



## Full wwPDB EM Validation Report ⓘ

Feb 25, 2024 – 08:06 AM EST

PDB ID : 6X6K  
EMDB ID : EMD-22076  
Title : Cryo-EM Structure of the Helicobacter pylori dCag3 OMC  
Authors : Sheedlo, M.J.; Chung, J.M.; Sawhney, N.; Durie, C.L.; Cover, T.L.; Ohi, M.D.;  
Lacy, D.B.  
Deposited on : 2020-05-28  
Resolution : 3.10 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:

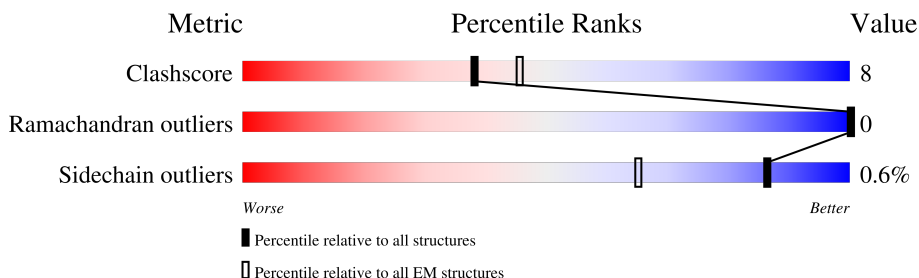
EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 Å.

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



| Metric                | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore            | 158937                   | 4297                     |
| 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | AT    | 278    | <div style="display: flex; justify-content: space-between;"> <span>38%</span> <span>53%</span> <span>11%</span> <span>•</span> <span>36%</span> </div> |
| 1   | BT    | 278    | <div style="display: flex; justify-content: space-between;"> <span>36%</span> <span>52%</span> <span>12%</span> <span>•</span> <span>36%</span> </div> |
| 1   | CT    | 278    | <div style="display: flex; justify-content: space-between;"> <span>36%</span> <span>51%</span> <span>12%</span> <span>•</span> <span>36%</span> </div> |
| 1   | DT    | 278    | <div style="display: flex; justify-content: space-between;"> <span>37%</span> <span>52%</span> <span>12%</span> <span>•</span> <span>36%</span> </div> |
| 1   | ET    | 278    | <div style="display: flex; justify-content: space-between;"> <span>36%</span> <span>53%</span> <span>11%</span> <span>•</span> <span>36%</span> </div> |
| 1   | FT    | 278    | <div style="display: flex; justify-content: space-between;"> <span>37%</span> <span>51%</span> <span>13%</span> <span>•</span> <span>36%</span> </div> |
| 1   | GT    | 278    | <div style="display: flex; justify-content: space-between;"> <span>38%</span> <span>53%</span> <span>10%</span> <span>•</span> <span>36%</span> </div> |
| 1   | HT    | 278    | <div style="display: flex; justify-content: space-between;"> <span>37%</span> <span>52%</span> <span>12%</span> <span>•</span> <span>36%</span> </div> |










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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | IT    | 278    |                  |
| 1   | JT    | 278    |                  |
| 1   | KT    | 278    |                  |
| 1   | LT    | 278    |                  |
| 1   | MT    | 278    |                  |
| 1   | NT    | 278    |                  |
| 2   | AX    | 522    |                  |
| 2   | BX    | 522    |                  |
| 2   | CX    | 522    |                  |
| 2   | DX    | 522    |                  |
| 2   | EX    | 522    |                  |
| 2   | FX    | 522    |                  |
| 2   | GX    | 522    |                  |
| 2   | HX    | 522    |                  |
| 2   | IX    | 522    |                  |
| 2   | JX    | 522    |                  |
| 2   | KX    | 522    |                  |
| 2   | LX    | 522    |                  |
| 2   | MX    | 522    |                  |
| 2   | NX    | 522    |                  |
| 3   | AY    | 1927   |                  |
| 3   | BY    | 1927   |                  |
| 3   | CY    | 1927   |                  |
| 3   | DY    | 1927   |                  |
| 3   | EY    | 1927   |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 3   | FY    | 1927   | <br>8% 89% |
| 3   | GY    | 1927   | <br>8% 89% |
| 3   | HY    | 1927   | <br>8% 89% |
| 3   | IY    | 1927   | <br>8% 89% |
| 3   | JY    | 1927   | <br>8% 89% |
| 3   | KY    | 1927   | <br>8% 89% |
| 3   | LY    | 1927   | <br>8% 89% |
| 3   | MY    | 1927   | <br>8% 89% |
| 3   | NY    | 1927   | <br>8% 89% |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 60970 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 Cag pathogenicity island protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 1   | AT    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |
| 1   | BT    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |
| 1   | CT    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |
| 1   | DT    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |
| 1   | ET    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |
| 1   | FT    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |
| 1   | GT    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |
| 1   | HT    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |
| 1   | IT    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |
| 1   | JT    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |
| 1   | KT    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |
| 1   | LT    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |
| 1   | MT    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |
| 1   | NT    | 179      | 1502  | 957 | 261 | 282 | 2 | 0       | 0     |

- Molecule 2 is a protein called Type IV secretion system apparatus protein CagX.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 2   | AX    | 155      | 1275  | 819 | 222 | 231 | 3 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | BX    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 819 | 222 | 231 | 3 |         |       |
| 2   | CX    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 819 | 222 | 231 | 3 |         |       |
| 2   | DX    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 819 | 222 | 231 | 3 |         |       |
| 2   | EX    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 819 | 222 | 231 | 3 |         |       |
| 2   | FX    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 819 | 222 | 231 | 3 |         |       |
| 2   | GX    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 819 | 222 | 231 | 3 |         |       |
| 2   | HX    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 819 | 222 | 231 | 3 |         |       |
| 2   | IX    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 819 | 222 | 231 | 3 |         |       |
| 2   | JX    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 819 | 222 | 231 | 3 |         |       |
| 2   | KX    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 819 | 222 | 231 | 3 |         |       |
| 2   | LX    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 819 | 222 | 231 | 3 |         |       |
| 2   | MX    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 819 | 222 | 231 | 3 |         |       |
| 2   | NX    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1275  | 819 | 222 | 231 | 3 |         |       |

- Molecule 3 is a protein called Cag pathogenicity island protein (Cag7).

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | AY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |
| 3   | BY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |
| 3   | CY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |
| 3   | DY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |
| 3   | EY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |
| 3   | FY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |

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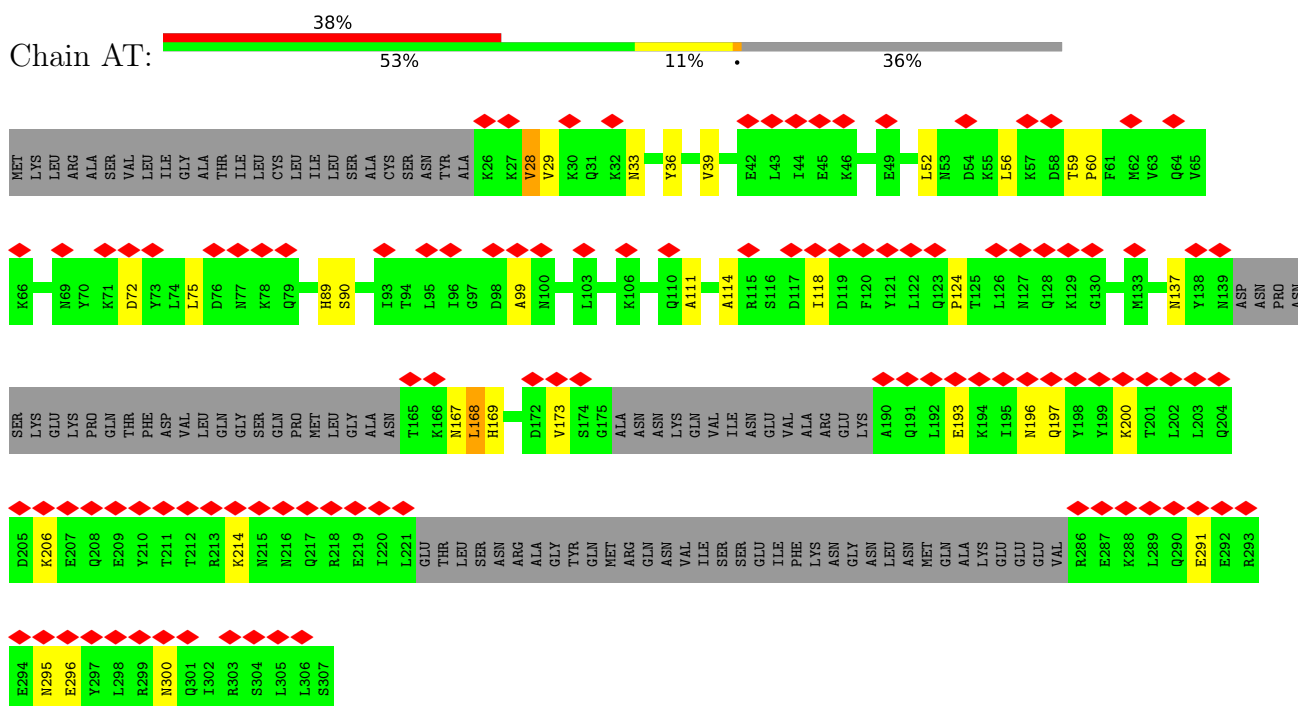
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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | GY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |
| 3   | HY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |
| 3   | IY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |
| 3   | JY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |
| 3   | KY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |
| 3   | LY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |
| 3   | MY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |
| 3   | NY    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1014 | 255 | 300 | 9 |         |       |

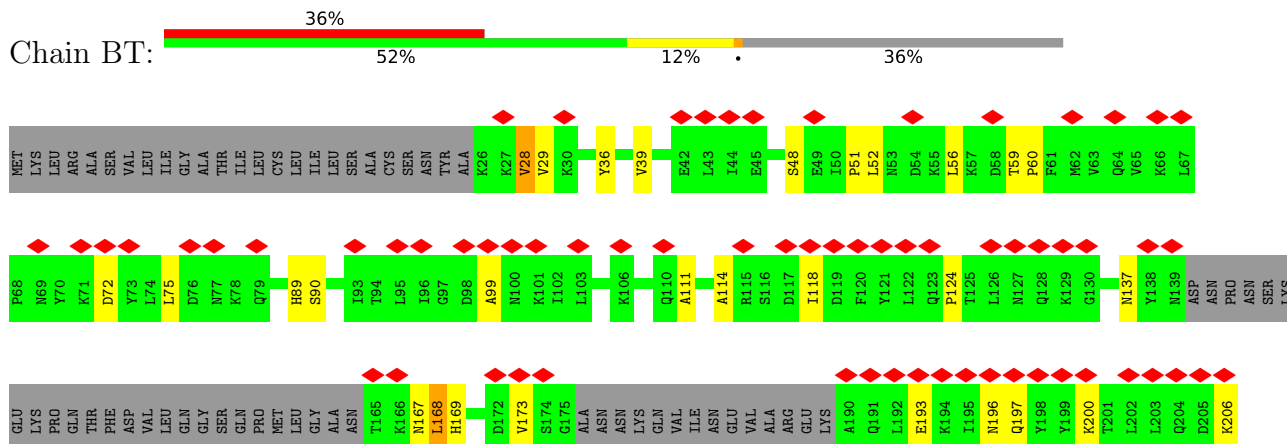
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

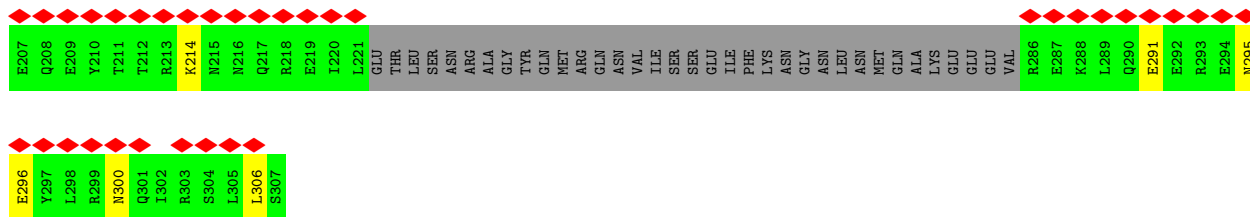
- Molecule 1: Cag pathogenicity island protein



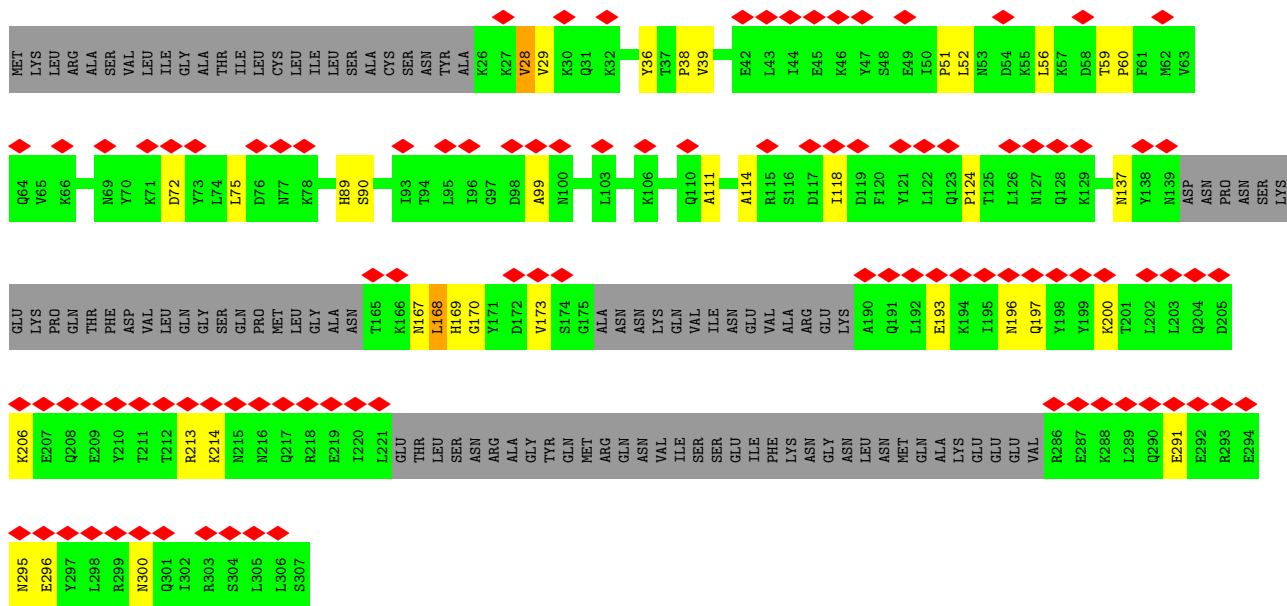
- Molecule 1: Cag pathogenicity island protein



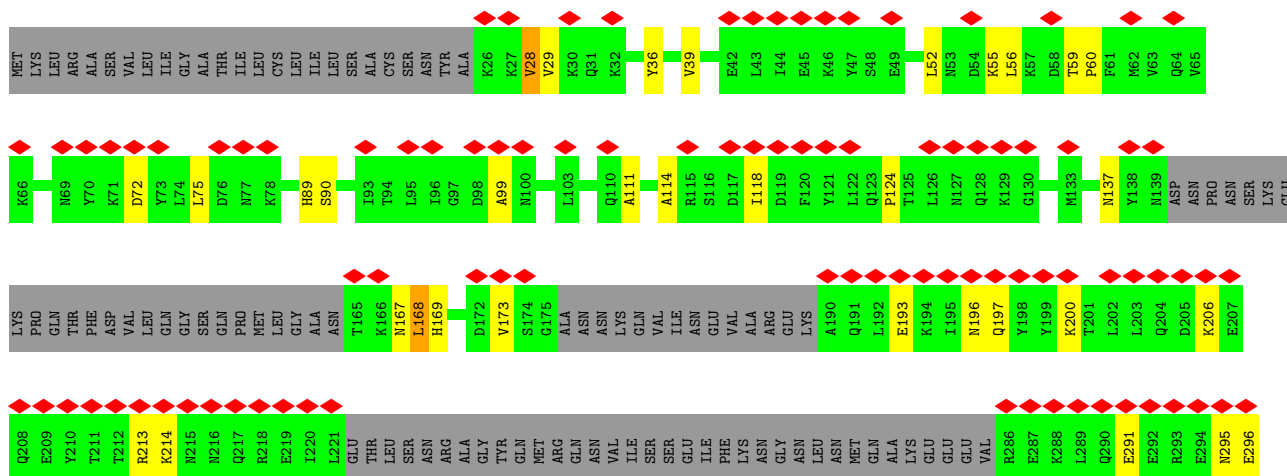
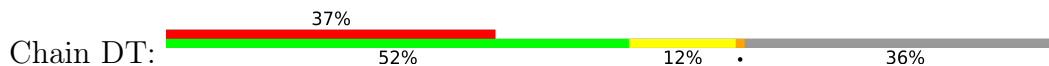


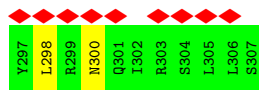


• Molecule 1: Cag pathogenicity island protein

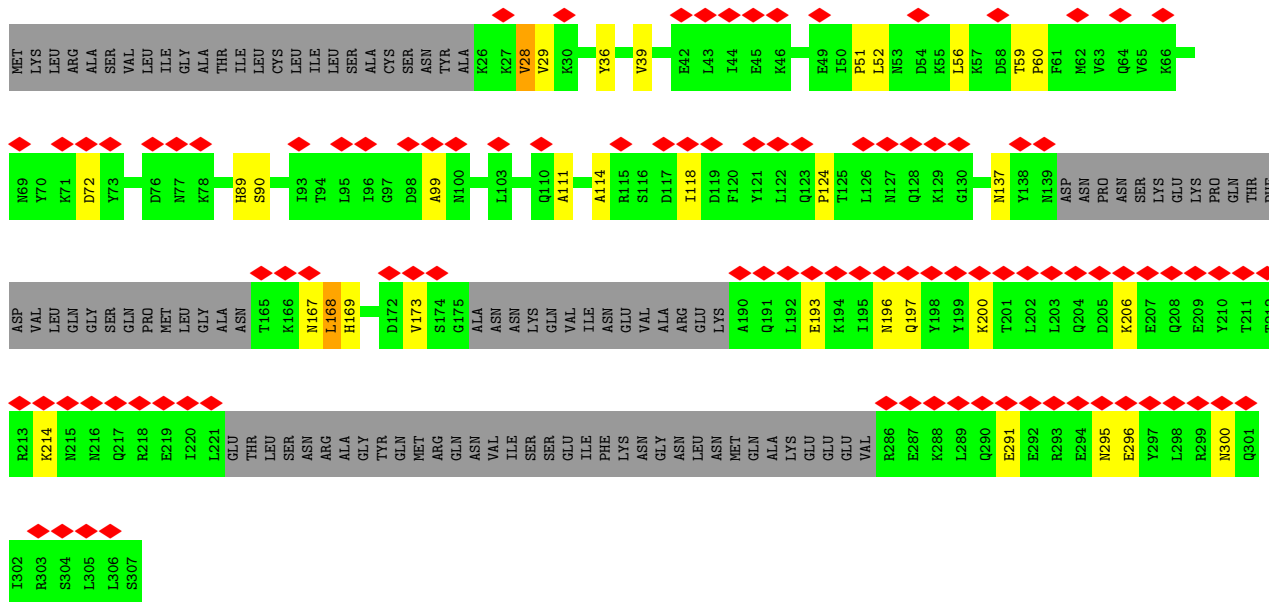


• Molecule 1: Cag pathogenicity island protein

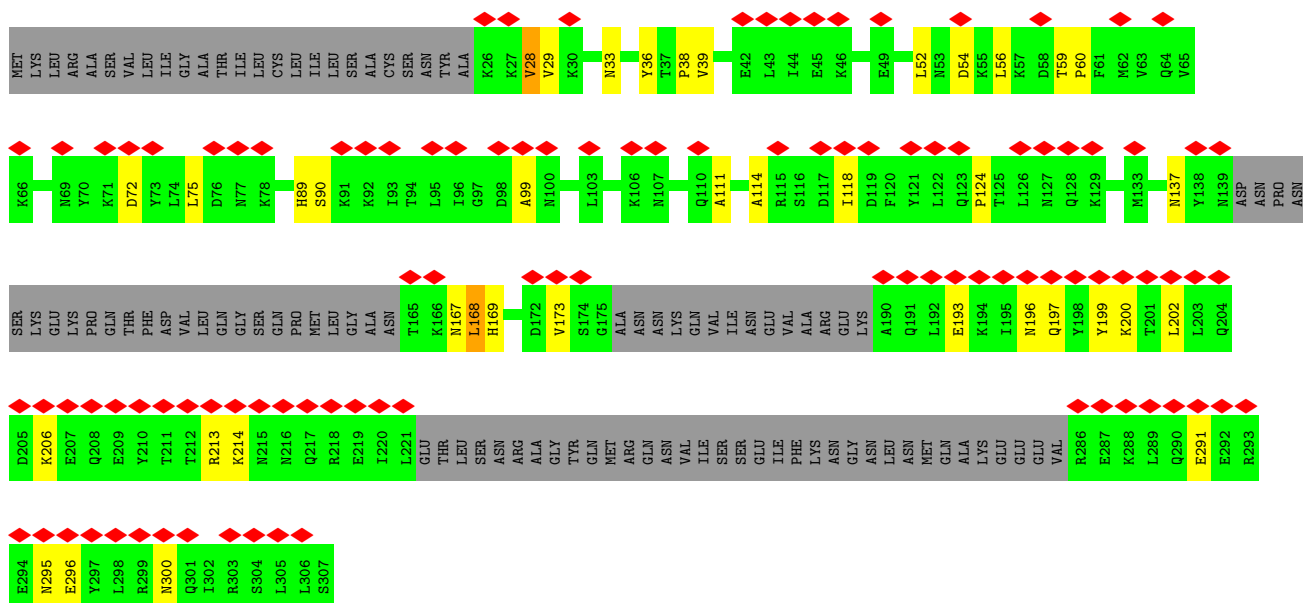




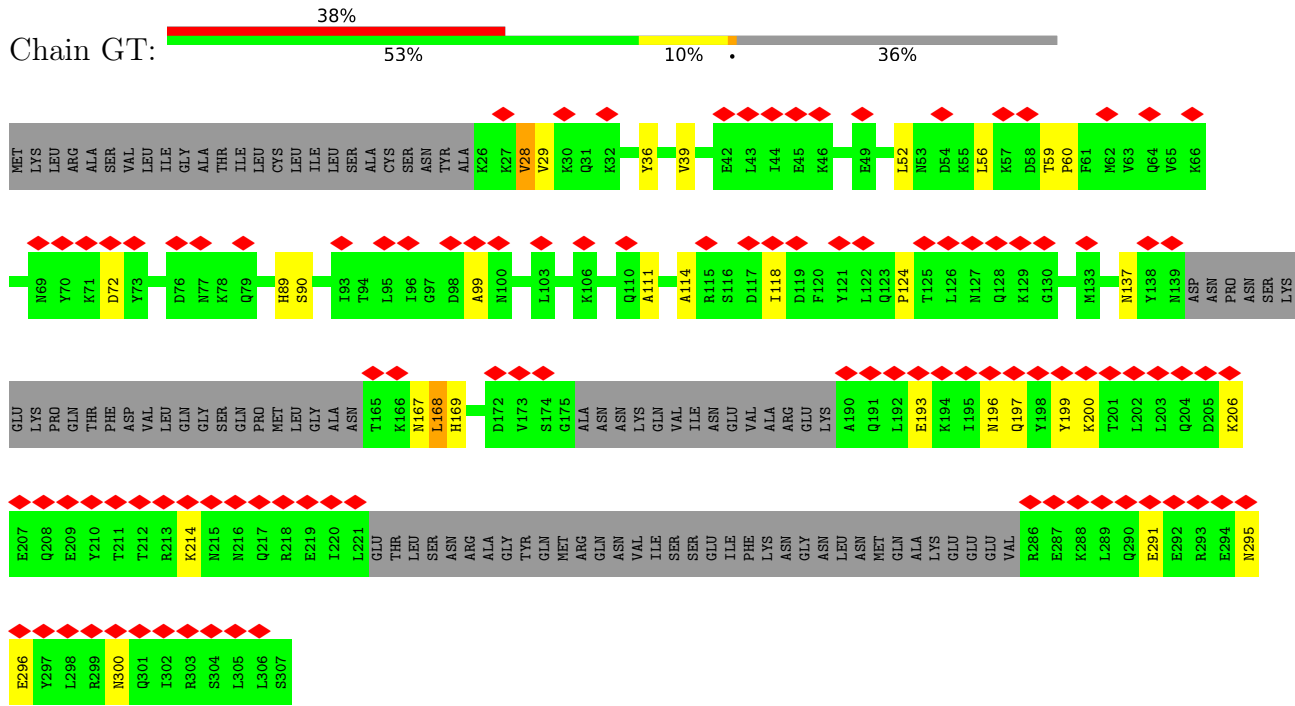
• Molecule 1: Cag pathogenicity island protein



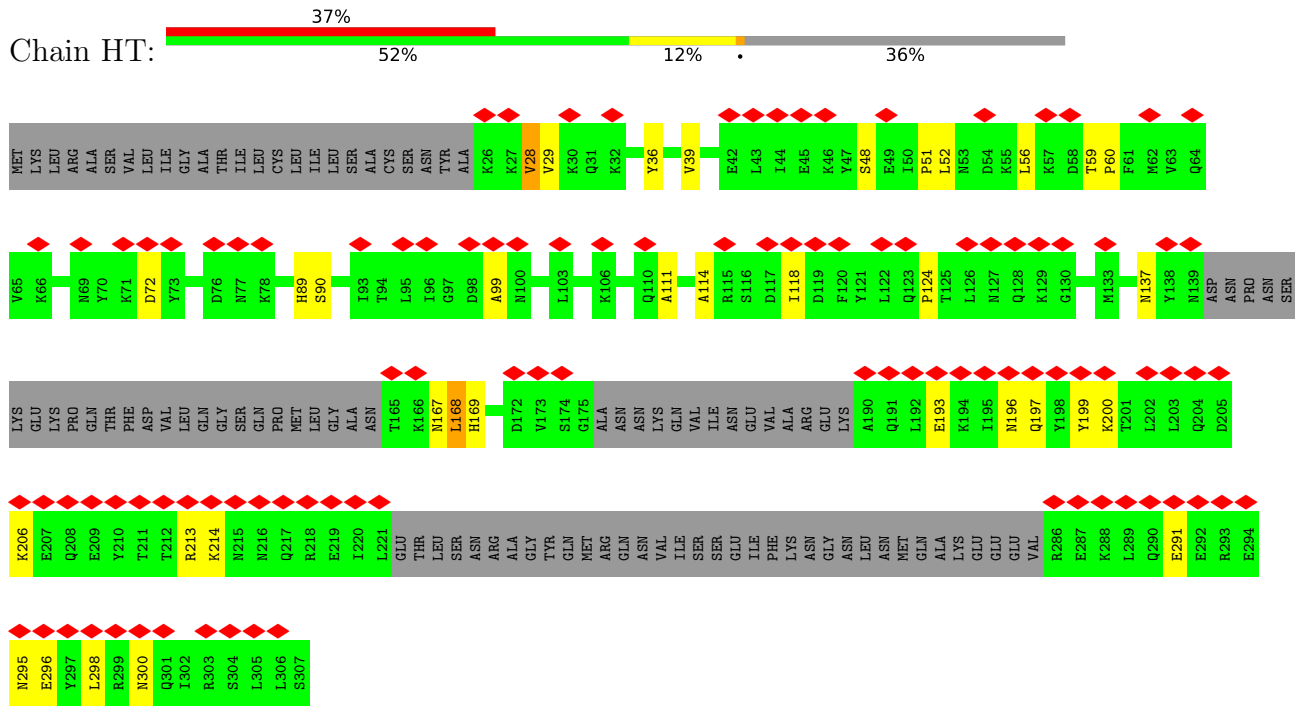
• Molecule 1: Cag pathogenicity island protein



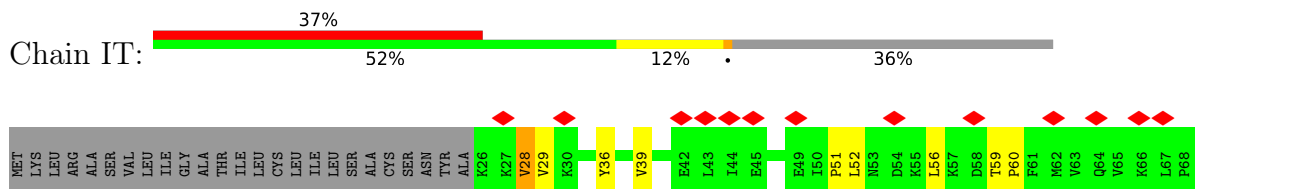
• Molecule 1: Cag pathogenicity island protein

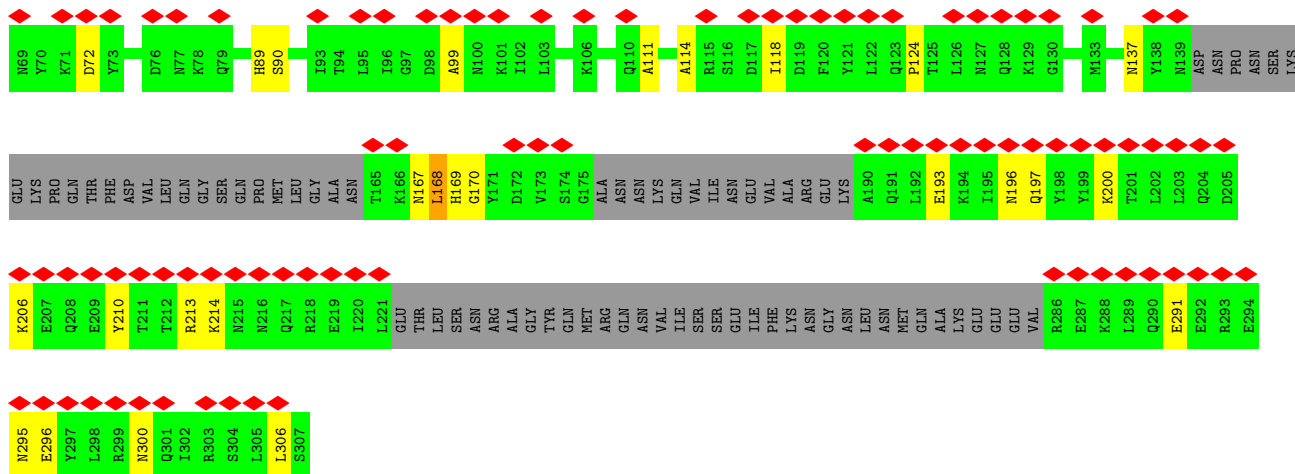


● Molecule 1: Cag pathogenicity island protein

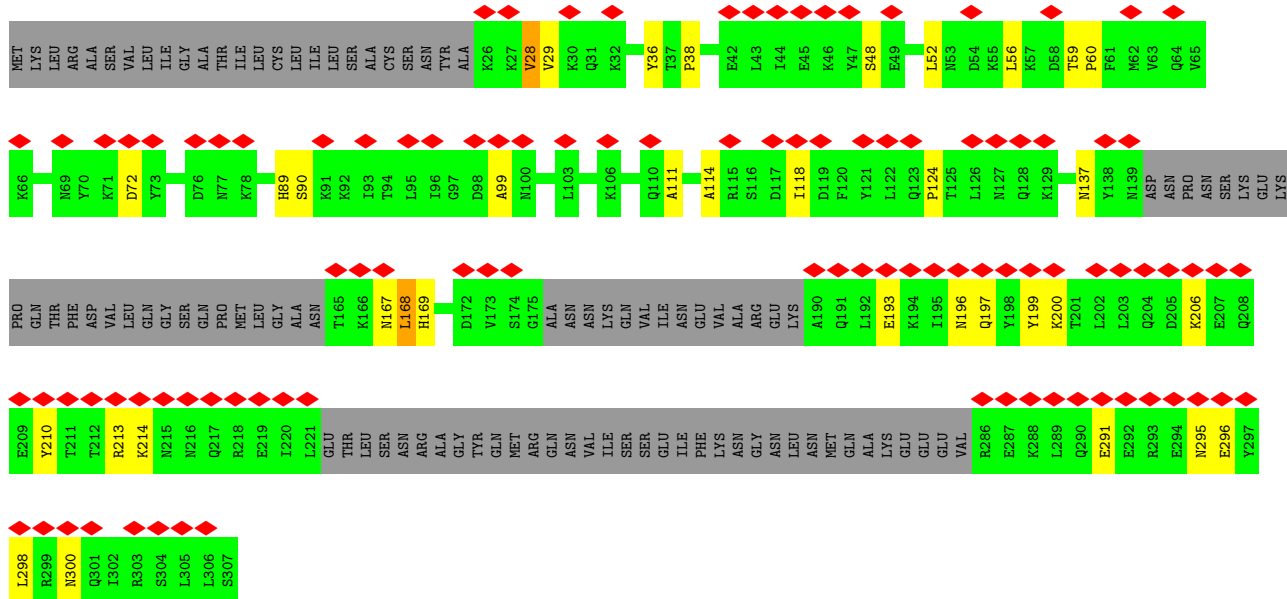


● Molecule 1: Cag pathogenicity island protein

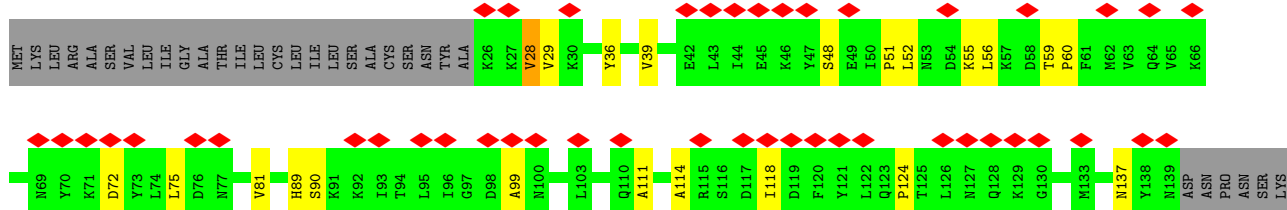


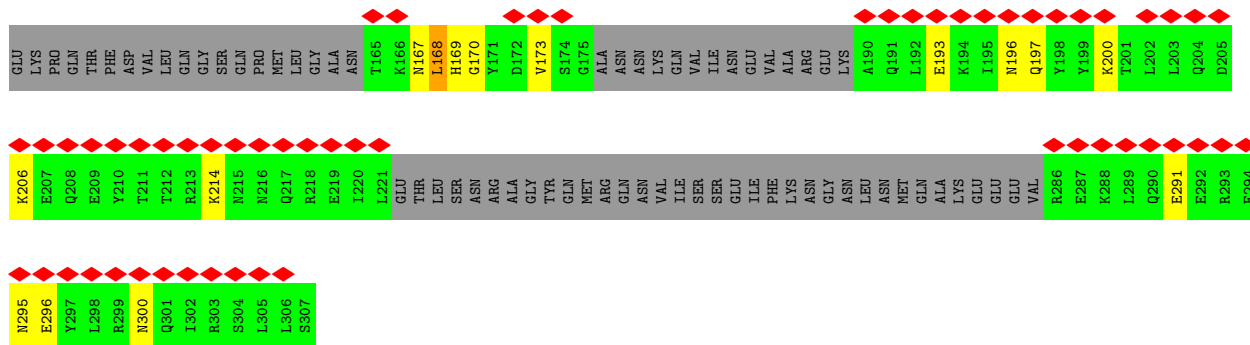


• Molecule 1: Cag pathogenicity island protein

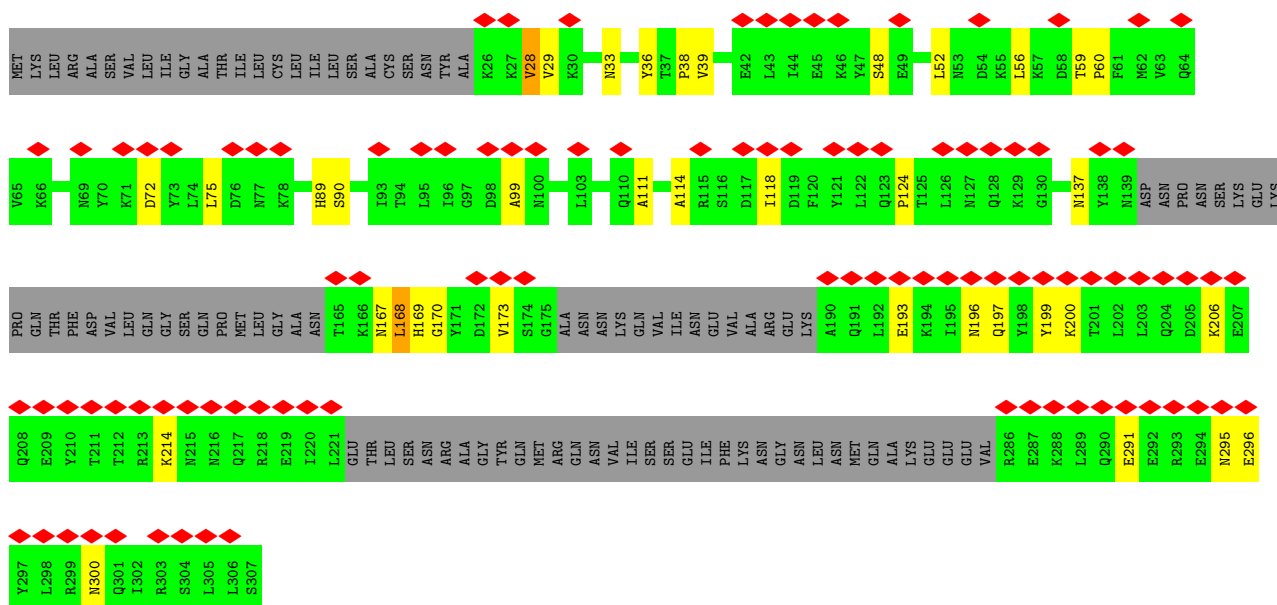


• Molecule 1: Cag pathogenicity island protein

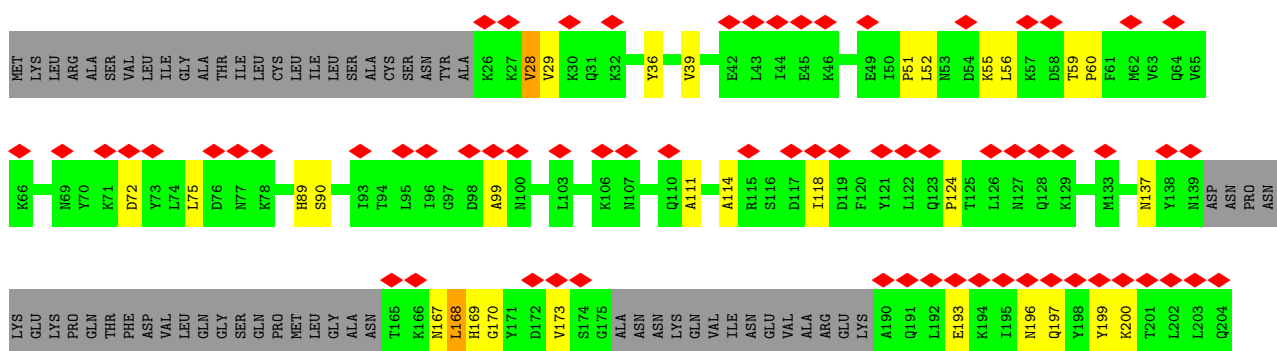




• Molecule 1: Cag pathogenicity island protein



• Molecule 1: Cag pathogenicity island protein

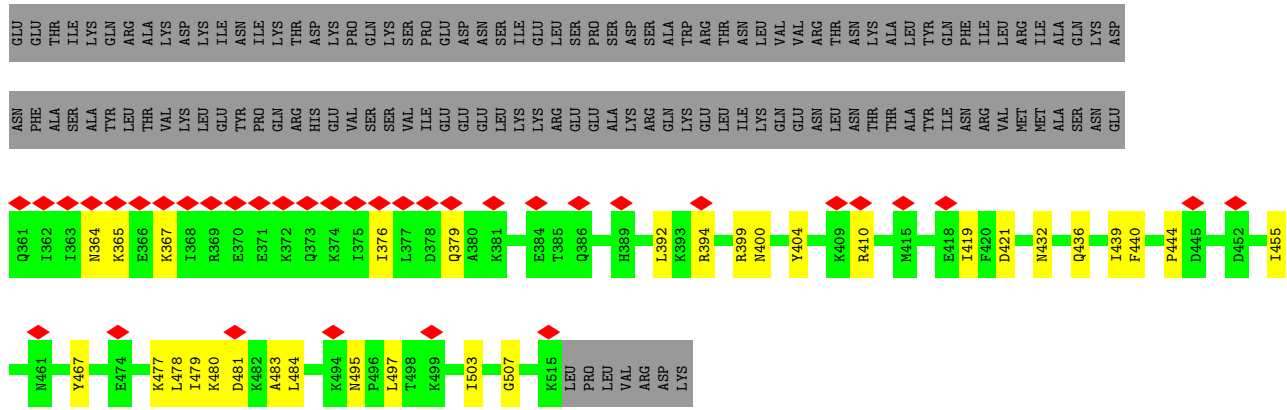




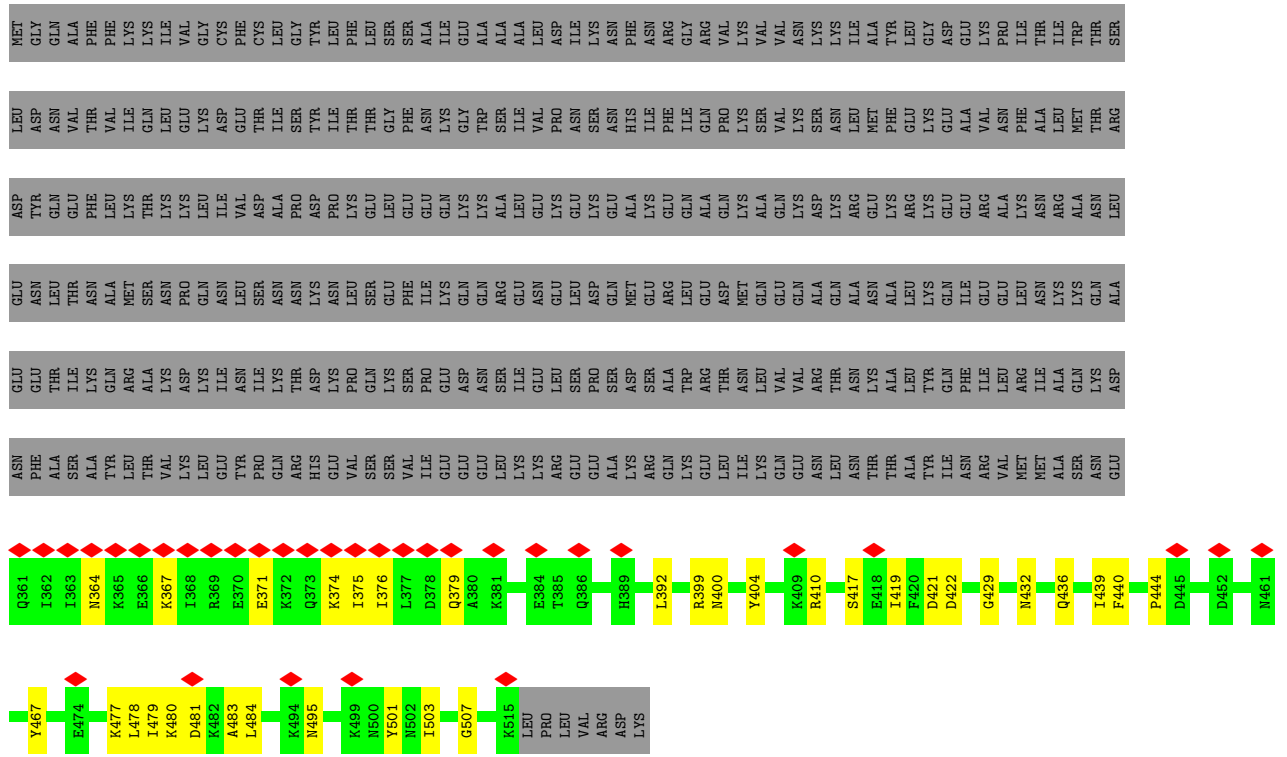




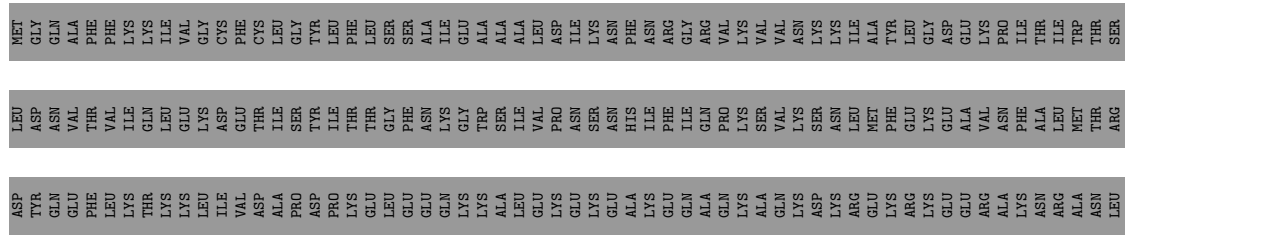




• Molecule 2: Type IV secretion system apparatus protein CagX

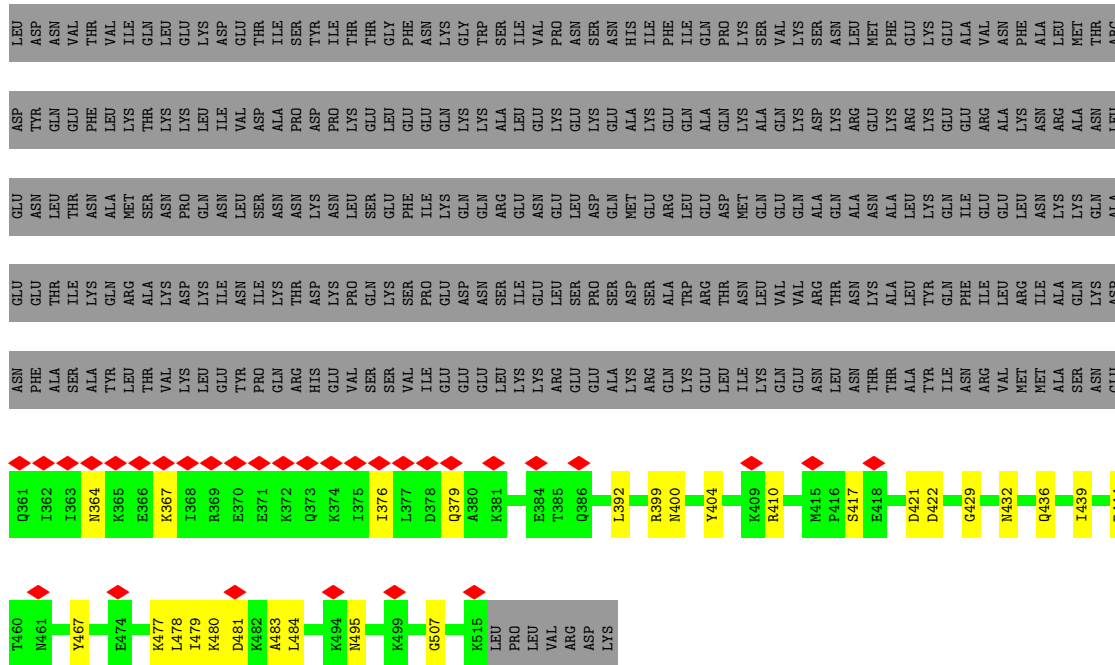


• Molecule 2: Type IV secretion system apparatus protein CagX

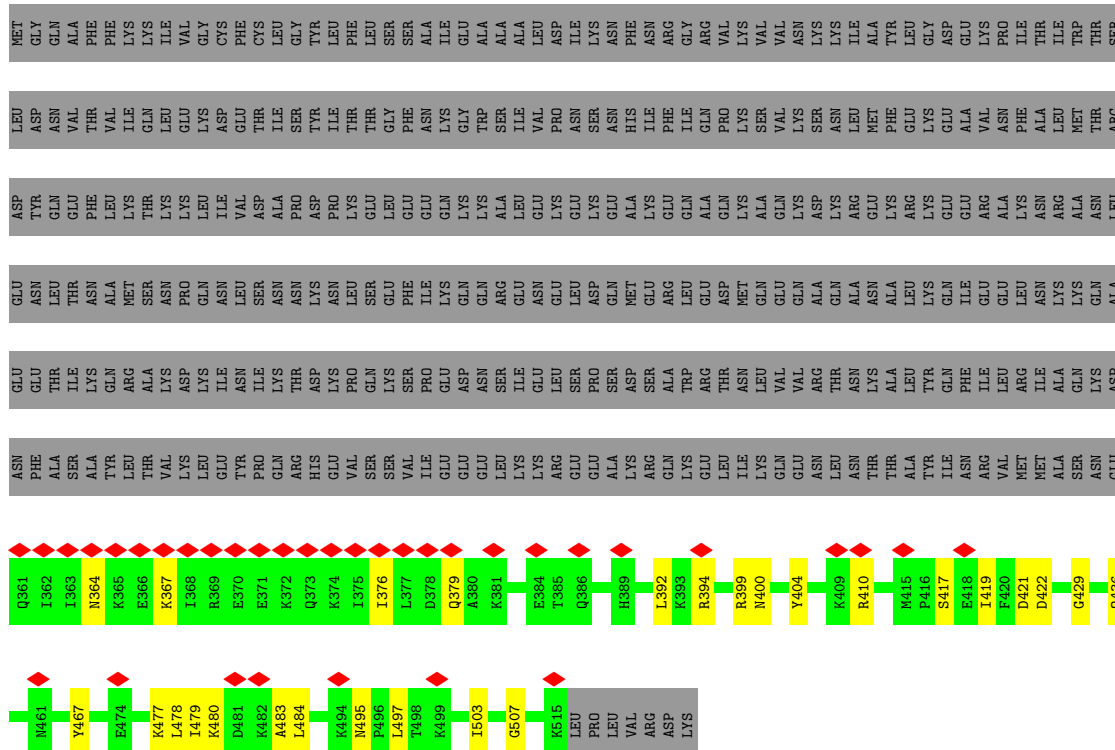








● Molecule 2: Type IV secretion system apparatus protein CagX

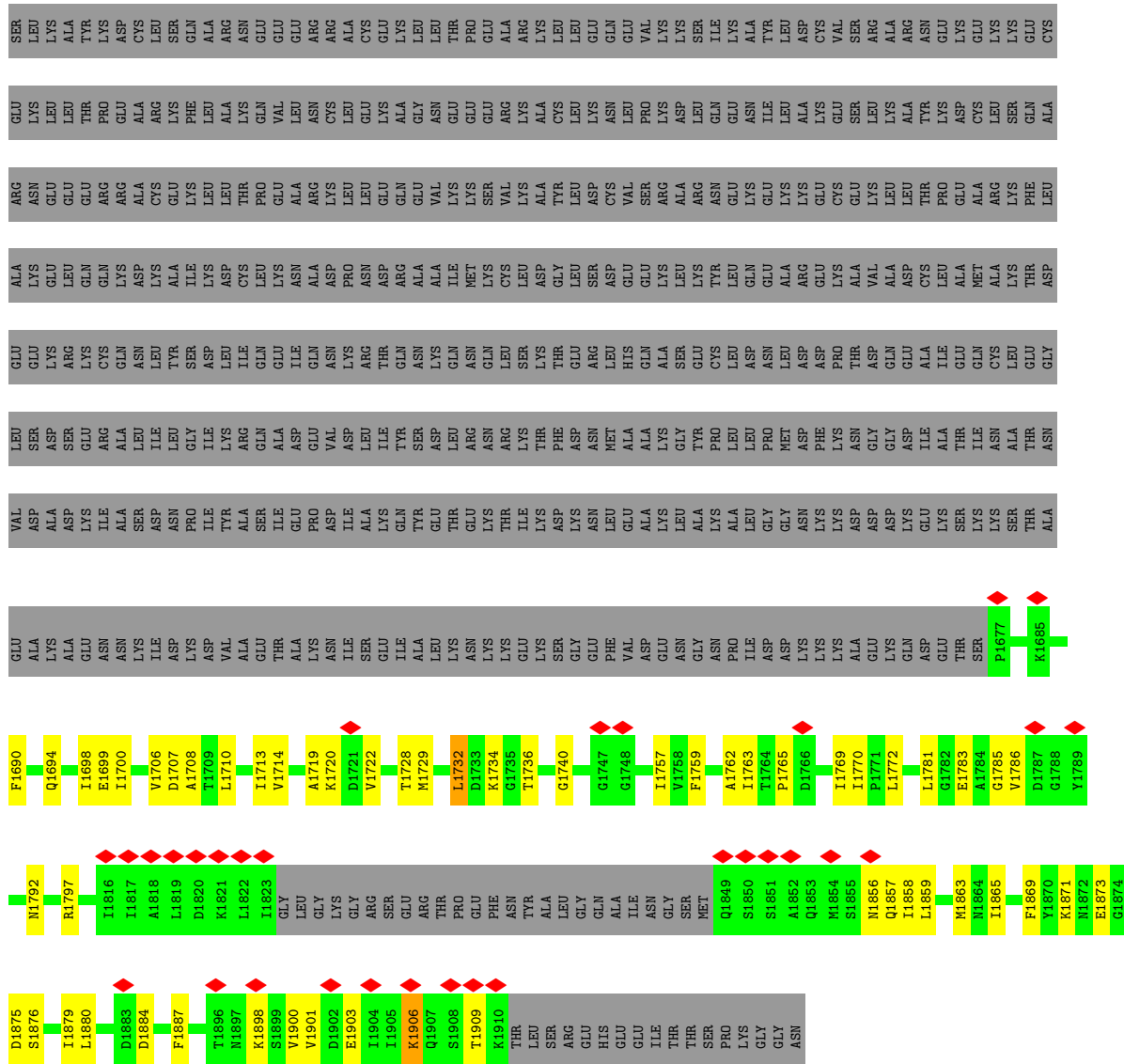


● Molecule 2: Type IV secretion system apparatus protein CagX

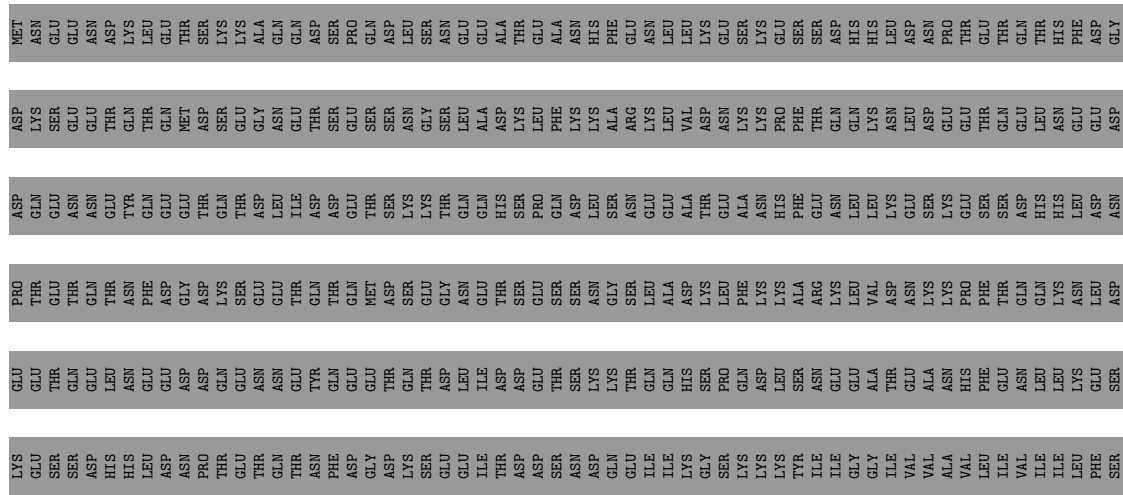








● Molecule 3: Cag pathogenicity island protein (Cag7)

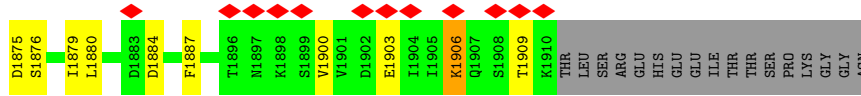












● Molecule 3: Cag pathogenicity island protein (Cag7)



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



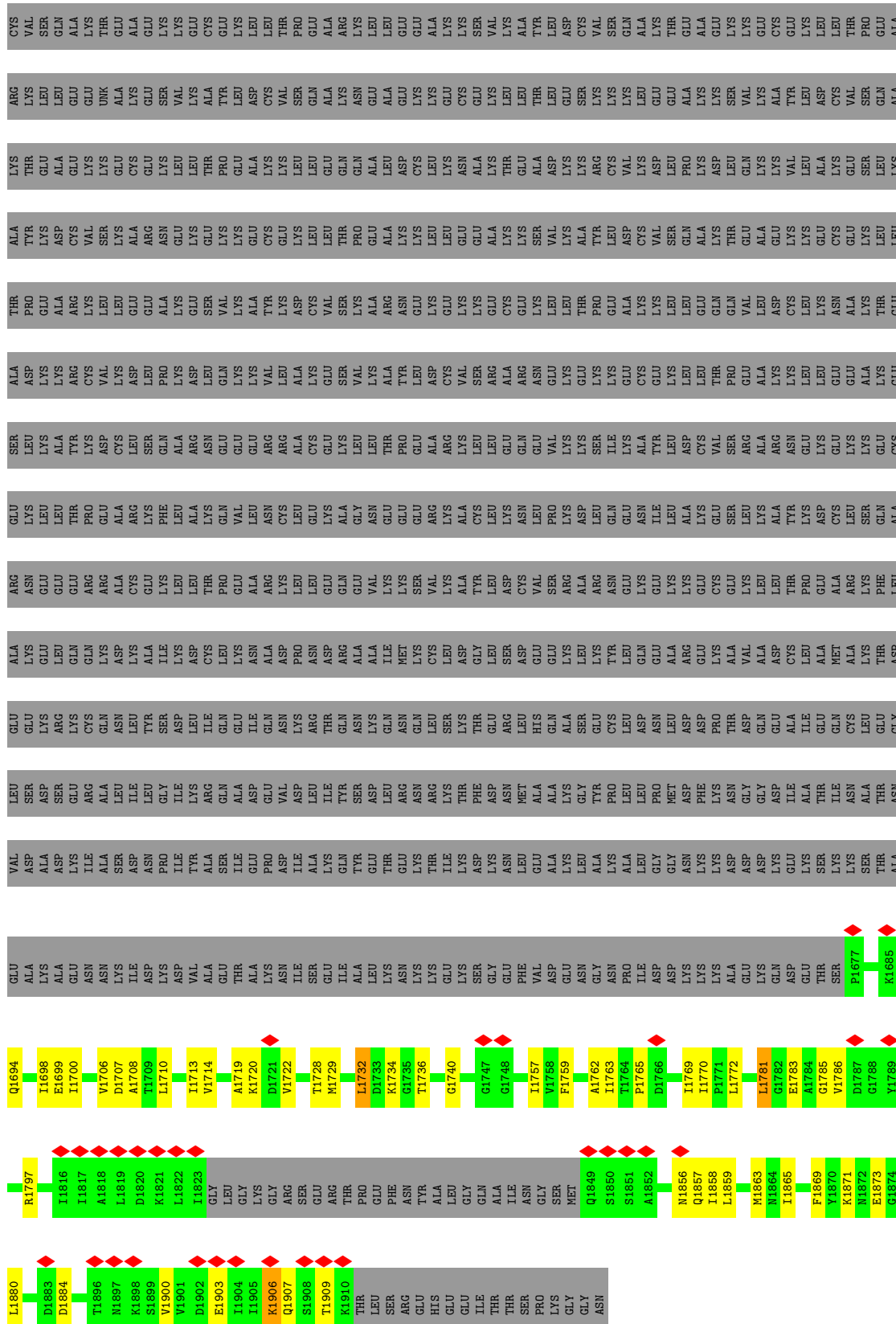












● Molecule 3: Cag pathogenicity island protein (Cag7)





























## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C14                              | Depositor |
| Number of particles used             | 7337                                    | 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 ( $e^-/\text{\AA}^2$ ) | 59.7                                    | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.049                                   | Depositor |
| Minimum map value                    | -0.036                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.002                                   | Depositor |
| Recommended contour level            | 0.015                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 510.0, 510.0, 510.0                     | wwPDB     |
| Map dimensions                       | 510, 510, 510                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.0, 1.0, 1.0                           | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 1   | AT    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 1   | BT    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 1   | CT    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 1   | DT    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 1   | ET    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 1   | FT    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 1   | GT    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 1   | HT    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 1   | IT    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 1   | JT    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 1   | KT    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 1   | LT    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 1   | MT    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 1   | NT    | 0.41         | 0/1525  | 0.71        | 4/2049 (0.2%) |
| 2   | AX    | 0.54         | 0/1301  | 0.69        | 0/1752        |
| 2   | BX    | 0.54         | 0/1301  | 0.69        | 0/1752        |
| 2   | CX    | 0.54         | 0/1301  | 0.69        | 0/1752        |
| 2   | DX    | 0.54         | 0/1301  | 0.69        | 0/1752        |
| 2   | EX    | 0.54         | 0/1301  | 0.69        | 0/1752        |
| 2   | FX    | 0.54         | 0/1301  | 0.69        | 1/1752 (0.1%) |
| 2   | GX    | 0.54         | 0/1301  | 0.69        | 0/1752        |
| 2   | HX    | 0.54         | 0/1301  | 0.69        | 0/1752        |
| 2   | IX    | 0.54         | 0/1301  | 0.69        | 0/1752        |
| 2   | JX    | 0.54         | 0/1301  | 0.69        | 0/1752        |
| 2   | KX    | 0.54         | 0/1301  | 0.69        | 1/1752 (0.1%) |
| 2   | LX    | 0.54         | 0/1301  | 0.69        | 1/1752 (0.1%) |
| 2   | MX    | 0.54         | 0/1301  | 0.69        | 1/1752 (0.1%) |
| 2   | NX    | 0.54         | 0/1301  | 0.69        | 1/1752 (0.1%) |
| 3   | AY    | 0.55         | 0/1602  | 0.72        | 3/2170 (0.1%) |
| 3   | BY    | 0.55         | 0/1602  | 0.72        | 4/2170 (0.2%) |
| 3   | CY    | 0.55         | 0/1602  | 0.72        | 4/2170 (0.2%) |
| 3   | DY    | 0.55         | 0/1602  | 0.72        | 3/2170 (0.1%) |
| 3   | EY    | 0.55         | 0/1602  | 0.72        | 3/2170 (0.1%) |
| 3   | FY    | 0.55         | 0/1602  | 0.72        | 4/2170 (0.2%) |

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 3   | GY    | 0.55         | 0/1602  | 0.72        | 4/2170 (0.2%)    |
| 3   | HY    | 0.55         | 0/1602  | 0.72        | 4/2170 (0.2%)    |
| 3   | IY    | 0.55         | 0/1602  | 0.72        | 4/2170 (0.2%)    |
| 3   | JY    | 0.55         | 0/1602  | 0.72        | 4/2170 (0.2%)    |
| 3   | KY    | 0.55         | 0/1602  | 0.72        | 4/2170 (0.2%)    |
| 3   | LY    | 0.55         | 0/1602  | 0.72        | 3/2170 (0.1%)    |
| 3   | MY    | 0.55         | 0/1602  | 0.72        | 4/2170 (0.2%)    |
| 3   | NY    | 0.55         | 0/1602  | 0.72        | 4/2170 (0.2%)    |
| All | All   | 0.50         | 0/61992 | 0.71        | 113/83594 (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 |
|-----|-------|---------------------|---------------------|
| 2   | AX    | 0                   | 1                   |
| 2   | BX    | 0                   | 1                   |
| 2   | CX    | 0                   | 1                   |
| 2   | DX    | 0                   | 1                   |
| 2   | EX    | 0                   | 1                   |
| 2   | FX    | 0                   | 1                   |
| 2   | GX    | 0                   | 1                   |
| 2   | HX    | 0                   | 1                   |
| 2   | IX    | 0                   | 1                   |
| 2   | JX    | 0                   | 1                   |
| 2   | KX    | 0                   | 1                   |
| 2   | LX    | 0                   | 1                   |
| 2   | MX    | 0                   | 1                   |
| 2   | NX    | 0                   | 1                   |
| All | All   | 0                   | 14                  |

There are no bond length outliers.

All (113) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 3   | MY    | 1772 | LEU  | CA-CB-CG | 7.79 | 133.22      | 115.30   |
| 3   | CY    | 1772 | LEU  | CA-CB-CG | 7.79 | 133.21      | 115.30   |
| 3   | KY    | 1772 | LEU  | CA-CB-CG | 7.78 | 133.20      | 115.30   |
| 3   | AY    | 1772 | LEU  | CA-CB-CG | 7.78 | 133.19      | 115.30   |
| 3   | HY    | 1772 | LEU  | CA-CB-CG | 7.78 | 133.20      | 115.30   |
| 3   | FY    | 1772 | LEU  | CA-CB-CG | 7.78 | 133.19      | 115.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | LY    | 1772 | LEU  | CA-CB-CG  | 7.77  | 133.18      | 115.30   |
| 3   | EY    | 1772 | LEU  | CA-CB-CG  | 7.77  | 133.18      | 115.30   |
| 3   | JY    | 1772 | LEU  | CA-CB-CG  | 7.77  | 133.17      | 115.30   |
| 3   | NY    | 1772 | LEU  | CA-CB-CG  | 7.77  | 133.17      | 115.30   |
| 3   | DY    | 1772 | LEU  | CA-CB-CG  | 7.77  | 133.17      | 115.30   |
| 3   | GY    | 1772 | LEU  | CA-CB-CG  | 7.76  | 133.16      | 115.30   |
| 3   | BY    | 1772 | LEU  | CA-CB-CG  | 7.76  | 133.15      | 115.30   |
| 3   | IY    | 1772 | LEU  | CA-CB-CG  | 7.76  | 133.15      | 115.30   |
| 1   | BT    | 168  | LEU  | CA-CB-CG  | 7.12  | 131.68      | 115.30   |
| 1   | LT    | 168  | LEU  | CA-CB-CG  | 7.12  | 131.68      | 115.30   |
| 1   | GT    | 168  | LEU  | CA-CB-CG  | 7.12  | 131.67      | 115.30   |
| 1   | IT    | 168  | LEU  | CA-CB-CG  | 7.12  | 131.67      | 115.30   |
| 1   | DT    | 168  | LEU  | CA-CB-CG  | 7.11  | 131.66      | 115.30   |
| 1   | NT    | 168  | LEU  | CA-CB-CG  | 7.11  | 131.66      | 115.30   |
| 1   | AT    | 168  | LEU  | CA-CB-CG  | 7.11  | 131.65      | 115.30   |
| 1   | FT    | 168  | LEU  | CA-CB-CG  | 7.11  | 131.65      | 115.30   |
| 1   | HT    | 168  | LEU  | CA-CB-CG  | 7.11  | 131.65      | 115.30   |
| 1   | JT    | 168  | LEU  | CA-CB-CG  | 7.11  | 131.64      | 115.30   |
| 1   | KT    | 168  | LEU  | CA-CB-CG  | 7.10  | 131.64      | 115.30   |
| 1   | ET    | 168  | LEU  | CA-CB-CG  | 7.10  | 131.63      | 115.30   |
| 1   | MT    | 168  | LEU  | CA-CB-CG  | 7.10  | 131.63      | 115.30   |
| 1   | CT    | 168  | LEU  | CA-CB-CG  | 7.09  | 131.61      | 115.30   |
| 1   | KT    | 72   | ASP  | CB-CG-OD2 | 6.55  | 124.20      | 118.30   |
| 1   | DT    | 72   | ASP  | CB-CG-OD2 | 6.50  | 124.15      | 118.30   |
| 1   | ET    | 72   | ASP  | CB-CG-OD2 | 6.50  | 124.15      | 118.30   |
| 1   | AT    | 72   | ASP  | CB-CG-OD2 | 6.50  | 124.15      | 118.30   |
| 1   | CT    | 72   | ASP  | CB-CG-OD2 | 6.49  | 124.14      | 118.30   |
| 1   | LT    | 72   | ASP  | CB-CG-OD2 | 6.49  | 124.14      | 118.30   |
| 1   | FT    | 72   | ASP  | CB-CG-OD2 | 6.48  | 124.13      | 118.30   |
| 1   | BT    | 72   | ASP  | CB-CG-OD2 | 6.48  | 124.13      | 118.30   |
| 1   | JT    | 72   | ASP  | CB-CG-OD2 | 6.47  | 124.12      | 118.30   |
| 1   | NT    | 72   | ASP  | CB-CG-OD2 | 6.46  | 124.11      | 118.30   |
| 1   | MT    | 72   | ASP  | CB-CG-OD2 | 6.45  | 124.10      | 118.30   |
| 1   | HT    | 72   | ASP  | CB-CG-OD2 | 6.45  | 124.10      | 118.30   |
| 1   | IT    | 72   | ASP  | CB-CG-OD2 | 6.44  | 124.09      | 118.30   |
| 1   | GT    | 72   | ASP  | CB-CG-OD2 | 6.43  | 124.08      | 118.30   |
| 3   | HY    | 1732 | LEU  | CB-CG-CD2 | -5.92 | 100.94      | 111.00   |
| 3   | AY    | 1732 | LEU  | CB-CG-CD2 | -5.91 | 100.95      | 111.00   |
| 3   | JY    | 1732 | LEU  | CB-CG-CD2 | -5.90 | 100.96      | 111.00   |
| 3   | MY    | 1732 | LEU  | CB-CG-CD2 | -5.90 | 100.97      | 111.00   |
| 3   | LY    | 1732 | LEU  | CB-CG-CD2 | -5.90 | 100.97      | 111.00   |
| 3   | GY    | 1732 | LEU  | CB-CG-CD2 | -5.90 | 100.97      | 111.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | KY    | 1732 | LEU  | CB-CG-CD2  | -5.89 | 100.98      | 111.00   |
| 3   | CY    | 1732 | LEU  | CB-CG-CD2  | -5.89 | 100.98      | 111.00   |
| 3   | BY    | 1732 | LEU  | CB-CG-CD2  | -5.89 | 100.99      | 111.00   |
| 3   | IY    | 1732 | LEU  | CB-CG-CD2  | -5.89 | 100.99      | 111.00   |
| 3   | NY    | 1732 | LEU  | CB-CG-CD2  | -5.89 | 100.99      | 111.00   |
| 3   | EY    | 1732 | LEU  | CB-CG-CD2  | -5.89 | 100.99      | 111.00   |
| 3   | FY    | 1732 | LEU  | CB-CG-CD2  | -5.88 | 101.01      | 111.00   |
| 3   | DY    | 1732 | LEU  | CB-CG-CD2  | -5.87 | 101.02      | 111.00   |
| 3   | KY    | 1772 | LEU  | CB-CG-CD1  | 5.49  | 120.34      | 111.00   |
| 3   | GY    | 1772 | LEU  | CB-CG-CD1  | 5.49  | 120.33      | 111.00   |
| 3   | CY    | 1772 | LEU  | CB-CG-CD1  | 5.49  | 120.33      | 111.00   |
| 3   | JY    | 1772 | LEU  | CB-CG-CD1  | 5.49  | 120.33      | 111.00   |
| 3   | EY    | 1772 | LEU  | CB-CG-CD1  | 5.48  | 120.31      | 111.00   |
| 3   | HY    | 1772 | LEU  | CB-CG-CD1  | 5.47  | 120.30      | 111.00   |
| 3   | AY    | 1772 | LEU  | CB-CG-CD1  | 5.46  | 120.29      | 111.00   |
| 3   | NY    | 1772 | LEU  | CB-CG-CD1  | 5.46  | 120.29      | 111.00   |
| 3   | MY    | 1772 | LEU  | CB-CG-CD1  | 5.46  | 120.29      | 111.00   |
| 3   | LY    | 1772 | LEU  | CB-CG-CD1  | 5.46  | 120.28      | 111.00   |
| 3   | BY    | 1772 | LEU  | CB-CG-CD1  | 5.46  | 120.28      | 111.00   |
| 3   | FY    | 1772 | LEU  | CB-CG-CD1  | 5.46  | 120.28      | 111.00   |
| 3   | IY    | 1772 | LEU  | CB-CG-CD1  | 5.44  | 120.25      | 111.00   |
| 3   | DY    | 1772 | LEU  | CB-CG-CD1  | 5.44  | 120.24      | 111.00   |
| 1   | MT    | 28   | VAL  | CG1-CB-CG2 | -5.27 | 102.47      | 110.90   |
| 1   | DT    | 28   | VAL  | CG1-CB-CG2 | -5.27 | 102.47      | 110.90   |
| 1   | BT    | 28   | VAL  | CG1-CB-CG2 | -5.25 | 102.50      | 110.90   |
| 1   | IT    | 28   | VAL  | CG1-CB-CG2 | -5.25 | 102.50      | 110.90   |
| 1   | AT    | 28   | VAL  | CG1-CB-CG2 | -5.25 | 102.50      | 110.90   |
| 1   | JT    | 28   | VAL  | CG1-CB-CG2 | -5.24 | 102.52      | 110.90   |
| 1   | LT    | 28   | VAL  | CG1-CB-CG2 | -5.24 | 102.52      | 110.90   |
| 1   | CT    | 28   | VAL  | CG1-CB-CG2 | -5.24 | 102.52      | 110.90   |
| 1   | NT    | 28   | VAL  | CG1-CB-CG2 | -5.24 | 102.53      | 110.90   |
| 1   | FT    | 28   | VAL  | CG1-CB-CG2 | -5.23 | 102.53      | 110.90   |
| 1   | ET    | 28   | VAL  | CG1-CB-CG2 | -5.23 | 102.53      | 110.90   |
| 1   | GT    | 28   | VAL  | CG1-CB-CG2 | -5.23 | 102.53      | 110.90   |
| 1   | KT    | 28   | VAL  | CG1-CB-CG2 | -5.22 | 102.55      | 110.90   |
| 1   | HT    | 28   | VAL  | CG1-CB-CG2 | -5.21 | 102.56      | 110.90   |
| 1   | IT    | 197  | GLN  | CA-CB-CG   | 5.20  | 124.84      | 113.40   |
| 1   | AT    | 197  | GLN  | CA-CB-CG   | 5.19  | 124.83      | 113.40   |
| 1   | DT    | 197  | GLN  | CA-CB-CG   | 5.19  | 124.81      | 113.40   |
| 1   | ET    | 197  | GLN  | CA-CB-CG   | 5.18  | 124.81      | 113.40   |
| 1   | LT    | 197  | GLN  | CA-CB-CG   | 5.18  | 124.80      | 113.40   |
| 1   | FT    | 197  | GLN  | CA-CB-CG   | 5.18  | 124.80      | 113.40   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | JT    | 197  | GLN  | CA-CB-CG  | 5.18  | 124.79      | 113.40   |
| 1   | HT    | 197  | GLN  | CA-CB-CG  | 5.17  | 124.79      | 113.40   |
| 1   | MT    | 197  | GLN  | CA-CB-CG  | 5.17  | 124.78      | 113.40   |
| 1   | BT    | 197  | GLN  | CA-CB-CG  | 5.17  | 124.78      | 113.40   |
| 1   | KT    | 197  | GLN  | CA-CB-CG  | 5.17  | 124.78      | 113.40   |
| 1   | CT    | 197  | GLN  | CA-CB-CG  | 5.17  | 124.77      | 113.40   |
| 1   | NT    | 197  | GLN  | CA-CB-CG  | 5.16  | 124.76      | 113.40   |
| 1   | GT    | 197  | GLN  | CA-CB-CG  | 5.16  | 124.75      | 113.40   |
| 2   | KX    | 422  | ASP  | CB-CG-OD2 | 5.03  | 122.82      | 118.30   |
| 3   | HY    | 1781 | LEU  | CA-CB-CG  | -5.02 | 103.75      | 115.30   |
| 2   | FX    | 422  | ASP  | CB-CG-OD2 | 5.02  | 122.82      | 118.30   |
| 3   | JY    | 1781 | LEU  | CA-CB-CG  | -5.02 | 103.76      | 115.30   |
| 3   | NY    | 1781 | LEU  | CA-CB-CG  | -5.02 | 103.76      | 115.30   |
| 2   | NX    | 422  | ASP  | CB-CG-OD2 | 5.01  | 122.81      | 118.30   |
| 3   | BY    | 1781 | LEU  | CA-CB-CG  | -5.01 | 103.79      | 115.30   |
| 2   | MX    | 422  | ASP  | CB-CG-OD2 | 5.01  | 122.81      | 118.30   |
| 3   | FY    | 1781 | LEU  | CA-CB-CG  | -5.00 | 103.79      | 115.30   |
| 3   | MY    | 1781 | LEU  | CA-CB-CG  | -5.00 | 103.79      | 115.30   |
| 3   | GY    | 1781 | LEU  | CA-CB-CG  | -5.00 | 103.79      | 115.30   |
| 3   | IY    | 1781 | LEU  | CA-CB-CG  | -5.00 | 103.79      | 115.30   |
| 3   | KY    | 1781 | LEU  | CA-CB-CG  | -5.00 | 103.79      | 115.30   |
| 3   | CY    | 1781 | LEU  | CA-CB-CG  | -5.00 | 103.80      | 115.30   |
| 2   | LX    | 422  | ASP  | CB-CG-OD2 | 5.00  | 122.80      | 118.30   |

There are no chirality outliers.

All (14) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | AX    | 479 | ILE  | Peptide |
| 2   | BX    | 479 | ILE  | Peptide |
| 2   | CX    | 479 | ILE  | Peptide |
| 2   | DX    | 479 | ILE  | Peptide |
| 2   | EX    | 479 | ILE  | Peptide |
| 2   | FX    | 479 | ILE  | Peptide |
| 2   | GX    | 479 | ILE  | Peptide |
| 2   | HX    | 479 | ILE  | Peptide |
| 2   | IX    | 479 | ILE  | Peptide |
| 2   | JX    | 479 | ILE  | Peptide |
| 2   | KX    | 479 | ILE  | Peptide |
| 2   | LX    | 479 | ILE  | Peptide |
| 2   | MX    | 479 | ILE  | Peptide |
| 2   | NX    | 479 | ILE  | Peptide |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AT    | 1502  | 0        | 1525     | 21      | 0            |
| 1   | BT    | 1502  | 0        | 1525     | 23      | 0            |
| 1   | CT    | 1502  | 0        | 1525     | 23      | 0            |
| 1   | DT    | 1502  | 0        | 1525     | 23      | 0            |
| 1   | ET    | 1502  | 0        | 1525     | 20      | 0            |
| 1   | FT    | 1502  | 0        | 1525     | 27      | 0            |
| 1   | GT    | 1502  | 0        | 1525     | 21      | 0            |
| 1   | HT    | 1502  | 0        | 1525     | 23      | 0            |
| 1   | IT    | 1502  | 0        | 1525     | 23      | 0            |
| 1   | JT    | 1502  | 0        | 1525     | 23      | 0            |
| 1   | KT    | 1502  | 0        | 1525     | 26      | 0            |
| 1   | LT    | 1502  | 0        | 1525     | 26      | 0            |
| 1   | MT    | 1502  | 0        | 1525     | 24      | 0            |
| 1   | NT    | 1502  | 0        | 1525     | 20      | 0            |
| 2   | AX    | 1275  | 0        | 1309     | 26      | 0            |
| 2   | BX    | 1275  | 0        | 1309     | 28      | 0            |
| 2   | CX    | 1275  | 0        | 1309     | 26      | 0            |
| 2   | DX    | 1275  | 0        | 1309     | 24      | 0            |
| 2   | EX    | 1275  | 0        | 1309     | 27      | 0            |
| 2   | FX    | 1275  | 0        | 1309     | 29      | 0            |
| 2   | GX    | 1275  | 0        | 1309     | 31      | 0            |
| 2   | HX    | 1275  | 0        | 1309     | 29      | 0            |
| 2   | IX    | 1275  | 0        | 1309     | 25      | 0            |
| 2   | JX    | 1275  | 0        | 1309     | 27      | 0            |
| 2   | KX    | 1275  | 0        | 1309     | 21      | 0            |
| 2   | LX    | 1275  | 0        | 1309     | 26      | 0            |
| 2   | MX    | 1275  | 0        | 1309     | 27      | 0            |
| 2   | NX    | 1275  | 0        | 1309     | 28      | 0            |
| 3   | AY    | 1578  | 0        | 1637     | 45      | 0            |
| 3   | BY    | 1578  | 0        | 1637     | 45      | 0            |
| 3   | CY    | 1578  | 0        | 1637     | 48      | 0            |
| 3   | DY    | 1578  | 0        | 1637     | 43      | 0            |
| 3   | EY    | 1578  | 0        | 1637     | 42      | 0            |
| 3   | FY    | 1578  | 0        | 1637     | 45      | 0            |
| 3   | GY    | 1578  | 0        | 1637     | 44      | 0            |
| 3   | HY    | 1578  | 0        | 1637     | 44      | 0            |
| 3   | IY    | 1578  | 0        | 1637     | 46      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | JY    | 1578  | 0        | 1637     | 42      | 0            |
| 3   | KY    | 1578  | 0        | 1637     | 42      | 0            |
| 3   | LY    | 1578  | 0        | 1637     | 41      | 0            |
| 3   | MY    | 1578  | 0        | 1637     | 43      | 0            |
| 3   | NY    | 1578  | 0        | 1637     | 42      | 0            |
| All | All   | 60970 | 0        | 62594    | 984     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (984) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:BX:444:PRO:O   | 2:CX:410:ARG:NH2  | 2.22                     | 0.73              |
| 2:HX:444:PRO:O   | 2:IX:410:ARG:NH2  | 2.21                     | 0.73              |
| 3:AY:1722:VAL:HB | 3:AY:1732:LEU:HB2 | 1.72                     | 0.72              |
| 3:DY:1722:VAL:HB | 3:DY:1732:LEU:HB2 | 1.72                     | 0.72              |
| 3:FY:1722:VAL:HB | 3:FY:1732:LEU:HB2 | 1.72                     | 0.72              |
| 3:CY:1722:VAL:HB | 3:CY:1732:LEU:HB2 | 1.72                     | 0.72              |
| 3:GY:1722:VAL:HB | 3:GY:1732:LEU:HB2 | 1.72                     | 0.72              |
| 3:BY:1722:VAL:HB | 3:BY:1732:LEU:HB2 | 1.72                     | 0.72              |
| 3:EY:1722:VAL:HB | 3:EY:1732:LEU:HB2 | 1.72                     | 0.72              |
| 3:IY:1722:VAL:HB | 3:IY:1732:LEU:HB2 | 1.72                     | 0.72              |
| 3:MY:1722:VAL:HB | 3:MY:1732:LEU:HB2 | 1.72                     | 0.72              |
| 3:NY:1722:VAL:HB | 3:NY:1732:LEU:HB2 | 1.72                     | 0.72              |
| 3:HY:1722:VAL:HB | 3:HY:1732:LEU:HB2 | 1.72                     | 0.71              |
| 3:KY:1700:ILE:O  | 3:KY:1876:SER:HA  | 1.90                     | 0.71              |
| 3:NY:1700:ILE:O  | 3:NY:1876:SER:HA  | 1.91                     | 0.71              |
| 3:KY:1722:VAL:HB | 3:KY:1732:LEU:HB2 | 1.72                     | 0.71              |
| 3:JY:1722:VAL:HB | 3:JY:1732:LEU:HB2 | 1.72                     | 0.71              |
| 3:LY:1700:ILE:O  | 3:LY:1876:SER:HA  | 1.91                     | 0.71              |
| 3:LY:1722:VAL:HB | 3:LY:1732:LEU:HB2 | 1.72                     | 0.71              |
| 3:AY:1700:ILE:O  | 3:AY:1876:SER:HA  | 1.91                     | 0.71              |
| 3:CY:1700:ILE:O  | 3:CY:1876:SER:HA  | 1.90                     | 0.71              |
| 3:IY:1700:ILE:O  | 3:IY:1876:SER:HA  | 1.90                     | 0.70              |
| 2:JX:480:LYS:HB2 | 2:JX:483:ALA:HB3  | 1.74                     | 0.70              |
| 2:LX:480:LYS:HB2 | 2:LX:483:ALA:HB3  | 1.74                     | 0.70              |
| 2:DX:480:LYS:HB2 | 2:DX:483:ALA:HB3  | 1.74                     | 0.70              |
| 3:FY:1700:ILE:O  | 3:FY:1876:SER:HA  | 1.91                     | 0.70              |
| 2:BX:480:LYS:HB2 | 2:BX:483:ALA:HB3  | 1.74                     | 0.70              |
| 2:CX:480:LYS:HB2 | 2:CX:483:ALA:HB3  | 1.74                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:EY:1700:ILE:O   | 3:EY:1876:SER:HA  | 1.90                     | 0.70              |
| 2:IX:480:LYS:HB2  | 2:IX:483:ALA:HB3  | 1.74                     | 0.70              |
| 2:NX:480:LYS:HB2  | 2:NX:483:ALA:HB3  | 1.74                     | 0.70              |
| 2:AX:480:LYS:HB2  | 2:AX:483:ALA:HB3  | 1.74                     | 0.70              |
| 3:BY:1700:ILE:O   | 3:BY:1876:SER:HA  | 1.90                     | 0.70              |
| 3:JY:1700:ILE:O   | 3:JY:1876:SER:HA  | 1.90                     | 0.70              |
| 3:MY:1700:ILE:O   | 3:MY:1876:SER:HA  | 1.91                     | 0.70              |
| 3:HY:1700:ILE:O   | 3:HY:1876:SER:HA  | 1.90                     | 0.70              |
| 2:KX:480:LYS:HB2  | 2:KX:483:ALA:HB3  | 1.74                     | 0.70              |
| 2:FX:480:LYS:HB2  | 2:FX:483:ALA:HB3  | 1.74                     | 0.70              |
| 2:GX:480:LYS:HB2  | 2:GX:483:ALA:HB3  | 1.74                     | 0.70              |
| 3:GY:1700:ILE:O   | 3:GY:1876:SER:HA  | 1.91                     | 0.70              |
| 2:EX:480:LYS:HB2  | 2:EX:483:ALA:HB3  | 1.74                     | 0.70              |
| 2:MX:480:LYS:HB2  | 2:MX:483:ALA:HB3  | 1.74                     | 0.70              |
| 3:DY:1700:ILE:O   | 3:DY:1876:SER:HA  | 1.91                     | 0.69              |
| 2:HX:480:LYS:HB2  | 2:HX:483:ALA:HB3  | 1.74                     | 0.69              |
| 2:KX:439:ILE:HG12 | 2:KX:478:LEU:HG   | 1.77                     | 0.67              |
| 2:EX:439:ILE:HG12 | 2:EX:478:LEU:HG   | 1.77                     | 0.67              |
| 2:FX:439:ILE:HG12 | 2:FX:478:LEU:HG   | 1.77                     | 0.67              |
| 2:LX:439:ILE:HG12 | 2:LX:478:LEU:HG   | 1.77                     | 0.67              |
| 2:HX:439:ILE:HG12 | 2:HX:478:LEU:HG   | 1.77                     | 0.67              |
| 2:IX:439:ILE:HG12 | 2:IX:478:LEU:HG   | 1.77                     | 0.67              |
| 2:NX:439:ILE:HG12 | 2:NX:478:LEU:HG   | 1.77                     | 0.67              |
| 2:DX:439:ILE:HG12 | 2:DX:478:LEU:HG   | 1.77                     | 0.67              |
| 2:KX:444:PRO:O    | 2:LX:410:ARG:NH2  | 2.28                     | 0.67              |
| 2:BX:439:ILE:HG12 | 2:BX:478:LEU:HG   | 1.77                     | 0.66              |
| 2:CX:439:ILE:HG12 | 2:CX:478:LEU:HG   | 1.77                     | 0.66              |
| 2:MX:439:ILE:HG12 | 2:MX:478:LEU:HG   | 1.77                     | 0.66              |
| 2:GX:439:ILE:HG12 | 2:GX:478:LEU:HG   | 1.77                     | 0.66              |
| 2:JX:439:ILE:HG12 | 2:JX:478:LEU:HG   | 1.77                     | 0.66              |
| 2:AX:439:ILE:HG12 | 2:AX:478:LEU:HG   | 1.77                     | 0.66              |
| 3:EY:1857:GLN:NE2 | 3:FY:1856:ASN:OD1 | 2.30                     | 0.65              |
| 3:IY:1857:GLN:NE2 | 3:JY:1856:ASN:OD1 | 2.30                     | 0.64              |
| 3:KY:1857:GLN:NE2 | 3:LY:1856:ASN:OD1 | 2.30                     | 0.64              |
| 3:GY:1857:GLN:NE2 | 3:HY:1856:ASN:OD1 | 2.31                     | 0.64              |
| 3:HY:1857:GLN:NE2 | 3:IY:1856:ASN:OD1 | 2.31                     | 0.64              |
| 2:AX:444:PRO:O    | 2:BX:410:ARG:NH2  | 2.30                     | 0.64              |
| 3:LY:1857:GLN:NE2 | 3:MY:1856:ASN:OD1 | 2.30                     | 0.64              |
| 3:DY:1857:GLN:NE2 | 3:EY:1856:ASN:OD1 | 2.31                     | 0.64              |
| 3:AY:1856:ASN:OD1 | 3:NY:1857:GLN:NE2 | 2.30                     | 0.63              |
| 1:ET:36:TYR:HB3   | 2:FX:404:TYR:HB3  | 1.78                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:FX:399:ARG:NH2   | 1:GT:169:HIS:O     | 2.31                     | 0.63              |
| 3:FY:1857:GLN:NE2  | 3:GY:1856:ASN:OD1  | 2.31                     | 0.63              |
| 3:JY:1857:GLN:NE2  | 3:KY:1856:ASN:OD1  | 2.32                     | 0.63              |
| 3:BY:1857:GLN:NE2  | 3:CY:1856:ASN:OD1  | 2.31                     | 0.63              |
| 3:AY:1857:GLN:NE2  | 3:BY:1856:ASN:OD1  | 2.31                     | 0.62              |
| 2:JX:444:PRO:O     | 2:KX:410:ARG:NH2   | 2.32                     | 0.62              |
| 3:MY:1857:GLN:NE2  | 3:NY:1856:ASN:OD1  | 2.32                     | 0.62              |
| 3:CY:1857:GLN:NE2  | 3:DY:1856:ASN:OD1  | 2.32                     | 0.61              |
| 1:JT:213:ARG:HH12  | 2:JX:364:ASN:HB3   | 1.64                     | 0.61              |
| 1:LT:39:VAL:HG11   | 2:MX:419:ILE:HG13  | 1.82                     | 0.61              |
| 2:EX:444:PRO:O     | 2:FX:410:ARG:NH2   | 2.33                     | 0.61              |
| 3:NY:1714:VAL:HG21 | 3:NY:1757:ILE:HD13 | 1.82                     | 0.61              |
| 1:CT:36:TYR:HB3    | 2:DX:404:TYR:HB3   | 1.83                     | 0.61              |
| 3:LY:1714:VAL:HG21 | 3:LY:1757:ILE:HD13 | 1.82                     | 0.61              |
| 3:MY:1714:VAL:HG21 | 3:MY:1757:ILE:HD13 | 1.83                     | 0.61              |
| 3:KY:1714:VAL:HG21 | 3:KY:1757:ILE:HD13 | 1.82                     | 0.61              |
| 1:IT:36:TYR:HB3    | 2:JX:404:TYR:HB3   | 1.82                     | 0.60              |
| 1:LT:39:VAL:HG21   | 2:MX:419:ILE:HD12  | 1.82                     | 0.60              |
| 1:MT:36:TYR:HB3    | 2:NX:404:TYR:HB3   | 1.82                     | 0.60              |
| 3:AY:1714:VAL:HG21 | 3:AY:1757:ILE:HD13 | 1.83                     | 0.60              |
| 3:JY:1714:VAL:HG21 | 3:JY:1757:ILE:HD13 | 1.83                     | 0.60              |
| 3:LY:1762:ALA:HB3  | 3:LY:1770:ILE:HB   | 1.84                     | 0.60              |
| 3:BY:1714:VAL:HG21 | 3:BY:1757:ILE:HD13 | 1.83                     | 0.60              |
| 1:GT:36:TYR:HB3    | 2:HX:404:TYR:HB3   | 1.81                     | 0.60              |
| 2:MX:444:PRO:O     | 2:NX:410:ARG:NH2   | 2.35                     | 0.60              |
| 3:NY:1762:ALA:HB3  | 3:NY:1770:ILE:HB   | 1.84                     | 0.60              |
| 2:CX:444:PRO:O     | 2:DX:410:ARG:NH2   | 2.34                     | 0.60              |
| 2:FX:444:PRO:O     | 2:GX:410:ARG:NH2   | 2.34                     | 0.60              |
| 2:GX:444:PRO:O     | 2:HX:410:ARG:NH2   | 2.35                     | 0.60              |
| 2:LX:444:PRO:O     | 2:MX:410:ARG:NH2   | 2.34                     | 0.60              |
| 3:BY:1762:ALA:HB3  | 3:BY:1770:ILE:HB   | 1.84                     | 0.60              |
| 3:IY:1714:VAL:HG21 | 3:IY:1757:ILE:HD13 | 1.83                     | 0.60              |
| 1:AT:36:TYR:HB3    | 2:BX:404:TYR:HB3   | 1.83                     | 0.60              |
| 3:JY:1762:ALA:HB3  | 3:JY:1770:ILE:HB   | 1.84                     | 0.60              |
| 3:MY:1762:ALA:HB3  | 3:MY:1770:ILE:HB   | 1.84                     | 0.60              |
| 3:CY:1714:VAL:HG21 | 3:CY:1757:ILE:HD13 | 1.83                     | 0.59              |
| 3:EY:1714:VAL:HG21 | 3:EY:1757:ILE:HD13 | 1.82                     | 0.59              |
| 3:HY:1714:VAL:HG21 | 3:HY:1757:ILE:HD13 | 1.83                     | 0.59              |
| 3:KY:1762:ALA:HB3  | 3:KY:1770:ILE:HB   | 1.84                     | 0.59              |
| 2:LX:399:ARG:NH2   | 1:MT:169:HIS:O     | 2.35                     | 0.59              |
| 1:ET:39:VAL:HG11   | 2:FX:419:ILE:HG13  | 1.83                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:IY:1762:ALA:HB3  | 3:IY:1770:ILE:HB   | 1.84                     | 0.59              |
| 1:LT:36:TYR:HB3    | 2:MX:404:TYR:HB3   | 1.84                     | 0.59              |
| 3:AY:1762:ALA:HB3  | 3:AY:1770:ILE:HB   | 1.84                     | 0.59              |
| 3:DY:1714:VAL:HG21 | 3:DY:1757:ILE:HD13 | 1.83                     | 0.59              |
| 3:GY:1714:VAL:HG21 | 3:GY:1757:ILE:HD13 | 1.82                     | 0.59              |
| 2:BX:399:ARG:NH2   | 1:CT:169:HIS:O     | 2.34                     | 0.59              |
| 3:FY:1714:VAL:HG21 | 3:FY:1757:ILE:HD13 | 1.83                     | 0.59              |
| 3:DY:1762:ALA:HB3  | 3:DY:1770:ILE:HB   | 1.84                     | 0.59              |
| 3:GY:1762:ALA:HB3  | 3:GY:1770:ILE:HB   | 1.84                     | 0.59              |
| 1:KT:36:TYR:HB3    | 2:LX:404:TYR:HB3   | 1.85                     | 0.59              |
| 1:MT:39:VAL:HG11   | 2:NX:419:ILE:HG13  | 1.84                     | 0.58              |
| 3:DY:1706:VAL:HB   | 3:DY:1871:LYS:HB3  | 1.86                     | 0.58              |
| 2:AX:410:ARG:NH2   | 2:NX:444:PRO:O     | 2.36                     | 0.58              |
| 3:AY:1706:VAL:HB   | 3:AY:1871:LYS:HB3  | 1.86                     | 0.58              |
| 3:BY:1706:VAL:HB   | 3:BY:1871:LYS:HB3  | 1.86                     | 0.58              |
| 3:EY:1762:ALA:HB3  | 3:EY:1770:ILE:HB   | 1.84                     | 0.58              |
| 2:IX:444:PRO:O     | 2:JX:410:ARG:NH2   | 2.37                     | 0.58              |
| 3:EY:1706:VAL:HB   | 3:EY:1871:LYS:HB3  | 1.86                     | 0.58              |
| 3:FY:1762:ALA:HB3  | 3:FY:1770:ILE:HB   | 1.84                     | 0.58              |
| 3:CY:1706:VAL:HB   | 3:CY:1871:LYS:HB3  | 1.86                     | 0.58              |
| 1:DT:36:TYR:HB3    | 2:EX:404:TYR:HB3   | 1.85                     | 0.58              |
| 3:FY:1706:VAL:HB   | 3:FY:1871:LYS:HB3  | 1.86                     | 0.58              |
| 2:AX:404:TYR:HB3   | 1:NT:36:TYR:HB3    | 1.84                     | 0.58              |
| 3:HY:1762:ALA:HB3  | 3:HY:1770:ILE:HB   | 1.84                     | 0.58              |
| 1:IT:39:VAL:HG11   | 2:JX:419:ILE:HG13  | 1.84                     | 0.57              |
| 3:MY:1706:VAL:HB   | 3:MY:1871:LYS:HB3  | 1.86                     | 0.57              |
| 3:NY:1706:VAL:HB   | 3:NY:1871:LYS:HB3  | 1.86                     | 0.57              |
| 1:AT:169:HIS:O     | 2:NX:399:ARG:NH2   | 2.37                     | 0.57              |
| 1:ET:39:VAL:HG21   | 2:FX:419:ILE:HD12  | 1.86                     | 0.57              |
| 3:GY:1706:VAL:HB   | 3:GY:1871:LYS:HB3  | 1.86                     | 0.57              |
| 3:CY:1762:ALA:HB3  | 3:CY:1770:ILE:HB   | 1.84                     | 0.57              |
| 1:BT:36:TYR:HB3    | 2:CX:404:TYR:HB3   | 1.86                     | 0.57              |
| 1:AT:39:VAL:HG11   | 2:BX:419:ILE:HG13  | 1.87                     | 0.57              |
| 1:MT:39:VAL:HG21   | 2:NX:419:ILE:HD12  | 1.86                     | 0.57              |
| 2:DX:399:ARG:NH2   | 1:ET:169:HIS:O     | 2.37                     | 0.57              |
| 3:KY:1706:VAL:HB   | 3:KY:1871:LYS:HB3  | 1.86                     | 0.57              |
| 2:DX:444:PRO:O     | 2:EX:410:ARG:NH2   | 2.37                     | 0.57              |
| 3:IY:1706:VAL:HB   | 3:IY:1871:LYS:HB3  | 1.86                     | 0.57              |
| 3:HY:1706:VAL:HB   | 3:HY:1871:LYS:HB3  | 1.86                     | 0.56              |
| 3:LY:1706:VAL:HB   | 3:LY:1871:LYS:HB3  | 1.86                     | 0.56              |
| 3:JY:1706:VAL:HB   | 3:JY:1871:LYS:HB3  | 1.86                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:MX:399:ARG:NH2   | 1:NT:169:HIS:O     | 2.39                     | 0.56              |
| 2:HX:399:ARG:NH2   | 1:IT:169:HIS:O     | 2.37                     | 0.56              |
| 1:KT:39:VAL:HG11   | 2:LX:419:ILE:HG13  | 1.86                     | 0.56              |
| 1:IT:39:VAL:HG21   | 2:JX:419:ILE:HD12  | 1.87                     | 0.56              |
| 2:AX:419:ILE:HG13  | 1:NT:39:VAL:HG11   | 1.88                     | 0.56              |
| 3:HY:1732:LEU:HD22 | 3:HY:1736:THR:HG21 | 1.89                     | 0.55              |
| 3:IY:1732:LEU:HD22 | 3:IY:1736:THR:HG21 | 1.89                     | 0.55              |
| 3:JY:1732:LEU:HD22 | 3:JY:1736:THR:HG21 | 1.89                     | 0.55              |
| 2:KX:507:GLY:HA2   | 1:LT:168:LEU:HD11  | 1.87                     | 0.55              |
| 2:AX:399:ARG:NH2   | 1:BT:169:HIS:O     | 2.38                     | 0.55              |
| 2:EX:399:ARG:NH2   | 1:FT:169:HIS:O     | 2.39                     | 0.55              |
| 3:LY:1732:LEU:HD22 | 3:LY:1736:THR:HG21 | 1.88                     | 0.55              |
| 3:GY:1732:LEU:HD22 | 3:GY:1736:THR:HG21 | 1.89                     | 0.55              |
| 3:KY:1732:LEU:HD22 | 3:KY:1736:THR:HG21 | 1.89                     | 0.55              |
| 3:MY:1732:LEU:HD22 | 3:MY:1736:THR:HG21 | 1.89                     | 0.55              |
| 3:FY:1732:LEU:HD22 | 3:FY:1736:THR:HG21 | 1.89                     | 0.54              |
| 3:NY:1732:LEU:HD22 | 3:NY:1736:THR:HG21 | 1.89                     | 0.54              |
| 1:LT:296:GLU:OE2   | 1:LT:300:ASN:ND2   | 2.41                     | 0.54              |
| 3:AY:1732:LEU:HD22 | 3:AY:1736:THR:HG21 | 1.89                     | 0.54              |
| 1:ET:296:GLU:OE2   | 1:ET:300:ASN:ND2   | 2.41                     | 0.54              |
| 1:FT:296:GLU:OE2   | 1:FT:300:ASN:ND2   | 2.41                     | 0.54              |
| 3:BY:1732:LEU:HD22 | 3:BY:1736:THR:HG21 | 1.88                     | 0.54              |
| 1:IT:296:GLU:OE2   | 1:IT:300:ASN:ND2   | 2.41                     | 0.54              |
| 1:MT:296:GLU:OE2   | 1:MT:300:ASN:ND2   | 2.41                     | 0.54              |
| 3:DY:1732:LEU:HD22 | 3:DY:1736:THR:HG21 | 1.88                     | 0.54              |
| 3:EY:1732:LEU:HD22 | 3:EY:1736:THR:HG21 | 1.89                     | 0.54              |
| 1:KT:296:GLU:OE2   | 1:KT:300:ASN:ND2   | 2.41                     | 0.54              |
| 1:FT:39:VAL:HG21   | 2:GX:419:ILE:HD12  | 1.89                     | 0.54              |
| 1:CT:296:GLU:OE2   | 1:CT:300:ASN:ND2   | 2.41                     | 0.54              |
| 3:CY:1732:LEU:HD22 | 3:CY:1736:THR:HG21 | 1.89                     | 0.54              |
| 3:HY:1859:LEU:O    | 3:HY:1863:MET:CB   | 2.56                     | 0.54              |
| 3:AY:1710:LEU:HD12 | 3:BY:1785:GLY:HA3  | 1.90                     | 0.54              |
| 3:CY:1710:LEU:HD12 | 3:DY:1785:GLY:HA3  | 1.90                     | 0.54              |
| 3:GY:1859:LEU:O    | 3:GY:1863:MET:CB   | 2.56                     | 0.54              |
| 1:HT:296:GLU:OE2   | 1:HT:300:ASN:ND2   | 2.41                     | 0.54              |
| 3:IY:1859:LEU:O    | 3:IY:1863:MET:CB   | 2.56                     | 0.54              |
| 1:NT:296:GLU:OE2   | 1:NT:300:ASN:ND2   | 2.41                     | 0.54              |
| 1:BT:296:GLU:OE2   | 1:BT:300:ASN:ND2   | 2.41                     | 0.54              |
| 2:IX:399:ARG:NH2   | 1:JT:169:HIS:O     | 2.41                     | 0.54              |
| 2:JX:399:ARG:NH2   | 1:KT:169:HIS:O     | 2.41                     | 0.54              |
| 3:JY:1710:LEU:HD12 | 3:KY:1785:GLY:HA3  | 1.90                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AY:1859:LEU:O    | 3:AY:1863:MET:CB   | 2.56                     | 0.53              |
| 1:JT:296:GLU:OE2   | 1:JT:300:ASN:ND2   | 2.41                     | 0.53              |
| 3:JY:1859:LEU:O    | 3:JY:1863:MET:CB   | 2.56                     | 0.53              |
| 3:LY:1710:LEU:HD12 | 3:MY:1785:GLY:HA3  | 1.90                     | 0.53              |
| 2:CX:399:ARG:NH2   | 1:DT:169:HIS:O     | 2.40                     | 0.53              |
| 3:CY:1859:LEU:O    | 3:CY:1863:MET:CB   | 2.56                     | 0.53              |
| 1:FT:39:VAL:HG11   | 2:GX:419:ILE:HG13  | 1.88                     | 0.53              |
| 1:GT:296:GLU:OE2   | 1:GT:300:ASN:ND2   | 2.41                     | 0.53              |
| 2:KX:399:ARG:NH2   | 1:LT:169:HIS:O     | 2.40                     | 0.53              |
| 1:DT:39:VAL:HG11   | 2:EX:419:ILE:HG13  | 1.89                     | 0.53              |
| 3:DY:1859:LEU:O    | 3:DY:1863:MET:CB   | 2.56                     | 0.53              |
| 3:FY:1859:LEU:O    | 3:FY:1863:MET:CB   | 2.56                     | 0.53              |
| 1:AT:296:GLU:OE2   | 1:AT:300:ASN:ND2   | 2.41                     | 0.53              |
| 3:AY:1785:GLY:HA3  | 3:NY:1710:LEU:HD12 | 1.91                     | 0.53              |
| 3:BY:1859:LEU:O    | 3:BY:1863:MET:CB   | 2.56                     | 0.53              |
| 1:DT:296:GLU:OE2   | 1:DT:300:ASN:ND2   | 2.41                     | 0.53              |
| 1:KT:39:VAL:HG21   | 2:LX:419:ILE:HD12  | 1.89                     | 0.53              |
| 2:BX:507:GLY:HA2   | 1:CT:168:LEU:HD11  | 1.90                     | 0.53              |
| 3:KY:1710:LEU:HD12 | 3:LY:1785:GLY:HA3  | 1.91                     | 0.53              |
| 3:KY:1859:LEU:O    | 3:KY:1863:MET:CB   | 2.56                     | 0.53              |
| 2:GX:376:ILE:HA    | 2:GX:379:GLN:HG2   | 1.91                     | 0.53              |
| 3:MY:1859:LEU:O    | 3:MY:1863:MET:CB   | 2.56                     | 0.53              |
| 2:AX:376:ILE:HA    | 2:AX:379:GLN:HG2   | 1.91                     | 0.53              |
| 2:BX:376:ILE:HA    | 2:BX:379:GLN:HG2   | 1.91                     | 0.53              |
| 2:FX:376:ILE:HA    | 2:FX:379:GLN:HG2   | 1.91                     | 0.53              |
| 2:GX:399:ARG:NH2   | 1:HT:169:HIS:O     | 2.42                     | 0.53              |
| 3:GY:1710:LEU:HD12 | 3:HY:1785:GLY:HA3  | 1.90                     | 0.53              |
| 1:HT:39:VAL:HG11   | 2:IX:419:ILE:HG13  | 1.90                     | 0.53              |
| 3:HY:1858:ILE:HG13 | 3:IY:1859:LEU:HD21 | 1.91                     | 0.53              |
| 2:MX:376:ILE:HA    | 2:MX:379:GLN:HG2   | 1.91                     | 0.53              |
| 3:MY:1710:LEU:HD12 | 3:NY:1785:GLY:HA3  | 1.91                     | 0.53              |
| 2:DX:376:ILE:HA    | 2:DX:379:GLN:HG2   | 1.91                     | 0.53              |
| 2:EX:376:ILE:HA    | 2:EX:379:GLN:HG2   | 1.91                     | 0.53              |
| 1:HT:111:ALA:O     | 1:IT:167:ASN:ND2   | 2.42                     | 0.53              |
| 1:LT:114:ALA:HB1   | 1:LT:118:ILE:HD11  | 1.91                     | 0.53              |
| 1:CT:114:ALA:HB1   | 1:CT:118:ILE:HD11  | 1.91                     | 0.52              |
| 1:DT:114:ALA:HB1   | 1:DT:118:ILE:HD11  | 1.92                     | 0.52              |
| 3:HY:1710:LEU:HD12 | 3:IY:1785:GLY:HA3  | 1.90                     | 0.52              |
| 2:IX:376:ILE:HA    | 2:IX:379:GLN:HG2   | 1.91                     | 0.52              |
| 1:JT:210:TYR:CD1   | 2:JX:368:ILE:HG13  | 2.45                     | 0.52              |
| 2:KX:376:ILE:HA    | 2:KX:379:GLN:HG2   | 1.91                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:LX:376:ILE:HA    | 2:LX:379:GLN:HG2   | 1.91                     | 0.52              |
| 2:CX:376:ILE:HA    | 2:CX:379:GLN:HG2   | 1.91                     | 0.52              |
| 3:DY:1710:LEU:HD12 | 3:EY:1785:GLY:HA3  | 1.90                     | 0.52              |
| 3:EY:1859:LEU:O    | 3:EY:1863:MET:CB   | 2.56                     | 0.52              |
| 1:FT:114:ALA:HB1   | 1:FT:118:ILE:HD11  | 1.92                     | 0.52              |
| 2:HX:376:ILE:HA    | 2:HX:379:GLN:HG2   | 1.91                     | 0.52              |
| 3:LY:1859:LEU:O    | 3:LY:1863:MET:CB   | 2.56                     | 0.52              |
| 1:NT:114:ALA:HB1   | 1:NT:118:ILE:HD11  | 1.92                     | 0.52              |
| 2:NX:376:ILE:HA    | 2:NX:379:GLN:HG2   | 1.91                     | 0.52              |
| 3:NY:1859:LEU:O    | 3:NY:1863:MET:CB   | 2.56                     | 0.52              |
| 1:AT:114:ALA:HB1   | 1:AT:118:ILE:HD11  | 1.92                     | 0.52              |
| 1:BT:111:ALA:O     | 1:CT:167:ASN:ND2   | 2.43                     | 0.52              |
| 1:ET:114:ALA:HB1   | 1:ET:118:ILE:HD11  | 1.91                     | 0.52              |
| 1:FT:36:TYR:HB3    | 2:GX:404:TYR:HB3   | 1.91                     | 0.52              |
| 1:GT:90:SER:HA     | 1:GT:137:ASN:HB2   | 1.92                     | 0.52              |
| 1:HT:90:SER:HA     | 1:HT:137:ASN:HB2   | 1.92                     | 0.52              |
| 1:MT:114:ALA:HB1   | 1:MT:118:ILE:HD11  | 1.91                     | 0.52              |
| 3:EY:1858:ILE:HG13 | 3:FY:1859:LEU:HD21 | 1.92                     | 0.52              |
| 1:GT:39:VAL:HG11   | 2:HX:419:ILE:HG13  | 1.91                     | 0.52              |
| 1:HT:114:ALA:HB1   | 1:HT:118:ILE:HD11  | 1.91                     | 0.52              |
| 1:JT:90:SER:HA     | 1:JT:137:ASN:HB2   | 1.92                     | 0.52              |
| 1:JT:114:ALA:HB1   | 1:JT:118:ILE:HD11  | 1.92                     | 0.52              |
| 2:JX:376:ILE:HA    | 2:JX:379:GLN:HG2   | 1.91                     | 0.52              |
| 1:KT:90:SER:HA     | 1:KT:137:ASN:HB2   | 1.92                     | 0.52              |
| 3:LY:1858:ILE:HG13 | 3:MY:1859:LEU:HD21 | 1.92                     | 0.52              |
| 3:EY:1710:LEU:HD12 | 3:FY:1785:GLY:HA3  | 1.91                     | 0.52              |
| 3:AY:1859:LEU:HD21 | 3:NY:1858:ILE:HG13 | 1.92                     | 0.52              |
| 3:AY:1858:ILE:HG13 | 3:BY:1859:LEU:HD21 | 1.92                     | 0.52              |
| 3:BY:1710:LEU:HD12 | 3:CY:1785:GLY:HA3  | 1.92                     | 0.52              |
| 1:GT:114:ALA:HB1   | 1:GT:118:ILE:HD11  | 1.91                     | 0.52              |
| 1:KT:114:ALA:HB1   | 1:KT:118:ILE:HD11  | 1.92                     | 0.52              |
| 1:BT:114:ALA:HB1   | 1:BT:118:ILE:HD11  | 1.92                     | 0.52              |
| 1:ET:111:ALA:O     | 1:FT:167:ASN:ND2   | 2.43                     | 0.52              |
| 1:IT:114:ALA:HB1   | 1:IT:118:ILE:HD11  | 1.91                     | 0.52              |
| 1:MT:90:SER:HA     | 1:MT:137:ASN:HB2   | 1.92                     | 0.52              |
| 1:FT:90:SER:HA     | 1:FT:137:ASN:HB2   | 1.92                     | 0.52              |
| 1:IT:90:SER:HA     | 1:IT:137:ASN:HB2   | 1.92                     | 0.52              |
| 1:ET:90:SER:HA     | 1:ET:137:ASN:HB2   | 1.92                     | 0.52              |
| 1:ET:193:GLU:HA    | 1:ET:196:ASN:HD22  | 1.75                     | 0.52              |
| 2:KX:439:ILE:HD12  | 2:KX:467:TYR:HD1   | 1.75                     | 0.52              |
| 1:LT:90:SER:HA     | 1:LT:137:ASN:HB2   | 1.92                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AT:39:VAL:HG21   | 2:BX:419:ILE:HD12  | 1.91                     | 0.51              |
| 3:KY:1858:ILE:HG13 | 3:LY:1859:LEU:HD21 | 1.92                     | 0.51              |
| 2:MX:439:ILE:HD12  | 2:MX:467:TYR:HD1   | 1.76                     | 0.51              |
| 1:FT:193:GLU:HA    | 1:FT:196:ASN:HD22  | 1.75                     | 0.51              |
| 1:IT:213:ARG:HH12  | 2:IX:364:ASN:HB3   | 1.76                     | 0.51              |
| 1:KT:193:GLU:HA    | 1:KT:196:ASN:HD22  | 1.75                     | 0.51              |
| 1:DT:193:GLU:HA    | 1:DT:196:ASN:HD22  | 1.75                     | 0.51              |
| 3:GY:1858:ILE:HG13 | 3:HY:1859:LEU:HD21 | 1.93                     | 0.51              |
| 3:IY:1710:LEU:HD12 | 3:JY:1785:GLY:HA3  | 1.92                     | 0.51              |
| 1:KT:111:ALA:O     | 1:LT:167:ASN:ND2   | 2.44                     | 0.51              |
| 2:AX:439:ILE:HD12  | 2:AX:467:TYR:HD1   | 1.76                     | 0.51              |
| 1:DT:90:SER:HA     | 1:DT:137:ASN:HB2   | 1.92                     | 0.51              |
| 1:JT:193:GLU:HA    | 1:JT:196:ASN:HD22  | 1.75                     | 0.51              |
| 1:NT:90:SER:HA     | 1:NT:137:ASN:HB2   | 1.92                     | 0.51              |
| 1:CT:90:SER:HA     | 1:CT:137:ASN:HB2   | 1.92                     | 0.51              |
| 3:FY:1710:LEU:HD12 | 3:GY:1785:GLY:HA3  | 1.92                     | 0.51              |
| 3:FY:1858:ILE:HG13 | 3:GY:1859:LEU:HD21 | 1.93                     | 0.51              |
| 1:GT:193:GLU:HA    | 1:GT:196:ASN:HD22  | 1.75                     | 0.51              |
| 2:IX:436:GLN:HB2   | 3:IY:1734:LYS:HG2  | 1.93                     | 0.51              |
| 3:IY:1858:ILE:HG13 | 3:JY:1859:LEU:HD21 | 1.93                     | 0.51              |
| 1:AT:193:GLU:HA    | 1:AT:196:ASN:HD22  | 1.75                     | 0.51              |
| 3:DY:1858:ILE:HG13 | 3:EY:1859:LEU:HD21 | 1.92                     | 0.51              |
| 2:IX:439:ILE:HD12  | 2:IX:467:TYR:HD1   | 1.76                     | 0.51              |
| 1:AT:90:SER:HA     | 1:AT:137:ASN:HB2   | 1.92                     | 0.51              |
| 2:AX:419:ILE:HD12  | 1:NT:39:VAL:HG21   | 1.91                     | 0.51              |
| 1:BT:193:GLU:HA    | 1:BT:196:ASN:HD22  | 1.75                     | 0.51              |
| 1:CT:193:GLU:HA    | 1:CT:196:ASN:HD22  | 1.75                     | 0.51              |
| 1:IT:210:TYR:CD1   | 2:IX:368:ILE:HG13  | 2.46                     | 0.51              |
| 1:MT:111:ALA:O     | 1:NT:167:ASN:ND2   | 2.44                     | 0.51              |
| 3:MY:1858:ILE:HG13 | 3:NY:1859:LEU:HD21 | 1.93                     | 0.51              |
| 1:DT:39:VAL:HG21   | 2:EX:419:ILE:HD12  | 1.92                     | 0.51              |
| 1:LT:193:GLU:HA    | 1:LT:196:ASN:HD22  | 1.75                     | 0.51              |
| 1:AT:111:ALA:O     | 1:BT:167:ASN:ND2   | 2.44                     | 0.50              |
| 1:IT:193:GLU:HA    | 1:IT:196:ASN:HD22  | 1.75                     | 0.50              |
| 1:BT:90:SER:HA     | 1:BT:137:ASN:HB2   | 1.92                     | 0.50              |
| 3:CY:1858:ILE:HG13 | 3:DY:1859:LEU:HD21 | 1.93                     | 0.50              |
| 1:DT:111:ALA:O     | 1:ET:167:ASN:ND2   | 2.44                     | 0.50              |
| 2:EX:439:ILE:HD12  | 2:EX:467:TYR:HD1   | 1.75                     | 0.50              |
| 2:FX:439:ILE:HD12  | 2:FX:467:TYR:HD1   | 1.76                     | 0.50              |
| 2:HX:439:ILE:HD12  | 2:HX:467:TYR:HD1   | 1.76                     | 0.50              |
| 3:JY:1858:ILE:HG13 | 3:KY:1859:LEU:HD21 | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CX:439:ILE:HD12  | 2:CX:467:TYR:HD1   | 1.76                     | 0.50              |
| 3:CY:1859:LEU:O    | 3:CY:1863:MET:HB2  | 2.11                     | 0.50              |
| 1:HT:39:VAL:HG21   | 2:IX:419:ILE:HD12  | 1.92                     | 0.50              |
| 2:JX:439:ILE:HD12  | 2:JX:467:TYR:HD1   | 1.76                     | 0.50              |
| 2:LX:439:ILE:HD12  | 2:LX:467:TYR:HD1   | 1.76                     | 0.50              |
| 3:BY:1858:ILE:HG13 | 3:CY:1859:LEU:HD21 | 1.93                     | 0.50              |
| 1:HT:193:GLU:HA    | 1:HT:196:ASN:HD22  | 1.75                     | 0.50              |
| 2:IX:507:GLY:HA2   | 1:JT:168:LEU:HD11  | 1.93                     | 0.50              |
| 3:NY:1859:LEU:O    | 3:NY:1863:MET:HB2  | 2.11                     | 0.50              |
| 2:AX:497:LEU:O     | 2:BX:432:ASN:ND2   | 2.37                     | 0.50              |
| 3:BY:1859:LEU:O    | 3:BY:1863:MET:HB2  | 2.11                     | 0.50              |
| 1:FT:111:ALA:O     | 1:GT:167:ASN:ND2   | 2.45                     | 0.50              |
| 3:FY:1740:GLY:HA2  | 3:FY:1759:PHE:HA   | 1.94                     | 0.50              |
| 3:HY:1859:LEU:O    | 3:HY:1863:MET:HB2  | 2.11                     | 0.50              |
| 3:IY:1763:ILE:HG12 | 3:IY:1769:ILE:HG22 | 1.94                     | 0.50              |
| 3:JY:1859:LEU:O    | 3:JY:1863:MET:HB2  | 2.11                     | 0.50              |
| 3:KY:1859:LEU:O    | 3:KY:1863:MET:HB2  | 2.11                     | 0.50              |
| 1:NT:193:GLU:HA    | 1:NT:196:ASN:HD22  | 1.75                     | 0.50              |
| 3:AY:1859:LEU:O    | 3:AY:1863:MET:HB2  | 2.11                     | 0.50              |
| 3:EY:1740:GLY:HA2  | 3:EY:1759:PHE:HA   | 1.94                     | 0.50              |
| 3:GY:1740:GLY:HA2  | 3:GY:1759:PHE:HA   | 1.94                     | 0.50              |
| 3:GY:1763:ILE:HG12 | 3:GY:1769:ILE:HG22 | 1.94                     | 0.50              |
| 3:KY:1763:ILE:HG12 | 3:KY:1769:ILE:HG22 | 1.94                     | 0.50              |
| 3:AY:1740:GLY:HA2  | 3:AY:1759:PHE:HA   | 1.94                     | 0.50              |
| 1:BT:39:VAL:HG11   | 2:CX:419:ILE:HG13  | 1.93                     | 0.50              |
| 2:BX:436:GLN:HB2   | 3:BY:1734:LYS:HG2  | 1.93                     | 0.50              |
| 2:DX:439:ILE:HD12  | 2:DX:467:TYR:HD1   | 1.76                     | 0.50              |
| 3:EY:1763:ILE:HG12 | 3:EY:1769:ILE:HG22 | 1.94                     | 0.50              |
| 2:NX:439:ILE:HD12  | 2:NX:467:TYR:HD1   | 1.76                     | 0.50              |
| 3:NY:1740:GLY:HA2  | 3:NY:1759:PHE:HA   | 1.94                     | 0.50              |
| 1:AT:167:ASN:ND2   | 1:NT:111:ALA:O     | 2.45                     | 0.49              |
| 3:BY:1740:GLY:HA2  | 3:BY:1759:PHE:HA   | 1.94                     | 0.49              |
| 3:DY:1740:GLY:HA2  | 3:DY:1759:PHE:HA   | 1.94                     | 0.49              |
| 3:HY:1740:GLY:HA2  | 3:HY:1759:PHE:HA   | 1.94                     | 0.49              |
| 3:HY:1763:ILE:HG12 | 3:HY:1769:ILE:HG22 | 1.94                     | 0.49              |
| 3:IY:1859:LEU:O    | 3:IY:1863:MET:HB2  | 2.12                     | 0.49              |
| 3:LY:1859:LEU:O    | 3:LY:1863:MET:HB2  | 2.12                     | 0.49              |
| 3:MY:1740:GLY:HA2  | 3:MY:1759:PHE:HA   | 1.94                     | 0.49              |
| 1:AT:28:VAL:HG23   | 1:AT:29:VAL:H      | 1.78                     | 0.49              |
| 3:CY:1740:GLY:HA2  | 3:CY:1759:PHE:HA   | 1.94                     | 0.49              |
| 2:FX:399:ARG:NH1   | 2:FX:495:ASN:OD1   | 2.46                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:HT:36:TYR:HB3    | 2:IX:404:TYR:HB3   | 1.92                     | 0.49              |
| 2:IX:455:ILE:HB    | 3:IY:1765:PRO:HB3  | 1.93                     | 0.49              |
| 2:IX:481:ASP:HB3   | 3:IY:1875:ASP:HA   | 1.95                     | 0.49              |
| 3:JY:1763:ILE:HG12 | 3:JY:1769:ILE:HG22 | 1.94                     | 0.49              |
| 3:LY:1763:ILE:HG12 | 3:LY:1769:ILE:HG22 | 1.94                     | 0.49              |
| 2:MX:399:ARG:NH1   | 2:MX:495:ASN:OD1   | 2.46                     | 0.49              |
| 2:EX:399:ARG:NH1   | 2:EX:495:ASN:OD1   | 2.46                     | 0.49              |
| 3:EY:1859:LEU:O    | 3:EY:1863:MET:HB2  | 2.11                     | 0.49              |
| 2:GX:439:ILE:HD12  | 2:GX:467:TYR:HD1   | 1.75                     | 0.49              |
| 3:LY:1740:GLY:HA2  | 3:LY:1759:PHE:HA   | 1.94                     | 0.49              |
| 3:FY:1763:ILE:HG12 | 3:FY:1769:ILE:HG22 | 1.94                     | 0.49              |
| 2:GX:399:ARG:NH1   | 2:GX:495:ASN:OD1   | 2.46                     | 0.49              |
| 1:IT:111:ALA:O     | 1:JT:167:ASN:ND2   | 2.45                     | 0.49              |
| 3:IY:1740:GLY:HA2  | 3:IY:1759:PHE:HA   | 1.94                     | 0.49              |
| 1:LT:111:ALA:O     | 1:MT:167:ASN:ND2   | 2.45                     | 0.49              |
| 3:NY:1763:ILE:HG12 | 3:NY:1769:ILE:HG22 | 1.94                     | 0.49              |
| 1:BT:28:VAL:HG23   | 1:BT:29:VAL:H      | 1.78                     | 0.49              |
| 2:BX:399:ARG:NH1   | 2:BX:495:ASN:OD1   | 2.46                     | 0.49              |
| 2:BX:439:ILE:HD12  | 2:BX:467:TYR:HD1   | 1.76                     | 0.49              |
| 2:CX:399:ARG:NH1   | 2:CX:495:ASN:OD1   | 2.46                     | 0.49              |
| 3:CY:1763:ILE:HG12 | 3:CY:1769:ILE:HG22 | 1.94                     | 0.49              |
| 1:FT:28:VAL:HG23   | 1:FT:29:VAL:H      | 1.78                     | 0.49              |
| 1:MT:193:GLU:HA    | 1:MT:196:ASN:HD22  | 1.75                     | 0.49              |
| 1:NT:28:VAL:HG23   | 1:NT:29:VAL:H      | 1.78                     | 0.49              |
| 2:NX:399:ARG:NH1   | 2:NX:495:ASN:OD1   | 2.46                     | 0.49              |
| 2:GX:400:ASN:HB3   | 2:GX:421:ASP:OD1   | 2.13                     | 0.49              |
| 2:JX:399:ARG:NH1   | 2:JX:495:ASN:OD1   | 2.46                     | 0.49              |
| 3:KY:1740:GLY:HA2  | 3:KY:1759:PHE:HA   | 1.94                     | 0.49              |
| 3:MY:1859:LEU:O    | 3:MY:1863:MET:HB2  | 2.12                     | 0.49              |
| 2:DX:400:ASN:HB3   | 2:DX:421:ASP:OD1   | 2.13                     | 0.49              |
| 1:GT:39:VAL:HG21   | 2:HX:419:ILE:HD12  | 1.95                     | 0.49              |
| 3:GY:1859:LEU:O    | 3:GY:1863:MET:HB2  | 2.11                     | 0.49              |
| 2:HX:400:ASN:HB3   | 2:HX:421:ASP:OD1   | 2.13                     | 0.49              |
| 3:JY:1740:GLY:HA2  | 3:JY:1759:PHE:HA   | 1.94                     | 0.49              |
| 1:KT:196:ASN:OD1   | 3:LY:1907:GLN:NE2  | 2.46                     | 0.49              |
| 2:DX:399:ARG:NH1   | 2:DX:495:ASN:OD1   | 2.46                     | 0.49              |
| 1:ET:28:VAL:HG23   | 1:ET:29:VAL:H      | 1.78                     | 0.49              |
| 2:CX:481:ASP:HB3   | 3:CY:1875:ASP:HA   | 1.94                     | 0.49              |
| 3:EY:1699:GLU:HG2  | 3:EY:1719:ALA:HB3  | 1.95                     | 0.49              |
| 3:FY:1699:GLU:HG2  | 3:FY:1719:ALA:HB3  | 1.95                     | 0.49              |
| 3:GY:1699:GLU:HG2  | 3:GY:1719:ALA:HB3  | 1.95                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:KX:399:ARG:NH1   | 2:KX:495:ASN:OD1   | 2.46                     | 0.49              |
| 1:CT:28:VAL:HG23   | 1:CT:29:VAL:H      | 1.78                     | 0.49              |
| 3:FY:1859:LEU:O    | 3:FY:1863:MET:HB2  | 2.11                     | 0.49              |
| 1:GT:28:VAL:HG23   | 1:GT:29:VAL:H      | 1.78                     | 0.49              |
| 2:HX:399:ARG:NH1   | 2:HX:495:ASN:OD1   | 2.46                     | 0.49              |
| 1:JT:99:ALA:HB2    | 1:JT:124:PRO:HB3   | 1.95                     | 0.49              |
| 1:JT:213:ARG:NH1   | 2:JX:364:ASN:HB3   | 2.28                     | 0.49              |
| 1:KT:28:VAL:HG23   | 1:KT:29:VAL:H      | 1.78                     | 0.49              |
| 3:MY:1698:ILE:HG23 | 3:MY:1722:VAL:HG21 | 1.95                     | 0.49              |
| 3:AY:1698:ILE:HG23 | 3:AY:1722:VAL:HG21 | 1.95                     | 0.48              |
| 2:CX:400:ASN:HB3   | 2:CX:421:ASP:OD1   | 2.13                     | 0.48              |
| 3:DY:1699:GLU:HG2  | 3:DY:1719:ALA:HB3  | 1.95                     | 0.48              |
| 3:HY:1699:GLU:HG2  | 3:HY:1719:ALA:HB3  | 1.95                     | 0.48              |
| 2:JX:507:GLY:HA2   | 1:KT:168:LEU:HD11  | 1.94                     | 0.48              |
| 2:LX:399:ARG:NH1   | 2:LX:495:ASN:OD1   | 2.46                     | 0.48              |
| 3:CY:1698:ILE:HG23 | 3:CY:1722:VAL:HG21 | 1.95                     | 0.48              |
| 3:EY:1698:ILE:HG23 | 3:EY:1722:VAL:HG21 | 1.95                     | 0.48              |
| 1:HT:99:ALA:HB2    | 1:HT:124:PRO:HB3   | 1.95                     | 0.48              |
| 3:HY:1698:ILE:HG23 | 3:HY:1722:VAL:HG21 | 1.95                     | 0.48              |
| 1:JT:28:VAL:HG23   | 1:JT:29:VAL:H      | 1.78                     | 0.48              |
| 3:KY:1698:ILE:HG23 | 3:KY:1722:VAL:HG21 | 1.95                     | 0.48              |
| 2:MX:400:ASN:HB3   | 2:MX:421:ASP:OD1   | 2.13                     | 0.48              |
| 2:NX:400:ASN:HB3   | 2:NX:421:ASP:OD1   | 2.13                     | 0.48              |
| 3:DY:1859:LEU:O    | 3:DY:1863:MET:HB2  | 2.12                     | 0.48              |
| 2:EX:400:ASN:HB3   | 2:EX:421:ASP:OD1   | 2.13                     | 0.48              |
| 3:FY:1698:ILE:HG23 | 3:FY:1722:VAL:HG21 | 1.95                     | 0.48              |
| 1:IT:28:VAL:HG23   | 1:IT:29:VAL:H      | 1.78                     | 0.48              |
| 3:IY:1699:GLU:HG2  | 3:IY:1719:ALA:HB3  | 1.95                     | 0.48              |
| 2:JX:364:ASN:HA    | 2:JX:367:LYS:HG2   | 1.96                     | 0.48              |
| 2:LX:400:ASN:HB3   | 2:LX:421:ASP:OD1   | 2.13                     | 0.48              |
| 3:LY:1873:GLU:HG2  | 3:MY:1781:LEU:HD22 | 1.95                     | 0.48              |
| 2:AX:400:ASN:HB3   | 2:AX:421:ASP:OD1   | 2.13                     | 0.48              |
| 3:BY:1763:ILE:HG12 | 3:BY:1769:ILE:HG22 | 1.94                     | 0.48              |
| 2:DX:364:ASN:HA    | 2:DX:367:LYS:HG2   | 1.96                     | 0.48              |
| 1:FT:99:ALA:HB2    | 1:FT:124:PRO:HB3   | 1.95                     | 0.48              |
| 2:KX:400:ASN:HB3   | 2:KX:421:ASP:OD1   | 2.13                     | 0.48              |
| 2:AX:364:ASN:HA    | 2:AX:367:LYS:HG2   | 1.96                     | 0.48              |
| 2:AX:399:ARG:NH1   | 2:AX:495:ASN:OD1   | 2.46                     | 0.48              |
| 3:CY:1699:GLU:HG2  | 3:CY:1719:ALA:HB3  | 1.95                     | 0.48              |
| 2:FX:364:ASN:HA    | 2:FX:367:LYS:HG2   | 1.96                     | 0.48              |
| 2:HX:364:ASN:HA    | 2:HX:367:LYS:HG2   | 1.96                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:HX:497:LEU:O     | 2:IX:432:ASN:ND2   | 2.38                     | 0.48              |
| 2:IX:400:ASN:HB3   | 2:IX:421:ASP:OD1   | 2.13                     | 0.48              |
| 3:IY:1873:GLU:HG2  | 3:JY:1781:LEU:HD22 | 1.95                     | 0.48              |
| 3:JY:1698:ILE:HG23 | 3:JY:1722:VAL:HG21 | 1.95                     | 0.48              |
| 1:MT:28:VAL:HG23   | 1:MT:29:VAL:H      | 1.78                     | 0.48              |
| 3:EY:1792:ASN:O    | 3:EY:1797:ARG:NH1  | 2.46                     | 0.48              |
| 2:FX:400:ASN:HB3   | 2:FX:421:ASP:OD1   | 2.13                     | 0.48              |
| 3:FY:1792:ASN:O    | 3:FY:1797:ARG:NH1  | 2.46                     | 0.48              |
| 3:JY:1699:GLU:HG2  | 3:JY:1719:ALA:HB3  | 1.95                     | 0.48              |
| 1:LT:99:ALA:HB2    | 1:LT:124:PRO:HB3   | 1.95                     | 0.48              |
| 2:LX:364:ASN:HA    | 2:LX:367:LYS:HG2   | 1.96                     | 0.48              |
| 3:MY:1763:ILE:HG12 | 3:MY:1769:ILE:HG22 | 1.94                     | 0.48              |
| 2:BX:400:ASN:HB3   | 2:BX:421:ASP:OD1   | 2.13                     | 0.48              |
| 3:JY:1792:ASN:O    | 3:JY:1797:ARG:NH1  | 2.46                     | 0.48              |
| 3:AY:1713:ILE:HD11 | 3:BY:1880:LEU:HD23 | 1.96                     | 0.48              |
| 3:CY:1873:GLU:HG2  | 3:DY:1781:LEU:HD22 | 1.95                     | 0.48              |
| 3:GY:1698:ILE:HG23 | 3:GY:1722:VAL:HG21 | 1.95                     | 0.48              |
| 3:HY:1713:ILE:HD11 | 3:IY:1880:LEU:HD23 | 1.96                     | 0.48              |
| 2:IX:399:ARG:NH1   | 2:IX:495:ASN:OD1   | 2.46                     | 0.48              |
| 2:JX:400:ASN:HB3   | 2:JX:421:ASP:OD1   | 2.13                     | 0.48              |
| 3:MY:1792:ASN:O    | 3:MY:1797:ARG:NH1  | 2.46                     | 0.48              |
| 3:BY:1699:GLU:HG2  | 3:BY:1719:ALA:HB3  | 1.95                     | 0.48              |
| 2:CX:364:ASN:HA    | 2:CX:367:LYS:HG2   | 1.96                     | 0.48              |
| 3:DY:1698:ILE:HG23 | 3:DY:1722:VAL:HG21 | 1.95                     | 0.48              |
| 3:GY:1792:ASN:O    | 3:GY:1797:ARG:NH1  | 2.46                     | 0.48              |
| 2:MX:364:ASN:HA    | 2:MX:367:LYS:HG2   | 1.96                     | 0.48              |
| 3:NY:1792:ASN:O    | 3:NY:1797:ARG:NH1  | 2.46                     | 0.48              |
| 3:AY:1763:ILE:HG12 | 3:AY:1769:ILE:HG22 | 1.94                     | 0.48              |
| 3:KY:1699:GLU:HG2  | 3:KY:1719:ALA:HB3  | 1.95                     | 0.48              |
| 3:LY:1792:ASN:O    | 3:LY:1797:ARG:NH1  | 2.46                     | 0.48              |
| 3:DY:1792:ASN:O    | 3:DY:1797:ARG:NH1  | 2.46                     | 0.47              |
| 3:EY:1873:GLU:HG2  | 3:FY:1781:LEU:HD22 | 1.96                     | 0.47              |
| 1:LT:28:VAL:HG23   | 1:LT:29:VAL:H      | 1.78                     | 0.47              |
| 3:LY:1707:ASP:HB2  | 3:MY:1783:GLU:HB2  | 1.96                     | 0.47              |
| 3:AY:1781:LEU:HD22 | 3:NY:1873:GLU:HG2  | 1.95                     | 0.47              |
| 3:AY:1792:ASN:O    | 3:AY:1797:ARG:NH1  | 2.46                     | 0.47              |
| 3:KY:1792:ASN:O    | 3:KY:1797:ARG:NH1  | 2.46                     | 0.47              |
| 2:BX:364:ASN:HA    | 2:BX:367:LYS:HG2   | 1.96                     | 0.47              |
| 3:BY:1698:ILE:HG23 | 3:BY:1722:VAL:HG21 | 1.95                     | 0.47              |
| 1:DT:28:VAL:HG23   | 1:DT:29:VAL:H      | 1.78                     | 0.47              |
| 3:DY:1763:ILE:HG12 | 3:DY:1769:ILE:HG22 | 1.94                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:HT:28:VAL:HG23   | 1:HT:29:VAL:H      | 1.78                     | 0.47              |
| 2:IX:364:ASN:HA    | 2:IX:367:LYS:HG2   | 1.96                     | 0.47              |
| 3:IY:1698:ILE:HG23 | 3:IY:1722:VAL:HG21 | 1.95                     | 0.47              |
| 3:LY:1698:ILE:HG23 | 3:LY:1722:VAL:HG21 | 1.95                     | 0.47              |
| 1:NT:52:LEU:HD12   | 1:NT:89:HIS:CD2    | 2.49                     | 0.47              |
| 3:NY:1698:ILE:HG23 | 3:NY:1722:VAL:HG21 | 1.95                     | 0.47              |
| 1:AT:99:ALA:HB2    | 1:AT:124:PRO:HB3   | 1.95                     | 0.47              |
| 3:AY:1699:GLU:HG2  | 3:AY:1719:ALA:HB3  | 1.95                     | 0.47              |
| 1:BT:48:SER:OG     | 1:CT:170:GLY:O     | 2.22                     | 0.47              |
| 3:BY:1873:GLU:HG2  | 3:CY:1781:LEU:HD22 | 1.95                     | 0.47              |
| 1:CT:99:ALA:HB2    | 1:CT:124:PRO:HB3   | 1.95                     | 0.47              |
| 1:IT:306:LEU:HD22  | 2:IX:384:GLU:HB2   | 1.97                     | 0.47              |
| 3:IY:1792:ASN:O    | 3:IY:1797:ARG:NH1  | 2.46                     | 0.47              |
| 3:LY:1699:GLU:HG2  | 3:LY:1719:ALA:HB3  | 1.95                     | 0.47              |
| 1:MT:52:LEU:HD12   | 1:MT:89:HIS:CD2    | 2.49                     | 0.47              |
| 3:AY:1783:GLU:HB2  | 3:NY:1707:ASP:HB2  | 1.96                     | 0.47              |
| 1:CT:52:LEU:HD12   | 1:CT:89:HIS:CD2    | 2.49                     | 0.47              |
| 2:GX:364:ASN:HA    | 2:GX:367:LYS:HG2   | 1.96                     | 0.47              |
| 3:GY:1713:ILE:HD11 | 3:HY:1880:LEU:HD23 | 1.97                     | 0.47              |
| 3:JY:1873:GLU:HG2  | 3:KY:1781:LEU:HD22 | 1.96                     | 0.47              |
| 1:LT:33:ASN:ND2    | 2:MX:407:PRO:O     | 2.47                     | 0.47              |
| 1:AT:52:LEU:HD12   | 1:AT:89:HIS:CD2    | 2.49                     | 0.47              |
| 3:BY:1713:ILE:HD11 | 3:CY:1880:LEU:HD23 | 1.97                     | 0.47              |
| 3:BY:1792:ASN:O    | 3:BY:1797:ARG:NH1  | 2.46                     | 0.47              |
| 1:DT:52:LEU:HD12   | 1:DT:89:HIS:CD2    | 2.49                     | 0.47              |
| 2:EX:364:ASN:HA    | 2:EX:367:LYS:HG2   | 1.96                     | 0.47              |
| 1:LT:52:LEU:HD12   | 1:LT:89:HIS:CD2    | 2.49                     | 0.47              |
| 1:BT:52:LEU:HD12   | 1:BT:89:HIS:CD2    | 2.49                     | 0.47              |
| 1:BT:99:ALA:HB2    | 1:BT:124:PRO:HB3   | 1.95                     | 0.47              |
| 1:ET:52:LEU:HD12   | 1:ET:89:HIS:CD2    | 2.49                     | 0.47              |
| 1:FT:199:TYR:HB3   | 2:FX:379:GLN:OE1   | 2.15                     | 0.47              |
| 3:FY:1873:GLU:HG2  | 3:GY:1781:LEU:HD22 | 1.96                     | 0.47              |
| 1:GT:99:ALA:HB2    | 1:GT:124:PRO:HB3   | 1.95                     | 0.47              |
| 1:IT:52:LEU:HD12   | 1:IT:89:HIS:CD2    | 2.49                     | 0.47              |
| 1:IT:99:ALA:HB2    | 1:IT:124:PRO:HB3   | 1.95                     | 0.47              |
| 1:KT:52:LEU:HD12   | 1:KT:89:HIS:CD2    | 2.50                     | 0.47              |
| 3:MY:1699:GLU:HG2  | 3:MY:1719:ALA:HB3  | 1.95                     | 0.47              |
| 1:NT:99:ALA:HB2    | 1:NT:124:PRO:HB3   | 1.95                     | 0.47              |
| 3:NY:1699:GLU:HG2  | 3:NY:1719:ALA:HB3  | 1.95                     | 0.47              |
| 1:DT:99:ALA:HB2    | 1:DT:124:PRO:HB3   | 1.95                     | 0.47              |
| 1:FT:52:LEU:HD12   | 1:FT:89:HIS:CD2    | 2.49                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:FT:60:PRO:HA     | 1:FT:137:ASN:O     | 2.15                     | 0.47              |
| 1:GT:60:PRO:HA     | 1:GT:137:ASN:O     | 2.15                     | 0.47              |
| 1:HT:52:LEU:HD12   | 1:HT:89:HIS:CD2    | 2.49                     | 0.47              |
| 1:IT:60:PRO:HA     | 1:IT:137:ASN:O     | 2.15                     | 0.47              |
| 1:JT:52:LEU:HD12   | 1:JT:89:HIS:CD2    | 2.49                     | 0.47              |
| 1:KT:99:ALA:HB2    | 1:KT:124:PRO:HB3   | 1.95                     | 0.47              |
| 2:BX:480:LYS:NZ    | 3:BY:1699:GLU:OE2  | 2.38                     | 0.47              |
| 3:DY:1713:ILE:HD11 | 3:EY:1880:LEU:HD23 | 1.96                     | 0.47              |
| 1:ET:60:PRO:HA     | 1:ET:137:ASN:O     | 2.15                     | 0.47              |
| 1:ET:99:ALA:HB2    | 1:ET:124:PRO:HB3   | 1.95                     | 0.47              |
| 2:GX:477:LYS:HD3   | 2:GX:484:LEU:HD11  | 1.96                     | 0.47              |
| 1:HT:60:PRO:HA     | 1:HT:137:ASN:O     | 2.15                     | 0.47              |
| 3:HY:1792:ASN:O    | 3:HY:1797:ARG:NH1  | 2.46                     | 0.47              |
| 1:MT:99:ALA:HB2    | 1:MT:124:PRO:HB3   | 1.95                     | 0.47              |
| 3:MY:1873:GLU:HG2  | 3:NY:1781:LEU:HD22 | 1.97                     | 0.47              |
| 3:CY:1713:ILE:HD11 | 3:DY:1880:LEU:HD23 | 1.97                     | 0.47              |
| 3:CY:1792:ASN:O    | 3:CY:1797:ARG:NH1  | 2.46                     | 0.47              |
| 1:DT:60:PRO:HA     | 1:DT:137:ASN:O     | 2.15                     | 0.47              |
| 2:EX:507:GLY:HA2   | 1:FT:168:LEU:HD11  | 1.97                     | 0.47              |
| 1:GT:52:LEU:HD12   | 1:GT:89:HIS:CD2    | 2.49                     | 0.47              |
| 2:HX:477:LYS:HD3   | 2:HX:484:LEU:HD11  | 1.96                     | 0.47              |
| 1:JT:60:PRO:HA     | 1:JT:137:ASN:O     | 2.15                     | 0.47              |
| 3:JY:1707:ASP:HB2  | 3:KY:1783:GLU:HB2  | 1.96                     | 0.47              |
| 2:KX:364:ASN:HA    | 2:KX:367:LYS:HG2   | 1.96                     | 0.47              |
| 2:NX:364:ASN:HA    | 2:NX:367:LYS:HG2   | 1.96                     | 0.47              |
| 1:CT:60:PRO:HA     | 1:CT:137:ASN:O     | 2.15                     | 0.46              |
| 3:GY:1707:ASP:HB2  | 3:HY:1783:GLU:HB2  | 1.96                     | 0.46              |
| 2:IX:477:LYS:HD3   | 2:IX:484:LEU:HD11  | 1.96                     | 0.46              |
| 1:LT:60:PRO:HA     | 1:LT:137:ASN:O     | 2.15                     | 0.46              |
| 1:GT:291:GLU:O     | 1:GT:295:ASN:HB2   | 2.16                     | 0.46              |
| 2:JX:477:LYS:HD3   | 2:JX:484:LEU:HD11  | 1.96                     | 0.46              |
| 3:MY:1707:ASP:HB2  | 3:NY:1783:GLU:HB2  | 1.97                     | 0.46              |
| 2:FX:417:SER:N     | 2:FX:429:GLY:O     | 2.44                     | 0.46              |
| 2:FX:477:LYS:HD3   | 2:FX:484:LEU:HD11  | 1.96                     | 0.46              |
| 3:FY:1713:ILE:HD11 | 3:GY:1880:LEU:HD23 | 1.97                     | 0.46              |
| 3:IY:1713:ILE:HD11 | 3:JY:1880:LEU:HD23 | 1.97                     | 0.46              |
| 1:KT:291:GLU:O     | 1:KT:295:ASN:HB2   | 2.16                     | 0.46              |
| 1:LT:291:GLU:O     | 1:LT:295:ASN:HB2   | 2.16                     | 0.46              |
| 1:AT:60:PRO:HA     | 1:AT:137:ASN:O     | 2.15                     | 0.46              |
| 1:CT:111:ALA:O     | 1:DT:167:ASN:ND2   | 2.49                     | 0.46              |
| 3:CY:1707:ASP:HB2  | 3:DY:1783:GLU:HB2  | 1.96                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:EX:477:LYS:HD3   | 2:EX:484:LEU:HD11  | 1.96                     | 0.46              |
| 1:FT:291:GLU:O     | 1:FT:295:ASN:HB2   | 2.16                     | 0.46              |
| 3:GY:1873:GLU:HG2  | 3:HY:1781:LEU:HD22 | 1.96                     | 0.46              |
| 1:HT:199:TYR:HB3   | 2:HX:379:GLN:OE1   | 2.16                     | 0.46              |
| 1:KT:60:PRO:HA     | 1:KT:137:ASN:O     | 2.15                     | 0.46              |
| 2:KX:477:LYS:HD3   | 2:KX:484:LEU:HD11  | 1.96                     | 0.46              |
| 1:BT:39:VAL:HG21   | 2:CX:419:ILE:HD12  | 1.97                     | 0.46              |
| 1:ET:291:GLU:O     | 1:ET:295:ASN:HB2   | 2.16                     | 0.46              |
| 2:MX:477:LYS:HD3   | 2:MX:484:LEU:HD11  | 1.96                     | 0.46              |
| 2:NX:477:LYS:HD3   | 2:NX:484:LEU:HD11  | 1.96                     | 0.46              |
| 1:HT:291:GLU:O     | 1:HT:295:ASN:HB2   | 2.16                     | 0.46              |
| 1:KT:51:PRO:HD3    | 2:KX:495:ASN:HB2   | 1.97                     | 0.46              |
| 1:KT:200:LYS:HD3   | 1:KT:200:LYS:HA    | 1.76                     | 0.46              |
| 2:LX:477:LYS:HD3   | 2:LX:484:LEU:HD11  | 1.96                     | 0.46              |
| 2:BX:455:ILE:HB    | 3:BY:1765:PRO:HB3  | 1.98                     | 0.46              |
| 3:FY:1707:ASP:HB2  | 3:GY:1783:GLU:HB2  | 1.97                     | 0.46              |
| 3:KY:1707:ASP:HB2  | 3:LY:1783:GLU:HB2  | 1.98                     | 0.46              |
| 3:KY:1873:GLU:HG2  | 3:LY:1781:LEU:HD22 | 1.98                     | 0.46              |
| 1:MT:291:GLU:O     | 1:MT:295:ASN:HB2   | 2.16                     | 0.46              |
| 2:MX:392:LEU:HD22  | 3:NY:1728:THR:HB   | 1.98                     | 0.46              |
| 2:AX:392:LEU:HD22  | 3:BY:1728:THR:HB   | 1.98                     | 0.46              |
| 1:BT:60:PRO:HA     | 1:BT:137:ASN:O     | 2.15                     | 0.46              |
| 2:DX:477:LYS:HD3   | 2:DX:484:LEU:HD11  | 1.96                     | 0.46              |
| 3:DY:1873:GLU:HG2  | 3:EY:1781:LEU:HD22 | 1.98                     | 0.46              |
| 1:MT:60:PRO:HA     | 1:MT:137:ASN:O     | 2.15                     | 0.46              |
| 2:AX:477:LYS:HD3   | 2:AX:484:LEU:HD11  | 1.96                     | 0.46              |
| 2:CX:436:GLN:HB2   | 3:CY:1734:LYS:HG2  | 1.98                     | 0.46              |
| 2:CX:477:LYS:HD3   | 2:CX:484:LEU:HD11  | 1.96                     | 0.46              |
| 1:DT:291:GLU:O     | 1:DT:295:ASN:HB2   | 2.16                     | 0.46              |
| 3:IY:1707:ASP:HB2  | 3:JY:1783:GLU:HB2  | 1.97                     | 0.46              |
| 3:JY:1713:ILE:HD11 | 3:KY:1880:LEU:HD23 | 1.97                     | 0.46              |
| 2:BX:477:LYS:HD3   | 2:BX:484:LEU:HD11  | 1.96                     | 0.46              |
| 3:KY:1713:ILE:HD11 | 3:LY:1880:LEU:HD23 | 1.97                     | 0.46              |
| 1:JT:291:GLU:O     | 1:JT:295:ASN:HB2   | 2.16                     | 0.45              |
| 1:NT:60:PRO:HA     | 1:NT:137:ASN:O     | 2.15                     | 0.45              |
| 3:AY:1880:LEU:HD23 | 3:NY:1713:ILE:HD11 | 1.98                     | 0.45              |
| 1:CT:291:GLU:O     | 1:CT:295:ASN:HB2   | 2.16                     | 0.45              |
| 3:MY:1713:ILE:HD11 | 3:NY:1880:LEU:HD23 | 1.97                     | 0.45              |
| 3:AY:1707:ASP:HB2  | 3:BY:1783:GLU:HB2  | 1.98                     | 0.45              |
| 3:DY:1707:ASP:HB2  | 3:EY:1783:GLU:HB2  | 1.98                     | 0.45              |
| 1:NT:200:LYS:HA    | 1:NT:200:LYS:HD3   | 1.76                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:BY:1707:ASP:HB2  | 3:CY:1783:GLU:HB2  | 1.97                     | 0.45              |
| 3:EY:1707:ASP:HB2  | 3:FY:1783:GLU:HB2  | 1.96                     | 0.45              |
| 3:EY:1713:ILE:HD11 | 3:FY:1880:LEU:HD23 | 1.98                     | 0.45              |
| 1:NT:291:GLU:O     | 1:NT:295:ASN:HB2   | 2.16                     | 0.45              |
| 1:BT:291:GLU:O     | 1:BT:295:ASN:HB2   | 2.16                     | 0.45              |
| 2:HX:392:LEU:HD22  | 3:IY:1728:THR:HB   | 1.97                     | 0.45              |
| 1:IT:291:GLU:O     | 1:IT:295:ASN:HB2   | 2.16                     | 0.45              |
| 1:LT:200:LYS:HD3   | 1:LT:200:LYS:HA    | 1.76                     | 0.45              |
| 2:AX:432:ASN:ND2   | 2:NX:497:LEU:O     | 2.38                     | 0.45              |
| 3:AY:1873:GLU:HG2  | 3:BY:1781:LEU:HD22 | 1.98                     | 0.45              |
| 1:CT:38:PRO:HG2    | 1:DT:55:LYS:HB2    | 1.97                     | 0.45              |
| 3:FY:1690:PHE:O    | 3:FY:1887:PHE:N    | 2.45                     | 0.45              |
| 3:HY:1873:GLU:HG2  | 3:IY:1781:LEU:HD22 | 1.97                     | 0.45              |
| 2:JX:481:ASP:HB3   | 3:JY:1875:ASP:HA   | 1.98                     | 0.45              |
| 1:CT:51:PRO:HD3    | 2:CX:495:ASN:HB2   | 1.99                     | 0.45              |
| 3:EY:1900:VAL:HA   | 3:EY:1903:GLU:HG3  | 1.99                     | 0.45              |
| 1:AT:291:GLU:O     | 1:AT:295:ASN:HB2   | 2.16                     | 0.45              |
| 3:AY:1900:VAL:HA   | 3:AY:1903:GLU:HG3  | 1.99                     | 0.45              |
| 1:GT:111:ALA:O     | 1:HT:167:ASN:ND2   | 2.50                     | 0.45              |
| 1:JT:36:TYR:HB3    | 2:KX:404:TYR:HB3   | 1.98                     | 0.45              |
| 3:FY:1900:VAL:HA   | 3:FY:1903:GLU:HG3  | 1.99                     | 0.45              |
| 2:LX:392:LEU:HD22  | 3:MY:1728:THR:HB   | 1.99                     | 0.45              |
| 3:NY:1690:PHE:O    | 3:NY:1887:PHE:N    | 2.45                     | 0.45              |
| 3:NY:1900:VAL:HA   | 3:NY:1903:GLU:HG3  | 1.99                     | 0.45              |
| 1:AT:200:LYS:HD3   | 1:AT:200:LYS:HA    | 1.76                     | 0.45              |
| 2:BX:392:LEU:HD22  | 3:CY:1728:THR:HB   | 1.99                     | 0.44              |
| 2:KX:417:SER:N     | 2:KX:429:GLY:O     | 2.44                     | 0.44              |
| 2:LX:497:LEU:O     | 2:MX:432:ASN:ND2   | 2.40                     | 0.44              |
| 3:LY:1713:ILE:HD11 | 3:MY:1880:LEU:HD23 | 1.98                     | 0.44              |
| 3:AY:1690:PHE:O    | 3:AY:1887:PHE:N    | 2.45                     | 0.44              |
| 3:DY:1900:VAL:HA   | 3:DY:1903:GLU:HG3  | 1.99                     | 0.44              |
| 3:HY:1707:ASP:HB2  | 3:IY:1783:GLU:HB2  | 1.98                     | 0.44              |
| 3:MY:1900:VAL:HA   | 3:MY:1903:GLU:HG3  | 1.99                     | 0.44              |
| 1:AT:75:LEU:HD23   | 1:AT:75:LEU:HA     | 1.86                     | 0.44              |
| 3:AY:1728:THR:HB   | 2:NX:392:LEU:HD22  | 1.99                     | 0.44              |
| 2:EX:497:LEU:O     | 2:FX:432:ASN:ND2   | 2.41                     | 0.44              |
| 3:KY:1732:LEU:HA   | 3:KY:1732:LEU:HD23 | 1.84                     | 0.44              |
| 2:NX:480:LYS:NZ    | 3:NY:1699:GLU:OE2  | 2.48                     | 0.44              |
| 2:AX:507:GLY:HA2   | 1:BT:168:LEU:HD11  | 1.99                     | 0.44              |
| 1:FT:33:ASN:ND2    | 2:GX:407:PRO:O     | 2.50                     | 0.44              |
| 2:FX:392:LEU:HD22  | 3:GY:1728:THR:HB   | 1.98                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LT:196:ASN:OD1   | 3:MY:1907:GLN:NE2  | 2.50                     | 0.44              |
| 1:MT:55:LYS:O      | 1:MT:59:THR:OG1    | 2.31                     | 0.44              |
| 1:MT:75:LEU:HA     | 1:MT:75:LEU:HD23   | 1.86                     | 0.44              |
| 3:LY:1900:VAL:HA   | 3:LY:1903:GLU:HG3  | 1.99                     | 0.44              |
| 3:BY:1900:VAL:HA   | 3:BY:1903:GLU:HG3  | 1.99                     | 0.44              |
| 2:GX:417:SER:N     | 2:GX:429:GLY:O     | 2.45                     | 0.44              |
| 1:HT:213:ARG:HH12  | 2:HX:364:ASN:HB3   | 1.83                     | 0.44              |
| 2:JX:436:GLN:HB2   | 3:JY:1734:LYS:HG2  | 1.99                     | 0.44              |
| 2:CX:455:ILE:HB    | 3:CY:1765:PRO:HB3  | 1.99                     | 0.44              |
| 3:GY:1900:VAL:HA   | 3:GY:1903:GLU:HG3  | 1.99                     | 0.44              |
| 1:AT:33:ASN:HD22   | 2:BX:406:ALA:HB1   | 1.83                     | 0.44              |
| 2:EX:481:ASP:OD1   | 2:EX:481:ASP:N     | 2.50                     | 0.44              |
| 1:MT:200:LYS:HD3   | 1:MT:200:LYS:HA    | 1.76                     | 0.44              |
| 3:MY:1690:PHE:O    | 3:MY:1887:PHE:N    | 2.45                     | 0.44              |
| 3:AY:1729:MET:HB3  | 2:NX:503:ILE:HG13  | 2.00                     | 0.44              |
| 1:FT:75:LEU:HD23   | 1:FT:75:LEU:HA     | 1.86                     | 0.44              |
| 1:JT:38:PRO:HG2    | 1:KT:55:LYS:HB2    | 2.00                     | 0.44              |
| 3:JY:1900:VAL:HA   | 3:JY:1903:GLU:HG3  | 1.99                     | 0.44              |
| 3:KY:1900:VAL:HA   | 3:KY:1903:GLU:HG3  | 1.99                     | 0.44              |
| 3:IY:1900:VAL:HA   | 3:IY:1903:GLU:HG3  | 1.99                     | 0.43              |
| 1:NT:75:LEU:HD23   | 1:NT:75:LEU:HA     | 1.86                     | 0.43              |
| 3:CY:1900:VAL:HA   | 3:CY:1903:GLU:HG3  | 1.99                     | 0.43              |
| 2:DX:503:ILE:HG13  | 3:EY:1729:MET:HB3  | 2.01                     | 0.43              |
| 1:FT:200:LYS:HA    | 1:FT:200:LYS:HD3   | 1.76                     | 0.43              |
| 2:GX:392:LEU:HD22  | 3:HY:1728:THR:HB   | 1.99                     | 0.43              |
| 2:DX:455:ILE:HB    | 3:DY:1765:PRO:HB3  | 2.00                     | 0.43              |
| 1:ET:200:LYS:HA    | 1:ET:200:LYS:HD3   | 1.76                     | 0.43              |
| 3:EY:1690:PHE:O    | 3:EY:1887:PHE:N    | 2.45                     | 0.43              |
| 2:FX:507:GLY:HA2   | 1:GT:168:LEU:HD11  | 2.00                     | 0.43              |
| 3:HY:1900:VAL:HA   | 3:HY:1903:GLU:HG3  | 1.99                     | 0.43              |
| 1:JT:111:ALA:O     | 1:KT:167:ASN:ND2   | 2.52                     | 0.43              |
| 3:JY:1732:LEU:HA   | 3:JY:1732:LEU:HD23 | 1.84                     | 0.43              |
| 1:LT:38:PRO:HA     | 2:MX:404:TYR:HA    | 2.00                     | 0.43              |
| 3:DY:1690:PHE:O    | 3:DY:1887:PHE:N    | 2.45                     | 0.43              |
| 3:GY:1708:ALA:HB3  | 3:GY:1869:PHE:HB3  | 2.01                     | 0.43              |
| 1:JT:199:TYR:HB3   | 2:JX:379:GLN:OE1   | 2.19                     | 0.43              |
| 3:MY:1708:ALA:HB3  | 3:MY:1869:PHE:HB3  | 2.01                     | 0.43              |
| 2:DX:503:ILE:HA    | 3:EY:1729:MET:HA   | 2.00                     | 0.43              |
| 1:FT:54:ASP:OD2    | 2:FX:404:TYR:OH    | 2.26                     | 0.43              |
| 1:FT:196:ASN:OD1   | 3:GY:1907:GLN:NE2  | 2.52                     | 0.43              |
| 3:FY:1732:LEU:HD23 | 3:FY:1732:LEU:HA   | 1.84                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:GT:200:LYS:HA   | 1:GT:200:LYS:HD3   | 1.76                     | 0.43              |
| 2:KX:481:ASP:HB3  | 3:KY:1875:ASP:HA   | 2.01                     | 0.43              |
| 3:MY:1906:LYS:HA  | 3:MY:1909:THR:HG22 | 2.01                     | 0.43              |
| 3:AY:1729:MET:HA  | 2:NX:503:ILE:HA    | 2.00                     | 0.43              |
| 3:AY:1906:LYS:HA  | 3:AY:1909:THR:HG22 | 2.01                     | 0.43              |
| 3:BY:1708:ALA:HB3 | 3:BY:1869:PHE:HB3  | 2.01                     | 0.43              |
| 3:DY:1708:ALA:HB3 | 3:DY:1869:PHE:HB3  | 2.01                     | 0.43              |
| 3:KY:1708:ALA:HB3 | 3:KY:1869:PHE:HB3  | 2.01                     | 0.43              |
| 3:KY:1906:LYS:HA  | 3:KY:1909:THR:HG22 | 2.01                     | 0.43              |
| 2:AX:394:ARG:HE   | 2:AX:394:ARG:HB3   | 1.67                     | 0.43              |
| 3:BY:1690:PHE:O   | 3:BY:1887:PHE:N    | 2.45                     | 0.43              |
| 3:CY:1690:PHE:O   | 3:CY:1887:PHE:N    | 2.45                     | 0.43              |
| 3:CY:1906:LYS:HA  | 3:CY:1909:THR:HG22 | 2.01                     | 0.43              |
| 2:DX:497:LEU:O    | 2:EX:432:ASN:ND2   | 2.39                     | 0.43              |
| 2:FX:481:ASP:OD1  | 2:FX:481:ASP:N     | 2.50                     | 0.43              |
| 1:GT:196:ASN:OD1  | 3:HY:1907:GLN:NE2  | 2.51                     | 0.43              |
| 2:GX:497:LEU:O    | 2:HX:432:ASN:ND2   | 2.39                     | 0.43              |
| 2:GX:507:GLY:HA2  | 1:HT:168:LEU:HD11  | 2.01                     | 0.43              |
| 1:HT:200:LYS:HA   | 1:HT:200:LYS:HD3   | 1.76                     | 0.43              |
| 3:IY:1708:ALA:HB3 | 3:IY:1869:PHE:HB3  | 2.01                     | 0.43              |
| 3:AY:1708:ALA:HB3 | 3:AY:1869:PHE:HB3  | 2.01                     | 0.43              |
| 1:BT:306:LEU:HD22 | 2:BX:384:GLU:HB2   | 2.00                     | 0.43              |
| 3:EY:1708:ALA:HB3 | 3:EY:1869:PHE:HB3  | 2.01                     | 0.43              |
| 1:HT:48:SER:OG    | 1:IT:170:GLY:O     | 2.34                     | 0.43              |
| 2:HX:507:GLY:HA2  | 1:IT:168:LEU:HD11  | 2.01                     | 0.43              |
| 2:LX:417:SER:N    | 2:LX:429:GLY:O     | 2.44                     | 0.43              |
| 1:BT:200:LYS:HA   | 1:BT:200:LYS:HD3   | 1.76                     | 0.43              |
| 1:DT:200:LYS:HA   | 1:DT:200:LYS:HD3   | 1.76                     | 0.43              |
| 2:DX:392:LEU:HD22 | 3:EY:1728:THR:HB   | 1.99                     | 0.43              |
| 1:ET:51:PRO:HD3   | 2:EX:495:ASN:HB2   | 2.01                     | 0.43              |
| 3:GY:1732:LEU:HA  | 3:GY:1732:LEU:HD23 | 1.84                     | 0.43              |
| 2:IX:480:LYS:NZ   | 3:IY:1699:GLU:OE2  | 2.41                     | 0.43              |
| 3:NY:1906:LYS:HA  | 3:NY:1909:THR:HG22 | 2.01                     | 0.43              |
| 3:BY:1906:LYS:HA  | 3:BY:1909:THR:HG22 | 2.01                     | 0.42              |
| 1:CT:39:VAL:HG11  | 2:DX:419:ILE:HG13  | 2.00                     | 0.42              |
| 3:EY:1906:LYS:HA  | 3:EY:1909:THR:HG22 | 2.01                     | 0.42              |
| 3:HY:1906:LYS:HA  | 3:HY:1909:THR:HG22 | 2.01                     | 0.42              |
| 3:IY:1732:LEU:HA  | 3:IY:1732:LEU:HD23 | 1.84                     | 0.42              |
| 2:JX:455:ILE:HB   | 3:JY:1765:PRO:HB3  | 2.00                     | 0.42              |
| 3:JY:1906:LYS:HA  | 3:JY:1909:THR:HG22 | 2.01                     | 0.42              |
| 3:LY:1906:LYS:HA  | 3:LY:1909:THR:HG22 | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:MX:503:ILE:HA    | 3:NY:1729:MET:HA   | 2.01                     | 0.42              |
| 3:FY:1720:LYS:HA   | 3:FY:1734:LYS:HE2  | 2.01                     | 0.42              |
| 3:HY:1732:LEU:HA   | 3:HY:1732:LEU:HD23 | 1.84                     | 0.42              |
| 3:NY:1708:ALA:HB3  | 3:NY:1869:PHE:HB3  | 2.01                     | 0.42              |
| 2:AX:436:GLN:HB2   | 3:AY:1734:LYS:HG2  | 2.01                     | 0.42              |
| 3:EY:1720:LYS:HA   | 3:EY:1734:LYS:HE2  | 2.01                     | 0.42              |
| 2:FX:503:ILE:HA    | 3:GY:1729:MET:HA   | 2.01                     | 0.42              |
| 3:FY:1708:ALA:HB3  | 3:FY:1869:PHE:HB3  | 2.01                     | 0.42              |
| 3:GY:1720:LYS:HA   | 3:GY:1734:LYS:HE2  | 2.01                     | 0.42              |
| 2:LX:507:GLY:HA2   | 1:MT:168:LEU:HD11  | 2.00                     | 0.42              |
| 3:DY:1720:LYS:HA   | 3:DY:1734:LYS:HE2  | 2.00                     | 0.42              |
| 2:EX:392:LEU:HD22  | 3:FY:1728:THR:HB   | 1.99                     | 0.42              |
| 3:GY:1903:GLU:HA   | 3:GY:1906:LYS:HG3  | 2.02                     | 0.42              |
| 3:HY:1720:LYS:HA   | 3:HY:1734:LYS:HE2  | 2.00                     | 0.42              |
| 2:JX:392:LEU:HD22  | 3:KY:1728:THR:HB   | 2.01                     | 0.42              |
| 1:KT:81:VAL:HG21   | 2:KX:459:MET:HE3   | 2.01                     | 0.42              |
| 2:LX:394:ARG:HE    | 2:LX:394:ARG:HB3   | 1.68                     | 0.42              |
| 2:MX:497:LEU:O     | 2:NX:432:ASN:ND2   | 2.40                     | 0.42              |
| 2:NX:440:PHE:CZ    | 3:NY:1873:GLU:HB3  | 2.55                     | 0.42              |
| 3:NY:1786:VAL:HG22 | 3:NY:1871:LYS:HE2  | 2.01                     | 0.42              |
| 3:IY:1903:GLU:HA   | 3:IY:1906:LYS:HG3  | 2.02                     | 0.42              |
| 3:KY:1786:VAL:HG22 | 3:KY:1871:LYS:HE2  | 2.01                     | 0.42              |
| 3:KY:1903:GLU:HA   | 3:KY:1906:LYS:HG3  | 2.02                     | 0.42              |
| 3:MY:1786:VAL:HG22 | 3:MY:1871:LYS:HE2  | 2.01                     | 0.42              |
| 1:NT:54:ASP:OD2    | 2:NX:404:TYR:OH    | 2.32                     | 0.42              |
| 2:BX:503:ILE:HG13  | 3:CY:1729:MET:HB3  | 2.02                     | 0.42              |
| 2:DX:436:GLN:HB2   | 3:DY:1734:LYS:HG2  | 2.01                     | 0.42              |
| 2:DX:507:GLY:HA2   | 1:ET:168:LEU:HD11  | 2.02                     | 0.42              |
| 2:EX:436:GLN:HB2   | 3:EY:1734:LYS:HG2  | 2.02                     | 0.42              |
| 3:EY:1903:GLU:HA   | 3:EY:1906:LYS:HG3  | 2.02                     | 0.42              |
| 2:FX:503:ILE:HG13  | 3:GY:1729:MET:HB3  | 2.02                     | 0.42              |
| 3:JY:1689:THR:O    | 3:JY:1724:ASN:ND2  | 2.34                     | 0.42              |
| 3:MY:1720:LYS:HA   | 3:MY:1734:LYS:HE2  | 2.00                     | 0.42              |
| 3:NY:1720:LYS:HA   | 3:NY:1734:LYS:HE2  | 2.00                     | 0.42              |
| 2:CX:440:PHE:CZ    | 3:CY:1873:GLU:HB3  | 2.54                     | 0.42              |
| 2:EX:503:ILE:HG13  | 3:FY:1729:MET:HB3  | 2.02                     | 0.42              |
| 2:GX:440:PHE:CZ    | 3:GY:1873:GLU:HB3  | 2.55                     | 0.42              |
| 3:IY:1720:LYS:HA   | 3:IY:1734:LYS:HE2  | 2.00                     | 0.42              |
| 1:JT:48:SER:OG     | 1:KT:170:GLY:O     | 2.28                     | 0.42              |
| 3:LY:1786:VAL:HG22 | 3:LY:1871:LYS:HE2  | 2.01                     | 0.42              |
| 2:AX:455:ILE:HB    | 3:AY:1765:PRO:HB3  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:IT:200:LYS:HA    | 1:IT:200:LYS:HD3   | 1.76                     | 0.42              |
| 2:IX:479:ILE:HG22  | 3:IY:1874:GLY:HA3  | 2.02                     | 0.42              |
| 3:AY:1720:LYS:HA   | 3:AY:1734:LYS:HE2  | 2.01                     | 0.42              |
| 3:CY:1720:LYS:HA   | 3:CY:1734:LYS:HE2  | 2.01                     | 0.42              |
| 2:DX:481:ASP:HB3   | 3:DY:1875:ASP:HA   | 2.01                     | 0.42              |
| 3:FY:1906:LYS:HA   | 3:FY:1909:THR:HG22 | 2.01                     | 0.42              |
| 2:GX:436:GLN:HB2   | 3:GY:1734:LYS:HG2  | 2.02                     | 0.42              |
| 1:JT:56:LEU:HD12   | 1:JT:59:THR:HB     | 2.02                     | 0.42              |
| 3:KY:1689:THR:O    | 3:KY:1724:ASN:ND2  | 2.34                     | 0.42              |
| 1:LT:199:TYR:HB3   | 2:LX:379:GLN:OE1   | 2.20                     | 0.42              |
| 3:LY:1708:ALA:HB3  | 3:LY:1869:PHE:HB3  | 2.01                     | 0.42              |
| 2:MX:503:ILE:HG13  | 3:NY:1729:MET:HB3  | 2.02                     | 0.42              |
| 2:AX:503:ILE:HA    | 3:BY:1729:MET:HA   | 2.01                     | 0.42              |
| 3:BY:1903:GLU:HA   | 3:BY:1906:LYS:HG3  | 2.01                     | 0.42              |
| 3:DY:1903:GLU:HA   | 3:DY:1906:LYS:HG3  | 2.02                     | 0.42              |
| 3:HY:1903:GLU:HA   | 3:HY:1906:LYS:HG3  | 2.02                     | 0.42              |
| 1:KT:75:LEU:HD23   | 1:KT:75:LEU:HA     | 1.86                     | 0.42              |
| 2:LX:503:ILE:HG13  | 3:MY:1729:MET:HB3  | 2.02                     | 0.42              |
| 3:LY:1720:LYS:HA   | 3:LY:1734:LYS:HE2  | 2.01                     | 0.42              |
| 3:MY:1903:GLU:HA   | 3:MY:1906:LYS:HG3  | 2.02                     | 0.42              |
| 3:AY:1786:VAL:HG22 | 3:AY:1871:LYS:HE2  | 2.01                     | 0.41              |
| 3:AY:1859:LEU:O    | 3:AY:1863:MET:HB3  | 2.20                     | 0.41              |
| 3:BY:1786:VAL:HG22 | 3:BY:1871:LYS:HE2  | 2.01                     | 0.41              |
| 1:CT:200:LYS:HA    | 1:CT:200:LYS:HD3   | 1.76                     | 0.41              |
| 2:CX:392:LEU:HD22  | 3:DY:1728:THR:HB   | 2.01                     | 0.41              |
| 2:CX:479:ILE:HG22  | 3:CY:1874:GLY:HA3  | 2.02                     | 0.41              |
| 2:GX:481:ASP:OD1   | 2:GX:481:ASP:N     | 2.50                     | 0.41              |
| 2:GX:503:ILE:HG13  | 3:HY:1729:MET:HB3  | 2.02                     | 0.41              |
| 3:HY:1708:ALA:HB3  | 3:HY:1869:PHE:HB3  | 2.01                     | 0.41              |
| 3:HY:1859:LEU:O    | 3:HY:1863:MET:HB3  | 2.20                     | 0.41              |
| 3:IY:1859:LEU:O    | 3:IY:1863:MET:HB3  | 2.20                     | 0.41              |
| 3:JY:1786:VAL:HG22 | 3:JY:1871:LYS:HE2  | 2.01                     | 0.41              |
| 3:JY:1903:GLU:HA   | 3:JY:1906:LYS:HG3  | 2.02                     | 0.41              |
| 2:KX:392:LEU:HD22  | 3:LY:1728:THR:HB   | 2.02                     | 0.41              |
| 2:LX:440:PHE:CZ    | 3:LY:1873:GLU:HB3  | 2.55                     | 0.41              |
| 2:LX:480:LYS:NZ    | 3:LY:1699:GLU:OE2  | 2.48                     | 0.41              |
| 3:MY:1898:LYS:HA   | 3:MY:1901:VAL:HG12 | 2.02                     | 0.41              |
| 3:NY:1859:LEU:O    | 3:NY:1863:MET:HB3  | 2.20                     | 0.41              |
| 3:AY:1732:LEU:HA   | 3:AY:1732:LEU:HD23 | 1.84                     | 0.41              |
| 2:BX:394:ARG:HE    | 2:BX:394:ARG:HB3   | 1.68                     | 0.41              |
| 3:CY:1708:ALA:HB3  | 3:CY:1869:PHE:HB3  | 2.01                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:FX:371:GLU:HA    | 2:FX:374:LYS:HG2   | 2.02                     | 0.41              |
| 3:FY:1903:GLU:HA   | 3:FY:1906:LYS:HG3  | 2.02                     | 0.41              |
| 3:IY:1890:VAL:HG12 | 3:JY:1683:ILE:HG13 | 2.02                     | 0.41              |
| 3:IY:1906:LYS:HA   | 3:IY:1909:THR:HG22 | 2.01                     | 0.41              |
| 3:JY:1720:LYS:HA   | 3:JY:1734:LYS:HE2  | 2.01                     | 0.41              |
| 1:KT:56:LEU:HD12   | 1:KT:59:THR:HB     | 2.02                     | 0.41              |
| 1:BT:51:PRO:HD3    | 2:BX:495:ASN:HB2   | 2.02                     | 0.41              |
| 3:BY:1720:LYS:HA   | 3:BY:1734:LYS:HE2  | 2.00                     | 0.41              |
| 2:CX:435:LEU:HD11  | 3:CY:1720:LYS:HE3  | 2.02                     | 0.41              |
| 3:EY:1859:LEU:O    | 3:EY:1863:MET:HB3  | 2.20                     | 0.41              |
| 2:FX:501:TYR:OH    | 1:GT:168:LEU:HB2   | 2.20                     | 0.41              |
| 1:GT:56:LEU:HD12   | 1:GT:59:THR:HB     | 2.02                     | 0.41              |
| 1:HT:56:LEU:HD12   | 1:HT:59:THR:HB     | 2.02                     | 0.41              |
| 2:HX:371:GLU:HA    | 2:HX:374:LYS:HG2   | 2.03                     | 0.41              |
| 1:IT:56:LEU:HD12   | 1:IT:59:THR:HB     | 2.02                     | 0.41              |
| 3:IY:1689:THR:O    | 3:IY:1724:ASN:ND2  | 2.34                     | 0.41              |
| 1:KT:48:SER:OG     | 1:LT:170:GLY:O     | 2.34                     | 0.41              |
| 2:MX:417:SER:N     | 2:MX:429:GLY:O     | 2.44                     | 0.41              |
| 3:NY:1797:ARG:HG3  | 3:NY:1865:ILE:HB   | 2.03                     | 0.41              |
| 1:BT:167:ASN:HB3   | 1:BT:173:VAL:HG11  | 2.03                     | 0.41              |
| 3:BY:1859:LEU:O    | 3:BY:1863:MET:HB3  | 2.20                     | 0.41              |
| 3:BY:1898:LYS:HA   | 3:BY:1901:VAL:HG12 | 2.02                     | 0.41              |
| 2:EX:503:ILE:HA    | 3:FY:1729:MET:HA   | 2.02                     | 0.41              |
| 1:FT:213:ARG:HH12  | 2:FX:364:ASN:HB3   | 1.86                     | 0.41              |
| 3:FY:1859:LEU:O    | 3:FY:1863:MET:HB3  | 2.20                     | 0.41              |
| 3:IY:1786:VAL:HG22 | 3:IY:1871:LYS:HE2  | 2.01                     | 0.41              |
| 3:JY:1708:ALA:HB3  | 3:JY:1869:PHE:HB3  | 2.01                     | 0.41              |
| 3:JY:1859:LEU:O    | 3:JY:1863:MET:HB3  | 2.20                     | 0.41              |
| 3:KY:1797:ARG:HG3  | 3:KY:1865:ILE:HB   | 2.03                     | 0.41              |
| 1:LT:48:SER:OG     | 1:MT:170:GLY:O     | 2.34                     | 0.41              |
| 1:MT:51:PRO:HD3    | 2:MX:495:ASN:HB2   | 2.03                     | 0.41              |
| 2:MX:507:GLY:HA2   | 1:NT:168:LEU:HD11  | 2.02                     | 0.41              |
| 1:CT:167:ASN:HB3   | 1:CT:173:VAL:HG11  | 2.03                     | 0.41              |
| 2:CX:450:MET:HE3   | 3:DY:1880:LEU:HD11 | 2.01                     | 0.41              |
| 1:DT:213:ARG:HH12  | 2:DX:364:ASN:HB3   | 1.85                     | 0.41              |
| 1:FT:56:LEU:HD12   | 1:FT:59:THR:HB     | 2.02                     | 0.41              |
| 2:GX:394:ARG:HE    | 2:GX:394:ARG:HB3   | 1.68                     | 0.41              |
| 3:GY:1906:LYS:HA   | 3:GY:1909:THR:HG22 | 2.01                     | 0.41              |
| 1:JT:298:LEU:HD13  | 2:JX:373:GLN:HE22  | 1.86                     | 0.41              |
| 3:JY:1797:ARG:HG3  | 3:JY:1865:ILE:HB   | 2.03                     | 0.41              |
| 3:KY:1720:LYS:HA   | 3:KY:1734:LYS:HE2  | 2.01                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:MY:1797:ARG:HG3  | 3:MY:1865:ILE:HB   | 2.03                     | 0.41              |
| 1:AT:167:ASN:HB3   | 1:AT:173:VAL:HG11  | 2.03                     | 0.41              |
| 3:CY:1797:ARG:HG3  | 3:CY:1865:ILE:HB   | 2.03                     | 0.41              |
| 2:HX:417:SER:N     | 2:HX:429:GLY:O     | 2.45                     | 0.41              |
| 3:KY:1898:LYS:HA   | 3:KY:1901:VAL:HG12 | 2.03                     | 0.41              |
| 1:LT:56:LEU:HD12   | 1:LT:59:THR:HB     | 2.02                     | 0.41              |
| 2:LX:503:ILE:HA    | 3:MY:1729:MET:HA   | 2.02                     | 0.41              |
| 3:LY:1890:VAL:HG12 | 3:MY:1683:ILE:HG13 | 2.03                     | 0.41              |
| 3:NY:1700:ILE:HG13 | 3:NY:1879:ILE:HG12 | 2.02                     | 0.41              |
| 3:NY:1898:LYS:HA   | 3:NY:1901:VAL:HG12 | 2.02                     | 0.41              |
| 3:AY:1797:ARG:HG3  | 3:AY:1865:ILE:HB   | 2.03                     | 0.41              |
| 2:BX:503:ILE:HA    | 3:CY:1729:MET:HA   | 2.02                     | 0.41              |
| 3:BY:1700:ILE:HG13 | 3:BY:1879:ILE:HG12 | 2.02                     | 0.41              |
| 3:BY:1797:ARG:HG3  | 3:BY:1865:ILE:HB   | 2.03                     | 0.41              |
| 3:CY:1732:LEU:HD23 | 3:CY:1732:LEU:HA   | 1.84                     | 0.41              |
| 1:DT:167:ASN:HB3   | 1:DT:173:VAL:HG11  | 2.03                     | 0.41              |
| 2:DX:371:GLU:HA    | 2:DX:374:LYS:HG2   | 2.02                     | 0.41              |
| 2:EX:440:PHE:CZ    | 3:EY:1873:GLU:HB3  | 2.56                     | 0.41              |
| 2:FX:440:PHE:CZ    | 3:FY:1873:GLU:HB3  | 2.55                     | 0.41              |
| 2:GX:503:ILE:HA    | 3:HY:1729:MET:HA   | 2.02                     | 0.41              |
| 3:GY:1786:VAL:HG22 | 3:GY:1871:LYS:HE2  | 2.01                     | 0.41              |
| 3:HY:1797:ARG:HG3  | 3:HY:1865:ILE:HB   | 2.03                     | 0.41              |
| 1:IT:51:PRO:HD3    | 2:IX:495:ASN:HB2   | 2.03                     | 0.41              |
| 2:JX:371:GLU:HA    | 2:JX:374:LYS:HG2   | 2.02                     | 0.41              |
| 3:JY:1700:ILE:HG13 | 3:JY:1879:ILE:HG12 | 2.02                     | 0.41              |
| 3:LY:1797:ARG:HG3  | 3:LY:1865:ILE:HB   | 2.03                     | 0.41              |
| 2:MX:440:PHE:CZ    | 3:MY:1873:GLU:HB3  | 2.55                     | 0.41              |
| 3:MY:1859:LEU:O    | 3:MY:1863:MET:HB3  | 2.20                     | 0.41              |
| 3:AY:1700:ILE:HG13 | 3:AY:1879:ILE:HG12 | 2.02                     | 0.41              |
| 3:AY:1898:LYS:HA   | 3:AY:1901:VAL:HG12 | 2.02                     | 0.41              |
| 2:BX:435:LEU:HD11  | 3:BY:1720:LYS:HE3  | 2.02                     | 0.41              |
| 1:CT:75:LEU:HD23   | 1:CT:75:LEU:HA     | 1.86                     | 0.41              |
| 1:CT:213:ARG:HH12  | 2:CX:364:ASN:HB3   | 1.85                     | 0.41              |
| 3:CY:1786:VAL:HG22 | 3:CY:1871:LYS:HE2  | 2.01                     | 0.41              |
| 3:DY:1859:LEU:O    | 3:DY:1863:MET:HB3  | 2.20                     | 0.41              |
| 3:DY:1906:LYS:HA   | 3:DY:1909:THR:HG22 | 2.01                     | 0.41              |
| 2:EX:455:ILE:HB    | 3:EY:1765:PRO:HB3  | 2.03                     | 0.41              |
| 3:EY:1890:VAL:HG12 | 3:FY:1683:ILE:HG13 | 2.02                     | 0.41              |
| 2:FX:436:GLN:HB2   | 3:FY:1734:LYS:HG2  | 2.02                     | 0.41              |
| 3:FY:1786:VAL:HG22 | 3:FY:1871:LYS:HE2  | 2.01                     | 0.41              |
| 3:IY:1797:ARG:HG3  | 3:IY:1865:ILE:HB   | 2.03                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:KY:1700:ILE:HG13 | 3:KY:1879:ILE:HG12 | 2.02                     | 0.41              |
| 3:LY:1700:ILE:HG13 | 3:LY:1879:ILE:HG12 | 2.02                     | 0.41              |
| 1:NT:167:ASN:HB3   | 1:NT:173:VAL:HG11  | 2.03                     | 0.41              |
| 2:NX:394:ARG:HE    | 2:NX:394:ARG:HB3   | 1.68                     | 0.41              |
| 1:BT:75:LEU:HA     | 1:BT:75:LEU:HD23   | 1.86                     | 0.41              |
| 2:BX:440:PHE:CZ    | 3:BY:1873:GLU:HB3  | 2.56                     | 0.41              |
| 3:CY:1694:GLN:N    | 3:CY:1884:ASP:OD2  | 2.54                     | 0.41              |
| 3:CY:1700:ILE:HG13 | 3:CY:1879:ILE:HG12 | 2.02                     | 0.41              |
| 3:CY:1903:GLU:HA   | 3:CY:1906:LYS:HG3  | 2.02                     | 0.41              |
| 1:DT:298:LEU:HD12  | 1:DT:298:LEU:HA    | 1.88                     | 0.41              |
| 3:DY:1694:GLN:N    | 3:DY:1884:ASP:OD2  | 2.54                     | 0.41              |
| 1:ET:167:ASN:HB3   | 1:ET:173:VAL:HG11  | 2.03                     | 0.41              |
| 3:EY:1786:VAL:HG22 | 3:EY:1871:LYS:HE2  | 2.01                     | 0.41              |
| 1:FT:38:PRO:HA     | 2:GX:404:TYR:HA    | 2.03                     | 0.41              |
| 3:FY:1689:THR:O    | 3:FY:1724:ASN:ND2  | 2.34                     | 0.41              |
| 1:GT:199:TYR:HB3   | 2:GX:379:GLN:OE1   | 2.21                     | 0.41              |
| 2:GX:455:ILE:HB    | 3:GY:1765:PRO:HB3  | 2.02                     | 0.41              |
| 2:GX:481:ASP:HB3   | 3:GY:1875:ASP:HA   | 2.02                     | 0.41              |
| 3:GY:1694:GLN:N    | 3:GY:1884:ASP:OD2  | 2.54                     | 0.41              |
| 1:HT:298:LEU:HA    | 1:HT:298:LEU:HD12  | 1.88                     | 0.41              |
| 2:HX:436:GLN:HB2   | 3:HY:1734:LYS:HG2  | 2.02                     | 0.41              |
| 2:HX:440:PHE:CZ    | 3:HY:1873:GLU:HB3  | 2.56                     | 0.41              |
| 2:HX:503:ILE:HA    | 3:IY:1729:MET:HA   | 2.02                     | 0.41              |
| 3:HY:1786:VAL:HG22 | 3:HY:1871:LYS:HE2  | 2.01                     | 0.41              |
| 3:IY:1700:ILE:HG13 | 3:IY:1879:ILE:HG12 | 2.02                     | 0.41              |
| 1:JT:200:LYS:HA    | 1:JT:200:LYS:HD3   | 1.76                     | 0.41              |
| 2:JX:440:PHE:CZ    | 3:JY:1873:GLU:HB3  | 2.56                     | 0.41              |
| 2:JX:497:LEU:O     | 2:KX:432:ASN:ND2   | 2.40                     | 0.41              |
| 3:JY:1898:LYS:HA   | 3:JY:1901:VAL:HG12 | 2.02                     | 0.41              |
| 2:KX:436:GLN:HB2   | 3:KY:1734:LYS:HG2  | 2.02                     | 0.41              |
| 2:KX:455:ILE:HB    | 3:KY:1765:PRO:HB3  | 2.01                     | 0.41              |
| 3:KY:1859:LEU:O    | 3:KY:1863:MET:HB3  | 2.20                     | 0.41              |
| 1:MT:56:LEU:HD12   | 1:MT:59:THR:HB     | 2.02                     | 0.41              |
| 1:MT:167:ASN:HB3   | 1:MT:173:VAL:HG11  | 2.03                     | 0.41              |
| 1:MT:199:TYR:HB3   | 2:MX:379:GLN:OE1   | 2.21                     | 0.41              |
| 3:MY:1700:ILE:HG13 | 3:MY:1879:ILE:HG12 | 2.02                     | 0.41              |
| 2:NX:436:GLN:HB2   | 3:NY:1734:LYS:HG2  | 2.02                     | 0.41              |
| 3:NY:1903:GLU:HA   | 3:NY:1906:LYS:HG3  | 2.02                     | 0.41              |
| 2:AX:440:PHE:CZ    | 3:AY:1873:GLU:HB3  | 2.56                     | 0.41              |
| 1:BT:56:LEU:HD12   | 1:BT:59:THR:HB     | 2.02                     | 0.41              |
| 3:BY:1890:VAL:HG12 | 3:CY:1683:ILE:HG13 | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CX:480:LYS:NZ    | 3:CY:1699:GLU:OE2  | 2.45                     | 0.41              |
| 2:CX:507:GLY:HA2   | 1:DT:168:LEU:HD11  | 2.03                     | 0.41              |
| 3:DY:1797:ARG:HG3  | 3:DY:1865:ILE:HB   | 2.03                     | 0.41              |
| 1:ET:56:LEU:HD12   | 1:ET:59:THR:HB     | 2.02                     | 0.41              |
| 3:FY:1694:GLN:N    | 3:FY:1884:ASP:OD2  | 2.54                     | 0.41              |
| 3:FY:1797:ARG:HG3  | 3:FY:1865:ILE:HB   | 2.03                     | 0.41              |
| 2:HX:365:LYS:HE2   | 2:HX:365:LYS:HB2   | 1.98                     | 0.41              |
| 1:LT:75:LEU:HD23   | 1:LT:75:LEU:HA     | 1.86                     | 0.41              |
| 3:LY:1689:THR:O    | 3:LY:1724:ASN:ND2  | 2.34                     | 0.41              |
| 2:AX:503:ILE:HG13  | 3:BY:1729:MET:HB3  | 2.03                     | 0.40              |
| 1:CT:56:LEU:HD12   | 1:CT:59:THR:HB     | 2.02                     | 0.40              |
| 1:DT:75:LEU:HD23   | 1:DT:75:LEU:HA     | 1.86                     | 0.40              |
| 3:DY:1898:LYS:HA   | 3:DY:1901:VAL:HG12 | 2.03                     | 0.40              |
| 2:EX:365:LYS:HE2   | 2:EX:365:LYS:HB2   | 1.98                     | 0.40              |
| 2:HX:455:ILE:HB    | 3:HY:1765:PRO:HB3  | 2.02                     | 0.40              |
| 1:LT:167:ASN:HB3   | 1:LT:173:VAL:HG11  | 2.03                     | 0.40              |
| 2:MX:436:GLN:HB2   | 3:MY:1734:LYS:HG2  | 2.02                     | 0.40              |
| 2:NX:394:ARG:HD2   | 2:NX:394:ARG:HA    | 1.93                     | 0.40              |
| 2:NX:417:SER:N     | 2:NX:429:GLY:O     | 2.45                     | 0.40              |
| 1:AT:168:LEU:HD11  | 2:NX:507:GLY:HA2   | 2.03                     | 0.40              |
| 3:CY:1859:LEU:O    | 3:CY:1863:MET:HB3  | 2.20                     | 0.40              |
| 3:EY:1797:ARG:HG3  | 3:EY:1865:ILE:HB   | 2.03                     | 0.40              |
| 3:GY:1859:LEU:O    | 3:GY:1863:MET:HB3  | 2.20                     | 0.40              |
| 3:HY:1700:ILE:HG13 | 3:HY:1879:ILE:HG12 | 2.02                     | 0.40              |
| 1:KT:167:ASN:HB3   | 1:KT:173:VAL:HG11  | 2.03                     | 0.40              |
| 1:AT:56:LEU:HD12   | 1:AT:59:THR:HB     | 2.02                     | 0.40              |
| 2:AX:417:SER:N     | 2:AX:429:GLY:O     | 2.45                     | 0.40              |
| 1:DT:56:LEU:HD12   | 1:DT:59:THR:HB     | 2.02                     | 0.40              |
| 3:DY:1786:VAL:HG22 | 3:DY:1871:LYS:HE2  | 2.01                     | 0.40              |
| 3:FY:1879:ILE:HD13 | 3:FY:1879:ILE:HA   | 1.86                     | 0.40              |
| 2:GX:365:LYS:HE2   | 2:GX:365:LYS:HB2   | 1.98                     | 0.40              |
| 3:GY:1797:ARG:HG3  | 3:GY:1865:ILE:HB   | 2.03                     | 0.40              |
| 3:IY:1694:GLN:N    | 3:IY:1884:ASP:OD2  | 2.54                     | 0.40              |
| 3:KY:1890:VAL:HG12 | 3:LY:1683:ILE:HG13 | 2.03                     | 0.40              |
| 2:LX:436:GLN:HB2   | 3:LY:1734:LYS:HG2  | 2.02                     | 0.40              |
| 2:AX:481:ASP:HB3   | 3:AY:1875:ASP:HA   | 2.02                     | 0.40              |
| 3:AY:1694:GLN:N    | 3:AY:1884:ASP:OD2  | 2.54                     | 0.40              |
| 2:DX:440:PHE:CZ    | 3:DY:1873:GLU:HB3  | 2.57                     | 0.40              |
| 2:EX:394:ARG:HE    | 2:EX:394:ARG:HB3   | 1.68                     | 0.40              |
| 3:EY:1879:ILE:HD13 | 3:EY:1879:ILE:HA   | 1.86                     | 0.40              |
| 1:FT:167:ASN:HB3   | 1:FT:173:VAL:HG11  | 2.03                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:FT:202:LEU:HD13  | 2:FX:375:ILE:HD11  | 2.04                     | 0.40              |
| 2:GX:371:GLU:HA    | 2:GX:374:LYS:HG2   | 2.03                     | 0.40              |
| 2:HX:481:ASP:HB3   | 3:HY:1875:ASP:HA   | 2.02                     | 0.40              |
| 3:LY:1898:LYS:HA   | 3:LY:1901:VAL:HG12 | 2.02                     | 0.40              |
| 3:AY:1903:GLU:HA   | 3:AY:1906:LYS:HG3  | 2.02                     | 0.40              |
| 3:DY:1700:ILE:HG13 | 3:DY:1879:ILE:HG12 | 2.02                     | 0.40              |
| 3:FY:1898:LYS:HA   | 3:FY:1901:VAL:HG12 | 2.02                     | 0.40              |
| 3:GY:1879:ILE:HD13 | 3:GY:1879:ILE:HA   | 1.86                     | 0.40              |
| 1:HT:51:PRO:HD3    | 2:HX:495:ASN:HB2   | 2.04                     | 0.40              |
| 3:HY:1898:LYS:HA   | 3:HY:1901:VAL:HG12 | 2.03                     | 0.40              |
| 3:IY:1898:LYS:HA   | 3:IY:1901:VAL:HG12 | 2.03                     | 0.40              |
| 2:LX:394:ARG:HD2   | 2:LX:394:ARG:HA    | 1.93                     | 0.40              |
| 2:NX:371:GLU:HA    | 2:NX:374:LYS:HG2   | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | AT    | 171/278 (62%) | 160 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | BT    | 171/278 (62%) | 160 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | CT    | 171/278 (62%) | 160 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | DT    | 171/278 (62%) | 160 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | ET    | 171/278 (62%) | 160 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | FT    | 171/278 (62%) | 160 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | GT    | 171/278 (62%) | 160 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | HT    | 171/278 (62%) | 160 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | IT    | 171/278 (62%) | 160 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | JT    | 171/278 (62%) | 160 (94%) | 11 (6%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | KT    | 171/278 (62%)  | 160 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | LT    | 171/278 (62%)  | 160 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | MT    | 171/278 (62%)  | 160 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | NT    | 171/278 (62%)  | 160 (94%) | 11 (6%) | 0        | 100         | 100 |
| 2   | AX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 2   | BX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 2   | CX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 2   | DX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 2   | EX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 2   | FX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 2   | GX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 2   | HX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 2   | IX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 2   | JX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 2   | KX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 2   | LX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 2   | MX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 2   | NX    | 153/522 (29%)  | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 3   | AY    | 205/1927 (11%) | 195 (95%) | 10 (5%) | 0        | 100         | 100 |
| 3   | BY    | 205/1927 (11%) | 195 (95%) | 10 (5%) | 0        | 100         | 100 |
| 3   | CY    | 205/1927 (11%) | 195 (95%) | 10 (5%) | 0        | 100         | 100 |
| 3   | DY    | 205/1927 (11%) | 195 (95%) | 10 (5%) | 0        | 100         | 100 |
| 3   | EY    | 205/1927 (11%) | 195 (95%) | 10 (5%) | 0        | 100         | 100 |
| 3   | FY    | 205/1927 (11%) | 195 (95%) | 10 (5%) | 0        | 100         | 100 |
| 3   | GY    | 205/1927 (11%) | 195 (95%) | 10 (5%) | 0        | 100         | 100 |
| 3   | HY    | 205/1927 (11%) | 195 (95%) | 10 (5%) | 0        | 100         | 100 |
| 3   | IY    | 205/1927 (11%) | 195 (95%) | 10 (5%) | 0        | 100         | 100 |
| 3   | JY    | 205/1927 (11%) | 195 (95%) | 10 (5%) | 0        | 100         | 100 |
| 3   | KY    | 205/1927 (11%) | 195 (95%) | 10 (5%) | 0        | 100         | 100 |
| 3   | LY    | 205/1927 (11%) | 195 (95%) | 10 (5%) | 0        | 100         | 100 |
| 3   | MY    | 205/1927 (11%) | 195 (95%) | 10 (5%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 3   | NY    | 205/1927 (11%)   | 195 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| All | All   | 7406/38178 (19%) | 7000 (94%) | 406 (6%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | AT    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 1   | BT    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 1   | CT    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 1   | DT    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 1   | ET    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 1   | FT    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 1   | GT    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 1   | HT    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 1   | IT    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 1   | JT    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 1   | KT    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 1   | LT    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 1   | MT    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 1   | NT    | 169/254 (66%) | 167 (99%)  | 2 (1%)   | 71          | 88  |
| 2   | AX    | 139/470 (30%) | 139 (100%) | 0        | 100         | 100 |
| 2   | BX    | 139/470 (30%) | 139 (100%) | 0        | 100         | 100 |
| 2   | CX    | 139/470 (30%) | 139 (100%) | 0        | 100         | 100 |
| 2   | DX    | 139/470 (30%) | 139 (100%) | 0        | 100         | 100 |
| 2   | EX    | 139/470 (30%) | 139 (100%) | 0        | 100         | 100 |
| 2   | FX    | 139/470 (30%) | 139 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 2   | GX    | 139/470 (30%)    | 139 (100%) | 0        | 100         | 100 |
| 2   | HX    | 139/470 (30%)    | 139 (100%) | 0        | 100         | 100 |
| 2   | IX    | 139/470 (30%)    | 139 (100%) | 0        | 100         | 100 |
| 2   | JX    | 139/470 (30%)    | 139 (100%) | 0        | 100         | 100 |
| 2   | KX    | 139/470 (30%)    | 139 (100%) | 0        | 100         | 100 |
| 2   | LX    | 139/470 (30%)    | 139 (100%) | 0        | 100         | 100 |
| 2   | MX    | 139/470 (30%)    | 139 (100%) | 0        | 100         | 100 |
| 2   | NX    | 139/470 (30%)    | 139 (100%) | 0        | 100         | 100 |
| 3   | AY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| 3   | BY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| 3   | CY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| 3   | DY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| 3   | EY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| 3   | FY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| 3   | GY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| 3   | HY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| 3   | IY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| 3   | JY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| 3   | KY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| 3   | LY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| 3   | MY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| 3   | NY    | 177/1724 (10%)   | 176 (99%)  | 1 (1%)   | 86          | 94  |
| All | All   | 6790/34272 (20%) | 6748 (99%) | 42 (1%)  | 86          | 94  |

All (42) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AT    | 206  | LYS  |
| 1   | AT    | 214  | LYS  |
| 3   | AY    | 1906 | LYS  |
| 1   | BT    | 206  | LYS  |
| 1   | BT    | 214  | LYS  |
| 3   | BY    | 1906 | LYS  |
| 1   | CT    | 206  | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CT    | 214  | LYS  |
| 3   | CY    | 1906 | LYS  |
| 1   | DT    | 206  | LYS  |
| 1   | DT    | 214  | LYS  |
| 3   | DY    | 1906 | LYS  |
| 1   | ET    | 206  | LYS  |
| 1   | ET    | 214  | LYS  |
| 3   | EY    | 1906 | LYS  |
| 1   | FT    | 206  | LYS  |
| 1   | FT    | 214  | LYS  |
| 3   | FY    | 1906 | LYS  |
| 1   | GT    | 206  | LYS  |
| 1   | GT    | 214  | LYS  |
| 3   | GY    | 1906 | LYS  |
| 1   | HT    | 206  | LYS  |
| 1   | HT    | 214  | LYS  |
| 3   | HY    | 1906 | LYS  |
| 1   | IT    | 206  | LYS  |
| 1   | IT    | 214  | LYS  |
| 3   | IY    | 1906 | LYS  |
| 1   | JT    | 206  | LYS  |
| 1   | JT    | 214  | LYS  |
| 3   | JY    | 1906 | LYS  |
| 1   | KT    | 206  | LYS  |
| 1   | KT    | 214  | LYS  |
| 3   | KY    | 1906 | LYS  |
| 1   | LT    | 206  | LYS  |
| 1   | LT    | 214  | LYS  |
| 3   | LY    | 1906 | LYS  |
| 1   | MT    | 206  | LYS  |
| 1   | MT    | 214  | LYS  |
| 3   | MY    | 1906 | LYS  |
| 1   | NT    | 206  | LYS  |
| 1   | NT    | 214  | LYS  |
| 3   | NY    | 1906 | LYS  |

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

### 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.

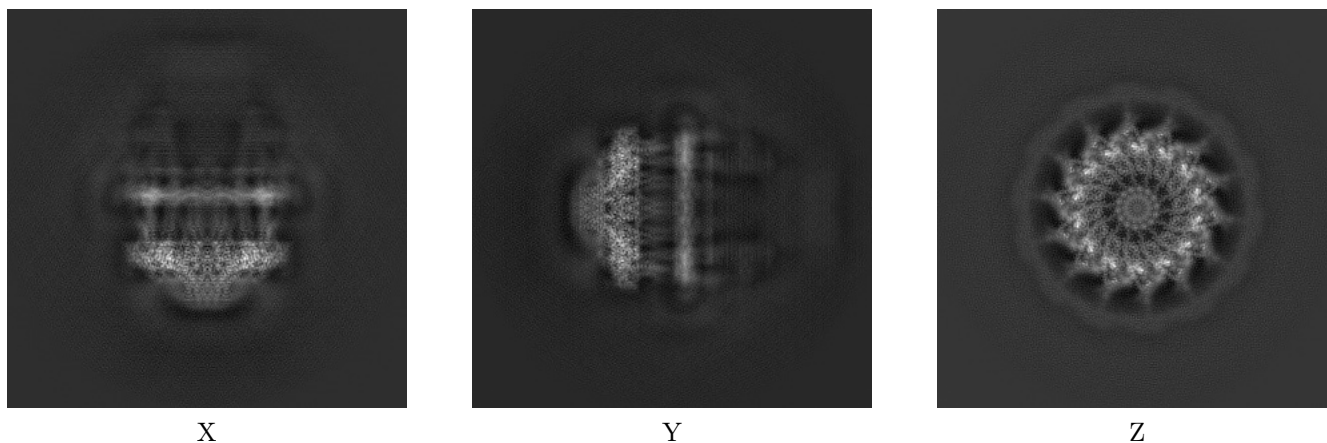
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22076. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

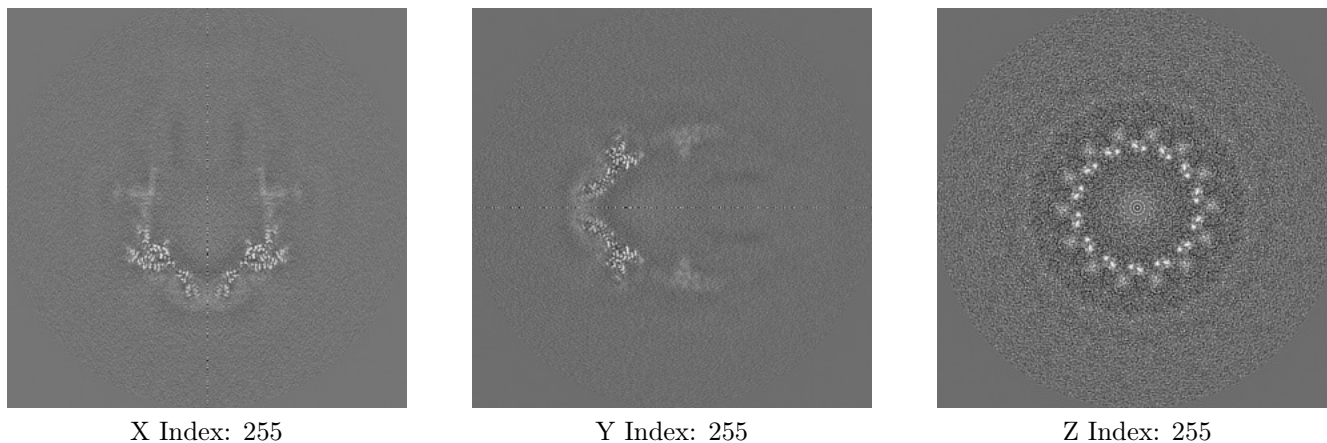
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

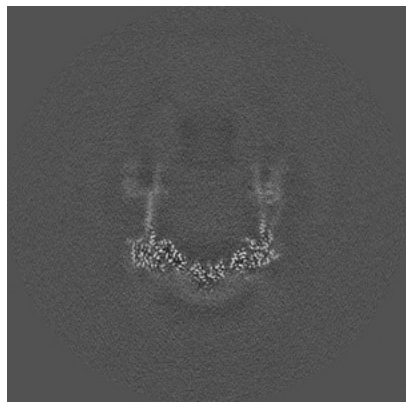
#### 6.2.1 Primary map



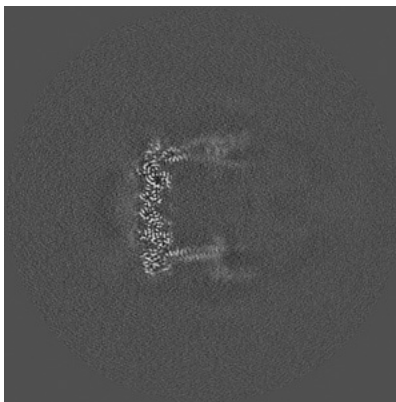
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

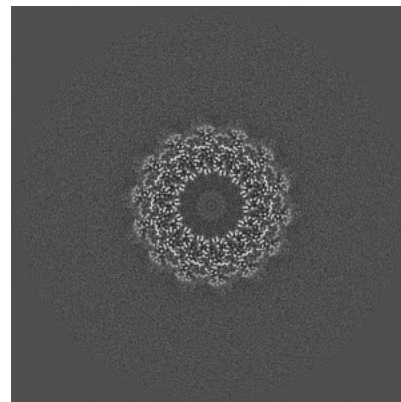
### 6.3.1 Primary map



X Index: 224



Y Index: 303

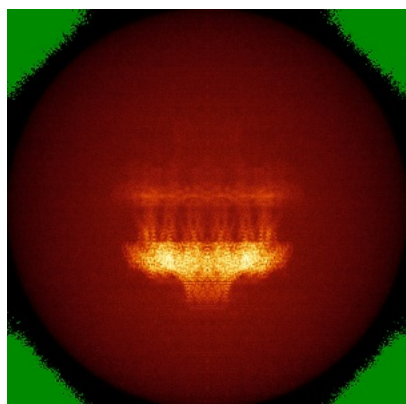


Z Index: 188

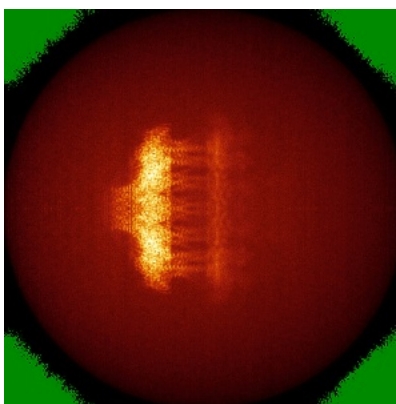
The images above show the largest variance slices of the map in three orthogonal directions.

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

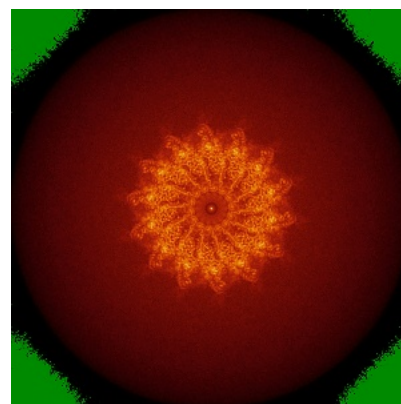
### 6.4.1 Primary map



X



Y

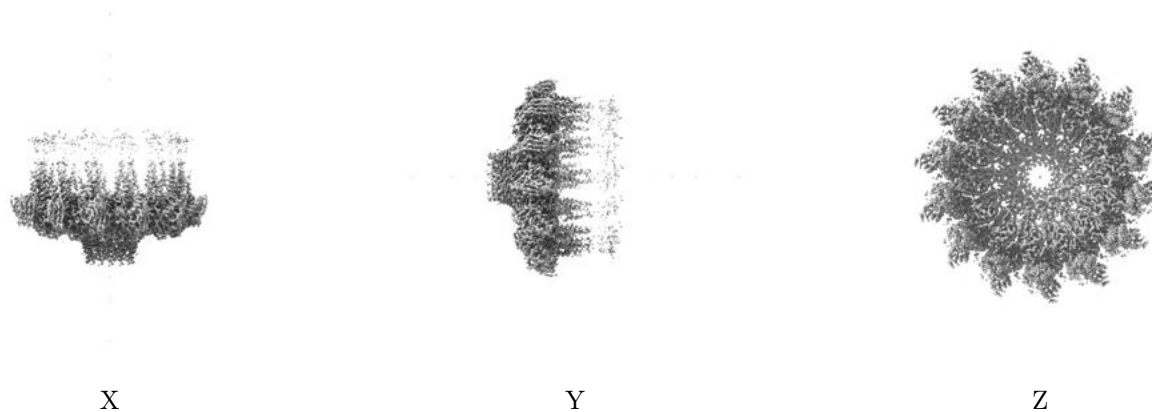


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

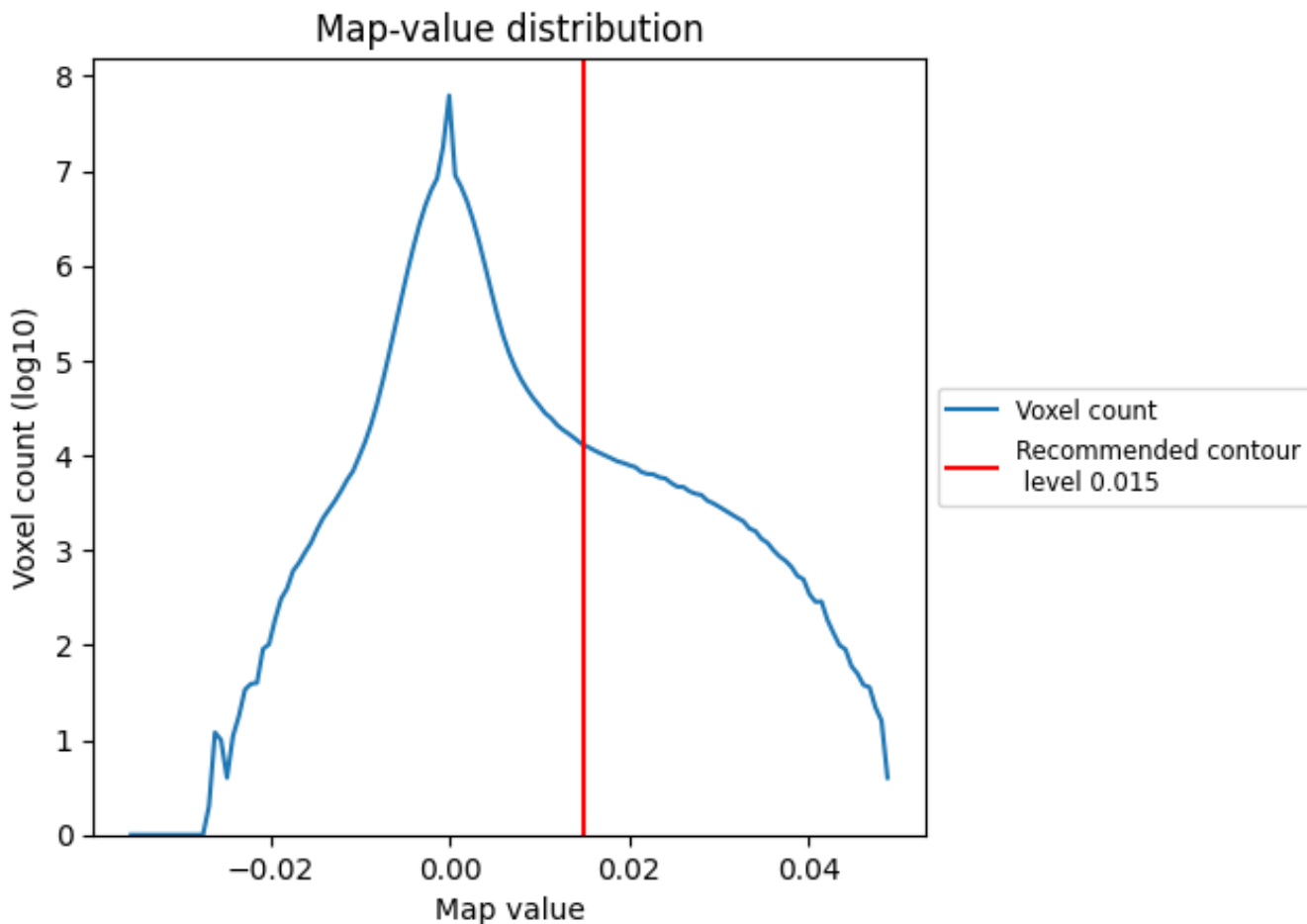
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

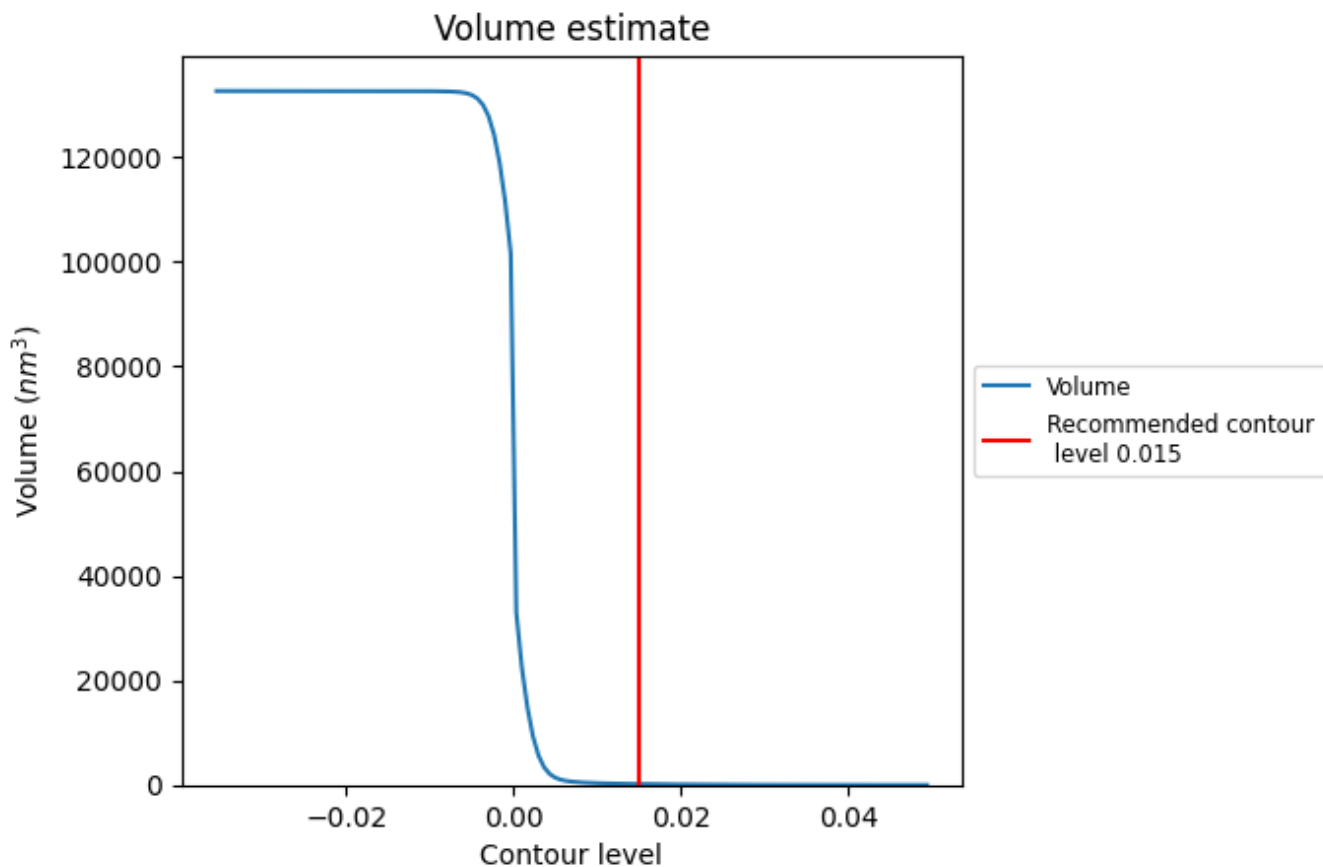
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

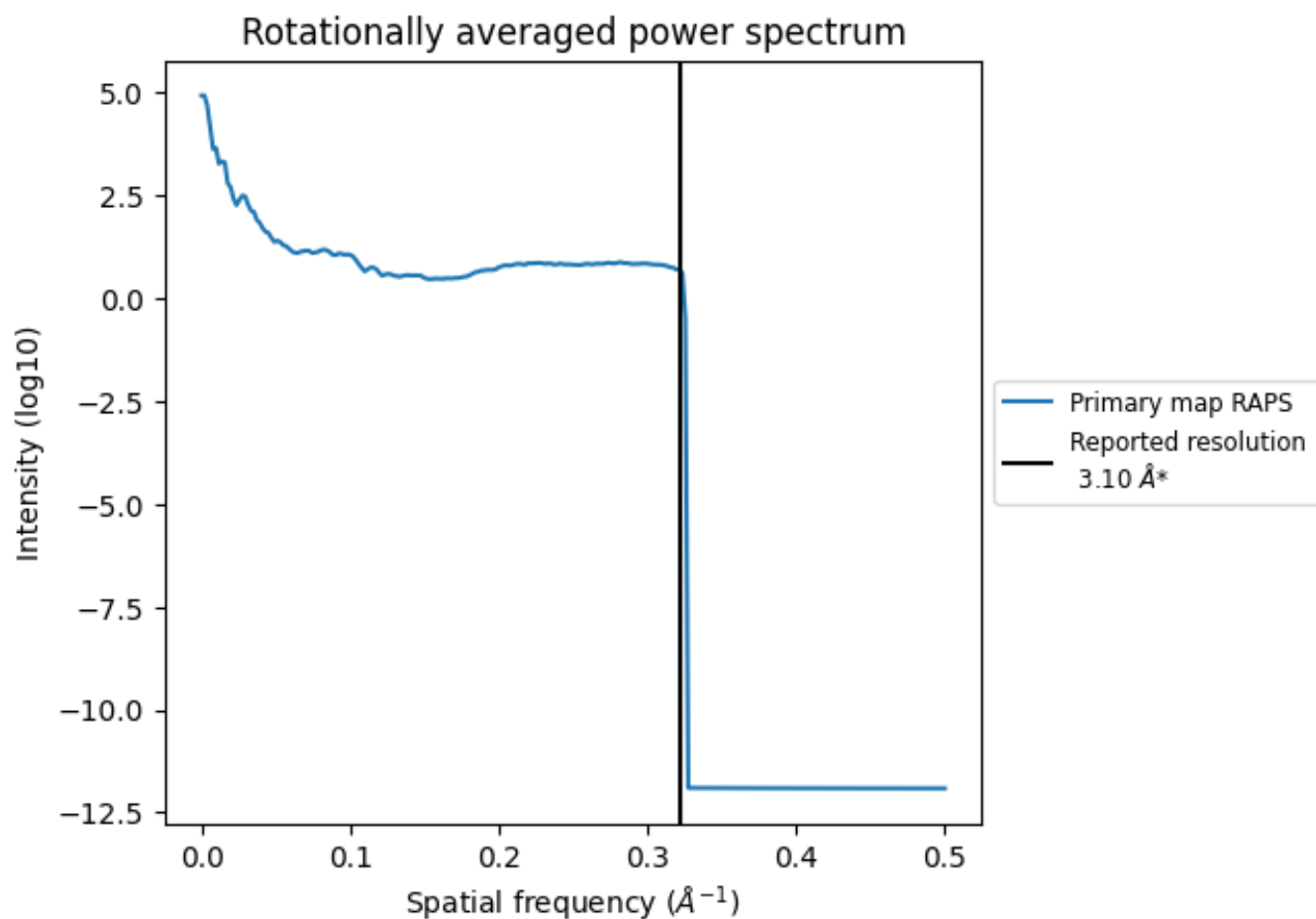
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm<sup>3</sup>; this corresponds to an approximate mass of 163 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



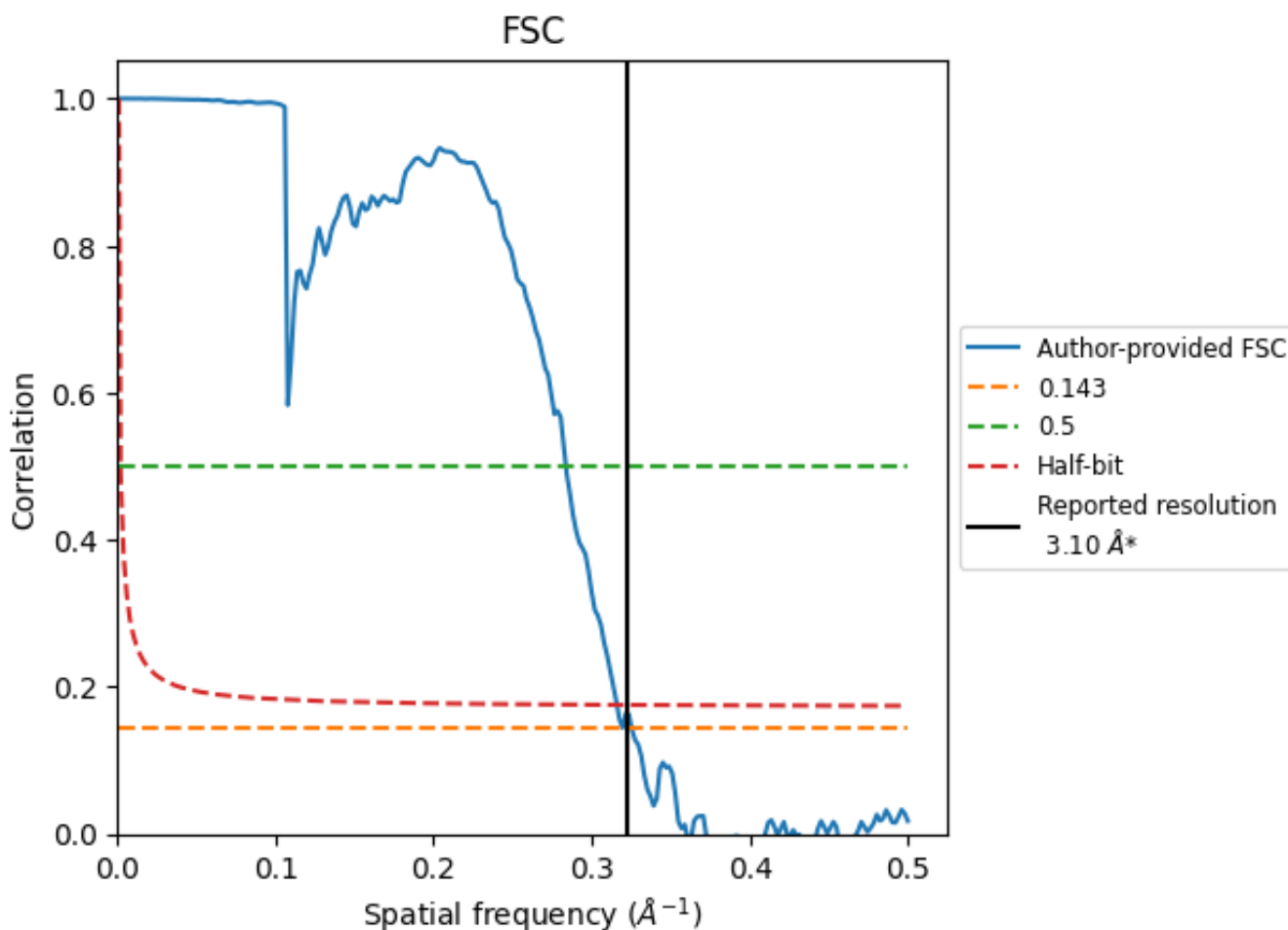
\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

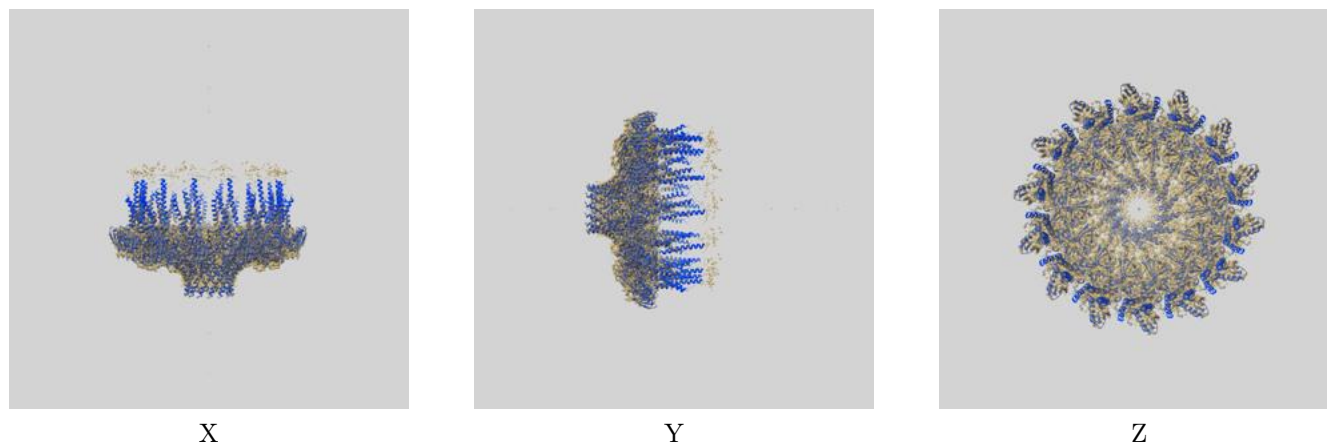
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.10                               | -    | -        |
| Author-provided FSC curve | 3.07                               | 3.52 | 3.16     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

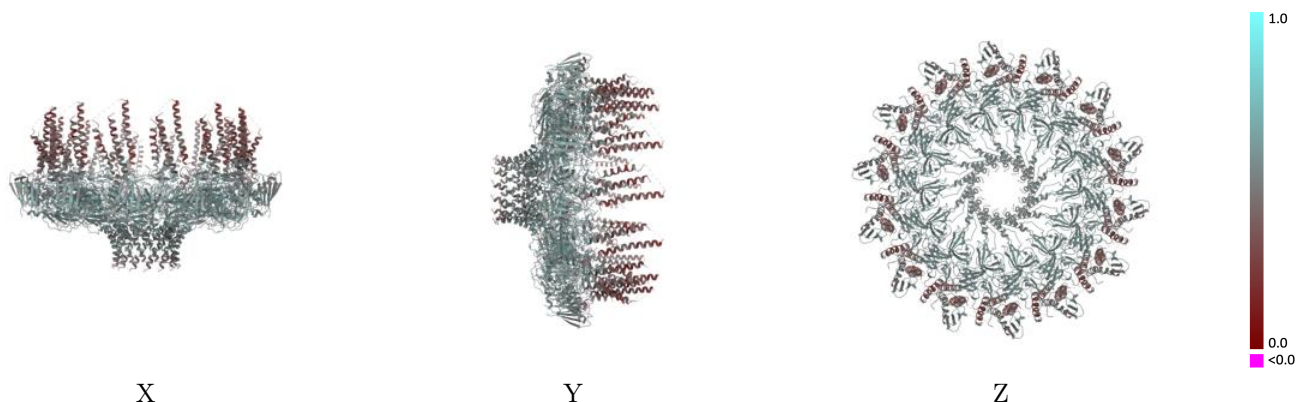
This section contains information regarding the fit between EMDB map EMD-22076 and PDB model 6X6K. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



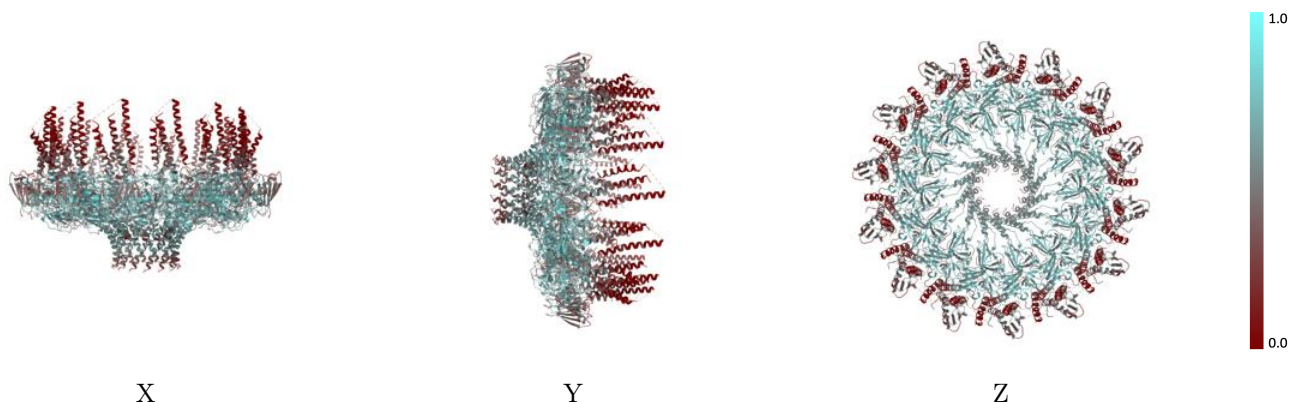
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



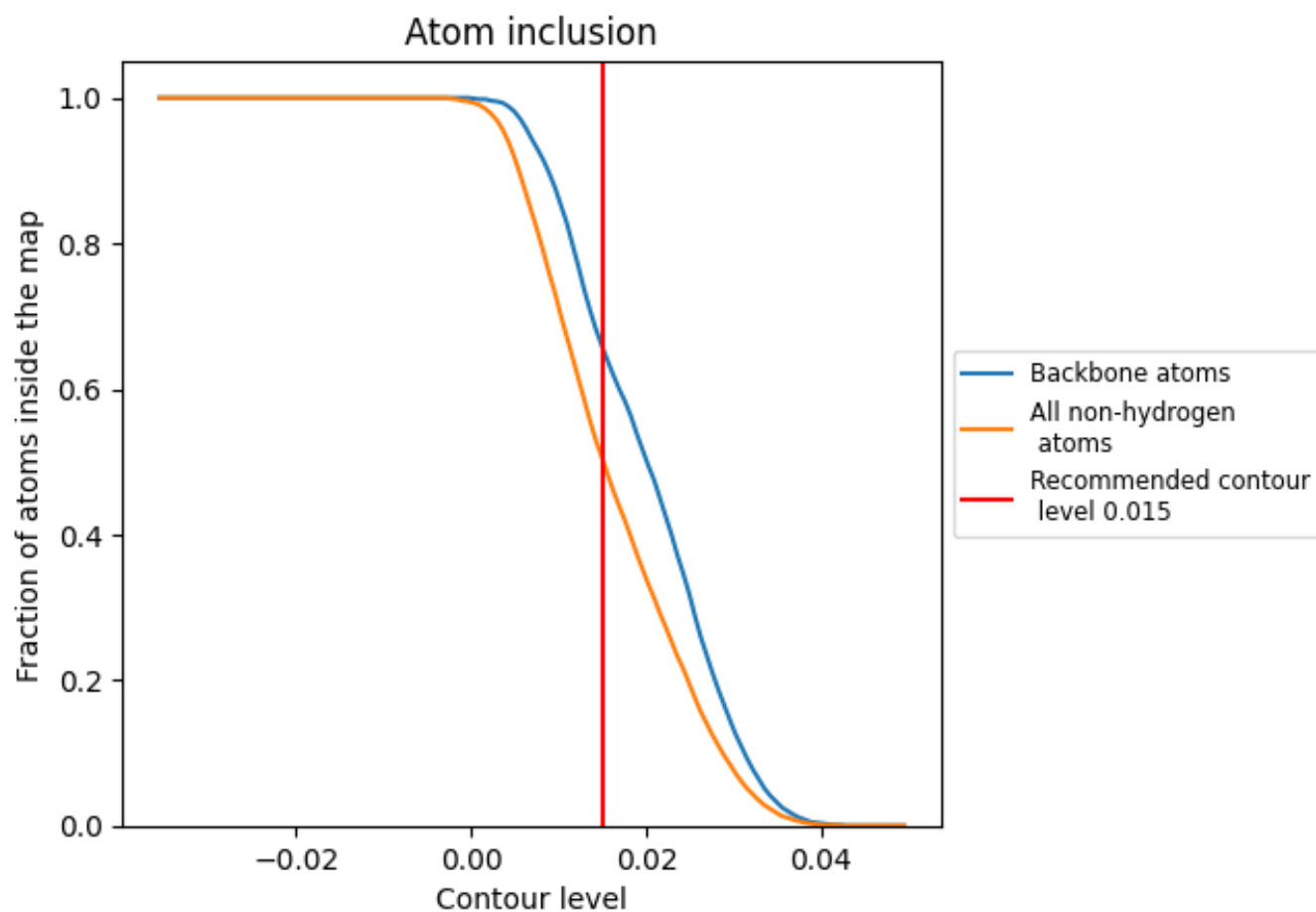
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

















The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| All   | 0.5050         | 0.5040  |
| AT    | 0.3380         | 0.4550  |
| AX    | 0.5770         | 0.5170  |
| AY    | 0.6070         | 0.5400  |
| BT    | 0.3390         | 0.4580  |
| BX    | 0.5750         | 0.5160  |
| BY    | 0.6070         | 0.5410  |
| CT    | 0.3350         | 0.4550  |
| CX    | 0.5740         | 0.5180  |
| CY    | 0.6040         | 0.5410  |
| DT    | 0.3390         | 0.4550  |
| DX    | 0.5720         | 0.5190  |
| DY    | 0.6020         | 0.5420  |
| ET    | 0.3400         | 0.4550  |
| EX    | 0.5790         | 0.5170  |
| EY    | 0.6040         | 0.5430  |
| FT    | 0.3360         | 0.4540  |
| FX    | 0.5780         | 0.5190  |
| FY    | 0.6050         | 0.5400  |
| GT    | 0.3330         | 0.4530  |
| GX    | 0.5800         | 0.5190  |
| GY    | 0.6090         | 0.5410  |
| HT    | 0.3370         | 0.4560  |
| HX    | 0.5770         | 0.5170  |
| HY    | 0.6060         | 0.5400  |
| IT    | 0.3370         | 0.4560  |
| IX    | 0.5710         | 0.5190  |
| IY    | 0.6070         | 0.5400  |
| JT    | 0.3350         | 0.4520  |
| JX    | 0.5740         | 0.5170  |
| JY    | 0.6050         | 0.5390  |
| KT    | 0.3360         | 0.4550  |
| KX    | 0.5730         | 0.5170  |
| KY    | 0.6020         | 0.5400  |
| LT    | 0.3370         | 0.4560  |



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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| LX    |  0.5790 |  0.5170 |
| LY    |  0.6050 |  0.5390 |
| MT    |  0.3350 |  0.4570 |
| MX    |  0.5770 |  0.5190 |
| MY    |  0.6050 |  0.5390 |
| NT    |  0.3390 |  0.4560 |
| NX    |  0.5790 |  0.5170 |
| NY    |  0.6090 |  0.5400 |