (93%) | 10 (7%) | 0        | 100         | 100 |
| 3   | BD    | 133/163 (82%) | 125 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 3   | Bd    | 136/163 (83%) | 125 (92%) | 11 (8%) | 0        | 100         | 100 |
| 3   | CD    | 133/163 (82%) | 128 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 3   | Cd    | 136/163 (83%) | 126 (93%) | 10 (7%) | 0        | 100         | 100 |
| 3   | DD    | 133/163 (82%) | 126 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 3   | Dd    | 136/163 (83%) | 127 (93%) | 9 (7%)  | 0        | 100         | 100 |
| 3   | ED    | 133/163 (82%) | 125 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 3   | Ed    | 136/163 (83%) | 129 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 3   | FD    | 133/163 (82%) | 126 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 3   | Fd    | 136/163 (83%) | 126 (93%) | 10 (7%) | 0        | 100         | 100 |
| 3   | GD    | 133/163 (82%) | 125 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 3   | Gd    | 136/163 (83%) | 128 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 3   | HD    | 133/163 (82%) | 128 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 3   | Hd    | 136/163 (83%) | 126 (93%) | 10 (7%) | 0        | 100         | 100 |
| 3   | ID    | 133/163 (82%) | 129 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 3   | Id    | 136/163 (83%) | 126 (93%) | 10 (7%) | 0        | 100         | 100 |
| 3   | JD    | 133/163 (82%) | 126 (95%) | 7 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3   | Jd    | 136/163 (83%) | 127 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 3   | KD    | 133/163 (82%) | 127 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 3   | Kd    | 136/163 (83%) | 130 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 3   | LD    | 133/163 (82%) | 126 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 3   | Ld    | 136/163 (83%) | 126 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 3   | MD    | 133/163 (82%) | 128 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 3   | Md    | 136/163 (83%) | 129 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 4   | AH    | 87/361 (24%)  | 79 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 4   | BH    | 87/361 (24%)  | 79 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 4   | CH    | 87/361 (24%)  | 77 (88%)  | 10 (12%) | 0        | 100         | 100 |
| 4   | DH    | 87/361 (24%)  | 79 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 4   | EH    | 87/361 (24%)  | 76 (87%)  | 11 (13%) | 0        | 100         | 100 |
| 4   | FH    | 87/361 (24%)  | 79 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 4   | GH    | 87/361 (24%)  | 79 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 4   | HH    | 87/361 (24%)  | 79 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 4   | IH    | 87/361 (24%)  | 79 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 4   | JH    | 87/361 (24%)  | 78 (90%)  | 9 (10%)  | 0        | 100         | 100 |
| 4   | KH    | 87/361 (24%)  | 79 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 4   | LH    | 87/361 (24%)  | 77 (88%)  | 10 (12%) | 0        | 100         | 100 |
| 4   | MH    | 87/361 (24%)  | 78 (90%)  | 9 (10%)  | 0        | 100         | 100 |
| 5   | AK    | 146/189 (77%) | 142 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 5   | BK    | 146/189 (77%) | 138 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 5   | CK    | 146/189 (77%) | 138 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 5   | DK    | 146/189 (77%) | 138 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 5   | EK    | 146/189 (77%) | 139 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 5   | FK    | 146/189 (77%) | 137 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 5   | GK    | 146/189 (77%) | 140 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 5   | HK    | 146/189 (77%) | 138 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 5   | IK    | 146/189 (77%) | 140 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 5   | JK    | 146/189 (77%) | 141 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 5   | KK    | 146/189 (77%) | 137 (94%) | 9 (6%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 5   | LK    | 146/189 (77%)     | 139 (95%)   | 7 (5%)   | 0        | 100         | 100 |
| 5   | MK    | 146/189 (77%)     | 136 (93%)   | 10 (7%)  | 0        | 100         | 100 |
| 6   | N     | 134/249 (54%)     | 123 (92%)   | 11 (8%)  | 0        | 100         | 100 |
| 6   | O     | 134/249 (54%)     | 124 (92%)   | 10 (8%)  | 0        | 100         | 100 |
| 6   | P     | 134/249 (54%)     | 126 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| 6   | Q     | 134/249 (54%)     | 127 (95%)   | 7 (5%)   | 0        | 100         | 100 |
| 6   | R     | 134/249 (54%)     | 126 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| 6   | S     | 134/249 (54%)     | 127 (95%)   | 7 (5%)   | 0        | 100         | 100 |
| 6   | T     | 134/249 (54%)     | 126 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| 6   | U     | 134/249 (54%)     | 128 (96%)   | 6 (4%)   | 0        | 100         | 100 |
| 6   | V     | 134/249 (54%)     | 126 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| 6   | W     | 134/249 (54%)     | 124 (92%)   | 10 (8%)  | 0        | 100         | 100 |
| 6   | X     | 134/249 (54%)     | 125 (93%)   | 9 (7%)   | 0        | 100         | 100 |
| 6   | Y     | 134/249 (54%)     | 125 (93%)   | 9 (7%)   | 0        | 100         | 100 |
| 6   | Z     | 134/249 (54%)     | 126 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| All | All   | 10816/18564 (58%) | 10205 (94%) | 611 (6%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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 |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2   | AC    | 169/257 (66%) | 157 (93%) | 12 (7%)  | 14          | 45 |
| 2   | BC    | 169/257 (66%) | 153 (90%) | 16 (10%) | 8           | 34 |
| 2   | CC    | 169/257 (66%) | 154 (91%) | 15 (9%)  | 9           | 37 |
| 2   | DC    | 169/257 (66%) | 149 (88%) | 20 (12%) | 5           | 26 |
| 2   | EC    | 169/257 (66%) | 152 (90%) | 17 (10%) | 7           | 31 |
| 2   | FC    | 169/257 (66%) | 155 (92%) | 14 (8%)  | 11          | 40 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2   | GC    | 169/257 (66%) | 153 (90%) | 16 (10%) | 8           | 34 |
| 2   | HC    | 169/257 (66%) | 156 (92%) | 13 (8%)  | 13          | 43 |
| 2   | IC    | 169/257 (66%) | 152 (90%) | 17 (10%) | 7           | 31 |
| 2   | JC    | 169/257 (66%) | 156 (92%) | 13 (8%)  | 13          | 43 |
| 2   | KC    | 169/257 (66%) | 154 (91%) | 15 (9%)  | 9           | 37 |
| 2   | LC    | 169/257 (66%) | 154 (91%) | 15 (9%)  | 9           | 37 |
| 2   | MC    | 169/257 (66%) | 157 (93%) | 12 (7%)  | 14          | 45 |
| 3   | AD    | 116/139 (84%) | 101 (87%) | 15 (13%) | 4           | 22 |
| 3   | Ad    | 119/139 (86%) | 105 (88%) | 14 (12%) | 5           | 26 |
| 3   | BD    | 116/139 (84%) | 99 (85%)  | 17 (15%) | 3           | 18 |
| 3   | Bd    | 119/139 (86%) | 106 (89%) | 13 (11%) | 6           | 29 |
| 3   | CD    | 116/139 (84%) | 93 (80%)  | 23 (20%) | 1           | 8  |
| 3   | Cd    | 119/139 (86%) | 109 (92%) | 10 (8%)  | 11          | 40 |
| 3   | DD    | 116/139 (84%) | 100 (86%) | 16 (14%) | 3           | 21 |
| 3   | Dd    | 119/139 (86%) | 104 (87%) | 15 (13%) | 4           | 23 |
| 3   | ED    | 116/139 (84%) | 98 (84%)  | 18 (16%) | 2           | 17 |
| 3   | Ed    | 119/139 (86%) | 108 (91%) | 11 (9%)  | 9           | 36 |
| 3   | FD    | 116/139 (84%) | 98 (84%)  | 18 (16%) | 2           | 17 |
| 3   | Fd    | 119/139 (86%) | 106 (89%) | 13 (11%) | 6           | 29 |
| 3   | GD    | 116/139 (84%) | 101 (87%) | 15 (13%) | 4           | 22 |
| 3   | Gd    | 119/139 (86%) | 101 (85%) | 18 (15%) | 3           | 17 |
| 3   | HD    | 116/139 (84%) | 95 (82%)  | 21 (18%) | 1           | 11 |
| 3   | Hd    | 119/139 (86%) | 102 (86%) | 17 (14%) | 3           | 19 |
| 3   | ID    | 116/139 (84%) | 102 (88%) | 14 (12%) | 5           | 24 |
| 3   | Id    | 119/139 (86%) | 110 (92%) | 9 (8%)   | 13          | 43 |
| 3   | JD    | 116/139 (84%) | 100 (86%) | 16 (14%) | 3           | 21 |
| 3   | Jd    | 119/139 (86%) | 105 (88%) | 14 (12%) | 5           | 26 |
| 3   | KD    | 116/139 (84%) | 105 (90%) | 11 (10%) | 8           | 34 |
| 3   | Kd    | 119/139 (86%) | 100 (84%) | 19 (16%) | 2           | 15 |
| 3   | LD    | 116/139 (84%) | 99 (85%)  | 17 (15%) | 3           | 18 |
| 3   | Ld    | 119/139 (86%) | 103 (87%) | 16 (13%) | 4           | 21 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3   | MD    | 116/139 (84%) | 102 (88%) | 14 (12%) | 5           | 24 |
| 3   | Md    | 119/139 (86%) | 97 (82%)  | 22 (18%) | 1           | 10 |
| 4   | AH    | 75/300 (25%)  | 65 (87%)  | 10 (13%) | 4           | 22 |
| 4   | BH    | 75/300 (25%)  | 64 (85%)  | 11 (15%) | 3           | 18 |
| 4   | CH    | 75/300 (25%)  | 67 (89%)  | 8 (11%)  | 6           | 30 |
| 4   | DH    | 75/300 (25%)  | 65 (87%)  | 10 (13%) | 4           | 22 |
| 4   | EH    | 75/300 (25%)  | 65 (87%)  | 10 (13%) | 4           | 22 |
| 4   | FH    | 75/300 (25%)  | 69 (92%)  | 6 (8%)   | 12          | 42 |
| 4   | GH    | 75/300 (25%)  | 66 (88%)  | 9 (12%)  | 5           | 25 |
| 4   | HH    | 75/300 (25%)  | 69 (92%)  | 6 (8%)   | 12          | 42 |
| 4   | IH    | 75/300 (25%)  | 65 (87%)  | 10 (13%) | 4           | 22 |
| 4   | JH    | 75/300 (25%)  | 64 (85%)  | 11 (15%) | 3           | 18 |
| 4   | KH    | 75/300 (25%)  | 67 (89%)  | 8 (11%)  | 6           | 30 |
| 4   | LH    | 75/300 (25%)  | 64 (85%)  | 11 (15%) | 3           | 18 |
| 4   | MH    | 75/300 (25%)  | 64 (85%)  | 11 (15%) | 3           | 18 |
| 5   | AK    | 126/163 (77%) | 108 (86%) | 18 (14%) | 3           | 19 |
| 5   | BK    | 126/163 (77%) | 106 (84%) | 20 (16%) | 2           | 16 |
| 5   | CK    | 126/163 (77%) | 105 (83%) | 21 (17%) | 2           | 14 |
| 5   | DK    | 126/163 (77%) | 110 (87%) | 16 (13%) | 4           | 23 |
| 5   | EK    | 126/163 (77%) | 109 (86%) | 17 (14%) | 4           | 21 |
| 5   | FK    | 126/163 (77%) | 103 (82%) | 23 (18%) | 1           | 10 |
| 5   | GK    | 126/163 (77%) | 107 (85%) | 19 (15%) | 3           | 17 |
| 5   | HK    | 126/163 (77%) | 104 (82%) | 22 (18%) | 2           | 12 |
| 5   | IK    | 126/163 (77%) | 114 (90%) | 12 (10%) | 8           | 34 |
| 5   | JK    | 126/163 (77%) | 110 (87%) | 16 (13%) | 4           | 23 |
| 5   | KK    | 126/163 (77%) | 112 (89%) | 14 (11%) | 6           | 28 |
| 5   | LK    | 126/163 (77%) | 111 (88%) | 15 (12%) | 5           | 25 |
| 5   | MK    | 126/163 (77%) | 112 (89%) | 14 (11%) | 6           | 28 |
| 6   | N     | 118/203 (58%) | 108 (92%) | 10 (8%)  | 10          | 40 |
| 6   | O     | 118/203 (58%) | 104 (88%) | 14 (12%) | 5           | 25 |
| 6   | P     | 118/203 (58%) | 108 (92%) | 10 (8%)  | 10          | 40 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|------------------|------------|------------|-------------|----|
| 6   | Q     | 118/203 (58%)    | 107 (91%)  | 11 (9%)    | 9           | 35 |
| 6   | R     | 118/203 (58%)    | 108 (92%)  | 10 (8%)    | 10          | 40 |
| 6   | S     | 118/203 (58%)    | 105 (89%)  | 13 (11%)   | 6           | 29 |
| 6   | T     | 118/203 (58%)    | 102 (86%)  | 16 (14%)   | 3           | 21 |
| 6   | U     | 118/203 (58%)    | 104 (88%)  | 14 (12%)   | 5           | 25 |
| 6   | V     | 118/203 (58%)    | 108 (92%)  | 10 (8%)    | 10          | 40 |
| 6   | W     | 118/203 (58%)    | 108 (92%)  | 10 (8%)    | 10          | 40 |
| 6   | X     | 118/203 (58%)    | 109 (92%)  | 9 (8%)     | 13          | 43 |
| 6   | Y     | 118/203 (58%)    | 108 (92%)  | 10 (8%)    | 10          | 40 |
| 6   | Z     | 118/203 (58%)    | 106 (90%)  | 12 (10%)   | 7           | 31 |
| All | All   | 9399/15613 (60%) | 8301 (88%) | 1098 (12%) | 9           | 26 |

All (1098) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 61  | GLU  |
| 2   | AC    | 72  | LEU  |
| 2   | AC    | 102 | GLU  |
| 2   | AC    | 137 | GLN  |
| 2   | AC    | 141 | ILE  |
| 2   | AC    | 173 | LYS  |
| 2   | AC    | 177 | CYS  |
| 2   | AC    | 190 | GLN  |
| 2   | AC    | 229 | THR  |
| 2   | AC    | 246 | VAL  |
| 2   | AC    | 258 | ASN  |
| 2   | AC    | 259 | SER  |
| 3   | AD    | 47  | SER  |
| 3   | AD    | 58  | VAL  |
| 3   | AD    | 61  | VAL  |
| 3   | AD    | 63  | THR  |
| 3   | AD    | 70  | THR  |
| 3   | AD    | 86  | ASP  |
| 3   | AD    | 108 | VAL  |
| 3   | AD    | 111 | LYS  |
| 3   | AD    | 115 | VAL  |
| 3   | AD    | 117 | VAL  |
| 3   | AD    | 123 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AD    | 126 | GLU  |
| 3   | AD    | 127 | SER  |
| 3   | AD    | 141 | LYS  |
| 3   | AD    | 157 | ARG  |
| 4   | AH    | 286 | GLU  |
| 4   | AH    | 288 | VAL  |
| 4   | AH    | 297 | VAL  |
| 4   | AH    | 307 | LEU  |
| 4   | AH    | 317 | ASN  |
| 4   | AH    | 318 | LEU  |
| 4   | AH    | 328 | SER  |
| 4   | AH    | 333 | ASP  |
| 4   | AH    | 343 | SER  |
| 4   | AH    | 349 | SER  |
| 5   | AK    | 43  | CYS  |
| 5   | AK    | 46  | ASP  |
| 5   | AK    | 66  | LYS  |
| 5   | AK    | 78  | ILE  |
| 5   | AK    | 83  | LEU  |
| 5   | AK    | 86  | ASP  |
| 5   | AK    | 91  | LEU  |
| 5   | AK    | 95  | SER  |
| 5   | AK    | 111 | LYS  |
| 5   | AK    | 115 | THR  |
| 5   | AK    | 116 | VAL  |
| 5   | AK    | 119 | TYR  |
| 5   | AK    | 120 | SER  |
| 5   | AK    | 125 | SER  |
| 5   | AK    | 153 | ILE  |
| 5   | AK    | 156 | THR  |
| 5   | AK    | 161 | SER  |
| 5   | AK    | 183 | THR  |
| 3   | Ad    | 38  | THR  |
| 3   | Ad    | 55  | MET  |
| 3   | Ad    | 63  | THR  |
| 3   | Ad    | 67  | LYS  |
| 3   | Ad    | 75  | ASN  |
| 3   | Ad    | 77  | TYR  |
| 3   | Ad    | 78  | ASN  |
| 3   | Ad    | 85  | VAL  |
| 3   | Ad    | 93  | GLU  |
| 3   | Ad    | 95  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Ad    | 111 | LYS  |
| 3   | Ad    | 117 | VAL  |
| 3   | Ad    | 127 | SER  |
| 3   | Ad    | 130 | GLU  |
| 2   | BC    | 79  | ILE  |
| 2   | BC    | 126 | ARG  |
| 2   | BC    | 128 | SER  |
| 2   | BC    | 143 | THR  |
| 2   | BC    | 148 | ARG  |
| 2   | BC    | 174 | GLU  |
| 2   | BC    | 177 | CYS  |
| 2   | BC    | 180 | THR  |
| 2   | BC    | 189 | ASP  |
| 2   | BC    | 221 | VAL  |
| 2   | BC    | 228 | HIS  |
| 2   | BC    | 229 | THR  |
| 2   | BC    | 246 | VAL  |
| 2   | BC    | 256 | ASN  |
| 2   | BC    | 258 | ASN  |
| 2   | BC    | 259 | SER  |
| 3   | BD    | 52  | MET  |
| 3   | BD    | 58  | VAL  |
| 3   | BD    | 61  | VAL  |
| 3   | BD    | 63  | THR  |
| 3   | BD    | 85  | VAL  |
| 3   | BD    | 87  | TRP  |
| 3   | BD    | 88  | SER  |
| 3   | BD    | 93  | GLU  |
| 3   | BD    | 108 | VAL  |
| 3   | BD    | 111 | LYS  |
| 3   | BD    | 112 | SER  |
| 3   | BD    | 115 | VAL  |
| 3   | BD    | 117 | VAL  |
| 3   | BD    | 127 | SER  |
| 3   | BD    | 133 | ARG  |
| 3   | BD    | 144 | SER  |
| 3   | BD    | 151 | SER  |
| 4   | BH    | 276 | SER  |
| 4   | BH    | 288 | VAL  |
| 4   | BH    | 298 | VAL  |
| 4   | BH    | 307 | LEU  |
| 4   | BH    | 318 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | BH    | 319 | THR  |
| 4   | BH    | 328 | SER  |
| 4   | BH    | 340 | MET  |
| 4   | BH    | 343 | SER  |
| 4   | BH    | 347 | LEU  |
| 4   | BH    | 349 | SER  |
| 5   | BK    | 43  | CYS  |
| 5   | BK    | 46  | ASP  |
| 5   | BK    | 66  | LYS  |
| 5   | BK    | 70  | VAL  |
| 5   | BK    | 76  | ILE  |
| 5   | BK    | 78  | ILE  |
| 5   | BK    | 86  | ASP  |
| 5   | BK    | 88  | SER  |
| 5   | BK    | 95  | SER  |
| 5   | BK    | 115 | THR  |
| 5   | BK    | 117 | THR  |
| 5   | BK    | 119 | TYR  |
| 5   | BK    | 120 | SER  |
| 5   | BK    | 125 | SER  |
| 5   | BK    | 134 | LEU  |
| 5   | BK    | 156 | THR  |
| 5   | BK    | 157 | GLN  |
| 5   | BK    | 168 | TYR  |
| 5   | BK    | 179 | ARG  |
| 5   | BK    | 183 | THR  |
| 3   | Bd    | 51  | SER  |
| 3   | Bd    | 61  | VAL  |
| 3   | Bd    | 62  | ILE  |
| 3   | Bd    | 63  | THR  |
| 3   | Bd    | 68  | ASP  |
| 3   | Bd    | 77  | TYR  |
| 3   | Bd    | 78  | ASN  |
| 3   | Bd    | 84  | SER  |
| 3   | Bd    | 85  | VAL  |
| 3   | Bd    | 115 | VAL  |
| 3   | Bd    | 117 | VAL  |
| 3   | Bd    | 127 | SER  |
| 3   | Bd    | 151 | SER  |
| 2   | CC    | 72  | LEU  |
| 2   | CC    | 91  | ASP  |
| 2   | CC    | 104 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CC    | 126 | ARG  |
| 2   | CC    | 173 | LYS  |
| 2   | CC    | 177 | CYS  |
| 2   | CC    | 180 | THR  |
| 2   | CC    | 189 | ASP  |
| 2   | CC    | 190 | GLN  |
| 2   | CC    | 221 | VAL  |
| 2   | CC    | 228 | HIS  |
| 2   | CC    | 229 | THR  |
| 2   | CC    | 234 | THR  |
| 2   | CC    | 239 | GLU  |
| 2   | CC    | 246 | VAL  |
| 3   | CD    | 31  | ASN  |
| 3   | CD    | 51  | SER  |
| 3   | CD    | 52  | MET  |
| 3   | CD    | 54  | GLU  |
| 3   | CD    | 59  | GLU  |
| 3   | CD    | 61  | VAL  |
| 3   | CD    | 70  | THR  |
| 3   | CD    | 84  | SER  |
| 3   | CD    | 85  | VAL  |
| 3   | CD    | 88  | SER  |
| 3   | CD    | 95  | THR  |
| 3   | CD    | 100 | LYS  |
| 3   | CD    | 108 | VAL  |
| 3   | CD    | 111 | LYS  |
| 3   | CD    | 117 | VAL  |
| 3   | CD    | 120 | SER  |
| 3   | CD    | 122 | SER  |
| 3   | CD    | 123 | THR  |
| 3   | CD    | 127 | SER  |
| 3   | CD    | 141 | LYS  |
| 3   | CD    | 147 | VAL  |
| 3   | CD    | 153 | VAL  |
| 3   | CD    | 157 | ARG  |
| 4   | CH    | 288 | VAL  |
| 4   | CH    | 307 | LEU  |
| 4   | CH    | 316 | THR  |
| 4   | CH    | 319 | THR  |
| 4   | CH    | 322 | SER  |
| 4   | CH    | 328 | SER  |
| 4   | CH    | 342 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | CH    | 349 | SER  |
| 5   | CK    | 43  | CYS  |
| 5   | CK    | 46  | ASP  |
| 5   | CK    | 76  | ILE  |
| 5   | CK    | 81  | SER  |
| 5   | CK    | 86  | ASP  |
| 5   | CK    | 115 | THR  |
| 5   | CK    | 116 | VAL  |
| 5   | CK    | 117 | THR  |
| 5   | CK    | 119 | TYR  |
| 5   | CK    | 120 | SER  |
| 5   | CK    | 125 | SER  |
| 5   | CK    | 128 | ARG  |
| 5   | CK    | 134 | LEU  |
| 5   | CK    | 156 | THR  |
| 5   | CK    | 161 | SER  |
| 5   | CK    | 166 | THR  |
| 5   | CK    | 168 | TYR  |
| 5   | CK    | 173 | ASP  |
| 5   | CK    | 175 | SER  |
| 5   | CK    | 179 | ARG  |
| 5   | CK    | 183 | THR  |
| 3   | Cd    | 38  | THR  |
| 3   | Cd    | 43  | GLU  |
| 3   | Cd    | 61  | VAL  |
| 3   | Cd    | 63  | THR  |
| 3   | Cd    | 71  | LEU  |
| 3   | Cd    | 78  | ASN  |
| 3   | Cd    | 85  | VAL  |
| 3   | Cd    | 111 | LYS  |
| 3   | Cd    | 138 | GLN  |
| 3   | Cd    | 141 | LYS  |
| 2   | DC    | 62  | THR  |
| 2   | DC    | 72  | LEU  |
| 2   | DC    | 91  | ASP  |
| 2   | DC    | 98  | SER  |
| 2   | DC    | 104 | ASN  |
| 2   | DC    | 119 | LEU  |
| 2   | DC    | 126 | ARG  |
| 2   | DC    | 127 | ILE  |
| 2   | DC    | 128 | SER  |
| 2   | DC    | 140 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | DC    | 143 | THR  |
| 2   | DC    | 157 | LYS  |
| 2   | DC    | 173 | LYS  |
| 2   | DC    | 177 | CYS  |
| 2   | DC    | 190 | GLN  |
| 2   | DC    | 231 | LEU  |
| 2   | DC    | 234 | THR  |
| 2   | DC    | 246 | VAL  |
| 2   | DC    | 256 | ASN  |
| 2   | DC    | 258 | ASN  |
| 3   | DD    | 31  | ASN  |
| 3   | DD    | 54  | GLU  |
| 3   | DD    | 63  | THR  |
| 3   | DD    | 70  | THR  |
| 3   | DD    | 85  | VAL  |
| 3   | DD    | 95  | THR  |
| 3   | DD    | 98  | ILE  |
| 3   | DD    | 108 | VAL  |
| 3   | DD    | 111 | LYS  |
| 3   | DD    | 120 | SER  |
| 3   | DD    | 122 | SER  |
| 3   | DD    | 133 | ARG  |
| 3   | DD    | 142 | LYS  |
| 3   | DD    | 144 | SER  |
| 3   | DD    | 151 | SER  |
| 3   | DD    | 157 | ARG  |
| 4   | DH    | 288 | VAL  |
| 4   | DH    | 297 | VAL  |
| 4   | DH    | 307 | LEU  |
| 4   | DH    | 314 | VAL  |
| 4   | DH    | 317 | ASN  |
| 4   | DH    | 318 | LEU  |
| 4   | DH    | 335 | THR  |
| 4   | DH    | 343 | SER  |
| 4   | DH    | 348 | VAL  |
| 4   | DH    | 349 | SER  |
| 5   | DK    | 43  | CYS  |
| 5   | DK    | 46  | ASP  |
| 5   | DK    | 69  | SER  |
| 5   | DK    | 81  | SER  |
| 5   | DK    | 88  | SER  |
| 5   | DK    | 92  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | DK    | 111 | LYS  |
| 5   | DK    | 115 | THR  |
| 5   | DK    | 119 | TYR  |
| 5   | DK    | 120 | SER  |
| 5   | DK    | 125 | SER  |
| 5   | DK    | 151 | SER  |
| 5   | DK    | 156 | THR  |
| 5   | DK    | 161 | SER  |
| 5   | DK    | 166 | THR  |
| 5   | DK    | 183 | THR  |
| 3   | Dd    | 38  | THR  |
| 3   | Dd    | 53  | LEU  |
| 3   | Dd    | 54  | GLU  |
| 3   | Dd    | 61  | VAL  |
| 3   | Dd    | 62  | ILE  |
| 3   | Dd    | 63  | THR  |
| 3   | Dd    | 68  | ASP  |
| 3   | Dd    | 75  | ASN  |
| 3   | Dd    | 78  | ASN  |
| 3   | Dd    | 93  | GLU  |
| 3   | Dd    | 111 | LYS  |
| 3   | Dd    | 117 | VAL  |
| 3   | Dd    | 118 | LEU  |
| 3   | Dd    | 144 | SER  |
| 3   | Dd    | 151 | SER  |
| 2   | EC    | 61  | GLU  |
| 2   | EC    | 72  | LEU  |
| 2   | EC    | 81  | GLU  |
| 2   | EC    | 97  | ASN  |
| 2   | EC    | 102 | GLU  |
| 2   | EC    | 105 | ILE  |
| 2   | EC    | 126 | ARG  |
| 2   | EC    | 139 | HIS  |
| 2   | EC    | 173 | LYS  |
| 2   | EC    | 177 | CYS  |
| 2   | EC    | 189 | ASP  |
| 2   | EC    | 199 | ILE  |
| 2   | EC    | 228 | HIS  |
| 2   | EC    | 229 | THR  |
| 2   | EC    | 238 | SER  |
| 2   | EC    | 244 | ASP  |
| 2   | EC    | 246 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | ED    | 39  | ILE  |
| 3   | ED    | 58  | VAL  |
| 3   | ED    | 61  | VAL  |
| 3   | ED    | 63  | THR  |
| 3   | ED    | 87  | TRP  |
| 3   | ED    | 88  | SER  |
| 3   | ED    | 94  | LEU  |
| 3   | ED    | 95  | THR  |
| 3   | ED    | 98  | ILE  |
| 3   | ED    | 108 | VAL  |
| 3   | ED    | 111 | LYS  |
| 3   | ED    | 120 | SER  |
| 3   | ED    | 122 | SER  |
| 3   | ED    | 123 | THR  |
| 3   | ED    | 124 | LYS  |
| 3   | ED    | 126 | GLU  |
| 3   | ED    | 127 | SER  |
| 3   | ED    | 151 | SER  |
| 4   | EH    | 297 | VAL  |
| 4   | EH    | 304 | ARG  |
| 4   | EH    | 307 | LEU  |
| 4   | EH    | 314 | VAL  |
| 4   | EH    | 316 | THR  |
| 4   | EH    | 318 | LEU  |
| 4   | EH    | 343 | SER  |
| 4   | EH    | 348 | VAL  |
| 4   | EH    | 349 | SER  |
| 4   | EH    | 357 | LEU  |
| 5   | EK    | 43  | CYS  |
| 5   | EK    | 46  | ASP  |
| 5   | EK    | 86  | ASP  |
| 5   | EK    | 111 | LYS  |
| 5   | EK    | 115 | THR  |
| 5   | EK    | 119 | TYR  |
| 5   | EK    | 120 | SER  |
| 5   | EK    | 125 | SER  |
| 5   | EK    | 152 | ARG  |
| 5   | EK    | 156 | THR  |
| 5   | EK    | 161 | SER  |
| 5   | EK    | 165 | ILE  |
| 5   | EK    | 166 | THR  |
| 5   | EK    | 168 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | EK    | 175 | SER  |
| 5   | EK    | 180 | VAL  |
| 5   | EK    | 183 | THR  |
| 3   | Ed    | 38  | THR  |
| 3   | Ed    | 62  | ILE  |
| 3   | Ed    | 72  | THR  |
| 3   | Ed    | 75  | ASN  |
| 3   | Ed    | 77  | TYR  |
| 3   | Ed    | 86  | ASP  |
| 3   | Ed    | 111 | LYS  |
| 3   | Ed    | 115 | VAL  |
| 3   | Ed    | 138 | GLN  |
| 3   | Ed    | 141 | LYS  |
| 3   | Ed    | 153 | VAL  |
| 2   | FC    | 72  | LEU  |
| 2   | FC    | 81  | GLU  |
| 2   | FC    | 119 | LEU  |
| 2   | FC    | 126 | ARG  |
| 2   | FC    | 134 | VAL  |
| 2   | FC    | 143 | THR  |
| 2   | FC    | 157 | LYS  |
| 2   | FC    | 173 | LYS  |
| 2   | FC    | 180 | THR  |
| 2   | FC    | 190 | GLN  |
| 2   | FC    | 228 | HIS  |
| 2   | FC    | 233 | VAL  |
| 2   | FC    | 246 | VAL  |
| 2   | FC    | 258 | ASN  |
| 3   | FD    | 31  | ASN  |
| 3   | FD    | 52  | MET  |
| 3   | FD    | 54  | GLU  |
| 3   | FD    | 63  | THR  |
| 3   | FD    | 69  | ASN  |
| 3   | FD    | 70  | THR  |
| 3   | FD    | 84  | SER  |
| 3   | FD    | 95  | THR  |
| 3   | FD    | 98  | ILE  |
| 3   | FD    | 100 | LYS  |
| 3   | FD    | 108 | VAL  |
| 3   | FD    | 111 | LYS  |
| 3   | FD    | 122 | SER  |
| 3   | FD    | 123 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | FD    | 127 | SER  |
| 3   | FD    | 142 | LYS  |
| 3   | FD    | 144 | SER  |
| 3   | FD    | 154 | VAL  |
| 4   | FH    | 282 | LEU  |
| 4   | FH    | 288 | VAL  |
| 4   | FH    | 312 | MET  |
| 4   | FH    | 316 | THR  |
| 4   | FH    | 317 | ASN  |
| 4   | FH    | 349 | SER  |
| 5   | FK    | 43  | CYS  |
| 5   | FK    | 46  | ASP  |
| 5   | FK    | 49  | CYS  |
| 5   | FK    | 60  | LEU  |
| 5   | FK    | 70  | VAL  |
| 5   | FK    | 75  | LEU  |
| 5   | FK    | 76  | ILE  |
| 5   | FK    | 77  | SER  |
| 5   | FK    | 81  | SER  |
| 5   | FK    | 86  | ASP  |
| 5   | FK    | 92  | ASN  |
| 5   | FK    | 95  | SER  |
| 5   | FK    | 111 | LYS  |
| 5   | FK    | 119 | TYR  |
| 5   | FK    | 120 | SER  |
| 5   | FK    | 125 | SER  |
| 5   | FK    | 137 | SER  |
| 5   | FK    | 156 | THR  |
| 5   | FK    | 161 | SER  |
| 5   | FK    | 173 | ASP  |
| 5   | FK    | 179 | ARG  |
| 5   | FK    | 181 | GLU  |
| 5   | FK    | 183 | THR  |
| 3   | Fd    | 38  | THR  |
| 3   | Fd    | 48  | VAL  |
| 3   | Fd    | 54  | GLU  |
| 3   | Fd    | 63  | THR  |
| 3   | Fd    | 67  | LYS  |
| 3   | Fd    | 71  | LEU  |
| 3   | Fd    | 72  | THR  |
| 3   | Fd    | 77  | TYR  |
| 3   | Fd    | 80  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Fd    | 111 | LYS  |
| 3   | Fd    | 115 | VAL  |
| 3   | Fd    | 117 | VAL  |
| 3   | Fd    | 127 | SER  |
| 2   | GC    | 97  | ASN  |
| 2   | GC    | 109 | VAL  |
| 2   | GC    | 134 | VAL  |
| 2   | GC    | 136 | LYS  |
| 2   | GC    | 173 | LYS  |
| 2   | GC    | 178 | ILE  |
| 2   | GC    | 180 | THR  |
| 2   | GC    | 189 | ASP  |
| 2   | GC    | 190 | GLN  |
| 2   | GC    | 213 | ARG  |
| 2   | GC    | 221 | VAL  |
| 2   | GC    | 228 | HIS  |
| 2   | GC    | 233 | VAL  |
| 2   | GC    | 234 | THR  |
| 2   | GC    | 246 | VAL  |
| 2   | GC    | 256 | ASN  |
| 3   | GD    | 31  | ASN  |
| 3   | GD    | 52  | MET  |
| 3   | GD    | 53  | LEU  |
| 3   | GD    | 61  | VAL  |
| 3   | GD    | 63  | THR  |
| 3   | GD    | 70  | THR  |
| 3   | GD    | 97  | ARG  |
| 3   | GD    | 108 | VAL  |
| 3   | GD    | 111 | LYS  |
| 3   | GD    | 117 | VAL  |
| 3   | GD    | 120 | SER  |
| 3   | GD    | 123 | THR  |
| 3   | GD    | 127 | SER  |
| 3   | GD    | 142 | LYS  |
| 3   | GD    | 157 | ARG  |
| 4   | GH    | 276 | SER  |
| 4   | GH    | 288 | VAL  |
| 4   | GH    | 304 | ARG  |
| 4   | GH    | 307 | LEU  |
| 4   | GH    | 328 | SER  |
| 4   | GH    | 342 | LYS  |
| 4   | GH    | 343 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | GH    | 345 | VAL  |
| 4   | GH    | 349 | SER  |
| 5   | GK    | 43  | CYS  |
| 5   | GK    | 46  | ASP  |
| 5   | GK    | 75  | LEU  |
| 5   | GK    | 76  | ILE  |
| 5   | GK    | 92  | ASN  |
| 5   | GK    | 111 | LYS  |
| 5   | GK    | 117 | THR  |
| 5   | GK    | 119 | TYR  |
| 5   | GK    | 120 | SER  |
| 5   | GK    | 125 | SER  |
| 5   | GK    | 137 | SER  |
| 5   | GK    | 141 | SER  |
| 5   | GK    | 152 | ARG  |
| 5   | GK    | 156 | THR  |
| 5   | GK    | 166 | THR  |
| 5   | GK    | 168 | TYR  |
| 5   | GK    | 173 | ASP  |
| 5   | GK    | 175 | SER  |
| 5   | GK    | 183 | THR  |
| 3   | Gd    | 36  | ASP  |
| 3   | Gd    | 61  | VAL  |
| 3   | Gd    | 62  | ILE  |
| 3   | Gd    | 68  | ASP  |
| 3   | Gd    | 71  | LEU  |
| 3   | Gd    | 75  | ASN  |
| 3   | Gd    | 77  | TYR  |
| 3   | Gd    | 78  | ASN  |
| 3   | Gd    | 82  | ARG  |
| 3   | Gd    | 85  | VAL  |
| 3   | Gd    | 93  | GLU  |
| 3   | Gd    | 108 | VAL  |
| 3   | Gd    | 111 | LYS  |
| 3   | Gd    | 117 | VAL  |
| 3   | Gd    | 122 | SER  |
| 3   | Gd    | 127 | SER  |
| 3   | Gd    | 141 | LYS  |
| 3   | Gd    | 156 | LEU  |
| 2   | HC    | 81  | GLU  |
| 2   | HC    | 99  | LEU  |
| 2   | HC    | 116 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | HC    | 126 | ARG  |
| 2   | HC    | 173 | LYS  |
| 2   | HC    | 177 | CYS  |
| 2   | HC    | 180 | THR  |
| 2   | HC    | 228 | HIS  |
| 2   | HC    | 229 | THR  |
| 2   | HC    | 233 | VAL  |
| 2   | HC    | 234 | THR  |
| 2   | HC    | 246 | VAL  |
| 2   | HC    | 266 | VAL  |
| 3   | HD    | 31  | ASN  |
| 3   | HD    | 47  | SER  |
| 3   | HD    | 58  | VAL  |
| 3   | HD    | 61  | VAL  |
| 3   | HD    | 63  | THR  |
| 3   | HD    | 70  | THR  |
| 3   | HD    | 84  | SER  |
| 3   | HD    | 85  | VAL  |
| 3   | HD    | 100 | LYS  |
| 3   | HD    | 108 | VAL  |
| 3   | HD    | 111 | LYS  |
| 3   | HD    | 115 | VAL  |
| 3   | HD    | 117 | VAL  |
| 3   | HD    | 119 | ILE  |
| 3   | HD    | 123 | THR  |
| 3   | HD    | 124 | LYS  |
| 3   | HD    | 126 | GLU  |
| 3   | HD    | 127 | SER  |
| 3   | HD    | 141 | LYS  |
| 3   | HD    | 146 | HIS  |
| 3   | HD    | 151 | SER  |
| 4   | HH    | 280 | LEU  |
| 4   | HH    | 288 | VAL  |
| 4   | HH    | 297 | VAL  |
| 4   | HH    | 317 | ASN  |
| 4   | HH    | 343 | SER  |
| 4   | HH    | 349 | SER  |
| 5   | HK    | 43  | CYS  |
| 5   | HK    | 46  | ASP  |
| 5   | HK    | 60  | LEU  |
| 5   | HK    | 67  | VAL  |
| 5   | HK    | 70  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | HK    | 81  | SER  |
| 5   | HK    | 92  | ASN  |
| 5   | HK    | 95  | SER  |
| 5   | HK    | 101 | GLU  |
| 5   | HK    | 116 | VAL  |
| 5   | HK    | 119 | TYR  |
| 5   | HK    | 120 | SER  |
| 5   | HK    | 125 | SER  |
| 5   | HK    | 150 | ASP  |
| 5   | HK    | 153 | ILE  |
| 5   | HK    | 156 | THR  |
| 5   | HK    | 159 | LEU  |
| 5   | HK    | 161 | SER  |
| 5   | HK    | 168 | TYR  |
| 5   | HK    | 173 | ASP  |
| 5   | HK    | 175 | SER  |
| 5   | HK    | 183 | THR  |
| 3   | Hd    | 29  | PRO  |
| 3   | Hd    | 35  | ASP  |
| 3   | Hd    | 38  | THR  |
| 3   | Hd    | 55  | MET  |
| 3   | Hd    | 57  | LYS  |
| 3   | Hd    | 60  | LYS  |
| 3   | Hd    | 77  | TYR  |
| 3   | Hd    | 85  | VAL  |
| 3   | Hd    | 93  | GLU  |
| 3   | Hd    | 111 | LYS  |
| 3   | Hd    | 122 | SER  |
| 3   | Hd    | 123 | THR  |
| 3   | Hd    | 126 | GLU  |
| 3   | Hd    | 138 | GLN  |
| 3   | Hd    | 152 | GLN  |
| 3   | Hd    | 153 | VAL  |
| 3   | Hd    | 161 | ILE  |
| 2   | IC    | 61  | GLU  |
| 2   | IC    | 72  | LEU  |
| 2   | IC    | 91  | ASP  |
| 2   | IC    | 99  | LEU  |
| 2   | IC    | 100 | VAL  |
| 2   | IC    | 119 | LEU  |
| 2   | IC    | 126 | ARG  |
| 2   | IC    | 140 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | IC    | 173 | LYS  |
| 2   | IC    | 177 | CYS  |
| 2   | IC    | 189 | ASP  |
| 2   | IC    | 226 | VAL  |
| 2   | IC    | 229 | THR  |
| 2   | IC    | 246 | VAL  |
| 2   | IC    | 256 | ASN  |
| 2   | IC    | 258 | ASN  |
| 2   | IC    | 266 | VAL  |
| 3   | ID    | 39  | ILE  |
| 3   | ID    | 61  | VAL  |
| 3   | ID    | 63  | THR  |
| 3   | ID    | 70  | THR  |
| 3   | ID    | 87  | TRP  |
| 3   | ID    | 108 | VAL  |
| 3   | ID    | 111 | LYS  |
| 3   | ID    | 115 | VAL  |
| 3   | ID    | 123 | THR  |
| 3   | ID    | 126 | GLU  |
| 3   | ID    | 133 | ARG  |
| 3   | ID    | 141 | LYS  |
| 3   | ID    | 144 | SER  |
| 3   | ID    | 151 | SER  |
| 4   | IH    | 288 | VAL  |
| 4   | IH    | 297 | VAL  |
| 4   | IH    | 299 | SER  |
| 4   | IH    | 307 | LEU  |
| 4   | IH    | 318 | LEU  |
| 4   | IH    | 319 | THR  |
| 4   | IH    | 343 | SER  |
| 4   | IH    | 348 | VAL  |
| 4   | IH    | 349 | SER  |
| 4   | IH    | 353 | LYS  |
| 5   | IK    | 43  | CYS  |
| 5   | IK    | 46  | ASP  |
| 5   | IK    | 70  | VAL  |
| 5   | IK    | 76  | ILE  |
| 5   | IK    | 101 | GLU  |
| 5   | IK    | 119 | TYR  |
| 5   | IK    | 146 | SER  |
| 5   | IK    | 152 | ARG  |
| 5   | IK    | 156 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | IK    | 168 | TYR  |
| 5   | IK    | 175 | SER  |
| 5   | IK    | 183 | THR  |
| 3   | Id    | 38  | THR  |
| 3   | Id    | 43  | GLU  |
| 3   | Id    | 63  | THR  |
| 3   | Id    | 75  | ASN  |
| 3   | Id    | 78  | ASN  |
| 3   | Id    | 82  | ARG  |
| 3   | Id    | 108 | VAL  |
| 3   | Id    | 111 | LYS  |
| 3   | Id    | 127 | SER  |
| 2   | JC    | 61  | GLU  |
| 2   | JC    | 143 | THR  |
| 2   | JC    | 149 | GLN  |
| 2   | JC    | 173 | LYS  |
| 2   | JC    | 177 | CYS  |
| 2   | JC    | 180 | THR  |
| 2   | JC    | 181 | GLU  |
| 2   | JC    | 189 | ASP  |
| 2   | JC    | 211 | LEU  |
| 2   | JC    | 228 | HIS  |
| 2   | JC    | 229 | THR  |
| 2   | JC    | 246 | VAL  |
| 2   | JC    | 258 | ASN  |
| 3   | JD    | 54  | GLU  |
| 3   | JD    | 63  | THR  |
| 3   | JD    | 70  | THR  |
| 3   | JD    | 85  | VAL  |
| 3   | JD    | 87  | TRP  |
| 3   | JD    | 108 | VAL  |
| 3   | JD    | 111 | LYS  |
| 3   | JD    | 117 | VAL  |
| 3   | JD    | 123 | THR  |
| 3   | JD    | 126 | GLU  |
| 3   | JD    | 127 | SER  |
| 3   | JD    | 144 | SER  |
| 3   | JD    | 147 | VAL  |
| 3   | JD    | 150 | ASN  |
| 3   | JD    | 153 | VAL  |
| 3   | JD    | 157 | ARG  |
| 4   | JH    | 288 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | JH    | 299 | SER  |
| 4   | JH    | 307 | LEU  |
| 4   | JH    | 314 | VAL  |
| 4   | JH    | 316 | THR  |
| 4   | JH    | 317 | ASN  |
| 4   | JH    | 323 | PRO  |
| 4   | JH    | 328 | SER  |
| 4   | JH    | 343 | SER  |
| 4   | JH    | 345 | VAL  |
| 4   | JH    | 349 | SER  |
| 5   | JK    | 43  | CYS  |
| 5   | JK    | 46  | ASP  |
| 5   | JK    | 70  | VAL  |
| 5   | JK    | 83  | LEU  |
| 5   | JK    | 86  | ASP  |
| 5   | JK    | 92  | ASN  |
| 5   | JK    | 111 | LYS  |
| 5   | JK    | 115 | THR  |
| 5   | JK    | 119 | TYR  |
| 5   | JK    | 120 | SER  |
| 5   | JK    | 122 | LYS  |
| 5   | JK    | 156 | THR  |
| 5   | JK    | 168 | TYR  |
| 5   | JK    | 179 | ARG  |
| 5   | JK    | 181 | GLU  |
| 5   | JK    | 183 | THR  |
| 3   | Jd    | 38  | THR  |
| 3   | Jd    | 62  | ILE  |
| 3   | Jd    | 63  | THR  |
| 3   | Jd    | 68  | ASP  |
| 3   | Jd    | 71  | LEU  |
| 3   | Jd    | 77  | TYR  |
| 3   | Jd    | 78  | ASN  |
| 3   | Jd    | 111 | LYS  |
| 3   | Jd    | 117 | VAL  |
| 3   | Jd    | 118 | LEU  |
| 3   | Jd    | 135 | ILE  |
| 3   | Jd    | 138 | GLN  |
| 3   | Jd    | 154 | VAL  |
| 3   | Jd    | 160 | LYS  |
| 2   | KC    | 61  | GLU  |
| 2   | KC    | 85  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | KC    | 130 | ARG  |
| 2   | KC    | 139 | HIS  |
| 2   | KC    | 157 | LYS  |
| 2   | KC    | 177 | CYS  |
| 2   | KC    | 180 | THR  |
| 2   | KC    | 190 | GLN  |
| 2   | KC    | 228 | HIS  |
| 2   | KC    | 239 | GLU  |
| 2   | KC    | 243 | ASP  |
| 2   | KC    | 246 | VAL  |
| 2   | KC    | 256 | ASN  |
| 2   | KC    | 258 | ASN  |
| 2   | KC    | 266 | VAL  |
| 3   | KD    | 39  | ILE  |
| 3   | KD    | 55  | MET  |
| 3   | KD    | 58  | VAL  |
| 3   | KD    | 63  | THR  |
| 3   | KD    | 94  | LEU  |
| 3   | KD    | 108 | VAL  |
| 3   | KD    | 111 | LYS  |
| 3   | KD    | 115 | VAL  |
| 3   | KD    | 117 | VAL  |
| 3   | KD    | 127 | SER  |
| 3   | KD    | 141 | LYS  |
| 4   | KH    | 288 | VAL  |
| 4   | KH    | 309 | ASN  |
| 4   | KH    | 314 | VAL  |
| 4   | KH    | 316 | THR  |
| 4   | KH    | 343 | SER  |
| 4   | KH    | 345 | VAL  |
| 4   | KH    | 349 | SER  |
| 4   | KH    | 359 | VAL  |
| 5   | KK    | 43  | CYS  |
| 5   | KK    | 46  | ASP  |
| 5   | KK    | 66  | LYS  |
| 5   | KK    | 86  | ASP  |
| 5   | KK    | 101 | GLU  |
| 5   | KK    | 119 | TYR  |
| 5   | KK    | 120 | SER  |
| 5   | KK    | 122 | LYS  |
| 5   | KK    | 125 | SER  |
| 5   | KK    | 132 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | KK    | 167 | SER  |
| 5   | KK    | 173 | ASP  |
| 5   | KK    | 175 | SER  |
| 5   | KK    | 183 | THR  |
| 3   | Kd    | 35  | ASP  |
| 3   | Kd    | 38  | THR  |
| 3   | Kd    | 43  | GLU  |
| 3   | Kd    | 62  | ILE  |
| 3   | Kd    | 63  | THR  |
| 3   | Kd    | 68  | ASP  |
| 3   | Kd    | 72  | THR  |
| 3   | Kd    | 75  | ASN  |
| 3   | Kd    | 78  | ASN  |
| 3   | Kd    | 84  | SER  |
| 3   | Kd    | 85  | VAL  |
| 3   | Kd    | 86  | ASP  |
| 3   | Kd    | 111 | LYS  |
| 3   | Kd    | 115 | VAL  |
| 3   | Kd    | 120 | SER  |
| 3   | Kd    | 126 | GLU  |
| 3   | Kd    | 127 | SER  |
| 3   | Kd    | 138 | GLN  |
| 3   | Kd    | 144 | SER  |
| 2   | LC    | 81  | GLU  |
| 2   | LC    | 104 | ASN  |
| 2   | LC    | 116 | THR  |
| 2   | LC    | 134 | VAL  |
| 2   | LC    | 153 | MET  |
| 2   | LC    | 173 | LYS  |
| 2   | LC    | 177 | CYS  |
| 2   | LC    | 180 | THR  |
| 2   | LC    | 189 | ASP  |
| 2   | LC    | 221 | VAL  |
| 2   | LC    | 228 | HIS  |
| 2   | LC    | 229 | THR  |
| 2   | LC    | 244 | ASP  |
| 2   | LC    | 246 | VAL  |
| 2   | LC    | 256 | ASN  |
| 3   | LD    | 54  | GLU  |
| 3   | LD    | 58  | VAL  |
| 3   | LD    | 61  | VAL  |
| 3   | LD    | 63  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | LD    | 70  | THR  |
| 3   | LD    | 84  | SER  |
| 3   | LD    | 85  | VAL  |
| 3   | LD    | 87  | TRP  |
| 3   | LD    | 98  | ILE  |
| 3   | LD    | 108 | VAL  |
| 3   | LD    | 111 | LYS  |
| 3   | LD    | 115 | VAL  |
| 3   | LD    | 120 | SER  |
| 3   | LD    | 123 | THR  |
| 3   | LD    | 127 | SER  |
| 3   | LD    | 133 | ARG  |
| 3   | LD    | 157 | ARG  |
| 4   | LH    | 286 | GLU  |
| 4   | LH    | 288 | VAL  |
| 4   | LH    | 293 | SER  |
| 4   | LH    | 297 | VAL  |
| 4   | LH    | 299 | SER  |
| 4   | LH    | 317 | ASN  |
| 4   | LH    | 318 | LEU  |
| 4   | LH    | 322 | SER  |
| 4   | LH    | 328 | SER  |
| 4   | LH    | 343 | SER  |
| 4   | LH    | 349 | SER  |
| 5   | LK    | 43  | CYS  |
| 5   | LK    | 46  | ASP  |
| 5   | LK    | 67  | VAL  |
| 5   | LK    | 70  | VAL  |
| 5   | LK    | 86  | ASP  |
| 5   | LK    | 95  | SER  |
| 5   | LK    | 107 | LYS  |
| 5   | LK    | 111 | LYS  |
| 5   | LK    | 115 | THR  |
| 5   | LK    | 119 | TYR  |
| 5   | LK    | 120 | SER  |
| 5   | LK    | 166 | THR  |
| 5   | LK    | 168 | TYR  |
| 5   | LK    | 170 | LEU  |
| 5   | LK    | 183 | THR  |
| 3   | Ld    | 35  | ASP  |
| 3   | Ld    | 36  | ASP  |
| 3   | Ld    | 48  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Ld    | 61  | VAL  |
| 3   | Ld    | 62  | ILE  |
| 3   | Ld    | 63  | THR  |
| 3   | Ld    | 72  | THR  |
| 3   | Ld    | 77  | TYR  |
| 3   | Ld    | 78  | ASN  |
| 3   | Ld    | 111 | LYS  |
| 3   | Ld    | 115 | VAL  |
| 3   | Ld    | 117 | VAL  |
| 3   | Ld    | 122 | SER  |
| 3   | Ld    | 127 | SER  |
| 3   | Ld    | 138 | GLN  |
| 3   | Ld    | 154 | VAL  |
| 2   | MC    | 91  | ASP  |
| 2   | MC    | 126 | ARG  |
| 2   | MC    | 134 | VAL  |
| 2   | MC    | 143 | THR  |
| 2   | MC    | 177 | CYS  |
| 2   | MC    | 211 | LEU  |
| 2   | MC    | 228 | HIS  |
| 2   | MC    | 229 | THR  |
| 2   | MC    | 246 | VAL  |
| 2   | MC    | 255 | LEU  |
| 2   | MC    | 258 | ASN  |
| 2   | MC    | 268 | LYS  |
| 3   | MD    | 58  | VAL  |
| 3   | MD    | 63  | THR  |
| 3   | MD    | 70  | THR  |
| 3   | MD    | 84  | SER  |
| 3   | MD    | 85  | VAL  |
| 3   | MD    | 108 | VAL  |
| 3   | MD    | 111 | LYS  |
| 3   | MD    | 117 | VAL  |
| 3   | MD    | 120 | SER  |
| 3   | MD    | 123 | THR  |
| 3   | MD    | 126 | GLU  |
| 3   | MD    | 146 | HIS  |
| 3   | MD    | 147 | VAL  |
| 3   | MD    | 150 | ASN  |
| 4   | MH    | 288 | VAL  |
| 4   | MH    | 297 | VAL  |
| 4   | MH    | 304 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | MH    | 307 | LEU  |
| 4   | MH    | 317 | ASN  |
| 4   | MH    | 318 | LEU  |
| 4   | MH    | 322 | SER  |
| 4   | MH    | 328 | SER  |
| 4   | MH    | 340 | MET  |
| 4   | MH    | 343 | SER  |
| 4   | MH    | 349 | SER  |
| 5   | MK    | 46  | ASP  |
| 5   | MK    | 50  | ASP  |
| 5   | MK    | 81  | SER  |
| 5   | MK    | 92  | ASN  |
| 5   | MK    | 115 | THR  |
| 5   | MK    | 116 | VAL  |
| 5   | MK    | 119 | TYR  |
| 5   | MK    | 120 | SER  |
| 5   | MK    | 125 | SER  |
| 5   | MK    | 141 | SER  |
| 5   | MK    | 156 | THR  |
| 5   | MK    | 161 | SER  |
| 5   | MK    | 173 | ASP  |
| 5   | MK    | 183 | THR  |
| 3   | Md    | 35  | ASP  |
| 3   | Md    | 38  | THR  |
| 3   | Md    | 48  | VAL  |
| 3   | Md    | 61  | VAL  |
| 3   | Md    | 67  | LYS  |
| 3   | Md    | 68  | ASP  |
| 3   | Md    | 71  | LEU  |
| 3   | Md    | 75  | ASN  |
| 3   | Md    | 77  | TYR  |
| 3   | Md    | 78  | ASN  |
| 3   | Md    | 82  | ARG  |
| 3   | Md    | 84  | SER  |
| 3   | Md    | 85  | VAL  |
| 3   | Md    | 88  | SER  |
| 3   | Md    | 92  | GLU  |
| 3   | Md    | 111 | LYS  |
| 3   | Md    | 117 | VAL  |
| 3   | Md    | 120 | SER  |
| 3   | Md    | 127 | SER  |
| 3   | Md    | 144 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Md    | 151 | SER  |
| 3   | Md    | 157 | ARG  |
| 6   | N     | 99  | ARG  |
| 6   | N     | 101 | SER  |
| 6   | N     | 108 | ASP  |
| 6   | N     | 118 | GLU  |
| 6   | N     | 119 | TYR  |
| 6   | N     | 130 | ASP  |
| 6   | N     | 134 | MET  |
| 6   | N     | 155 | LEU  |
| 6   | N     | 162 | THR  |
| 6   | N     | 210 | ASP  |
| 6   | O     | 99  | ARG  |
| 6   | O     | 101 | SER  |
| 6   | O     | 108 | ASP  |
| 6   | O     | 110 | GLN  |
| 6   | O     | 117 | VAL  |
| 6   | O     | 130 | ASP  |
| 6   | O     | 143 | ILE  |
| 6   | O     | 162 | THR  |
| 6   | O     | 174 | SER  |
| 6   | O     | 181 | LEU  |
| 6   | O     | 189 | MET  |
| 6   | O     | 202 | ARG  |
| 6   | O     | 219 | ILE  |
| 6   | O     | 226 | ASN  |
| 6   | P     | 99  | ARG  |
| 6   | P     | 101 | SER  |
| 6   | P     | 110 | GLN  |
| 6   | P     | 115 | GLN  |
| 6   | P     | 121 | ASP  |
| 6   | P     | 124 | THR  |
| 6   | P     | 155 | LEU  |
| 6   | P     | 174 | SER  |
| 6   | P     | 196 | ASN  |
| 6   | P     | 210 | ASP  |
| 6   | Q     | 99  | ARG  |
| 6   | Q     | 108 | ASP  |
| 6   | Q     | 110 | GLN  |
| 6   | Q     | 130 | ASP  |
| 6   | Q     | 143 | ILE  |
| 6   | Q     | 162 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | Q     | 174 | SER  |
| 6   | Q     | 181 | LEU  |
| 6   | Q     | 189 | MET  |
| 6   | Q     | 196 | ASN  |
| 6   | Q     | 210 | ASP  |
| 6   | R     | 99  | ARG  |
| 6   | R     | 118 | GLU  |
| 6   | R     | 130 | ASP  |
| 6   | R     | 143 | ILE  |
| 6   | R     | 154 | LEU  |
| 6   | R     | 155 | LEU  |
| 6   | R     | 169 | THR  |
| 6   | R     | 174 | SER  |
| 6   | R     | 210 | ASP  |
| 6   | R     | 226 | ASN  |
| 6   | S     | 99  | ARG  |
| 6   | S     | 101 | SER  |
| 6   | S     | 108 | ASP  |
| 6   | S     | 110 | GLN  |
| 6   | S     | 130 | ASP  |
| 6   | S     | 165 | VAL  |
| 6   | S     | 174 | SER  |
| 6   | S     | 182 | SER  |
| 6   | S     | 189 | MET  |
| 6   | S     | 196 | ASN  |
| 6   | S     | 210 | ASP  |
| 6   | S     | 212 | ASN  |
| 6   | S     | 223 | SER  |
| 6   | T     | 99  | ARG  |
| 6   | T     | 101 | SER  |
| 6   | T     | 108 | ASP  |
| 6   | T     | 110 | GLN  |
| 6   | T     | 118 | GLU  |
| 6   | T     | 119 | TYR  |
| 6   | T     | 121 | ASP  |
| 6   | T     | 130 | ASP  |
| 6   | T     | 134 | MET  |
| 6   | T     | 140 | LEU  |
| 6   | T     | 143 | ILE  |
| 6   | T     | 155 | LEU  |
| 6   | T     | 162 | THR  |
| 6   | T     | 196 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | T     | 210 | ASP  |
| 6   | T     | 219 | ILE  |
| 6   | U     | 99  | ARG  |
| 6   | U     | 101 | SER  |
| 6   | U     | 117 | VAL  |
| 6   | U     | 119 | TYR  |
| 6   | U     | 130 | ASP  |
| 6   | U     | 139 | ARG  |
| 6   | U     | 140 | LEU  |
| 6   | U     | 143 | ILE  |
| 6   | U     | 144 | CYS  |
| 6   | U     | 155 | LEU  |
| 6   | U     | 169 | THR  |
| 6   | U     | 174 | SER  |
| 6   | U     | 196 | ASN  |
| 6   | U     | 210 | ASP  |
| 6   | V     | 99  | ARG  |
| 6   | V     | 110 | GLN  |
| 6   | V     | 130 | ASP  |
| 6   | V     | 134 | MET  |
| 6   | V     | 143 | ILE  |
| 6   | V     | 154 | LEU  |
| 6   | V     | 162 | THR  |
| 6   | V     | 174 | SER  |
| 6   | V     | 210 | ASP  |
| 6   | V     | 211 | LYS  |
| 6   | W     | 99  | ARG  |
| 6   | W     | 101 | SER  |
| 6   | W     | 110 | GLN  |
| 6   | W     | 121 | ASP  |
| 6   | W     | 143 | ILE  |
| 6   | W     | 154 | LEU  |
| 6   | W     | 162 | THR  |
| 6   | W     | 174 | SER  |
| 6   | W     | 210 | ASP  |
| 6   | W     | 212 | ASN  |
| 6   | X     | 99  | ARG  |
| 6   | X     | 108 | ASP  |
| 6   | X     | 110 | GLN  |
| 6   | X     | 119 | TYR  |
| 6   | X     | 130 | ASP  |
| 6   | X     | 143 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | X     | 162 | THR  |
| 6   | X     | 174 | SER  |
| 6   | X     | 210 | ASP  |
| 6   | Y     | 99  | ARG  |
| 6   | Y     | 101 | SER  |
| 6   | Y     | 108 | ASP  |
| 6   | Y     | 124 | THR  |
| 6   | Y     | 129 | THR  |
| 6   | Y     | 130 | ASP  |
| 6   | Y     | 155 | LEU  |
| 6   | Y     | 169 | THR  |
| 6   | Y     | 174 | SER  |
| 6   | Y     | 210 | ASP  |
| 6   | Z     | 99  | ARG  |
| 6   | Z     | 101 | SER  |
| 6   | Z     | 108 | ASP  |
| 6   | Z     | 118 | GLU  |
| 6   | Z     | 130 | ASP  |
| 6   | Z     | 139 | ARG  |
| 6   | Z     | 140 | LEU  |
| 6   | Z     | 143 | ILE  |
| 6   | Z     | 162 | THR  |
| 6   | Z     | 165 | VAL  |
| 6   | Z     | 174 | SER  |
| 6   | Z     | 181 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AC    | 103 | HIS  |
| 3   | AD    | 152 | GLN  |
| 5   | AK    | 147 | GLN  |
| 3   | Ad    | 152 | GLN  |
| 2   | BC    | 82  | GLN  |
| 2   | BC    | 103 | HIS  |
| 3   | BD    | 138 | GLN  |
| 3   | BD    | 152 | GLN  |
| 3   | Bd    | 78  | ASN  |
| 3   | Bd    | 152 | GLN  |
| 2   | CC    | 103 | HIS  |
| 2   | CC    | 228 | HIS  |
| 3   | CD    | 152 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | CK    | 147 | GLN  |
| 3   | Cd    | 78  | ASN  |
| 3   | Cd    | 152 | GLN  |
| 2   | DC    | 103 | HIS  |
| 3   | DD    | 152 | GLN  |
| 3   | Dd    | 152 | GLN  |
| 2   | EC    | 103 | HIS  |
| 3   | ED    | 138 | GLN  |
| 3   | ED    | 152 | GLN  |
| 4   | EH    | 341 | GLN  |
| 5   | EK    | 100 | ASN  |
| 5   | EK    | 147 | GLN  |
| 3   | Ed    | 31  | ASN  |
| 3   | Ed    | 32  | ASN  |
| 2   | FC    | 256 | ASN  |
| 2   | FC    | 258 | ASN  |
| 3   | FD    | 32  | ASN  |
| 3   | FD    | 138 | GLN  |
| 3   | FD    | 152 | GLN  |
| 3   | Fd    | 32  | ASN  |
| 2   | GC    | 103 | HIS  |
| 3   | GD    | 138 | GLN  |
| 3   | GD    | 152 | GLN  |
| 4   | GH    | 351 | HIS  |
| 3   | Gd    | 78  | ASN  |
| 3   | HD    | 138 | GLN  |
| 3   | HD    | 152 | GLN  |
| 5   | HK    | 61  | ASN  |
| 2   | IC    | 103 | HIS  |
| 3   | ID    | 138 | GLN  |
| 3   | ID    | 152 | GLN  |
| 3   | Id    | 80  | GLN  |
| 3   | Id    | 103 | HIS  |
| 3   | Id    | 152 | GLN  |
| 2   | JC    | 103 | HIS  |
| 2   | JC    | 241 | HIS  |
| 3   | JD    | 138 | GLN  |
| 3   | JD    | 152 | GLN  |
| 4   | JH    | 351 | HIS  |
| 5   | JK    | 87  | GLN  |
| 3   | Jd    | 31  | ASN  |
| 3   | Jd    | 32  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Jd    | 78  | ASN  |
| 2   | KC    | 103 | HIS  |
| 3   | KD    | 152 | GLN  |
| 3   | Kd    | 32  | ASN  |
| 3   | Kd    | 152 | GLN  |
| 2   | LC    | 103 | HIS  |
| 3   | LD    | 138 | GLN  |
| 3   | LD    | 152 | GLN  |
| 5   | LK    | 87  | GLN  |
| 3   | Ld    | 32  | ASN  |
| 3   | Ld    | 152 | GLN  |
| 2   | MC    | 103 | HIS  |
| 3   | MD    | 138 | GLN  |
| 3   | Md    | 32  | ASN  |
| 3   | Md    | 78  | ASN  |
| 6   | N     | 112 | GLN  |
| 6   | N     | 150 | ASN  |
| 6   | N     | 156 | ASN  |
| 6   | N     | 177 | HIS  |
| 6   | N     | 212 | ASN  |
| 6   | N     | 232 | GLN  |
| 6   | O     | 141 | ASN  |
| 6   | O     | 212 | ASN  |
| 6   | O     | 232 | GLN  |
| 6   | P     | 112 | GLN  |
| 6   | P     | 141 | ASN  |
| 6   | P     | 149 | ASN  |
| 6   | P     | 212 | ASN  |
| 6   | P     | 232 | GLN  |
| 6   | Q     | 112 | GLN  |
| 6   | Q     | 150 | ASN  |
| 6   | Q     | 232 | GLN  |
| 6   | R     | 112 | GLN  |
| 6   | R     | 149 | ASN  |
| 6   | R     | 156 | ASN  |
| 6   | R     | 177 | HIS  |
| 6   | R     | 212 | ASN  |
| 6   | R     | 232 | GLN  |
| 6   | S     | 112 | GLN  |
| 6   | S     | 141 | ASN  |
| 6   | S     | 150 | ASN  |
| 6   | S     | 156 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | S     | 185 | GLN  |
| 6   | S     | 212 | ASN  |
| 6   | S     | 232 | GLN  |
| 6   | T     | 112 | GLN  |
| 6   | T     | 141 | ASN  |
| 6   | T     | 149 | ASN  |
| 6   | T     | 150 | ASN  |
| 6   | T     | 212 | ASN  |
| 6   | T     | 232 | GLN  |
| 6   | U     | 112 | GLN  |
| 6   | U     | 141 | ASN  |
| 6   | U     | 150 | ASN  |
| 6   | U     | 185 | GLN  |
| 6   | U     | 212 | ASN  |
| 6   | U     | 232 | GLN  |
| 6   | V     | 112 | GLN  |
| 6   | V     | 141 | ASN  |
| 6   | V     | 150 | ASN  |
| 6   | V     | 212 | ASN  |
| 6   | V     | 232 | GLN  |
| 6   | W     | 112 | GLN  |
| 6   | W     | 141 | ASN  |
| 6   | W     | 177 | HIS  |
| 6   | W     | 232 | GLN  |
| 6   | X     | 112 | GLN  |
| 6   | X     | 150 | ASN  |
| 6   | X     | 212 | ASN  |
| 6   | X     | 232 | GLN  |
| 6   | Y     | 112 | GLN  |
| 6   | Y     | 141 | ASN  |
| 6   | Y     | 150 | ASN  |
| 6   | Y     | 212 | ASN  |
| 6   | Y     | 232 | GLN  |
| 6   | Z     | 112 | GLN  |
| 6   | Z     | 141 | ASN  |
| 6   | Z     | 149 | ASN  |
| 6   | Z     | 212 | ASN  |
| 6   | Z     | 232 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22070. 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

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal surface views

This section was not generated.

### 6.5 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.