



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:05 AM UTC

PDB ID : 6SIC / pdb\_00006sic  
EMDB ID : EMD-10209  
Title : Cryo-EM structure of the Type III-B Cmr-beta bound to cognate target RNA  
Authors : Sofos, N.; Montoya, G.; Stella, S.  
Deposited on : 2019-08-09  
Resolution : 3.52 Å(reported)  
Based on initial model : 6S8B

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:

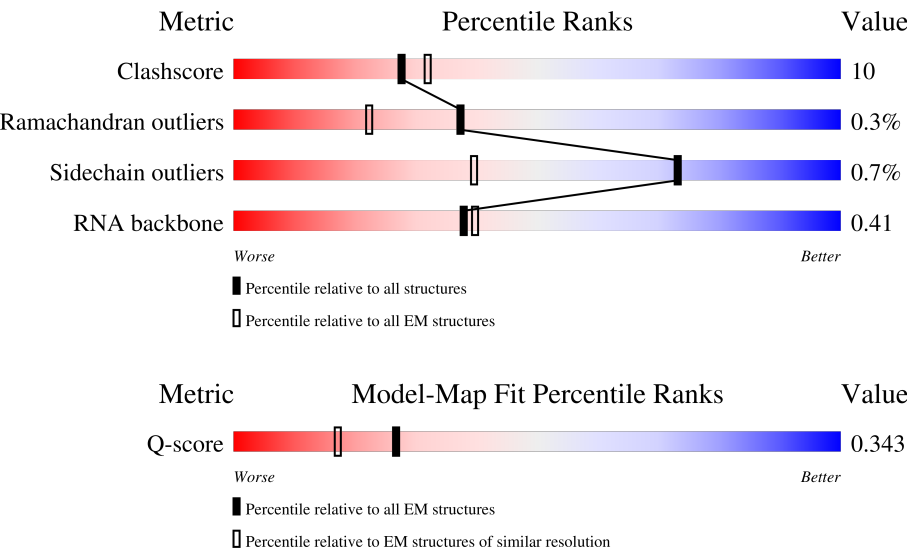
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 3.52 Å.

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



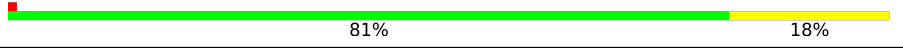
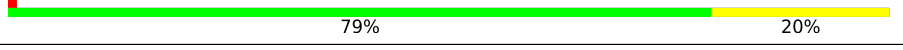
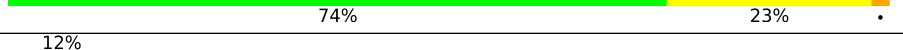
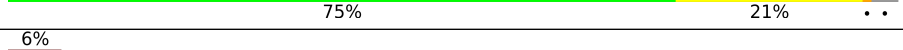
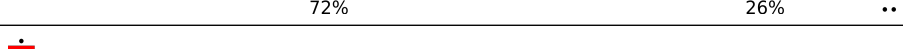
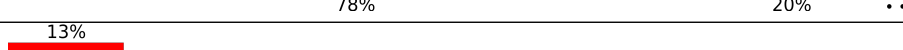
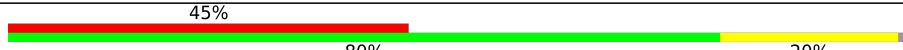
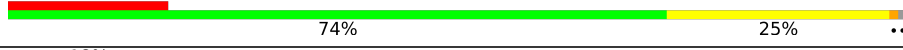
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 13017 ( 3.02 - 4.02 )                                    |

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   | A     | 155    |                  |
| 1   | B     | 155    |                  |
| 1   | C     | 155    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | D     | 286    |    |
| 2   | E     | 286    |    |
| 2   | F     | 286    |    |
| 2   | G     | 286    |    |
| 3   | H     | 313    |    |
| 4   | I     | 296    |    |
| 5   | J     | 476    |    |
| 6   | K     | 1037   |    |
| 7   | L     | 174    |    |
| 7   | M     | 174    |    |
| 7   | N     | 174    |    |
| 7   | O     | 174    |  |
| 7   | P     | 174    |  |
| 7   | Q     | 174    |  |
| 7   | R     | 174    |  |
| 7   | S     | 174    |  |
| 7   | T     | 174    |  |
| 7   | W     | 174    |  |
| 7   | X     | 174    |  |
| 7   | l     | 174    |  |
| 7   | m     | 174    |  |
| 7   | n     | 174    |  |
| 7   | o     | 174    |  |
| 7   | p     | 174    |  |
| 7   | q     | 174    |  |

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| Mol | Chain | Length | Quality of chain                                                    |
|-----|-------|--------|---------------------------------------------------------------------|
| 7   | r     | 174    | <div><div>5%</div><div>76%</div><div>23%</div><div>.</div></div>    |
| 7   | s     | 174    | <div><div>48%</div><div>74%</div><div>26%</div><div>.</div></div>   |
| 7   | t     | 174    | <div><div>11%</div><div>69%</div><div>28%</div><div>...</div></div> |
| 7   | w     | 174    | <div><div>21%</div><div>71%</div><div>26%</div><div>...</div></div> |
| 7   | x     | 174    | <div><div>86%</div><div>41%</div><div>58%</div><div>.</div></div>   |
| 8   | U     | 46     | <div><div>48%</div><div>39%</div><div>9%</div><div>.</div></div>    |
| 9   | V     | 51     | <div><div>45%</div><div>39%</div><div>10%</div><div>6%</div></div>  |

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 62079 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 CRISPR-associated protein, Cmr5 family.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1253  | 817 | 205 | 230 | 1 |         |       |
| 1   | B     | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1261  | 823 | 206 | 231 | 1 |         |       |
| 1   | C     | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1261  | 823 | 206 | 231 | 1 |         |       |

- Molecule 2 is a protein called CRISPR-associated RAMP protein, Cmr4 family.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | D     | 285      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2274  | 1478 | 369 | 425 | 2 |         |       |
| 2   | E     | 285      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2274  | 1478 | 369 | 425 | 2 |         |       |
| 2   | F     | 285      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2274  | 1478 | 369 | 425 | 2 |         |       |
| 2   | G     | 285      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2273  | 1478 | 369 | 424 | 2 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| D     | 31      | ALA      | ASP    | engineered mutation | UNP F0NDX6 |
| E     | 31      | ALA      | ASP    | engineered mutation | UNP F0NDX6 |
| F     | 31      | ALA      | ASP    | engineered mutation | UNP F0NDX6 |
| G     | 31      | ALA      | ASP    | engineered mutation | UNP F0NDX6 |

- Molecule 3 is a protein called CRISPR-associated protein, Cmr3 family.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | H     | 312      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2528  | 1630 | 418 | 473 | 7 |         |       |

- Molecule 4 is a protein called CRISPR-associated RAMP protein, Cmr6 family.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | I     | 284      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2282  | 1470 | 381 | 427 | 4 |         |       |

There are 13 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| I     | 284     | ALA      | -      | expression tag | UNP F0NDX3 |
| I     | 285     | ALA      | -      | expression tag | UNP F0NDX3 |
| I     | 286     | ALA      | -      | expression tag | UNP F0NDX3 |
| I     | 287     | HIS      | -      | expression tag | UNP F0NDX3 |
| I     | 288     | HIS      | -      | expression tag | UNP F0NDX3 |
| I     | 289     | HIS      | -      | expression tag | UNP F0NDX3 |
| I     | 290     | HIS      | -      | expression tag | UNP F0NDX3 |
| I     | 291     | HIS      | -      | expression tag | UNP F0NDX3 |
| I     | 292     | HIS      | -      | expression tag | UNP F0NDX3 |
| I     | 293     | HIS      | -      | expression tag | UNP F0NDX3 |
| I     | 294     | HIS      | -      | expression tag | UNP F0NDX3 |
| I     | 295     | HIS      | -      | expression tag | UNP F0NDX3 |
| I     | 296     | HIS      | -      | expression tag | UNP F0NDX3 |

- Molecule 5 is a protein called CRISPR-associated RAMP protein, Cmr1 family.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | J     | 475      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3889  | 2517 | 632 | 727 | 13 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| J     | 1       | MET      | -      | initiating methionine | UNP F0NDX4 |
| J     | 2       | GLU      | -      | expression tag        | UNP F0NDX4 |
| J     | 3       | GLU      | -      | expression tag        | UNP F0NDX4 |
| J     | 4       | LEU      | -      | expression tag        | UNP F0NDX4 |
| J     | 5       | LEU      | -      | expression tag        | UNP F0NDX4 |

- Molecule 6 is a protein called CRISPR-associated protein, Cmr2 family.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 6   | K     | 1009     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8282  | 5360 | 1366 | 1532 | 24 |         |       |

- Molecule 7 is a protein called CRISPR-associated protein CmrX.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | L     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | M     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | N     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | O     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | P     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | Q     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | R     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | S     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | T     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | W     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | l     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | m     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | n     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | o     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | p     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | q     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | r     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | s     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | t     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | w     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |
| 7   | X     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | x     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1378  | 880 | 227 | 269 | 2 |         |       |

- Molecule 8 is a RNA chain called Cognate target RNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 8   | U     | 42       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 886   | 398 | 152 | 295 | 41 |         |       |

- Molecule 9 is a RNA chain called crRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | V     | 48       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1025  | 461 | 192 | 325 | 47 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference    |
|-------|---------|----------|--------|----------|--------------|
| V     | 1       | A        | C      | conflict | GB 323473489 |
| V     | 3       | U        | G      | conflict | GB 323473489 |

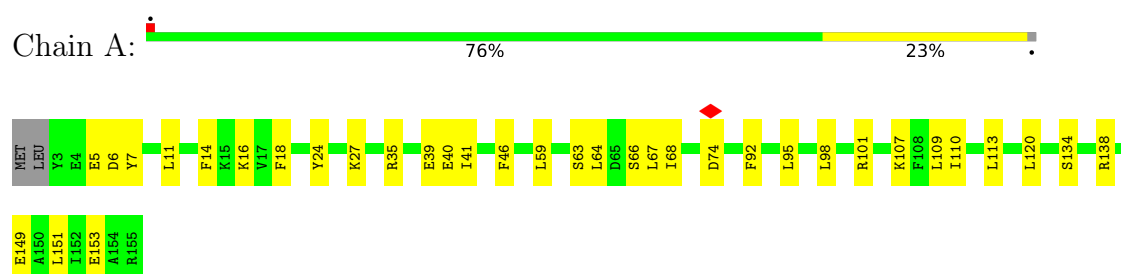
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 10  | K     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

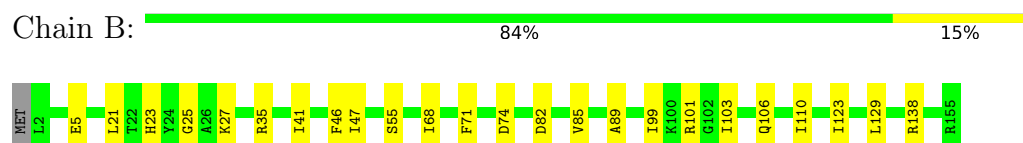
### 3 Residue-property plots [i](#)

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

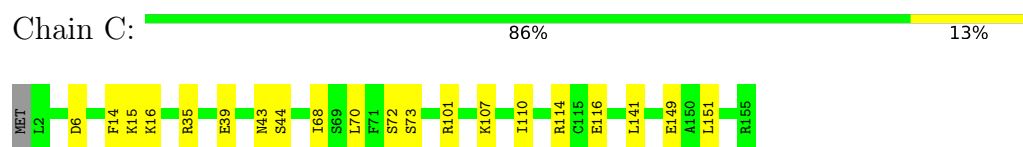
- Molecule 1: CRISPR-associated protein, Cmr5 family



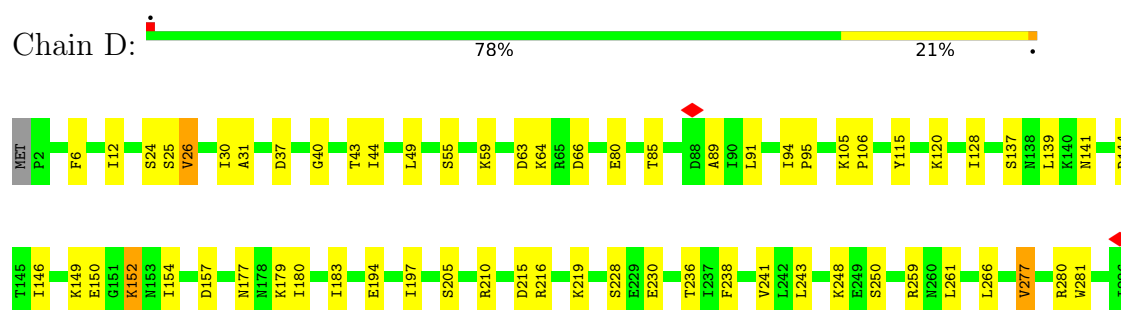
- Molecule 1: CRISPR-associated protein, Cmr5 family



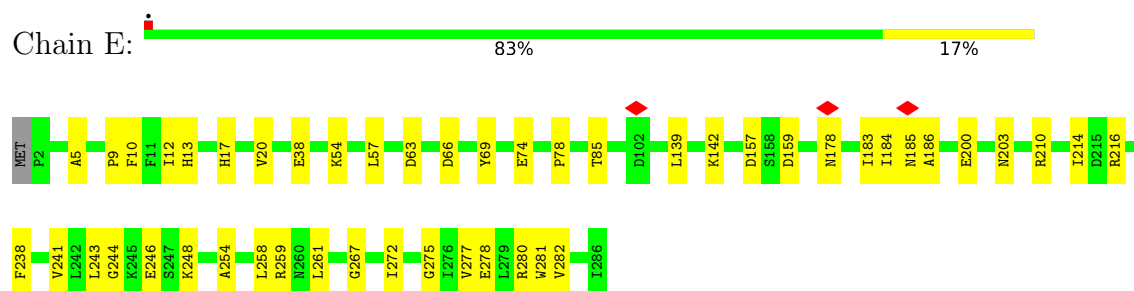
- Molecule 1: CRISPR-associated protein, Cmr5 family



- Molecule 2: CRISPR-associated RAMP protein, Cmr4 family



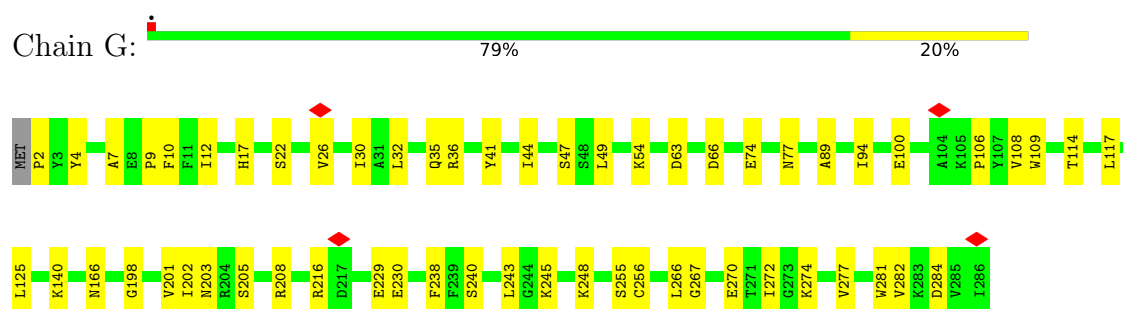
- Molecule 2: CRISPR-associated RAMP protein, Cmr4 family



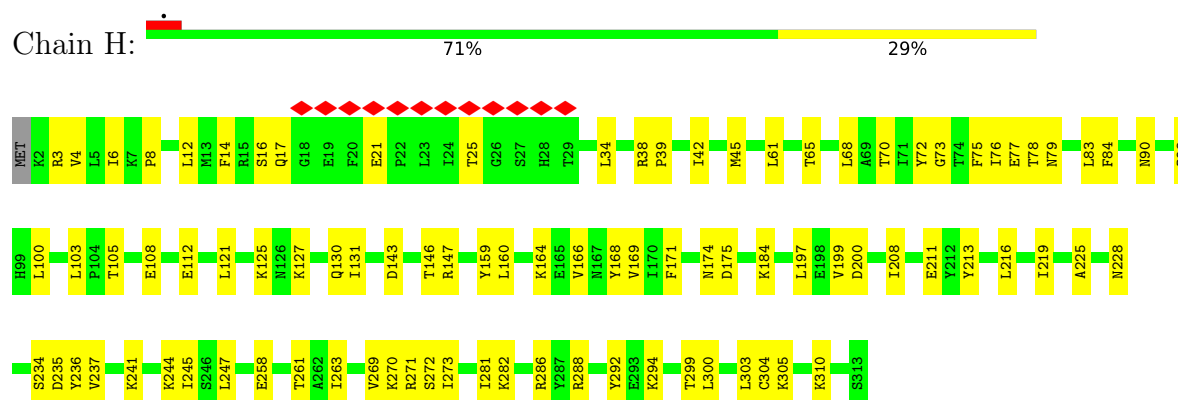
- Molecule 2: CRISPR-associated RAMP protein, Cmr4 family



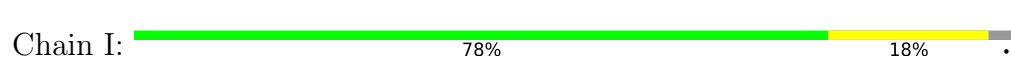
- Molecule 2: CRISPR-associated RAMP protein, Cmr4 family

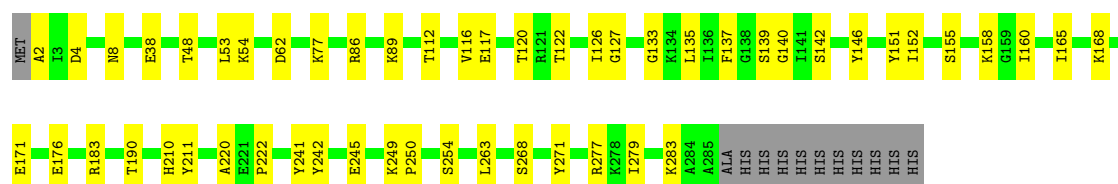


- Molecule 3: CRISPR-associated protein, Cmr3 family

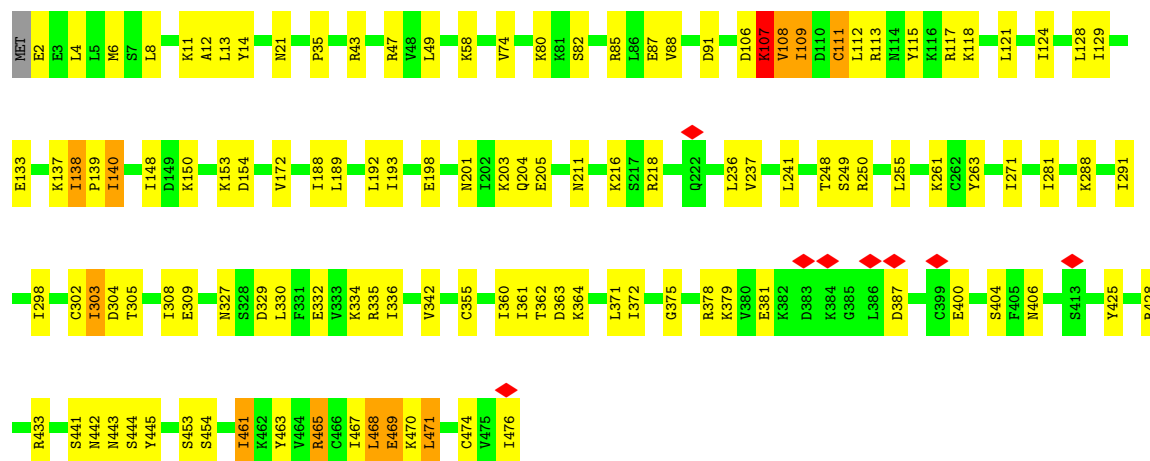


- Molecule 4: CRISPR-associated RAMP protein, Cmr6 family

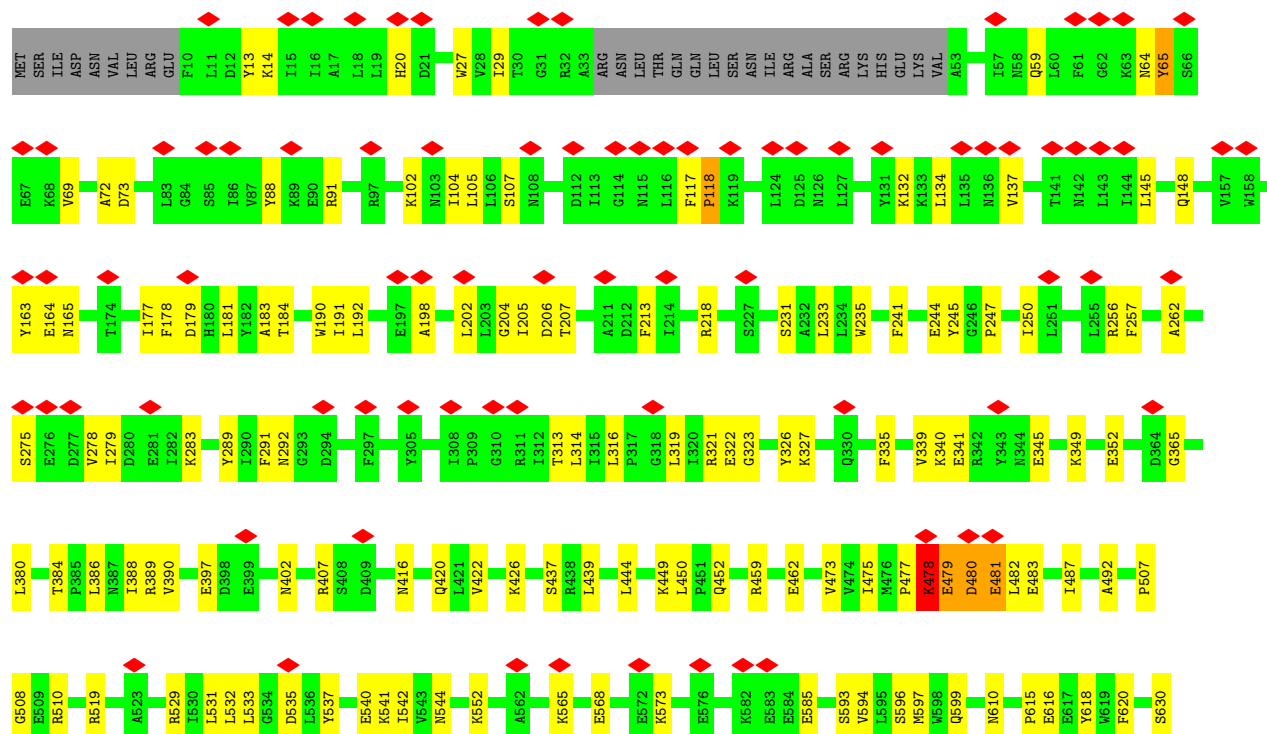
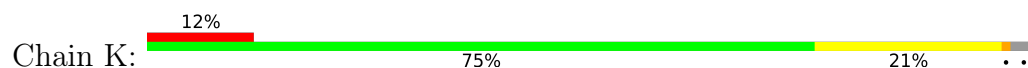


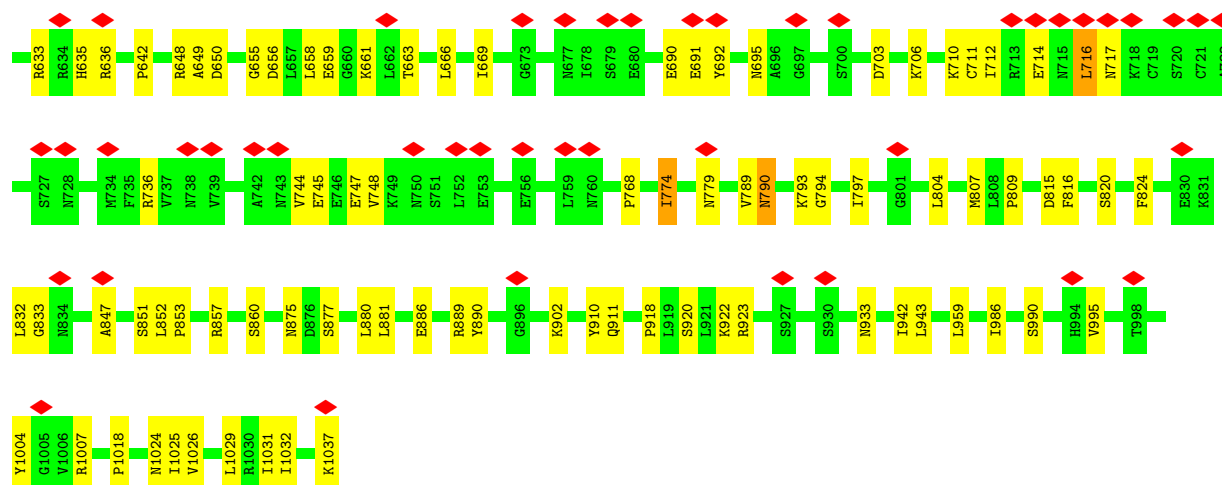


- Molecule 5: CRISPR-associated RAMP protein, Cmr1 family

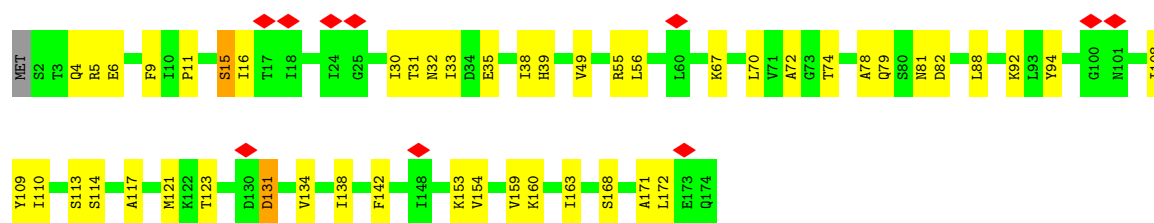


- Molecule 6: CRISPR-associated protein, Cmr2 family

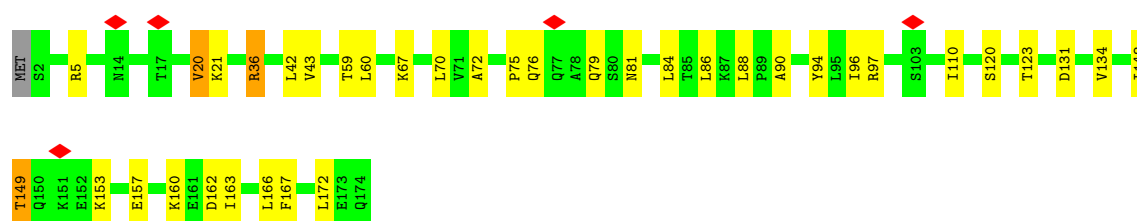
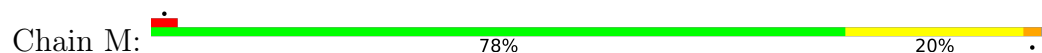




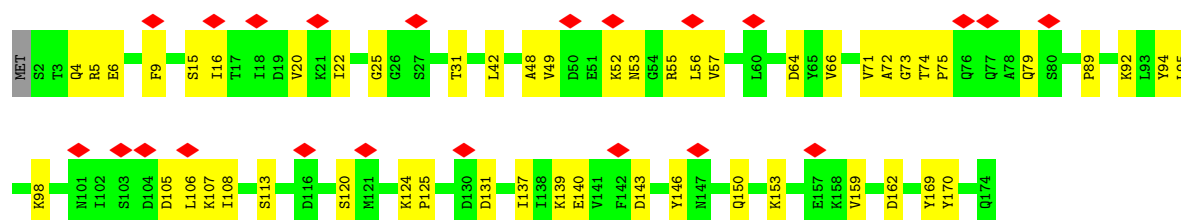
• Molecule 7: CRISPR-associated protein CmrX



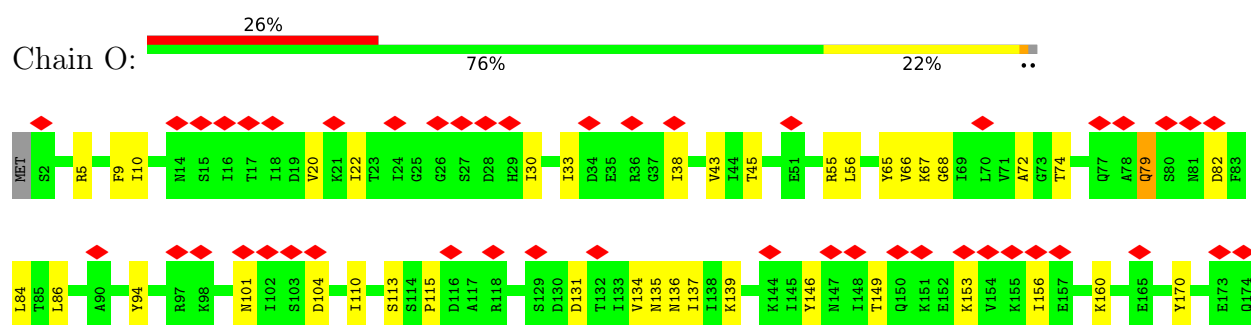
• Molecule 7: CRISPR-associated protein CmrX



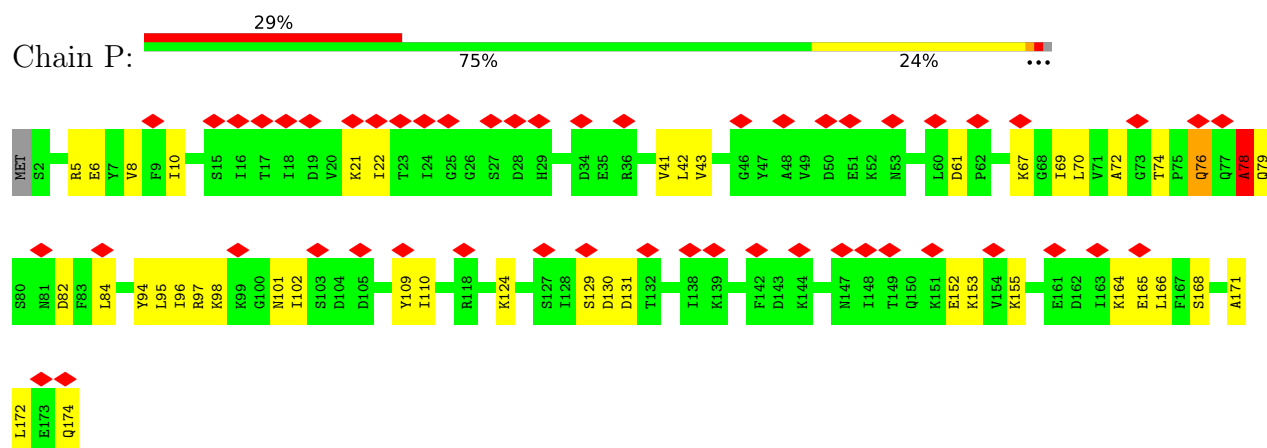
• Molecule 7: CRISPR-associated protein CmrX



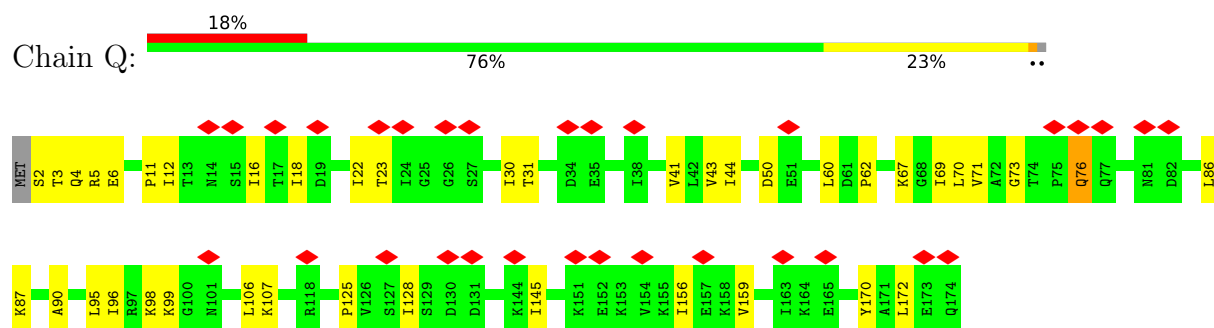
• Molecule 7: CRISPR-associated protein CmrX



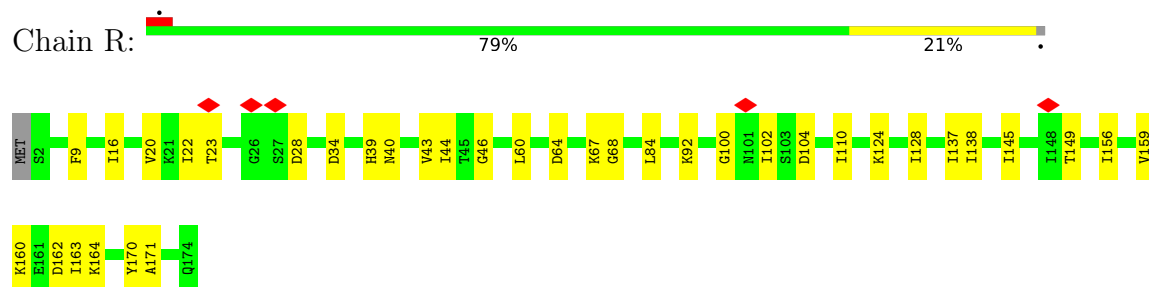
• Molecule 7: CRISPR-associated protein CmrX



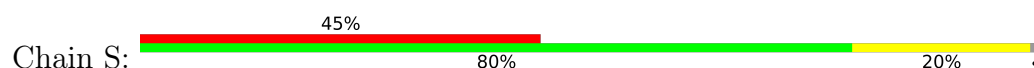
• Molecule 7: CRISPR-associated protein CmrX

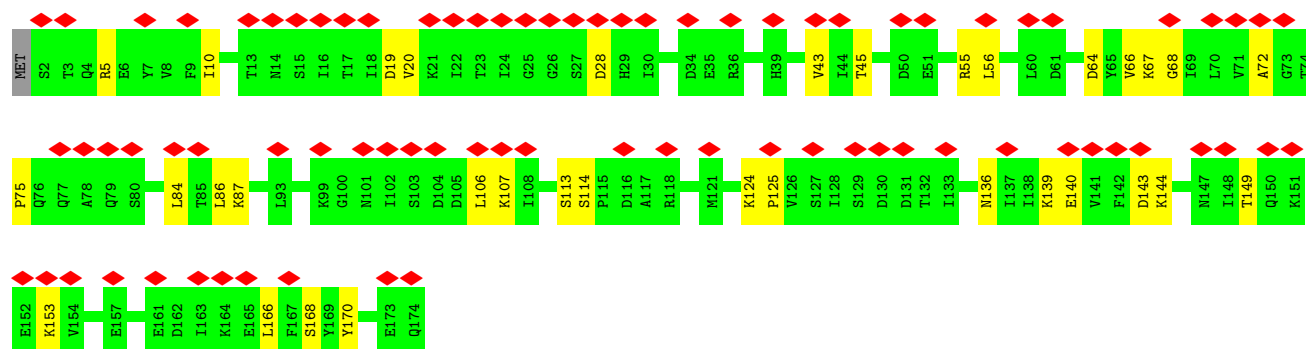


• Molecule 7: CRISPR-associated protein CmrX

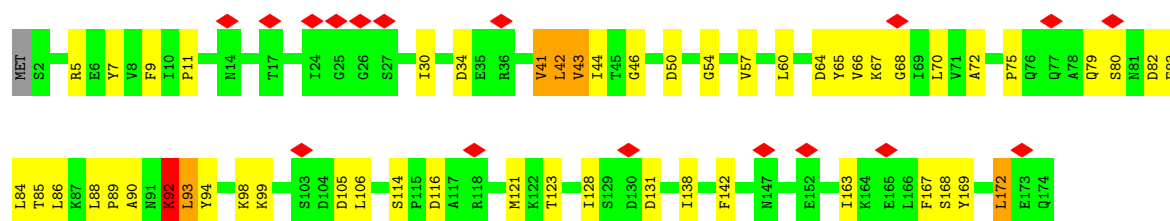


• Molecule 7: CRISPR-associated protein CmrX

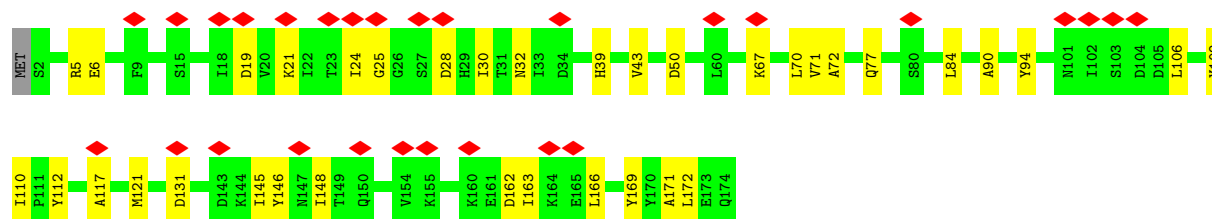
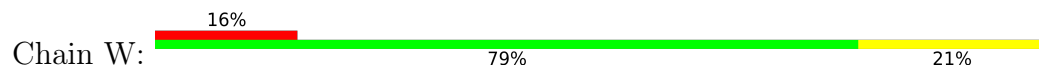




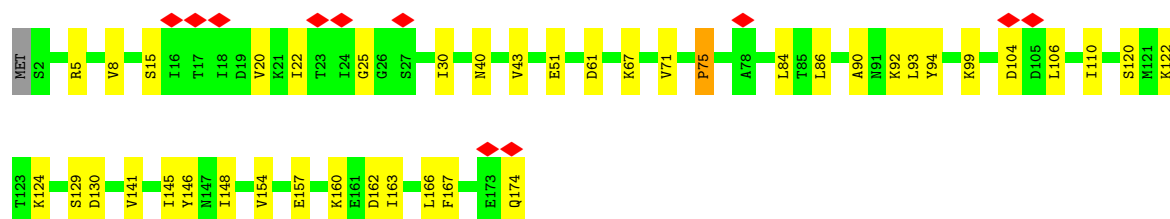
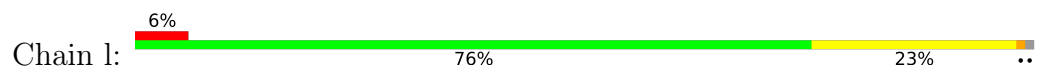
• Molecule 7: CRISPR-associated protein CmrX



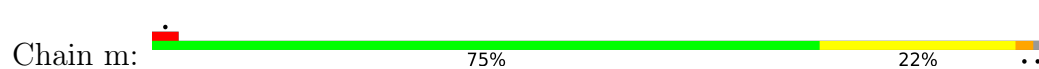
• Molecule 7: CRISPR-associated protein CmrX

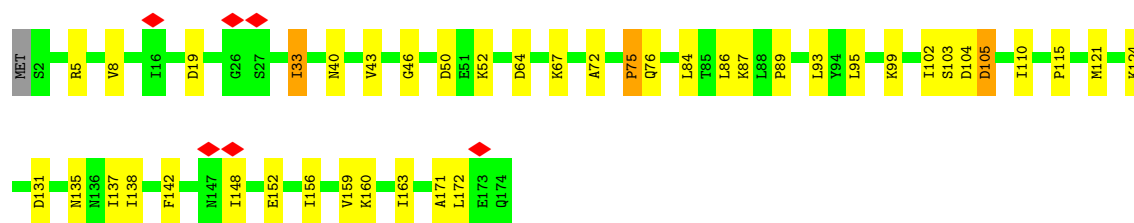


• Molecule 7: CRISPR-associated protein CmrX

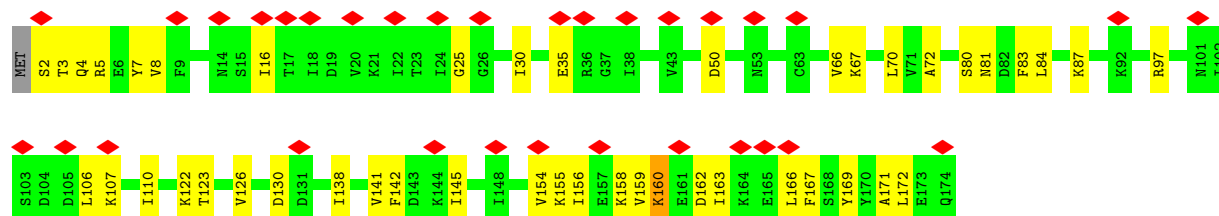
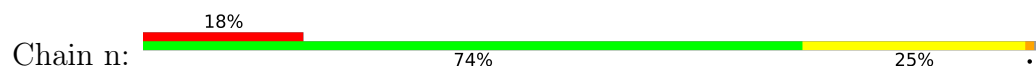


• Molecule 7: CRISPR-associated protein CmrX

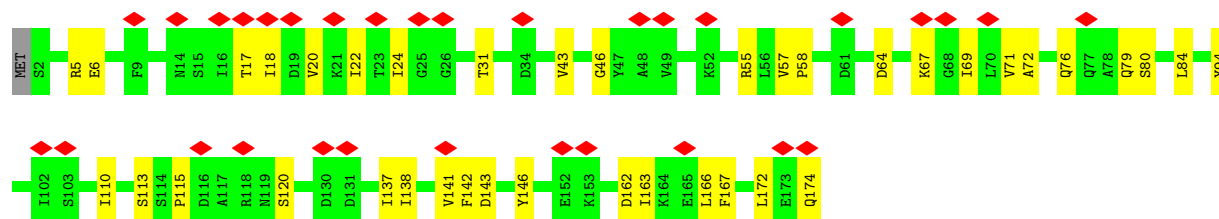
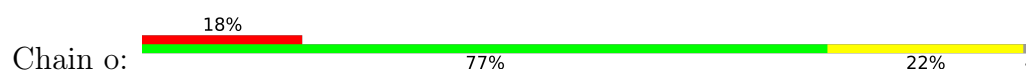




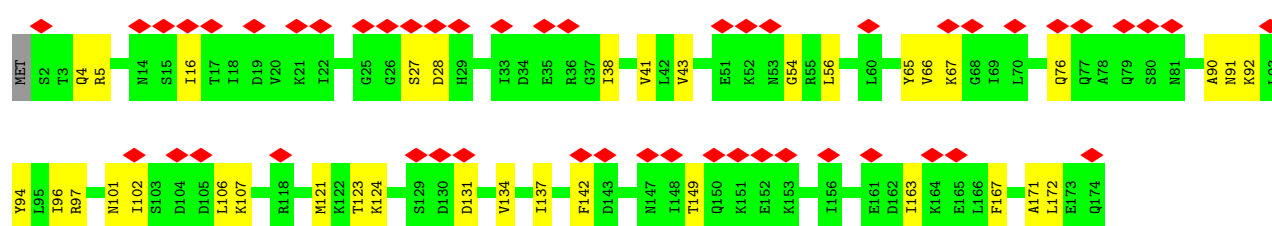
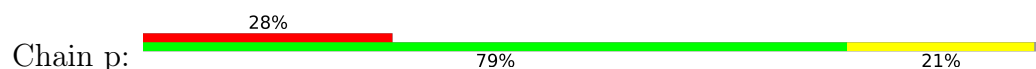
• Molecule 7: CRISPR-associated protein CmrX



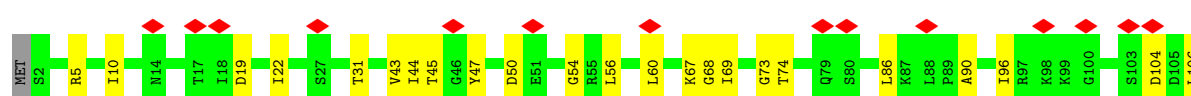
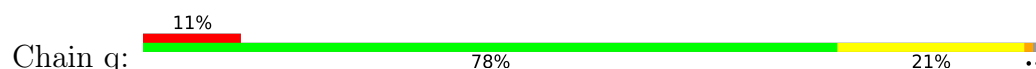
• Molecule 7: CRISPR-associated protein CmrX

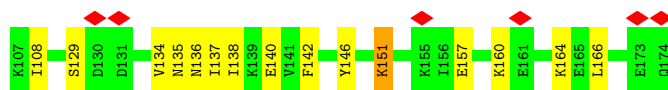


• Molecule 7: CRISPR-associated protein CmrX

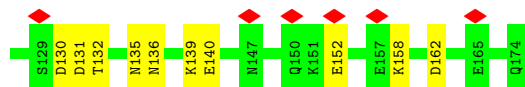
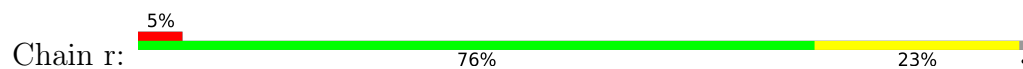


• Molecule 7: CRISPR-associated protein CmrX

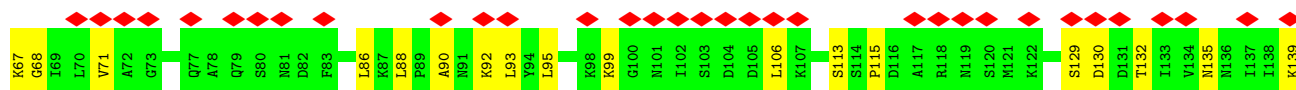
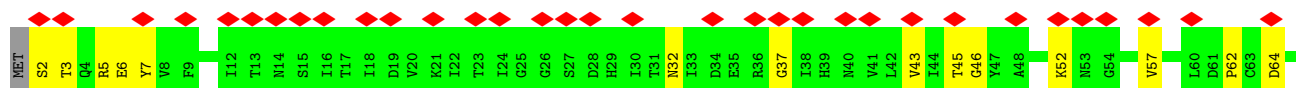
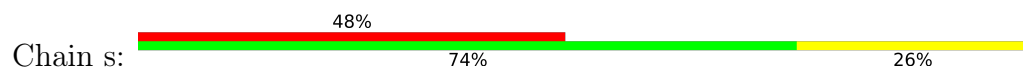




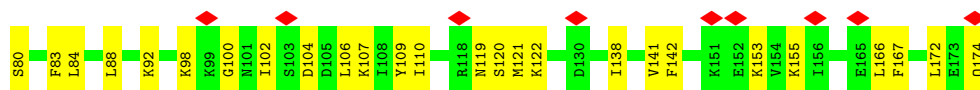
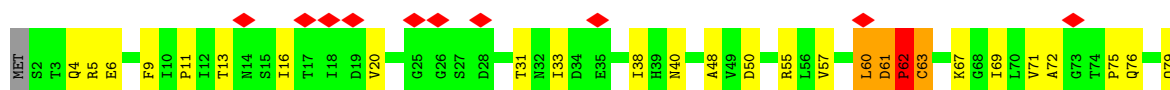
- Molecule 7: CRISPR-associated protein CmrX



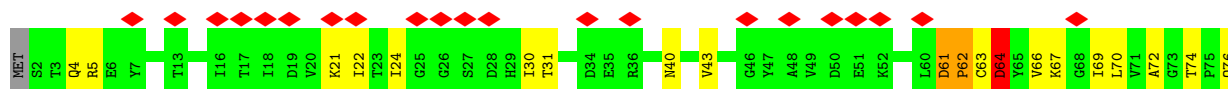
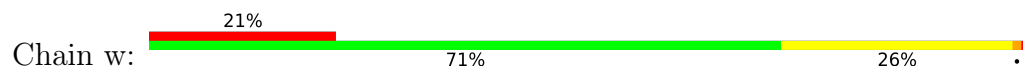
- Molecule 7: CRISPR-associated protein CmrX

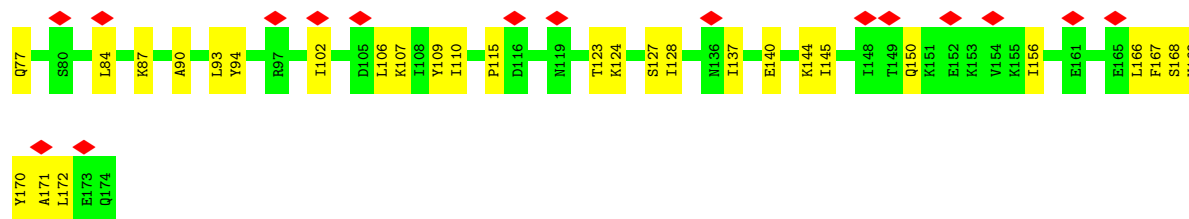


- Molecule 7: CRISPR-associated protein CmrX

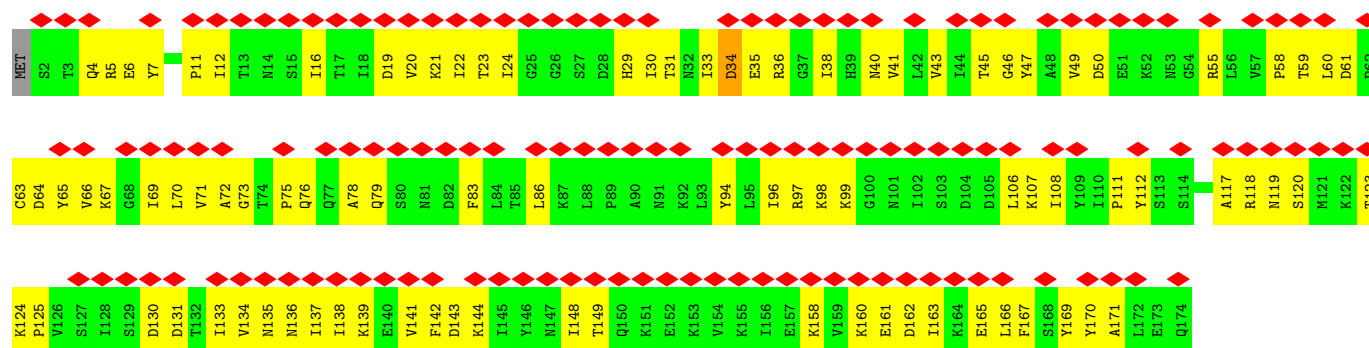
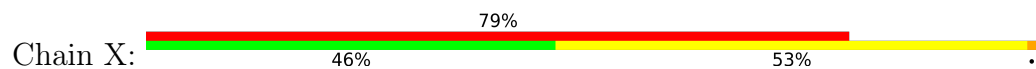


- Molecule 7: CRISPR-associated protein CmrX

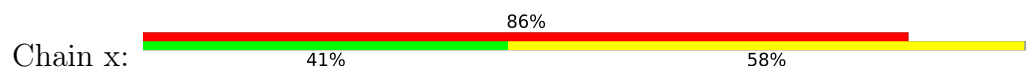




• Molecule 7: CRISPR-associated protein CmrX



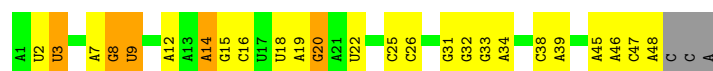
• Molecule 7: CRISPR-associated protein CmrX



• Molecule 8: Cognate target RNA



• Molecule 9: crRNA



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 30455                                   | 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 ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 1700                                    | Depositor |
| Maximum defocus (nm)                 | 2600                                    | Depositor |
| Magnification                        | 96000                                   | Depositor |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 19.604                                  | Depositor |
| Minimum map value                    | -9.825                                  | Depositor |
| Average map value                    | -0.007                                  | Depositor |
| Map value standard deviation         | 0.637                                   | Depositor |
| Recommended contour level            | 2.25                                    | Depositor |
| Map size (Å)                         | 480.0, 480.0, 480.0                     | wwPDB     |
| Map dimensions                       | 480, 480, 480                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.0, 1.0, 1.0                           | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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   | A     | 0.53         | 0/1275        | 0.66        | 0/1716         |
| 1   | B     | 0.51         | 0/1283        | 0.72        | 0/1727         |
| 1   | C     | 0.54         | 0/1283        | 0.66        | 0/1727         |
| 2   | D     | 0.60         | 0/2318        | 0.72        | 2/3134 (0.1%)  |
| 2   | E     | 0.59         | 0/2318        | 0.73        | 1/3134 (0.0%)  |
| 2   | F     | 0.61         | 1/2318 (0.0%) | 0.75        | 0/3134         |
| 2   | G     | 0.53         | 0/2317        | 0.72        | 1/3133 (0.0%)  |
| 3   | H     | 0.40         | 0/2574        | 0.70        | 2/3469 (0.1%)  |
| 4   | I     | 0.55         | 0/2325        | 0.69        | 0/3138         |
| 5   | J     | 0.51         | 0/3956        | 0.81        | 7/5319 (0.1%)  |
| 6   | K     | 0.34         | 0/8452        | 0.72        | 6/11416 (0.1%) |
| 7   | L     | 0.36         | 0/1400        | 0.80        | 1/1895 (0.1%)  |
| 7   | M     | 0.38         | 0/1400        | 0.81        | 3/1895 (0.2%)  |
| 7   | N     | 0.31         | 0/1400        | 0.75        | 0/1895         |
| 7   | O     | 0.30         | 0/1400        | 0.71        | 2/1895 (0.1%)  |
| 7   | P     | 0.33         | 0/1400        | 0.74        | 1/1895 (0.1%)  |
| 7   | Q     | 0.31         | 0/1400        | 0.81        | 2/1895 (0.1%)  |
| 7   | R     | 0.33         | 0/1400        | 0.75        | 2/1895 (0.1%)  |
| 7   | S     | 0.32         | 0/1400        | 0.74        | 0/1895         |
| 7   | T     | 0.35         | 0/1400        | 0.87        | 3/1895 (0.2%)  |
| 7   | W     | 0.31         | 0/1400        | 0.76        | 1/1895 (0.1%)  |
| 7   | X     | 0.19         | 0/1400        | 0.50        | 0/1895         |
| 7   | l     | 0.36         | 0/1400        | 0.78        | 2/1895 (0.1%)  |
| 7   | m     | 0.38         | 0/1400        | 0.82        | 2/1895 (0.1%)  |
| 7   | n     | 0.32         | 0/1400        | 0.83        | 3/1895 (0.2%)  |
| 7   | o     | 0.31         | 0/1400        | 0.81        | 1/1895 (0.1%)  |
| 7   | p     | 0.31         | 0/1400        | 0.77        | 1/1895 (0.1%)  |
| 7   | q     | 0.32         | 0/1400        | 0.80        | 2/1895 (0.1%)  |
| 7   | r     | 0.35         | 0/1400        | 0.78        | 3/1895 (0.2%)  |
| 7   | s     | 0.30         | 0/1400        | 0.81        | 2/1895 (0.1%)  |
| 7   | t     | 0.57         | 1/1400 (0.1%) | 0.90        | 4/1895 (0.2%)  |
| 7   | w     | 0.63         | 2/1400 (0.1%) | 1.05        | 7/1895 (0.4%)  |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 7   | x     | 0.18         | 0/1400         | 0.49        | 0/1895          |
| 8   | U     | 0.48         | 0/989          | 0.49        | 0/1538          |
| 9   | V     | 0.64         | 0/1149         | 0.51        | 0/1789          |
| All | All   | 0.43         | 4/63357 (0.0%) | 0.75        | 61/86064 (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   | D     | 0                   | 1                   |
| 2   | F     | 0                   | 1                   |
| 5   | J     | 0                   | 2                   |
| 6   | K     | 0                   | 5                   |
| 7   | L     | 0                   | 1                   |
| 7   | N     | 0                   | 2                   |
| 7   | P     | 0                   | 2                   |
| 7   | W     | 0                   | 1                   |
| 7   | X     | 0                   | 1                   |
| 7   | m     | 0                   | 1                   |
| 7   | n     | 0                   | 1                   |
| 7   | p     | 0                   | 1                   |
| 7   | q     | 0                   | 1                   |
| 7   | r     | 0                   | 1                   |
| All | All   | 0                   | 21                  |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7   | t     | 62  | PRO  | N-CA  | 17.33 | 1.69        | 1.47     |
| 7   | w     | 62  | PRO  | N-CA  | 17.09 | 1.70        | 1.47     |
| 7   | w     | 61  | ASP  | C-N   | 10.15 | 1.45        | 1.34     |
| 2   | F     | 40  | GLY  | C-N   | -6.77 | 1.20        | 1.33     |

All (61) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | w     | 61  | ASP  | CA-C-N | 18.24 | 138.84      | 119.87   |
| 7   | w     | 61  | ASP  | C-N-CA | 18.24 | 138.84      | 119.87   |
| 7   | t     | 61  | ASP  | CA-C-N | 13.27 | 136.43      | 119.84   |
| 7   | t     | 61  | ASP  | C-N-CA | 13.27 | 136.43      | 119.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | l     | 154 | VAL  | N-CA-C  | -9.73 | 103.99      | 113.53   |
| 7   | n     | 154 | VAL  | N-CA-C  | -8.92 | 104.45      | 113.10   |
| 7   | s     | 52  | LYS  | N-CA-C  | -8.32 | 105.13      | 114.62   |
| 5   | J     | 107 | LYS  | N-CA-C  | -8.06 | 103.04      | 113.12   |
| 2   | E     | 272 | ILE  | N-CA-C  | -8.04 | 104.87      | 112.83   |
| 7   | w     | 62  | PRO  | CA-N-CD | -7.78 | 101.11      | 112.00   |
| 6   | K     | 748 | VAL  | N-CA-C  | -7.19 | 104.26      | 111.88   |
| 7   | L     | 154 | VAL  | N-CA-C  | -7.16 | 104.33      | 111.77   |
| 5   | J     | 362 | THR  | CA-C-N  | 7.12  | 135.14      | 121.54   |
| 5   | J     | 362 | THR  | C-N-CA  | 7.12  | 135.14      | 121.54   |
| 7   | t     | 62  | PRO  | CA-N-CD | -6.87 | 102.38      | 112.00   |
| 6   | K     | 745 | GLU  | N-CA-C  | -6.81 | 104.66      | 114.12   |
| 7   | w     | 62  | PRO  | N-CA-C  | -6.78 | 105.69      | 114.03   |
| 7   | q     | 151 | LYS  | N-CA-C  | -6.59 | 106.19      | 114.56   |
| 5   | J     | 355 | CYS  | N-CA-C  | -6.52 | 106.53      | 114.75   |
| 7   | o     | 24  | ILE  | N-CA-C  | -6.36 | 106.50      | 113.43   |
| 7   | s     | 154 | VAL  | N-CA-C  | -6.36 | 103.39      | 112.35   |
| 7   | n     | 160 | LYS  | CA-C-N  | 6.15  | 130.44      | 120.60   |
| 7   | n     | 160 | LYS  | C-N-CA  | 6.15  | 130.44      | 120.60   |
| 7   | t     | 63  | CYS  | N-CA-C  | -5.98 | 107.81      | 114.62   |
| 7   | Q     | 99  | LYS  | N-CA-C  | -5.93 | 107.27      | 114.75   |
| 7   | m     | 104 | ASP  | CA-C-N  | 5.93  | 132.87      | 121.54   |
| 7   | m     | 104 | ASP  | C-N-CA  | 5.93  | 132.87      | 121.54   |
| 5   | J     | 387 | ASP  | N-CA-C  | -5.78 | 106.87      | 114.04   |
| 5   | J     | 124 | ILE  | CA-C-N  | 5.77  | 130.77      | 122.35   |
| 5   | J     | 124 | ILE  | C-N-CA  | 5.77  | 130.77      | 122.35   |
| 7   | r     | 79  | GLN  | CA-C-N  | 5.70  | 132.71      | 123.93   |
| 7   | r     | 79  | GLN  | C-N-CA  | 5.70  | 132.71      | 123.93   |
| 7   | Q     | 76  | GLN  | N-CA-CB | -5.66 | 107.72      | 114.17   |
| 7   | W     | 19  | ASP  | N-CA-C  | -5.63 | 104.29      | 113.19   |
| 7   | T     | 92  | LYS  | N-CA-C  | -5.59 | 104.65      | 112.25   |
| 7   | r     | 152 | GLU  | N-CA-C  | -5.58 | 107.12      | 114.04   |
| 7   | O     | 79  | GLN  | CA-C-N  | 5.52  | 130.48      | 122.36   |
| 7   | O     | 79  | GLN  | C-N-CA  | 5.52  | 130.48      | 122.36   |
| 2   | G     | 272 | ILE  | N-CA-C  | -5.52 | 105.51      | 113.07   |
| 6   | K     | 473 | VAL  | N-CA-C  | -5.49 | 107.92      | 113.47   |
| 7   | w     | 115 | PRO  | CA-C-N  | 5.36  | 130.43      | 122.82   |
| 7   | w     | 115 | PRO  | C-N-CA  | 5.36  | 130.43      | 122.82   |
| 7   | P     | 78  | ALA  | N-CA-C  | -5.31 | 104.59      | 111.71   |
| 3   | H     | 25  | THR  | N-CA-C  | -5.30 | 108.07      | 114.75   |
| 6   | K     | 478 | LYS  | N-CA-C  | -5.30 | 104.41      | 112.04   |
| 2   | D     | 24  | SER  | N-CA-C  | 5.21  | 117.01      | 110.91   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | p     | 54  | GLY  | N-CA-C  | 5.19  | 118.29      | 111.03   |
| 6   | K     | 365 | GLY  | CA-C-N  | 5.14  | 131.36      | 121.54   |
| 6   | K     | 365 | GLY  | C-N-CA  | 5.14  | 131.36      | 121.54   |
| 7   | M     | 149 | THR  | CA-C-N  | 5.13  | 131.34      | 121.54   |
| 7   | M     | 149 | THR  | C-N-CA  | 5.13  | 131.34      | 121.54   |
| 7   | l     | 15  | SER  | N-CA-C  | -5.11 | 106.29      | 112.88   |
| 7   | T     | 172 | LEU  | CA-C-N  | 5.07  | 131.22      | 121.54   |
| 7   | T     | 172 | LEU  | C-N-CA  | 5.07  | 131.22      | 121.54   |
| 7   | q     | 19  | ASP  | N-CA-C  | -5.06 | 106.95      | 114.64   |
| 7   | R     | 149 | THR  | CA-C-N  | 5.05  | 129.50      | 122.08   |
| 7   | R     | 149 | THR  | C-N-CA  | 5.05  | 129.50      | 122.08   |
| 2   | D     | 26  | VAL  | N-CA-C  | -5.03 | 108.37      | 113.20   |
| 7   | M     | 36  | ARG  | N-CA-C  | -5.01 | 106.09      | 113.61   |
| 7   | w     | 64  | ASP  | CB-CA-C | 5.01  | 118.77      | 109.54   |
| 3   | H     | 146 | THR  | N-CA-C  | -5.00 | 108.91      | 114.62   |

There are no chirality outliers.

All (21) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | D     | 31  | ALA  | Peptide |
| 2   | F     | 105 | LYS  | Peptide |
| 5   | J     | 303 | ILE  | Peptide |
| 5   | J     | 363 | ASP  | Peptide |
| 6   | K     | 118 | PRO  | Peptide |
| 6   | K     | 593 | SER  | Peptide |
| 6   | K     | 65  | TYR  | Peptide |
| 6   | K     | 736 | ARG  | Peptide |
| 6   | K     | 790 | ASN  | Peptide |
| 7   | L     | 15  | SER  | Peptide |
| 7   | N     | 52  | LYS  | Peptide |
| 7   | N     | 53  | ASN  | Peptide |
| 7   | P     | 76  | GLN  | Peptide |
| 7   | P     | 78  | ALA  | Peptide |
| 7   | W     | 50  | ASP  | Peptide |
| 7   | X     | 34  | ASP  | Peptide |
| 7   | m     | 76  | GLN  | Peptide |
| 7   | n     | 130 | ASP  | Peptide |
| 7   | p     | 76  | GLN  | Peptide |
| 7   | q     | 142 | PHE  | Peptide |
| 7   | r     | 103 | SER  | Peptide |

## 5.2 Too-close contacts ⓘ

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   | A     | 1253  | 0        | 1287     | 24      | 0            |
| 1   | B     | 1261  | 0        | 1298     | 16      | 0            |
| 1   | C     | 1261  | 0        | 1298     | 16      | 0            |
| 2   | D     | 2274  | 0        | 2342     | 41      | 0            |
| 2   | E     | 2274  | 0        | 2342     | 32      | 0            |
| 2   | F     | 2274  | 0        | 2342     | 34      | 0            |
| 2   | G     | 2273  | 0        | 2339     | 37      | 0            |
| 3   | H     | 2528  | 0        | 2582     | 82      | 0            |
| 4   | I     | 2282  | 0        | 2331     | 37      | 0            |
| 5   | J     | 3889  | 0        | 3973     | 114     | 0            |
| 6   | K     | 8282  | 0        | 8426     | 131     | 0            |
| 7   | L     | 1378  | 0        | 1418     | 28      | 0            |
| 7   | M     | 1378  | 0        | 1418     | 24      | 0            |
| 7   | N     | 1378  | 0        | 1417     | 30      | 0            |
| 7   | O     | 1378  | 0        | 1417     | 27      | 0            |
| 7   | P     | 1378  | 0        | 1418     | 28      | 0            |
| 7   | Q     | 1378  | 0        | 1417     | 23      | 0            |
| 7   | R     | 1378  | 0        | 1417     | 23      | 0            |
| 7   | S     | 1378  | 0        | 1417     | 21      | 0            |
| 7   | T     | 1378  | 0        | 1418     | 50      | 0            |
| 7   | W     | 1378  | 0        | 1418     | 20      | 0            |
| 7   | X     | 1378  | 0        | 1418     | 96      | 0            |
| 7   | l     | 1378  | 0        | 1417     | 26      | 0            |
| 7   | m     | 1378  | 0        | 1417     | 22      | 0            |
| 7   | n     | 1378  | 0        | 1418     | 27      | 0            |
| 7   | o     | 1378  | 0        | 1418     | 24      | 0            |
| 7   | p     | 1378  | 0        | 1417     | 19      | 0            |
| 7   | q     | 1378  | 0        | 1418     | 26      | 0            |
| 7   | r     | 1378  | 0        | 1418     | 23      | 0            |
| 7   | s     | 1378  | 0        | 1418     | 26      | 0            |
| 7   | t     | 1378  | 0        | 1418     | 38      | 0            |
| 7   | w     | 1378  | 0        | 1417     | 46      | 0            |
| 7   | x     | 1378  | 0        | 1418     | 102     | 0            |
| 8   | U     | 886   | 0        | 450      | 9       | 0            |
| 9   | V     | 1025  | 0        | 520      | 20      | 0            |
| 10  | K     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 62079 | 0        | 62717    | 1203    | 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 10.

All (1203) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:H:108:GLU:CG   | 7:X:94:TYR:HE1   | 1.28                     | 1.42              |
| 7:w:64:ASP:OD1   | 7:w:170:TYR:CD2  | 1.73                     | 1.42              |
| 7:w:62:PRO:N     | 7:w:62:PRO:CA    | 1.70                     | 1.39              |
| 7:w:64:ASP:OD1   | 7:w:170:TYR:CG   | 1.75                     | 1.38              |
| 3:H:108:GLU:HG2  | 7:X:94:TYR:CE1   | 1.57                     | 1.36              |
| 7:t:62:PRO:N     | 7:t:62:PRO:CA    | 1.69                     | 1.35              |
| 3:H:304:CYS:SG   | 7:X:63:CYS:CB    | 2.19                     | 1.29              |
| 3:H:108:GLU:OE2  | 7:X:94:TYR:HD1   | 1.17                     | 1.27              |
| 5:J:360:ILE:HD12 | 5:J:471:LEU:CD2  | 1.68                     | 1.22              |
| 3:H:108:GLU:CG   | 7:X:94:TYR:CE1   | 2.18                     | 1.21              |
| 3:H:108:GLU:OE2  | 7:X:94:TYR:CD1   | 1.95                     | 1.19              |
| 3:H:304:CYS:SG   | 7:X:63:CYS:SG    | 1.33                     | 1.19              |
| 5:J:360:ILE:CD1  | 5:J:471:LEU:CD2  | 2.21                     | 1.19              |
| 5:J:360:ILE:CD1  | 5:J:471:LEU:HD23 | 1.72                     | 1.18              |
| 3:H:79:ASN:OD1   | 7:x:36:ARG:NH1   | 1.79                     | 1.15              |
| 3:H:304:CYS:CB   | 7:X:63:CYS:HB3   | 1.77                     | 1.14              |
| 5:J:107:LYS:HE3  | 5:J:107:LYS:HA   | 1.25                     | 1.14              |
| 7:T:43:VAL:HG22  | 7:T:67:LYS:HG2   | 1.29                     | 1.11              |
| 7:w:64:ASP:OD1   | 7:w:170:TYR:CE2  | 2.03                     | 1.11              |
| 3:H:304:CYS:HB2  | 7:X:63:CYS:HB3   | 1.21                     | 1.10              |
| 5:J:115:TYR:CB   | 5:J:117:ARG:HE   | 1.63                     | 1.10              |
| 3:H:304:CYS:HB2  | 7:X:63:CYS:CB    | 1.82                     | 1.08              |
| 7:w:64:ASP:OD1   | 7:w:170:TYR:CD1  | 2.06                     | 1.08              |
| 7:T:92:LYS:NZ    | 7:t:121:MET:O    | 1.86                     | 1.08              |
| 7:T:89:PRO:HD2   | 7:T:92:LYS:HZ2   | 1.17                     | 1.07              |
| 7:T:43:VAL:CG2   | 7:T:67:LYS:HG2   | 1.83                     | 1.07              |
| 5:J:115:TYR:CB   | 5:J:117:ARG:NE   | 2.11                     | 1.06              |
| 3:H:304:CYS:CB   | 7:X:63:CYS:SG    | 2.42                     | 1.06              |
| 5:J:115:TYR:HB3  | 5:J:117:ARG:NE   | 1.35                     | 1.04              |
| 3:H:304:CYS:CB   | 7:X:63:CYS:CB    | 2.34                     | 1.04              |
| 3:H:105:THR:HG21 | 7:x:63:CYS:SG    | 2.01                     | 1.00              |
| 7:x:123:THR:HA   | 7:x:171:ALA:O    | 1.64                     | 0.97              |
| 5:J:360:ILE:HD13 | 5:J:471:LEU:HD23 | 1.43                     | 0.96              |
| 3:H:108:GLU:CD   | 7:X:94:TYR:CD1   | 2.46                     | 0.92              |
| 5:J:360:ILE:HD12 | 5:J:471:LEU:HD21 | 1.48                     | 0.92              |
| 7:w:64:ASP:CG    | 7:w:170:TYR:CG   | 2.48                     | 0.91              |
| 5:J:404:SER:HG   | 5:J:463:TYR:HD2  | 0.94                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:327:ASN:HD21 | 5:J:461:ILE:HD11 | 1.35                     | 0.90              |
| 5:J:465:ARG:NH1  | 5:J:465:ARG:HB3  | 1.86                     | 0.90              |
| 3:H:108:GLU:HG2  | 7:X:94:TYR:HE1   | 0.72                     | 0.89              |
| 3:H:108:GLU:CD   | 7:X:94:TYR:CE1   | 2.52                     | 0.88              |
| 3:H:304:CYS:SG   | 7:X:63:CYS:HB3   | 2.13                     | 0.86              |
| 6:K:478:LYS:O    | 6:K:478:LYS:NZ   | 2.08                     | 0.85              |
| 5:J:330:LEU:CD1  | 5:J:465:ARG:HG2  | 2.05                     | 0.85              |
| 7:w:64:ASP:OD1   | 7:w:170:TYR:CZ   | 2.30                     | 0.85              |
| 7:X:138:ILE:HA   | 7:X:142:PHE:HB2  | 1.59                     | 0.84              |
| 7:w:64:ASP:OD1   | 7:w:170:TYR:CE1  | 2.31                     | 0.83              |
| 5:J:332:GLU:HG2  | 5:J:469:GLU:CA   | 2.08                     | 0.82              |
| 3:H:305:LYS:HD3  | 7:x:94:TYR:CE2   | 2.14                     | 0.82              |
| 7:T:89:PRO:CD    | 7:T:92:LYS:HZ2   | 1.91                     | 0.82              |
| 5:J:361:ILE:HD11 | 5:J:467:ILE:HD13 | 1.62                     | 0.82              |
| 7:w:64:ASP:CG    | 7:w:170:TYR:CD2  | 2.58                     | 0.82              |
| 7:X:22:ILE:HG21  | 7:X:73:GLY:HA3   | 1.63                     | 0.81              |
| 3:H:305:LYS:HD3  | 7:x:94:TYR:HE2   | 1.47                     | 0.80              |
| 5:J:330:LEU:HD13 | 5:J:465:ARG:HG2  | 1.62                     | 0.80              |
| 7:X:66:VAL:HG22  | 7:X:169:TYR:HB2  | 1.64                     | 0.80              |
| 6:K:478:LYS:HA   | 6:K:478:LYS:HE2  | 1.63                     | 0.80              |
| 6:K:481:GLU:HA   | 6:K:481:GLU:OE1  | 1.80                     | 0.80              |
| 3:H:305:LYS:HB3  | 7:x:94:TYR:CE2   | 2.18                     | 0.79              |
| 5:J:329:ASP:OD2  | 5:J:465:ARG:HG3  | 1.81                     | 0.79              |
| 7:x:87:LYS:HB2   | 7:x:107:LYS:HG2  | 1.65                     | 0.79              |
| 5:J:332:GLU:HG2  | 5:J:469:GLU:HA   | 1.67                     | 0.77              |
| 7:T:89:PRO:HD2   | 7:T:92:LYS:NZ    | 1.98                     | 0.76              |
| 7:x:138:ILE:HA   | 7:x:142:PHE:HB2  | 1.66                     | 0.76              |
| 7:T:94:TYR:HD1   | 7:t:62:PRO:HG3   | 1.51                     | 0.75              |
| 7:X:96:ILE:HG22  | 7:X:97:ARG:HG3   | 1.69                     | 0.74              |
| 3:H:105:THR:CG2  | 7:x:63:CYS:SG    | 2.75                     | 0.74              |
| 7:x:128:ILE:HB   | 7:x:164:LYS:HA   | 1.69                     | 0.73              |
| 5:J:465:ARG:HB3  | 5:J:465:ARG:CZ   | 2.18                     | 0.73              |
| 5:J:404:SER:OG   | 5:J:463:TYR:HD2  | 1.69                     | 0.72              |
| 7:X:5:ARG:HE     | 7:X:30:ILE:HG12  | 1.53                     | 0.72              |
| 3:H:108:GLU:CD   | 7:X:94:TYR:HD1   | 1.90                     | 0.72              |
| 7:X:134:VAL:HG21 | 7:X:163:ILE:HG21 | 1.70                     | 0.71              |
| 7:m:84:LEU:HB2   | 7:m:110:ILE:HB   | 1.73                     | 0.71              |
| 5:J:106:ASP:HA   | 5:J:109:ILE:HG13 | 1.74                     | 0.69              |
| 7:R:9:PHE:HA     | 7:R:68:GLY:HA3   | 1.73                     | 0.69              |
| 7:q:5:ARG:HA     | 7:q:73:GLY:H     | 1.57                     | 0.69              |
| 7:x:31:THR:HG21  | 7:x:69:ILE:HB    | 1.72                     | 0.69              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 7:w:64:ASP:HA   | 7:w:170:TYR:CE2  | 2.27                     | 0.69              |
| 7:X:38:ILE:HD12 | 7:X:41:VAL:HG21  | 1.74                     | 0.69              |
| 7:x:6:GLU:HA    | 7:x:109:TYR:H    | 1.59                     | 0.68              |
| 7:P:43:VAL:HG22 | 7:P:67:LYS:HG2   | 1.75                     | 0.68              |
| 2:D:12:ILE:HB   | 2:D:238:PHE:HB2  | 1.75                     | 0.68              |
| 7:N:75:PRO:HB2  | 7:N:79:GLN:HB2   | 1.76                     | 0.68              |
| 7:N:92:LYS:HE3  | 7:n:122:LYS:HA   | 1.75                     | 0.68              |
| 7:o:5:ARG:HA    | 7:o:72:ALA:HA    | 1.76                     | 0.68              |
| 5:J:115:TYR:HB3 | 5:J:117:ARG:HE   | 0.68                     | 0.67              |
| 7:t:50:ASP:HB3  | 7:t:55:ARG:H     | 1.59                     | 0.67              |
| 6:K:65:TYR:HB3  | 6:K:69:VAL:HG12  | 1.76                     | 0.67              |
| 7:R:20:VAL:HG22 | 7:R:22:ILE:H     | 1.58                     | 0.67              |
| 7:T:43:VAL:HG21 | 7:T:67:LYS:HG2   | 1.74                     | 0.67              |
| 7:X:5:ARG:HG3   | 7:X:106:LEU:HD21 | 1.75                     | 0.67              |
| 7:t:61:ASP:OD2  | 7:t:63:CYS:HB2   | 1.95                     | 0.67              |
| 7:w:137:ILE:HA  | 7:w:140:GLU:HG2  | 1.76                     | 0.66              |
| 1:A:39:GLU:OE1  | 8:U:23:G:N2      | 2.28                     | 0.66              |
| 7:t:84:LEU:HB2  | 7:t:110:ILE:HB   | 1.78                     | 0.65              |
| 5:J:107:LYS:HE3 | 5:J:107:LYS:CA   | 2.16                     | 0.65              |
| 2:D:216:ARG:NH2 | 9:V:32:G:OP2     | 2.29                     | 0.65              |
| 7:P:6:GLU:HG2   | 7:P:109:TYR:HB2  | 1.79                     | 0.65              |
| 7:q:157:GLU:HA  | 7:q:160:LYS:HB3  | 1.79                     | 0.65              |
| 7:S:67:LYS:HD2  | 7:S:168:SER:H    | 1.62                     | 0.65              |
| 7:l:20:VAL:HG22 | 7:l:22:ILE:H     | 1.62                     | 0.64              |
| 7:r:96:ILE:HG22 | 7:r:97:ARG:HG2   | 1.79                     | 0.64              |
| 7:l:20:VAL:HA   | 7:l:75:PRO:HA    | 1.79                     | 0.64              |
| 7:n:163:ILE:HA  | 7:n:167:PHE:HB2  | 1.78                     | 0.64              |
| 2:G:12:ILE:HB   | 2:G:238:PHE:HB2  | 1.79                     | 0.64              |
| 3:H:219:ILE:HB  | 3:H:263:ILE:HB   | 1.80                     | 0.64              |
| 6:K:573:LYS:NZ  | 6:K:635:HIS:O    | 2.31                     | 0.64              |
| 7:t:67:LYS:HD2  | 7:t:167:PHE:HA   | 1.80                     | 0.64              |
| 7:t:62:PRO:N    | 7:t:62:PRO:C     | 2.53                     | 0.64              |
| 7:M:88:LEU:HD12 | 7:M:90:ALA:H     | 1.63                     | 0.64              |
| 7:x:9:PHE:HD1   | 7:x:11:PRO:HD3   | 1.63                     | 0.64              |
| 7:W:5:ARG:HA    | 7:W:72:ALA:HA    | 1.79                     | 0.64              |
| 7:Q:43:VAL:HG22 | 7:Q:67:LYS:HG2   | 1.80                     | 0.63              |
| 5:J:471:LEU:O   | 5:J:474:CYS:N    | 2.28                     | 0.63              |
| 2:F:182:SER:HB3 | 7:M:36:ARG:HH22  | 1.63                     | 0.63              |
| 3:H:305:LYS:CD  | 7:x:94:TYR:HE2   | 2.10                     | 0.63              |
| 7:X:5:ARG:N     | 7:X:107:LYS:O    | 2.29                     | 0.63              |
| 3:H:211:GLU:HA  | 3:H:271:ARG:HB2  | 1.79                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:16:LYS:NZ    | 1:C:70:LEU:O      | 2.31                     | 0.63              |
| 7:M:149:THR:HA   | 7:M:153:LYS:HB2   | 1.81                     | 0.63              |
| 7:O:10:ILE:HG12  | 7:O:68:GLY:HA2    | 1.81                     | 0.63              |
| 7:X:86:LEU:HA    | 7:x:117:ALA:HB2   | 1.80                     | 0.63              |
| 7:S:10:ILE:HG12  | 7:S:68:GLY:HA2    | 1.80                     | 0.62              |
| 7:l:43:VAL:HB    | 7:l:94:TYR:HD2    | 1.64                     | 0.62              |
| 7:q:50:ASP:HB3   | 7:q:54:GLY:HA2    | 1.79                     | 0.62              |
| 7:W:84:LEU:HB2   | 7:W:110:ILE:HB    | 1.81                     | 0.62              |
| 7:T:5:ARG:HA     | 7:T:72:ALA:HA     | 1.81                     | 0.62              |
| 7:p:38:ILE:HD12  | 7:p:41:VAL:HG21   | 1.81                     | 0.62              |
| 7:X:46:GLY:N     | 7:X:64:ASP:O      | 2.26                     | 0.62              |
| 2:F:27:GLU:HG3   | 2:F:28:GLU:HG3    | 1.81                     | 0.62              |
| 3:H:225:ALA:HB1  | 3:H:228:ASN:HB2   | 1.80                     | 0.62              |
| 7:t:102:ILE:HG22 | 7:t:104:ASP:H     | 1.63                     | 0.62              |
| 7:x:12:ILE:HG23  | 7:x:133:ILE:HG12  | 1.81                     | 0.62              |
| 5:J:465:ARG:C    | 5:J:465:ARG:HH11  | 2.07                     | 0.62              |
| 7:M:84:LEU:HB2   | 7:M:110:ILE:HB    | 1.81                     | 0.62              |
| 2:E:12:ILE:HB    | 2:E:238:PHE:HB2   | 1.81                     | 0.62              |
| 7:m:5:ARG:HA     | 7:m:72:ALA:HA     | 1.81                     | 0.62              |
| 3:H:6:ILE:HB     | 3:H:168:TYR:HB2   | 1.82                     | 0.62              |
| 7:p:4:GLN:HB3    | 7:p:107:LYS:HE2   | 1.82                     | 0.62              |
| 7:x:29:HIS:HB2   | 7:x:71:VAL:HA     | 1.82                     | 0.62              |
| 3:H:90:ASN:H     | 3:H:241:LYS:HD2   | 1.65                     | 0.61              |
| 7:x:5:ARG:NH1    | 7:x:28:ASP:O      | 2.32                     | 0.61              |
| 6:K:257:PHE:HB2  | 6:K:779:ASN:HB3   | 1.82                     | 0.61              |
| 7:N:20:VAL:HG22  | 7:N:22:ILE:H      | 1.65                     | 0.61              |
| 5:J:329:ASP:HB3  | 5:J:330:LEU:HD22  | 1.83                     | 0.61              |
| 5:J:330:LEU:HD13 | 5:J:465:ARG:CG    | 2.30                     | 0.61              |
| 7:l:120:SER:O    | 7:l:174:GLN:NE2   | 2.33                     | 0.61              |
| 2:F:203:ASN:OD1  | 2:F:208:ARG:NH2   | 2.33                     | 0.61              |
| 2:E:74:GLU:HB2   | 2:E:78:PRO:HB3    | 1.82                     | 0.61              |
| 7:Q:18:ILE:HG12  | 7:Q:76:GLN:HG3    | 1.82                     | 0.61              |
| 7:T:7:TYR:HD1    | 7:T:42:LEU:HD23   | 1.65                     | 0.61              |
| 2:G:284:ASP:HA   | 7:n:97:ARG:HG2    | 1.83                     | 0.61              |
| 7:T:7:TYR:CD1    | 7:T:42:LEU:HD23   | 2.36                     | 0.60              |
| 7:X:24:ILE:HG23  | 7:X:29:HIS:HE1    | 1.66                     | 0.60              |
| 7:x:137:ILE:HA   | 7:x:140:GLU:HB2   | 1.83                     | 0.60              |
| 6:K:910:TYR:HB2  | 6:K:1031:ILE:HG12 | 1.82                     | 0.60              |
| 7:O:79:GLN:NE2   | 7:O:82:ASP:OD1    | 2.35                     | 0.60              |
| 2:F:12:ILE:HB    | 2:F:238:PHE:HB2   | 1.83                     | 0.60              |
| 7:s:67:LYS:HD2   | 7:s:167:PHE:HA    | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:281:ILE:O    | 5:J:443:ASN:ND2  | 2.35                     | 0.60              |
| 5:J:334:LYS:HB2  | 5:J:476:ILE:HD13 | 1.82                     | 0.60              |
| 7:l:90:ALA:HB3   | 7:l:104:ASP:HA   | 1.82                     | 0.60              |
| 5:J:332:GLU:HG2  | 5:J:469:GLU:CB   | 2.32                     | 0.60              |
| 5:J:335:ARG:NH1  | 5:J:445:TYR:OH   | 2.35                     | 0.60              |
| 7:O:5:ARG:HE     | 7:O:30:ILE:HG13  | 1.67                     | 0.60              |
| 7:q:22:ILE:HB    | 7:q:74:THR:H     | 1.67                     | 0.60              |
| 3:H:108:GLU:OE1  | 7:X:98:LYS:HE3   | 1.99                     | 0.60              |
| 7:X:49:VAL:HG22  | 7:X:171:ALA:HA   | 1.82                     | 0.60              |
| 7:X:70:LEU:HD13  | 7:X:108:ILE:HG12 | 1.84                     | 0.60              |
| 7:X:117:ALA:O    | 7:X:118:ARG:NH2  | 2.28                     | 0.60              |
| 2:G:270:GLU:OE2  | 3:H:147:ARG:NH1  | 2.33                     | 0.60              |
| 3:H:98:GLN:NE2   | 7:x:96:ILE:HG12  | 2.17                     | 0.60              |
| 2:F:177:ASN:HB3  | 2:F:179:LYS:HE2  | 1.83                     | 0.60              |
| 3:H:237:VAL:HG12 | 3:H:269:VAL:HG12 | 1.84                     | 0.60              |
| 7:P:5:ARG:HA     | 7:P:72:ALA:HA    | 1.83                     | 0.60              |
| 7:t:33:ILE:HG13  | 7:t:38:ILE:HG12  | 1.84                     | 0.60              |
| 7:T:50:ASP:HB3   | 7:T:54:GLY:HA2   | 1.83                     | 0.60              |
| 7:x:44:ILE:HD12  | 7:x:47:TYR:HD2   | 1.66                     | 0.60              |
| 2:G:4:TYR:H      | 2:G:245:LYS:HG2  | 1.64                     | 0.60              |
| 7:n:3:THR:OG1    | 7:n:5:ARG:NH1    | 2.35                     | 0.60              |
| 2:E:85:THR:HB    | 2:E:243:LEU:HB2  | 1.84                     | 0.59              |
| 3:H:72:TYR:HB2   | 3:H:171:PHE:HB2  | 1.83                     | 0.59              |
| 7:w:62:PRO:N     | 7:w:62:PRO:C     | 2.57                     | 0.59              |
| 7:w:67:LYS:NZ    | 7:w:166:LEU:O    | 2.34                     | 0.59              |
| 2:E:69:TYR:HB3   | 2:E:74:GLU:HG2   | 1.83                     | 0.59              |
| 3:H:244:LYS:HE2  | 6:K:437:SER:HA   | 1.84                     | 0.59              |
| 7:t:40:ASN:HD21  | 7:t:100:GLY:H    | 1.50                     | 0.59              |
| 7:x:89:PRO:HA    | 7:x:105:ASP:HA   | 1.84                     | 0.59              |
| 3:H:100:LEU:HB3  | 3:H:303:LEU:HD22 | 1.85                     | 0.59              |
| 7:Q:22:ILE:HB    | 7:Q:73:GLY:HA2   | 1.82                     | 0.59              |
| 6:K:712:ILE:O    | 6:K:717:ASN:ND2  | 2.36                     | 0.59              |
| 6:K:860:SER:HB2  | 6:K:880:LEU:HD23 | 1.85                     | 0.59              |
| 7:p:5:ARG:HH22   | 7:p:27:SER:HB2   | 1.66                     | 0.59              |
| 7:m:124:LYS:NZ   | 7:m:172:LEU:O    | 2.33                     | 0.59              |
| 7:x:58:PRO:HG3   | 7:x:112:TYR:HE1  | 1.66                     | 0.59              |
| 7:N:49:VAL:HG21  | 7:N:169:TYR:HB2  | 1.85                     | 0.59              |
| 7:S:84:LEU:HB2   | 7:s:115:PRO:HG2  | 1.85                     | 0.59              |
| 7:X:23:THR:HG22  | 7:X:24:ILE:HG12  | 1.84                     | 0.59              |
| 1:A:67:LEU:HD11  | 1:A:92:PHE:HB2   | 1.85                     | 0.59              |
| 5:J:372:ILE:O    | 5:J:428:ARG:NH2  | 2.36                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:T:43:VAL:HG12  | 7:T:43:VAL:O     | 2.01                     | 0.59              |
| 7:T:89:PRO:HA    | 7:T:105:ASP:HA   | 1.83                     | 0.59              |
| 7:o:20:VAL:HG22  | 7:o:22:ILE:H     | 1.67                     | 0.59              |
| 5:J:87:GLU:HB2   | 5:J:211:ASN:HB2  | 1.84                     | 0.59              |
| 6:K:537:TYR:HB3  | 6:K:541:LYS:HB3  | 1.85                     | 0.59              |
| 7:l:43:VAL:HG22  | 7:l:67:LYS:HG2   | 1.85                     | 0.59              |
| 7:o:18:ILE:HG22  | 7:o:76:GLN:HG3   | 1.85                     | 0.58              |
| 2:D:177:ASN:OD1  | 2:D:179:LYS:NZ   | 2.36                     | 0.58              |
| 7:r:11:PRO:HB2   | 7:r:13:THR:H     | 1.68                     | 0.58              |
| 7:t:88:LEU:HB2   | 7:t:106:LEU:HB2  | 1.84                     | 0.58              |
| 7:o:84:LEU:HB3   | 7:o:110:ILE:HB   | 1.86                     | 0.58              |
| 7:X:34:ASP:O     | 7:X:36:ARG:N     | 2.36                     | 0.58              |
| 3:H:98:GLN:HE21  | 7:x:96:ILE:HG12  | 1.68                     | 0.58              |
| 7:l:162:ASP:O    | 7:l:166:LEU:N    | 2.36                     | 0.58              |
| 1:A:120:LEU:HD13 | 1:C:15:LYS:HG3   | 1.84                     | 0.58              |
| 5:J:201:ASN:OD1  | 5:J:203:LYS:NZ   | 2.36                     | 0.58              |
| 7:n:162:ASP:O    | 7:n:167:PHE:N    | 2.36                     | 0.58              |
| 7:s:32:ASN:HB2   | 7:s:99:LYS:HZ1   | 1.67                     | 0.58              |
| 1:B:68:ILE:HG23  | 1:B:110:ILE:HD12 | 1.85                     | 0.58              |
| 6:K:666:LEU:HB3  | 6:K:669:ILE:HB   | 1.85                     | 0.58              |
| 3:H:299:THR:OG1  | 3:H:310:LYS:NZ   | 2.36                     | 0.58              |
| 7:P:129:SER:HA   | 7:P:164:LYS:HE3  | 1.85                     | 0.58              |
| 7:x:7:TYR:HE1    | 7:x:42:LEU:HB3   | 1.67                     | 0.58              |
| 7:X:133:ILE:O    | 7:X:137:ILE:HG12 | 2.04                     | 0.58              |
| 3:H:208:ILE:O    | 3:H:213:TYR:OH   | 2.20                     | 0.57              |
| 5:J:360:ILE:HD12 | 5:J:471:LEU:HD22 | 1.76                     | 0.57              |
| 5:J:4:LEU:HD23   | 7:p:91:ASN:HD22  | 1.69                     | 0.57              |
| 6:K:478:LYS:CE   | 6:K:507:PRO:O    | 2.52                     | 0.57              |
| 2:E:157:ASP:O    | 2:E:178:ASN:ND2  | 2.36                     | 0.57              |
| 2:E:214:ILE:O    | 2:E:216:ARG:NH1  | 2.37                     | 0.57              |
| 6:K:218:ARG:HB2  | 6:K:519:ARG:HH22 | 1.69                     | 0.57              |
| 2:D:43:THR:OG1   | 2:D:89:ALA:O     | 2.19                     | 0.57              |
| 7:x:40:ASN:H     | 7:x:97:ARG:HB2   | 1.69                     | 0.57              |
| 2:D:49:LEU:HD11  | 2:D:89:ALA:HB2   | 1.85                     | 0.57              |
| 7:L:121:MET:HE3  | 7:L:172:LEU:HD21 | 1.85                     | 0.57              |
| 7:s:57:VAL:HG22  | 7:s:113:SER:HB2  | 1.86                     | 0.57              |
| 3:H:234:SER:O    | 3:H:270:LYS:NZ   | 2.36                     | 0.57              |
| 7:x:17:THR:HG23  | 7:x:18:ILE:H     | 1.69                     | 0.57              |
| 6:K:816:PHE:O    | 6:K:820:SER:N    | 2.37                     | 0.57              |
| 7:P:96:ILE:HG22  | 7:P:97:ARG:HG3   | 1.86                     | 0.57              |
| 7:T:43:VAL:HG22  | 7:T:67:LYS:CG    | 2.18                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:q:43:VAL:HG22  | 7:q:67:LYS:HG2   | 1.87                     | 0.57              |
| 7:t:120:SER:O    | 7:t:174:GLN:NE2  | 2.38                     | 0.57              |
| 4:I:86:ARG:O     | 4:I:89:LYS:NZ    | 2.34                     | 0.57              |
| 4:I:117:GLU:OE1  | 4:I:277:ARG:NH1  | 2.38                     | 0.57              |
| 5:J:91:ASP:OD2   | 7:p:101:ASN:ND2  | 2.37                     | 0.57              |
| 6:K:165:ASN:HB2  | 6:K:847:ALA:HB1  | 1.87                     | 0.57              |
| 7:X:130:ASP:O    | 7:X:133:ILE:N    | 2.31                     | 0.57              |
| 2:D:6:PHE:HE1    | 2:D:250:SER:HB3  | 1.70                     | 0.57              |
| 2:F:259:ARG:HG3  | 7:M:94:TYR:HE1   | 1.69                     | 0.57              |
| 7:q:96:ILE:HD11  | 7:q:166:LEU:HD21 | 1.87                     | 0.57              |
| 7:t:20:VAL:HA    | 7:t:75:PRO:HA    | 1.87                     | 0.57              |
| 7:X:162:ASP:HA   | 7:X:165:GLU:HG2  | 1.86                     | 0.57              |
| 5:J:304:ASP:N    | 5:J:304:ASP:OD1  | 2.38                     | 0.56              |
| 7:s:172:LEU:HD12 | 7:s:174:GLN:H    | 1.69                     | 0.56              |
| 7:P:84:LEU:HD23  | 7:P:110:ILE:HD11 | 1.85                     | 0.56              |
| 7:x:133:ILE:HA   | 7:x:136:ASN:HD21 | 1.70                     | 0.56              |
| 2:G:36:ARG:NH2   | 2:G:230:GLU:OE1  | 2.38                     | 0.56              |
| 6:K:690:GLU:OE2  | 6:K:710:LYS:NZ   | 2.39                     | 0.56              |
| 7:L:6:GLU:HA     | 7:L:109:TYR:H    | 1.70                     | 0.56              |
| 7:T:7:TYR:CD1    | 7:T:42:LEU:CD2   | 2.89                     | 0.56              |
| 7:T:65:TYR:HE2   | 7:T:67:LYS:HE2   | 1.69                     | 0.56              |
| 7:q:31:THR:O     | 7:q:146:TYR:OH   | 2.19                     | 0.56              |
| 7:w:63:CYS:SG    | 7:w:170:TYR:OH   | 2.61                     | 0.56              |
| 7:X:38:ILE:HD11  | 7:X:166:LEU:HG   | 1.88                     | 0.56              |
| 2:E:38:GLU:OE2   | 2:F:235:LYS:NZ   | 2.38                     | 0.56              |
| 2:G:44:ILE:HB    | 2:G:89:ALA:HB3   | 1.88                     | 0.56              |
| 7:o:31:THR:O     | 7:o:146:TYR:OH   | 2.24                     | 0.56              |
| 3:H:3:ARG:NH1    | 3:H:77:GLU:OE1   | 2.39                     | 0.56              |
| 7:W:5:ARG:NH2    | 7:W:28:ASP:OD2   | 2.38                     | 0.56              |
| 7:w:90:ALA:HA    | 7:w:93:LEU:HD13  | 1.88                     | 0.56              |
| 7:Q:4:GLN:HG2    | 7:Q:107:LYS:HB3  | 1.87                     | 0.56              |
| 2:D:105:LYS:HD3  | 2:D:106:PRO:HD2  | 1.86                     | 0.56              |
| 2:D:259:ARG:HH11 | 7:o:94:TYR:HE1   | 1.54                     | 0.56              |
| 2:E:9:PRO:HA     | 2:E:241:VAL:HA   | 1.88                     | 0.56              |
| 3:H:4:VAL:HG22   | 3:H:199:VAL:HG22 | 1.88                     | 0.56              |
| 4:I:77:LYS:NZ    | 8:U:12:G:OP2     | 2.38                     | 0.56              |
| 7:x:12:ILE:HD11  | 7:x:129:SER:H    | 1.71                     | 0.56              |
| 6:K:13:TYR:OH    | 6:K:64:ASN:ND2   | 2.39                     | 0.56              |
| 6:K:105:LEU:HD12 | 6:K:853:PRO:HD2  | 1.88                     | 0.56              |
| 7:s:37:GLY:HA2   | 7:s:159:VAL:HG23 | 1.86                     | 0.56              |
| 7:s:141:VAL:HA   | 7:s:144:LYS:HE3  | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:t:11:PRO:HB2   | 7:t:13:THR:H     | 1.71                     | 0.56              |
| 7:X:5:ARG:HA     | 7:X:72:ALA:HA    | 1.87                     | 0.56              |
| 7:R:102:ILE:HG22 | 7:R:104:ASP:H    | 1.71                     | 0.56              |
| 7:r:42:LEU:HD13  | 7:r:93:LEU:HD12  | 1.86                     | 0.56              |
| 6:K:104:ILE:O    | 6:K:692:TYR:OH   | 2.19                     | 0.56              |
| 7:L:5:ARG:HA     | 7:L:72:ALA:HA    | 1.87                     | 0.56              |
| 7:N:64:ASP:HA    | 7:N:170:TYR:HD2  | 1.70                     | 0.56              |
| 7:Q:87:LYS:HA    | 7:Q:107:LYS:HA   | 1.88                     | 0.56              |
| 7:X:6:GLU:O      | 7:X:70:LEU:HA    | 2.06                     | 0.56              |
| 2:D:266:LEU:HD12 | 2:D:277:VAL:HG21 | 1.88                     | 0.55              |
| 6:K:59:GLN:HB3   | 6:K:132:LYS:HE3  | 1.88                     | 0.55              |
| 7:O:45:THR:HA    | 7:O:65:TYR:HA    | 1.88                     | 0.55              |
| 7:O:136:ASN:HA   | 7:O:139:LYS:HB2  | 1.88                     | 0.55              |
| 7:O:146:TYR:O    | 7:O:149:THR:OG1  | 2.24                     | 0.55              |
| 7:o:138:ILE:O    | 7:o:143:ASP:N    | 2.38                     | 0.55              |
| 6:K:72:ALA:HB2   | 6:K:191:ILE:HG13 | 1.88                     | 0.55              |
| 6:K:459:ARG:NH2  | 6:K:462:GLU:OE1  | 2.35                     | 0.55              |
| 7:P:10:ILE:HD11  | 7:P:69:ILE:HG12  | 1.88                     | 0.55              |
| 7:X:31:THR:HG21  | 7:X:69:ILE:HG23  | 1.88                     | 0.55              |
| 7:X:119:ASN:C    | 7:x:87:LYS:HE3   | 2.31                     | 0.55              |
| 6:K:478:LYS:HE2  | 6:K:507:PRO:O    | 2.06                     | 0.55              |
| 7:s:90:ALA:HA    | 7:s:93:LEU:HD13  | 1.88                     | 0.55              |
| 7:t:4:GLN:NE2    | 7:t:109:TYR:OH   | 2.39                     | 0.55              |
| 7:X:11:PRO:HD2   | 7:X:16:ILE:HD11  | 1.88                     | 0.55              |
| 2:E:200:GLU:OE2  | 2:E:203:ASN:ND2  | 2.40                     | 0.55              |
| 5:J:107:LYS:HA   | 5:J:107:LYS:CE   | 2.11                     | 0.55              |
| 5:J:107:LYS:HG2  | 7:T:94:TYR:HA    | 1.87                     | 0.55              |
| 7:L:88:LEU:HD12  | 7:L:108:ILE:HD13 | 1.89                     | 0.55              |
| 7:S:5:ARG:HH22   | 7:S:28:ASP:HB3   | 1.72                     | 0.55              |
| 7:T:163:ILE:HA   | 7:T:167:PHE:HD2  | 1.71                     | 0.55              |
| 7:n:25:GLY:H     | 7:n:72:ALA:HB1   | 1.70                     | 0.55              |
| 7:x:133:ILE:O    | 7:x:137:ILE:HG13 | 2.06                     | 0.55              |
| 7:n:50:ASP:HA    | 7:n:172:LEU:HD12 | 1.89                     | 0.55              |
| 5:J:400:GLU:OE2  | 5:J:406:ASN:ND2  | 2.40                     | 0.55              |
| 6:K:691:GLU:O    | 6:K:695:ASN:ND2  | 2.40                     | 0.55              |
| 6:K:793:LYS:HB2  | 6:K:809:PRO:HG3  | 1.89                     | 0.55              |
| 7:L:55:ARG:NH1   | 7:L:82:ASP:OD2   | 2.40                     | 0.55              |
| 7:R:60:LEU:HD22  | 7:r:44:ILE:HD12  | 1.89                     | 0.55              |
| 7:t:67:LYS:NZ    | 7:t:166:LEU:O    | 2.35                     | 0.55              |
| 2:G:2:PRO:O      | 3:H:184:LYS:NZ   | 2.32                     | 0.54              |
| 5:J:21:ASN:ND2   | 5:J:198:GLU:OE1  | 2.40                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:K:537:TYR:HB2  | 6:K:542:ILE:HG13 | 1.88                     | 0.54              |
| 6:K:599:GLN:OE1  | 6:K:790:ASN:ND2  | 2.40                     | 0.54              |
| 7:P:21:LYS:HE3   | 7:P:76:GLN:HA    | 1.89                     | 0.54              |
| 7:S:64:ASP:HA    | 7:S:170:TYR:HD2  | 1.72                     | 0.54              |
| 7:s:5:ARG:HH11   | 7:s:106:LEU:HB3  | 1.72                     | 0.54              |
| 7:t:5:ARG:HA     | 7:t:72:ALA:HA    | 1.89                     | 0.54              |
| 7:x:133:ILE:HA   | 7:x:136:ASN:ND2  | 2.23                     | 0.54              |
| 3:H:235:ASP:O    | 3:H:272:SER:OG   | 2.24                     | 0.54              |
| 5:J:453:SER:OG   | 5:J:454:SER:N    | 2.38                     | 0.54              |
| 7:N:150:GLN:H    | 7:N:153:LYS:HB2  | 1.70                     | 0.54              |
| 7:T:57:VAL:HG11  | 7:T:172:LEU:HD13 | 1.89                     | 0.54              |
| 7:T:138:ILE:HA   | 7:T:142:PHE:HB2  | 1.90                     | 0.54              |
| 7:L:15:SER:H     | 7:L:16:ILE:HG23  | 1.72                     | 0.54              |
| 7:X:5:ARG:HG2    | 7:X:106:LEU:HD11 | 1.88                     | 0.54              |
| 7:X:86:LEU:HD12  | 7:x:121:MET:HE3  | 1.88                     | 0.54              |
| 6:K:450:LEU:HD23 | 6:K:452:GLN:HE21 | 1.73                     | 0.54              |
| 7:L:32:ASN:HB2   | 7:L:39:HIS:HB2   | 1.88                     | 0.54              |
| 7:R:60:LEU:HD11  | 7:r:110:ILE:HD11 | 1.90                     | 0.54              |
| 7:m:46:GLY:N     | 7:m:64:ASP:O     | 2.40                     | 0.54              |
| 7:x:31:THR:HA    | 7:x:40:ASN:HB2   | 1.89                     | 0.54              |
| 7:N:55:ARG:HB2   | 7:N:113:SER:HB2  | 1.90                     | 0.54              |
| 7:m:43:VAL:HG22  | 7:m:67:LYS:HG2   | 1.90                     | 0.54              |
| 7:X:12:ILE:N     | 7:X:169:TYR:OH   | 2.41                     | 0.54              |
| 2:D:128:ILE:HG21 | 2:D:241:VAL:HG11 | 1.90                     | 0.54              |
| 7:L:78:ALA:O     | 7:L:81:ASN:ND2   | 2.41                     | 0.54              |
| 2:E:159:ASP:OD1  | 2:E:159:ASP:N    | 2.38                     | 0.54              |
| 7:P:153:LYS:HB3  | 7:P:155:LYS:HG2  | 1.90                     | 0.54              |
| 5:J:465:ARG:HB3  | 5:J:465:ARG:HH11 | 1.70                     | 0.54              |
| 6:K:102:LYS:HD3  | 6:K:107:SER:HB3  | 1.90                     | 0.54              |
| 7:X:120:SER:OG   | 7:x:105:ASP:OD2  | 2.16                     | 0.54              |
| 7:x:148:ILE:HD12 | 7:x:148:ILE:H    | 1.72                     | 0.54              |
| 1:C:44:SER:HB3   | 4:I:135:LEU:HD11 | 1.90                     | 0.54              |
| 5:J:330:LEU:HD12 | 5:J:465:ARG:HG2  | 1.90                     | 0.54              |
| 6:K:349:LYS:HA   | 6:K:352:GLU:HG2  | 1.90                     | 0.54              |
| 6:K:478:LYS:HE2  | 6:K:507:PRO:C    | 2.33                     | 0.54              |
| 7:T:41:VAL:HG22  | 7:T:68:GLY:O     | 2.06                     | 0.54              |
| 7:r:43:VAL:HG22  | 7:r:67:LYS:HG2   | 1.90                     | 0.54              |
| 2:F:48:SER:OG    | 9:V:15:G:OP1     | 2.26                     | 0.53              |
| 4:I:126:ILE:HG12 | 4:I:152:ILE:HG12 | 1.89                     | 0.53              |
| 7:N:106:LEU:HD13 | 7:N:108:ILE:HD11 | 1.88                     | 0.53              |
| 7:t:98:LYS:O     | 8:U:4:U:O2'      | 2.27                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:x:33:ILE:HG13  | 7:x:38:ILE:HA     | 1.91                     | 0.53              |
| 7:Q:3:THR:O      | 7:Q:5:ARG:NH1     | 2.42                     | 0.53              |
| 7:T:114:SER:OG   | 7:T:116:ASP:OD1   | 2.26                     | 0.53              |
| 7:W:5:ARG:NH2    | 7:W:28:ASP:O      | 2.41                     | 0.53              |
| 7:N:31:THR:O     | 7:N:146:TYR:OH    | 2.24                     | 0.53              |
| 7:r:136:ASN:O    | 7:r:140:GLU:N     | 2.39                     | 0.53              |
| 7:w:64:ASP:OD2   | 7:w:123:THR:HG21  | 2.08                     | 0.53              |
| 7:X:165:GLU:HG3  | 7:X:166:LEU:HD22  | 1.89                     | 0.53              |
| 7:x:155:LYS:HE2  | 7:x:158:LYS:HD2   | 1.90                     | 0.53              |
| 5:J:112:LEU:CD1  | 5:J:189:LEU:HD11  | 2.38                     | 0.53              |
| 7:R:44:ILE:HG12  | 7:r:60:LEU:HD13   | 1.90                     | 0.53              |
| 7:W:162:ASP:O    | 7:W:166:LEU:N     | 2.35                     | 0.53              |
| 7:l:5:ARG:HE     | 7:l:30:ILE:HG13   | 1.72                     | 0.53              |
| 7:w:64:ASP:HA    | 7:w:170:TYR:CD2   | 2.44                     | 0.53              |
| 7:w:67:LYS:HG3   | 7:w:167:PHE:HA    | 1.91                     | 0.53              |
| 7:x:6:GLU:HG3    | 7:x:71:VAL:O      | 2.08                     | 0.53              |
| 7:x:7:TYR:CE1    | 7:x:42:LEU:HB3    | 2.43                     | 0.53              |
| 7:x:122:LYS:HB3  | 7:x:173:GLU:HB2   | 1.90                     | 0.53              |
| 5:J:336:ILE:HA   | 5:J:476:ILE:HD11  | 1.91                     | 0.53              |
| 7:S:19:ASP:OD1   | 7:S:144:LYS:NZ    | 2.42                     | 0.53              |
| 2:D:55:SER:O     | 2:D:59:LYS:NZ     | 2.39                     | 0.53              |
| 5:J:249:SER:OG   | 5:J:250:ARG:NH1   | 2.41                     | 0.53              |
| 6:K:1018:PRO:HD2 | 6:K:1024:ASN:HD21 | 1.73                     | 0.53              |
| 7:Q:41:VAL:O     | 7:Q:96:ILE:N      | 2.40                     | 0.53              |
| 2:G:17:HIS:HB2   | 2:G:274:LYS:HD2   | 1.91                     | 0.53              |
| 3:H:16:SER:HB2   | 3:H:34:LEU:HG     | 1.90                     | 0.53              |
| 3:H:100:LEU:HD23 | 3:H:103:LEU:HD13  | 1.89                     | 0.53              |
| 4:I:2:ALA:N      | 4:I:4:ASP:OD1     | 2.41                     | 0.53              |
| 7:W:30:ILE:HB    | 7:W:70:LEU:HD11   | 1.91                     | 0.53              |
| 7:n:155:LYS:HB3  | 7:n:158:LYS:HE3   | 1.90                     | 0.53              |
| 7:x:149:THR:HG22 | 7:x:150:GLN:HG3   | 1.89                     | 0.53              |
| 5:J:107:LYS:HD3  | 7:T:94:TYR:HA     | 1.90                     | 0.53              |
| 6:K:851:SER:OG   | 6:K:852:LEU:N     | 2.42                     | 0.53              |
| 7:L:123:THR:OG1  | 7:l:92:LYS:NZ     | 2.37                     | 0.53              |
| 7:N:89:PRO:HA    | 7:N:105:ASP:HA    | 1.91                     | 0.53              |
| 7:T:128:ILE:HG21 | 7:T:163:ILE:HG22  | 1.91                     | 0.53              |
| 7:Q:11:PRO:HD2   | 7:Q:16:ILE:HD11   | 1.89                     | 0.53              |
| 7:W:84:LEU:HG    | 7:W:112:TYR:HB2   | 1.90                     | 0.53              |
| 3:H:3:ARG:NH2    | 3:H:200:ASP:OD2   | 2.42                     | 0.52              |
| 4:I:268:SER:HA   | 5:J:85:ARG:HG3    | 1.91                     | 0.52              |
| 1:A:95:LEU:HD22  | 1:A:109:LEU:HD11  | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:38:GLU:OE2   | 2:F:120:LYS:NZ   | 2.41                     | 0.52              |
| 2:G:89:ALA:HA    | 2:G:240:SER:HB2  | 1.90                     | 0.52              |
| 6:K:649:ALA:HB3  | 6:K:804:LEU:HB3  | 1.91                     | 0.52              |
| 7:R:46:GLY:N     | 7:R:64:ASP:O     | 2.39                     | 0.52              |
| 7:R:156:ILE:O    | 7:R:160:LYS:N    | 2.39                     | 0.52              |
| 7:T:46:GLY:N     | 7:T:64:ASP:O     | 2.40                     | 0.52              |
| 2:F:88:ASP:OD2   | 2:G:274:LYS:NZ   | 2.42                     | 0.52              |
| 5:J:237:VAL:HG13 | 5:J:241:LEU:HD13 | 1.91                     | 0.52              |
| 7:Q:50:ASP:HA    | 7:Q:172:LEU:HB2  | 1.91                     | 0.52              |
| 7:S:113:SER:OG   | 7:S:114:SER:N    | 2.43                     | 0.52              |
| 7:T:89:PRO:CD    | 7:T:92:LYS:NZ    | 2.64                     | 0.52              |
| 7:o:17:THR:HG22  | 7:o:18:ILE:HG13  | 1.90                     | 0.52              |
| 7:s:155:LYS:HG3  | 7:s:158:LYS:HD3  | 1.90                     | 0.52              |
| 5:J:129:ILE:HG22 | 5:J:139:PRO:HA   | 1.92                     | 0.52              |
| 7:O:5:ARG:HA     | 7:O:72:ALA:HA    | 1.92                     | 0.52              |
| 7:R:16:ILE:HD11  | 7:R:137:ILE:HD11 | 1.91                     | 0.52              |
| 7:w:43:VAL:HG22  | 7:w:67:LYS:HD3   | 1.90                     | 0.52              |
| 4:I:127:GLY:HA3  | 4:I:142:SER:HB3  | 1.91                     | 0.52              |
| 7:n:2:SER:OG     | 7:n:3:THR:N      | 2.43                     | 0.52              |
| 2:D:85:THR:HB    | 2:D:243:LEU:HB2  | 1.91                     | 0.52              |
| 4:I:4:ASP:O      | 4:I:8:ASN:ND2    | 2.42                     | 0.52              |
| 5:J:375:GLY:O    | 5:J:378:ARG:NH1  | 2.42                     | 0.52              |
| 6:K:478:LYS:HE2  | 6:K:478:LYS:CA   | 2.36                     | 0.52              |
| 7:M:86:LEU:HB3   | 7:m:115:PRO:HB2  | 1.91                     | 0.52              |
| 7:Q:31:THR:HG21  | 7:Q:69:ILE:HB    | 1.92                     | 0.52              |
| 7:W:71:VAL:HG11  | 7:W:145:ILE:HG13 | 1.92                     | 0.52              |
| 7:l:40:ASN:HD21  | 7:l:99:LYS:H     | 1.57                     | 0.52              |
| 7:X:124:LYS:HD2  | 7:X:125:PRO:HD2  | 1.92                     | 0.52              |
| 3:H:78:THR:HG22  | 3:H:166:VAL:HG22 | 1.92                     | 0.52              |
| 4:I:4:ASP:OD1    | 4:I:4:ASP:N      | 2.43                     | 0.52              |
| 6:K:322:GLU:OE2  | 6:K:327:LYS:NZ   | 2.43                     | 0.52              |
| 7:r:4:GLN:HG3    | 7:r:107:LYS:HB3  | 1.91                     | 0.52              |
| 7:w:43:VAL:HB    | 7:w:94:TYR:HD2   | 1.75                     | 0.52              |
| 2:G:166:ASN:ND2  | 2:G:201:VAL:O    | 2.42                     | 0.52              |
| 7:R:84:LEU:HB2   | 7:R:110:ILE:HB   | 1.90                     | 0.52              |
| 7:X:59:THR:OG1   | 7:X:60:LEU:N     | 2.43                     | 0.52              |
| 7:X:97:ARG:HH21  | 7:X:166:LEU:HD21 | 1.74                     | 0.52              |
| 7:x:64:ASP:HA    | 7:x:170:TYR:CD2  | 2.44                     | 0.52              |
| 2:D:210:ARG:NH1  | 9:V:33:G:O6      | 2.43                     | 0.52              |
| 5:J:302:CYS:SG   | 5:J:303:ILE:N    | 2.80                     | 0.52              |
| 7:X:7:TYR:HB3    | 7:X:111:PRO:HD3  | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:X:19:ASP:OD1   | 7:X:20:VAL:N     | 2.41                     | 0.52              |
| 1:B:85:VAL:O     | 1:B:89:ALA:N     | 2.38                     | 0.51              |
| 5:J:108:VAL:HG22 | 5:J:140:ILE:HD11 | 1.91                     | 0.51              |
| 7:N:22:ILE:HG23  | 7:N:25:GLY:HA3   | 1.91                     | 0.51              |
| 7:T:66:VAL:HG12  | 7:T:169:TYR:HB2  | 1.92                     | 0.51              |
| 7:n:30:ILE:HD11  | 7:n:70:LEU:HD12  | 1.92                     | 0.51              |
| 7:w:5:ARG:HA     | 7:w:72:ALA:HA    | 1.93                     | 0.51              |
| 7:w:5:ARG:HD3    | 7:w:106:LEU:HD22 | 1.92                     | 0.51              |
| 6:K:204:GLY:HA2  | 6:K:313:THR:HA   | 1.93                     | 0.51              |
| 7:L:38:ILE:HD11  | 7:L:159:VAL:HG13 | 1.92                     | 0.51              |
| 7:M:162:ASP:O    | 7:M:166:LEU:N    | 2.43                     | 0.51              |
| 1:A:41:ILE:HD11  | 1:A:46:PHE:HD1   | 1.75                     | 0.51              |
| 7:n:123:THR:HG22 | 7:n:172:LEU:HD23 | 1.91                     | 0.51              |
| 7:x:128:ILE:HG12 | 7:x:167:PHE:O    | 2.11                     | 0.51              |
| 5:J:237:VAL:O    | 5:J:241:LEU:N    | 2.43                     | 0.51              |
| 5:J:332:GLU:HG2  | 5:J:469:GLU:HB3  | 1.91                     | 0.51              |
| 7:S:139:LYS:HA   | 7:S:143:ASP:HB2  | 1.92                     | 0.51              |
| 6:K:487:ILE:HG12 | 6:K:492:ALA:HB3  | 1.93                     | 0.51              |
| 7:M:21:LYS:H     | 7:M:76:GLN:H     | 1.57                     | 0.51              |
| 7:T:79:GLN:NE2   | 7:T:82:ASP:OD2   | 2.42                     | 0.51              |
| 6:K:250:ILE:HG13 | 6:K:314:LEU:HG   | 1.92                     | 0.51              |
| 7:L:55:ARG:HB2   | 7:L:113:SER:HB2  | 1.92                     | 0.51              |
| 7:t:80:SER:HA    | 7:t:83:PHE:HB2   | 1.91                     | 0.51              |
| 7:w:4:GLN:HA     | 7:w:107:LYS:HB2  | 1.93                     | 0.51              |
| 7:x:83:PHE:CD1   | 7:x:111:PRO:HA   | 2.45                     | 0.51              |
| 4:I:54:LYS:HB2   | 5:J:188:ILE:HD11 | 1.93                     | 0.51              |
| 6:K:529:ARG:HA   | 6:K:532:LEU:HB3  | 1.91                     | 0.51              |
| 7:L:5:ARG:HE     | 7:L:30:ILE:HG13  | 1.75                     | 0.51              |
| 7:P:152:GLU:HG2  | 7:q:151:LYS:HG3  | 1.92                     | 0.51              |
| 7:q:10:ILE:HD11  | 7:q:69:ILE:HG12  | 1.92                     | 0.51              |
| 7:x:133:ILE:HD12 | 7:x:136:ASN:HD21 | 1.74                     | 0.51              |
| 7:N:95:LEU:O     | 7:N:98:LYS:NZ    | 2.44                     | 0.51              |
| 7:O:101:ASN:ND2  | 7:O:104:ASP:OD1  | 2.44                     | 0.51              |
| 7:x:6:GLU:OE2    | 7:x:71:VAL:HB    | 2.11                     | 0.51              |
| 1:A:149:GLU:HG3  | 1:B:55:SER:HB2   | 1.92                     | 0.51              |
| 6:K:241:PHE:O    | 6:K:245:TYR:N    | 2.40                     | 0.51              |
| 6:K:596:SER:OG   | 6:K:597:MET:N    | 2.43                     | 0.51              |
| 7:N:56:LEU:HD22  | 7:N:66:VAL:HG11  | 1.93                     | 0.51              |
| 7:P:61:ASP:HB2   | 7:p:92:LYS:HB3   | 1.92                     | 0.51              |
| 7:S:67:LYS:NZ    | 7:S:166:LEU:O    | 2.37                     | 0.51              |
| 7:x:4:GLN:HG2    | 7:x:107:LYS:HB2  | 1.93                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:68:ILE:HG23  | 1:A:110:ILE:HD12  | 1.92                     | 0.51              |
| 4:I:139:SER:OG   | 4:I:140:GLY:N     | 2.44                     | 0.51              |
| 7:l:71:VAL:HG21  | 7:l:145:ILE:HD13  | 1.93                     | 0.51              |
| 7:s:5:ARG:HB2    | 7:s:106:LEU:HB2   | 1.92                     | 0.51              |
| 2:D:25:SER:OG    | 2:D:26:VAL:N      | 2.38                     | 0.50              |
| 6:K:630:SER:HA   | 6:K:633:ARG:HH21  | 1.75                     | 0.50              |
| 7:s:93:LEU:HD21  | 7:s:106:LEU:HD11  | 1.94                     | 0.50              |
| 7:w:66:VAL:HG22  | 7:w:169:TYR:HB2   | 1.93                     | 0.50              |
| 4:I:142:SER:OG   | 4:I:151:TYR:O     | 2.29                     | 0.50              |
| 7:N:5:ARG:HA     | 7:N:72:ALA:HA     | 1.93                     | 0.50              |
| 7:q:5:ARG:HH11   | 7:q:106:LEU:HD13  | 1.76                     | 0.50              |
| 1:A:134:SER:O    | 1:A:138:ARG:NE    | 2.44                     | 0.50              |
| 2:G:74:GLU:HG3   | 2:G:77:ASN:H      | 1.76                     | 0.50              |
| 2:G:100:GLU:HG3  | 2:G:106:PRO:HA    | 1.92                     | 0.50              |
| 7:S:55:ARG:HB2   | 7:S:113:SER:HB2   | 1.93                     | 0.50              |
| 7:x:35:GLU:HA    | 7:x:153:LYS:NZ    | 2.26                     | 0.50              |
| 3:H:108:GLU:HG3  | 7:X:94:TYR:CE1    | 2.33                     | 0.50              |
| 7:L:113:SER:OG   | 7:L:114:SER:N     | 2.43                     | 0.50              |
| 7:R:23:THR:HG23  | 7:R:145:ILE:HG22  | 1.93                     | 0.50              |
| 7:T:9:PHE:HD2    | 7:T:11:PRO:HD3    | 1.76                     | 0.50              |
| 9:V:47:C:H2'     | 9:V:48:A:H8       | 1.75                     | 0.50              |
| 7:X:61:ASP:HB3   | 7:X:64:ASP:HB3    | 1.92                     | 0.50              |
| 2:G:22:SER:HB3   | 2:G:35:GLN:HA     | 1.93                     | 0.50              |
| 6:K:942:ILE:HG12 | 6:K:1025:ILE:HG23 | 1.93                     | 0.50              |
| 7:P:129:SER:OG   | 7:P:130:ASP:N     | 2.44                     | 0.50              |
| 7:R:138:ILE:HD11 | 7:R:163:ILE:HG13  | 1.94                     | 0.50              |
| 2:E:5:ALA:HB2    | 2:E:246:GLU:HA    | 1.94                     | 0.50              |
| 5:J:11:LYS:HD3   | 5:J:205:GLU:HG2   | 1.94                     | 0.50              |
| 6:K:648:ARG:HH11 | 6:K:877:SER:HB3   | 1.77                     | 0.50              |
| 7:O:22:ILE:HD12  | 7:O:74:THR:H      | 1.76                     | 0.50              |
| 7:Q:125:PRO:HA   | 7:Q:170:TYR:HA    | 1.93                     | 0.50              |
| 7:T:34:ASP:OD2   | 7:T:99:LYS:NZ     | 2.38                     | 0.50              |
| 7:o:120:SER:O    | 7:o:174:GLN:NE2   | 2.43                     | 0.50              |
| 7:x:50:ASP:O     | 7:x:52:LYS:N      | 2.45                     | 0.50              |
| 5:J:248:THR:OG1  | 5:J:433:ARG:NH1   | 2.45                     | 0.50              |
| 7:P:41:VAL:O     | 7:P:96:ILE:N      | 2.43                     | 0.50              |
| 7:X:47:TYR:HD1   | 7:X:58:PRO:HA     | 1.76                     | 0.50              |
| 7:X:162:ASP:OD1  | 7:X:163:ILE:N     | 2.44                     | 0.50              |
| 3:H:14:PHE:HB2   | 3:H:34:LEU:HB2    | 1.94                     | 0.50              |
| 5:J:58:LYS:NZ    | 5:J:309:GLU:OE2   | 2.40                     | 0.50              |
| 6:K:986:ILE:O    | 6:K:990:SER:OG    | 2.30                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:n:66:VAL:HG22  | 7:n:169:TYR:HB2  | 1.93                     | 0.50              |
| 7:x:12:ILE:HD11  | 7:x:128:ILE:HA   | 1.94                     | 0.50              |
| 5:J:336:ILE:HG23 | 5:J:342:VAL:HG21 | 1.93                     | 0.50              |
| 6:K:380:LEU:HD22 | 6:K:439:LEU:HD23 | 1.94                     | 0.50              |
| 7:t:138:ILE:HA   | 7:t:142:PHE:HD2  | 1.77                     | 0.50              |
| 7:X:67:LYS:HE3   | 7:X:167:PHE:HA   | 1.94                     | 0.50              |
| 1:A:64:LEU:HD22  | 1:A:113:LEU:HD22 | 1.94                     | 0.49              |
| 7:T:42:LEU:HD21  | 7:T:44:ILE:HD11  | 1.94                     | 0.49              |
| 1:A:16:LYS:NZ    | 1:A:74:ASP:OD1   | 2.38                     | 0.49              |
| 2:G:266:LEU:HD12 | 2:G:277:VAL:HG21 | 1.94                     | 0.49              |
| 2:D:80:GLU:HB3   | 2:F:218:LYS:HD3  | 1.94                     | 0.49              |
| 7:O:43:VAL:HG22  | 7:O:67:LYS:HG2   | 1.93                     | 0.49              |
| 7:R:44:ILE:HG23  | 7:r:60:LEU:HD22  | 1.93                     | 0.49              |
| 7:l:163:ILE:HA   | 7:l:167:PHE:HD2  | 1.77                     | 0.49              |
| 7:m:131:ASP:O    | 7:m:135:ASN:N    | 2.45                     | 0.49              |
| 7:r:158:LYS:O    | 7:r:162:ASP:N    | 2.45                     | 0.49              |
| 7:s:7:TYR:OH     | 7:s:68:GLY:N     | 2.45                     | 0.49              |
| 7:X:131:ASP:O    | 7:X:135:ASN:HB2  | 2.12                     | 0.49              |
| 2:D:149:LYS:HE2  | 2:D:152:LYS:HD3  | 1.95                     | 0.49              |
| 3:H:130:GLN:O    | 3:H:164:LYS:NZ   | 2.45                     | 0.49              |
| 3:H:282:LYS:O    | 3:H:286:ARG:N    | 2.40                     | 0.49              |
| 6:K:616:GLU:HA   | 6:K:620:PHE:HB2  | 1.95                     | 0.49              |
| 7:N:9:PHE:HB3    | 7:N:56:LEU:HD11  | 1.94                     | 0.49              |
| 7:Q:60:LEU:HD22  | 7:q:44:ILE:HG23  | 1.93                     | 0.49              |
| 1:C:6:ASP:OD1    | 1:C:101:ARG:NH1  | 2.34                     | 0.49              |
| 5:J:461:ILE:HG23 | 5:J:461:ILE:O    | 2.13                     | 0.49              |
| 7:N:15:SER:H     | 7:N:16:ILE:HD12  | 1.78                     | 0.49              |
| 7:T:80:SER:HA    | 7:T:83:PHE:H     | 1.77                     | 0.49              |
| 6:K:416:ASN:O    | 6:K:420:GLN:N    | 2.45                     | 0.49              |
| 6:K:475:ILE:HA   | 6:K:510:ARG:HG2  | 1.95                     | 0.49              |
| 7:P:67:LYS:NZ    | 7:P:166:LEU:O    | 2.35                     | 0.49              |
| 7:S:84:LEU:HD12  | 7:S:86:LEU:HD22  | 1.94                     | 0.49              |
| 7:W:43:VAL:HG22  | 7:W:67:LYS:HG2   | 1.95                     | 0.49              |
| 1:C:114:ARG:HH12 | 7:s:45:THR:HG21  | 1.78                     | 0.49              |
| 2:G:108:VAL:HG23 | 2:G:109:TRP:HD1  | 1.76                     | 0.49              |
| 5:J:379:LYS:NZ   | 5:J:381:GLU:OE1  | 2.41                     | 0.49              |
| 6:K:552:LYS:HB3  | 6:K:594:VAL:HG22 | 1.95                     | 0.49              |
| 7:N:139:LYS:HA   | 7:N:143:ASP:HB2  | 1.95                     | 0.49              |
| 7:p:121:MET:HE3  | 7:p:172:LEU:HD21 | 1.94                     | 0.49              |
| 7:q:136:ASN:O    | 7:q:140:GLU:N    | 2.32                     | 0.49              |
| 2:D:128:ILE:HG22 | 2:D:243:LEU:HD21 | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:248:LYS:HB3  | 7:O:94:TYR:HD1   | 1.77                     | 0.49              |
| 2:G:255:SER:OG   | 2:G:256:CYS:N    | 2.46                     | 0.49              |
| 4:I:62:ASP:OD1   | 4:I:62:ASP:N     | 2.44                     | 0.49              |
| 5:J:121:LEU:HD23 | 5:J:128:LEU:HD11 | 1.94                     | 0.49              |
| 5:J:150:LYS:NZ   | 5:J:154:ASP:OD2  | 2.39                     | 0.49              |
| 7:M:43:VAL:HG22  | 7:M:67:LYS:HG2   | 1.95                     | 0.49              |
| 7:X:40:ASN:HD21  | 7:X:99:LYS:H     | 1.61                     | 0.49              |
| 7:W:121:MET:HB3  | 7:W:172:LEU:HD11 | 1.94                     | 0.49              |
| 7:t:153:LYS:HE2  | 7:t:155:LYS:HB2  | 1.94                     | 0.49              |
| 4:I:116:VAL:HG22 | 4:I:279:ILE:HG12 | 1.94                     | 0.49              |
| 7:n:7:TYR:OH     | 7:n:66:VAL:O     | 2.31                     | 0.49              |
| 7:p:16:ILE:HD11  | 7:p:137:ILE:HD11 | 1.94                     | 0.48              |
| 6:K:27:TRP:CE2   | 6:K:117:PHE:HB3  | 2.48                     | 0.48              |
| 7:O:115:PRO:HG2  | 7:o:84:LEU:HD11  | 1.94                     | 0.48              |
| 7:n:156:ILE:O    | 7:n:160:LYS:N    | 2.47                     | 0.48              |
| 1:A:24:TYR:OH    | 1:A:153:GLU:OE1  | 2.32                     | 0.48              |
| 7:O:9:PHE:HA     | 7:O:68:GLY:HA3   | 1.94                     | 0.48              |
| 7:P:172:LEU:HB3  | 7:P:174:GLN:HG3  | 1.95                     | 0.48              |
| 7:Q:90:ALA:HB2   | 7:Q:106:LEU:HG   | 1.95                     | 0.48              |
| 7:R:40:ASN:HD21  | 7:R:100:GLY:H    | 1.60                     | 0.48              |
| 2:D:30:ILE:HG13  | 2:D:228:SER:HB2  | 1.96                     | 0.48              |
| 3:H:17:GLN:HG2   | 9:V:3:U:H5       | 1.78                     | 0.48              |
| 3:H:84:PHE:HD1   | 3:H:216:LEU:HD11 | 1.78                     | 0.48              |
| 3:H:281:ILE:HD12 | 3:H:286:ARG:HD3  | 1.95                     | 0.48              |
| 7:m:93:LEU:HB3   | 7:m:95:LEU:HG    | 1.95                     | 0.48              |
| 7:X:5:ARG:NH1    | 7:X:72:ALA:HB2   | 2.28                     | 0.48              |
| 6:K:642:PRO:HD2  | 6:K:1037:LYS:HB2 | 1.94                     | 0.48              |
| 7:n:5:ARG:HB2    | 7:n:106:LEU:HD21 | 1.94                     | 0.48              |
| 5:J:138:ILE:HG13 | 7:t:62:PRO:HB2   | 1.96                     | 0.48              |
| 7:L:4:GLN:OE1    | 7:L:74:THR:OG1   | 2.30                     | 0.48              |
| 7:n:4:GLN:HG2    | 7:n:107:LYS:HB3  | 1.95                     | 0.48              |
| 7:x:49:VAL:HG12  | 7:x:170:TYR:O    | 2.14                     | 0.48              |
| 2:G:26:VAL:HG22  | 6:K:911:GLN:HE21 | 1.79                     | 0.48              |
| 7:L:35:GLU:HA    | 7:L:153:LYS:HZ3  | 1.77                     | 0.48              |
| 7:S:87:LYS:HE2   | 7:S:107:LYS:HB2  | 1.95                     | 0.48              |
| 7:x:93:LEU:HD23  | 7:x:93:LEU:H     | 1.79                     | 0.48              |
| 1:A:18:PHE:O     | 1:A:27:LYS:NZ    | 2.46                     | 0.48              |
| 7:r:130:ASP:OD2  | 7:r:132:THR:OG1  | 2.31                     | 0.48              |
| 3:H:70:THR:HG23  | 3:H:294:LYS:HA   | 1.95                     | 0.48              |
| 6:K:177:ILE:O    | 6:K:181:LEU:N    | 2.42                     | 0.48              |
| 6:K:478:LYS:HE3  | 6:K:507:PRO:O    | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:94:ILE:HA     | 2:D:236:THR:HG23  | 1.96                     | 0.48              |
| 2:E:74:GLU:O      | 9:V:18:U:O2'      | 2.30                     | 0.48              |
| 2:E:254:ALA:HA    | 2:E:258:LEU:HD12  | 1.96                     | 0.48              |
| 2:F:216:ARG:NH1   | 9:V:20:G:OP1      | 2.36                     | 0.48              |
| 6:K:319:LEU:HB3   | 6:K:326:TYR:HB3   | 1.95                     | 0.48              |
| 7:N:64:ASP:HA     | 7:N:170:TYR:CD2   | 2.48                     | 0.48              |
| 7:P:67:LYS:HD2    | 7:P:168:SER:H     | 1.79                     | 0.48              |
| 7:T:90:ALA:HB2    | 7:T:106:LEU:HG    | 1.95                     | 0.48              |
| 7:m:50:ASP:OD1    | 7:m:52:LYS:NZ     | 2.46                     | 0.48              |
| 7:n:126:VAL:HG21  | 7:n:171:ALA:HB3   | 1.94                     | 0.48              |
| 7:q:10:ILE:HD12   | 7:q:68:GLY:HA2    | 1.95                     | 0.48              |
| 7:s:152:GLU:OE2   | 7:s:153:LYS:NZ    | 2.47                     | 0.48              |
| 7:X:20:VAL:HG22   | 7:X:75:PRO:HB3    | 1.95                     | 0.48              |
| 7:X:40:ASN:ND2    | 7:X:98:LYS:HA     | 2.29                     | 0.48              |
| 5:J:305:THR:HG22  | 5:J:308:ILE:HD12  | 1.95                     | 0.47              |
| 6:K:190:TRP:HZ2   | 6:K:202:LEU:HG    | 1.79                     | 0.47              |
| 6:K:565:LYS:HA    | 6:K:568:GLU:HB2   | 1.96                     | 0.47              |
| 7:O:56:LEU:HD21   | 7:O:66:VAL:HG11   | 1.95                     | 0.47              |
| 7:l:122:LYS:O     | 7:l:124:LYS:NZ    | 2.44                     | 0.47              |
| 7:s:46:GLY:N      | 7:s:64:ASP:O      | 2.47                     | 0.47              |
| 7:x:67:LYS:HE2    | 7:x:167:PHE:HA    | 1.95                     | 0.47              |
| 2:E:13:HIS:HB2    | 2:E:278:GLU:HB3   | 1.95                     | 0.47              |
| 7:R:43:VAL:HG22   | 7:R:67:LYS:HG2    | 1.96                     | 0.47              |
| 7:r:20:VAL:HG23   | 7:r:75:PRO:HA     | 1.97                     | 0.47              |
| 7:w:62:PRO:N      | 7:w:63:CYS:N      | 2.62                     | 0.47              |
| 7:X:125:PRO:HB3   | 7:X:170:TYR:CE1   | 2.49                     | 0.47              |
| 1:A:35:ARG:NH2    | 8:U:23:G:OP2      | 2.45                     | 0.47              |
| 3:H:305:LYS:CD    | 7:x:94:TYR:CE2    | 2.89                     | 0.47              |
| 4:I:48:THR:HA     | 4:I:53:LEU:HD11   | 1.97                     | 0.47              |
| 6:K:479:GLU:HB3   | 6:K:480:ASP:H     | 1.60                     | 0.47              |
| 6:K:1029:LEU:HD23 | 6:K:1032:ILE:HD12 | 1.95                     | 0.47              |
| 7:X:33:ILE:HG13   | 7:X:148:ILE:HG21  | 1.96                     | 0.47              |
| 7:x:153:LYS:NZ    | 7:x:155:LYS:HB3   | 2.30                     | 0.47              |
| 3:H:261:THR:HG23  | 6:K:437:SER:HB2   | 1.95                     | 0.47              |
| 6:K:29:ILE:HG23   | 6:K:91:ARG:HB2    | 1.94                     | 0.47              |
| 6:K:615:PRO:HA    | 6:K:618:TYR:HD2   | 1.79                     | 0.47              |
| 7:Q:2:SER:OG      | 7:Q:3:THR:N       | 2.44                     | 0.47              |
| 7:r:24:ILE:HA     | 7:r:29:HIS:HE2    | 1.80                     | 0.47              |
| 7:x:58:PRO:HG3    | 7:x:112:TYR:CE1   | 2.47                     | 0.47              |
| 1:B:21:LEU:O      | 1:B:27:LYS:NZ     | 2.37                     | 0.47              |
| 2:G:208:ARG:HG2   | 2:G:230:GLU:HG2   | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:H:38:ARG:HH12  | 3:H:245:ILE:HB   | 1.78                     | 0.47              |
| 3:H:305:LYS:CB   | 7:x:94:TYR:CE2   | 2.93                     | 0.47              |
| 6:K:118:PRO:HD3  | 6:K:163:TYR:HA   | 1.96                     | 0.47              |
| 7:X:61:ASP:HB2   | 7:x:92:LYS:HB3   | 1.95                     | 0.47              |
| 1:B:99:ILE:HG23  | 1:B:106:GLN:HB2  | 1.97                     | 0.47              |
| 2:F:57:LEU:HD21  | 2:F:261:LEU:HD13 | 1.97                     | 0.47              |
| 6:K:289:TYR:O    | 6:K:292:ASN:ND2  | 2.47                     | 0.47              |
| 7:Q:6:GLU:N      | 7:Q:71:VAL:O     | 2.45                     | 0.47              |
| 7:R:34:ASP:OD1   | 7:R:39:HIS:NE2   | 2.48                     | 0.47              |
| 7:x:6:GLU:CB     | 7:x:109:TYR:HB2  | 2.44                     | 0.47              |
| 1:A:59:LEU:HD22  | 1:A:64:LEU:HD21  | 1.96                     | 0.47              |
| 2:D:91:LEU:HA    | 2:D:238:PHE:HD1  | 1.79                     | 0.47              |
| 5:J:332:GLU:CG   | 5:J:469:GLU:HB3  | 2.44                     | 0.47              |
| 6:K:920:SER:OG   | 6:K:923:ARG:NH2  | 2.41                     | 0.47              |
| 7:T:67:LYS:HE3   | 7:T:168:SER:H    | 1.79                     | 0.47              |
| 7:x:4:GLN:NE2    | 7:x:107:LYS:HD2  | 2.30                     | 0.47              |
| 6:K:596:SER:OG   | 6:K:597:MET:SD   | 2.73                     | 0.47              |
| 7:p:65:TYR:HE2   | 7:p:67:LYS:HE3   | 1.80                     | 0.47              |
| 2:D:30:ILE:HD13  | 2:D:230:GLU:HG3  | 1.96                     | 0.47              |
| 4:I:112:THR:HG23 | 4:I:283:LYS:HA   | 1.97                     | 0.47              |
| 7:s:129:SER:OG   | 7:s:130:ASP:N    | 2.46                     | 0.47              |
| 3:H:143:ASP:OD1  | 3:H:143:ASP:N    | 2.45                     | 0.47              |
| 5:J:121:LEU:HD21 | 5:J:193:ILE:HG12 | 1.96                     | 0.47              |
| 5:J:327:ASN:HD21 | 5:J:461:ILE:CD1  | 2.19                     | 0.47              |
| 6:K:206:ASP:O    | 6:K:389:ARG:N    | 2.42                     | 0.47              |
| 6:K:340:LYS:NZ   | 6:K:388:ILE:O    | 2.48                     | 0.47              |
| 7:o:163:ILE:HA   | 7:o:167:PHE:HD2  | 1.79                     | 0.47              |
| 7:w:124:LYS:N    | 7:w:171:ALA:O    | 2.48                     | 0.47              |
| 7:w:127:SER:HA   | 7:w:168:SER:HA   | 1.96                     | 0.47              |
| 7:X:20:VAL:HG13  | 7:X:75:PRO:HA    | 1.97                     | 0.47              |
| 2:D:64:LYS:NZ    | 7:O:170:TYR:OH   | 2.45                     | 0.46              |
| 2:G:267:GLY:O    | 9:V:8:G:N2       | 2.48                     | 0.46              |
| 3:H:21:GLU:OE2   | 6:K:875:ASN:ND2  | 2.48                     | 0.46              |
| 7:Q:23:THR:HG23  | 7:Q:145:ILE:HA   | 1.96                     | 0.46              |
| 7:q:129:SER:HA   | 7:q:164:LYS:HG2  | 1.97                     | 0.46              |
| 7:X:45:THR:HA    | 7:X:65:TYR:HA    | 1.97                     | 0.46              |
| 7:x:44:ILE:O     | 7:x:65:TYR:HA    | 2.14                     | 0.46              |
| 2:G:216:ARG:NH1  | 9:V:14:A:OP1     | 2.44                     | 0.46              |
| 3:H:83:LEU:HD21  | 3:H:127:LYS:HD2  | 1.98                     | 0.46              |
| 4:I:165:ILE:HD11 | 4:I:254:SER:HB2  | 1.96                     | 0.46              |
| 5:J:13:LEU:HA    | 5:J:205:GLU:H    | 1.78                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:L:79:GLN:NE2   | 7:L:82:ASP:OD1   | 2.42                     | 0.46              |
| 7:t:6:GLU:N      | 7:t:71:VAL:O     | 2.40                     | 0.46              |
| 2:E:9:PRO:HG2    | 2:E:282:VAL:HB   | 1.98                     | 0.46              |
| 5:J:360:ILE:HD13 | 5:J:471:LEU:CD2  | 2.16                     | 0.46              |
| 7:T:123:THR:OG1  | 7:t:92:LYS:NZ    | 2.46                     | 0.46              |
| 7:q:134:VAL:HG11 | 7:q:164:LYS:HG3  | 1.96                     | 0.46              |
| 7:r:90:ALA:HB1   | 7:r:102:ILE:HB   | 1.96                     | 0.46              |
| 7:w:123:THR:HA   | 7:w:172:LEU:HA   | 1.96                     | 0.46              |
| 7:x:90:ALA:HA    | 7:x:93:LEU:HD21  | 1.97                     | 0.46              |
| 6:K:669:ILE:HD11 | 6:K:923:ARG:HG3  | 1.96                     | 0.46              |
| 7:R:156:ILE:HA   | 7:R:159:VAL:HG12 | 1.98                     | 0.46              |
| 7:q:86:LEU:HB2   | 7:q:108:ILE:HB   | 1.97                     | 0.46              |
| 7:w:4:GLN:HG3    | 7:w:107:LYS:HD3  | 1.98                     | 0.46              |
| 2:F:284:ASP:OD1  | 2:F:285:VAL:N    | 2.49                     | 0.46              |
| 5:J:49:LEU:HD11  | 5:J:298:ILE:HD13 | 1.97                     | 0.46              |
| 6:K:205:ILE:HG12 | 6:K:390:VAL:HG22 | 1.96                     | 0.46              |
| 6:K:402:ASN:HB3  | 6:K:407:ARG:HB3  | 1.97                     | 0.46              |
| 7:X:141:VAL:HA   | 7:X:144:LYS:HB3  | 1.97                     | 0.46              |
| 6:K:540:GLU:O    | 6:K:544:ASN:ND2  | 2.49                     | 0.46              |
| 7:o:43:VAL:HG22  | 7:o:67:LYS:HG2   | 1.96                     | 0.46              |
| 2:E:259:ARG:HG3  | 7:L:94:TYR:HE1   | 1.81                     | 0.46              |
| 4:I:220:ALA:O    | 5:J:425:TYR:OH   | 2.33                     | 0.46              |
| 7:L:49:VAL:HG12  | 7:L:171:ALA:HA   | 1.98                     | 0.46              |
| 7:w:61:ASP:OD1   | 7:w:62:PRO:HD2   | 2.15                     | 0.46              |
| 7:w:84:LEU:HB2   | 7:w:110:ILE:HB   | 1.96                     | 0.46              |
| 7:x:24:ILE:HD11  | 7:x:27:SER:HA    | 1.96                     | 0.46              |
| 7:x:35:GLU:HA    | 7:x:153:LYS:HZ3  | 1.80                     | 0.46              |
| 1:C:39:GLU:OE1   | 1:C:43:ASN:ND2   | 2.48                     | 0.46              |
| 2:D:137:SER:OG   | 2:D:141:ASN:OD1  | 2.34                     | 0.46              |
| 5:J:35:PRO:HG3   | 5:J:88:VAL:HB    | 1.98                     | 0.46              |
| 6:K:321:ARG:HG2  | 6:K:323:GLY:H    | 1.80                     | 0.46              |
| 6:K:477:PRO:O    | 6:K:508:GLY:N    | 2.48                     | 0.46              |
| 7:r:46:GLY:N     | 7:r:64:ASP:O     | 2.49                     | 0.46              |
| 7:x:42:LEU:O     | 7:x:67:LYS:HA    | 2.16                     | 0.46              |
| 7:x:86:LEU:HD23  | 7:x:87:LYS:N     | 2.30                     | 0.46              |
| 1:B:82:ASP:HA    | 1:B:85:VAL:HB    | 1.98                     | 0.46              |
| 1:C:35:ARG:HH21  | 8:U:17:C:H2'     | 1.81                     | 0.46              |
| 2:G:30:ILE:HG21  | 2:G:230:GLU:HG3  | 1.97                     | 0.46              |
| 5:J:118:LYS:HB3  | 5:J:133:GLU:HG2  | 1.98                     | 0.46              |
| 7:X:136:ASN:O    | 7:X:139:LYS:HB3  | 2.16                     | 0.46              |
| 7:x:50:ASP:OD1   | 7:x:55:ARG:N     | 2.40                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:159:ASP:N    | 2:F:159:ASP:OD1  | 2.49                     | 0.46              |
| 7:O:43:VAL:HB    | 7:O:94:TYR:HD2   | 1.81                     | 0.46              |
| 7:Q:156:ILE:HA   | 7:Q:159:VAL:HG22 | 1.98                     | 0.46              |
| 2:D:261:LEU:HD23 | 2:D:281:TRP:HZ2  | 1.81                     | 0.45              |
| 2:F:19:HIS:HB2   | 2:F:231:TYR:HD1  | 1.81                     | 0.45              |
| 5:J:80:LYS:HD3   | 5:J:218:ARG:HD3  | 1.97                     | 0.45              |
| 7:M:148:ILE:HG22 | 7:M:153:LYS:HG2  | 1.98                     | 0.45              |
| 7:r:20:VAL:HA    | 7:r:76:GLN:H     | 1.81                     | 0.45              |
| 7:x:140:GLU:O    | 7:x:144:LYS:HD2  | 2.15                     | 0.45              |
| 2:D:144:ASP:OD1  | 2:D:144:ASP:N    | 2.47                     | 0.45              |
| 2:E:184:ILE:HD12 | 2:E:186:ALA:HB3  | 1.98                     | 0.45              |
| 4:I:250:PRO:O    | 4:I:254:SER:N    | 2.43                     | 0.45              |
| 5:J:465:ARG:NH1  | 5:J:465:ARG:C    | 2.74                     | 0.45              |
| 7:L:117:ALA:HA   | 7:l:86:LEU:HA    | 1.99                     | 0.45              |
| 7:Q:95:LEU:HD23  | 7:Q:98:LYS:HE2   | 1.98                     | 0.45              |
| 7:l:157:GLU:HA   | 7:l:160:LYS:HG2  | 1.98                     | 0.45              |
| 7:p:163:ILE:HA   | 7:p:167:PHE:HD2  | 1.82                     | 0.45              |
| 2:E:5:ALA:N      | 2:E:244:GLY:O    | 2.50                     | 0.45              |
| 2:F:36:ARG:HH12  | 2:F:206:LEU:HD11 | 1.80                     | 0.45              |
| 5:J:107:LYS:O    | 5:J:111:CYS:SG   | 2.75                     | 0.45              |
| 5:J:330:LEU:CD1  | 5:J:465:ARG:CG   | 2.86                     | 0.45              |
| 6:K:279:ILE:O    | 6:K:283:LYS:N    | 2.41                     | 0.45              |
| 7:r:132:THR:HA   | 7:r:135:ASN:HD22 | 1.81                     | 0.45              |
| 7:t:4:GLN:HE22   | 7:t:107:LYS:HD2  | 1.81                     | 0.45              |
| 7:X:130:ASP:O    | 7:X:133:ILE:HG22 | 2.16                     | 0.45              |
| 7:X:134:VAL:HA   | 7:X:137:ILE:HB   | 1.99                     | 0.45              |
| 2:D:194:GLU:HB2  | 2:D:197:ILE:HG22 | 1.98                     | 0.45              |
| 6:K:178:PHE:HA   | 6:K:181:LEU:HB2  | 1.98                     | 0.45              |
| 6:K:422:VAL:O    | 6:K:426:LYS:N    | 2.45                     | 0.45              |
| 7:N:4:GLN:HG3    | 7:N:107:LYS:HB3  | 1.97                     | 0.45              |
| 7:m:137:ILE:HG21 | 7:m:163:ILE:HG21 | 1.97                     | 0.45              |
| 7:x:134:VAL:HG22 | 7:x:163:ILE:HD11 | 1.97                     | 0.45              |
| 5:J:107:LYS:NZ   | 7:T:98:LYS:NZ    | 2.65                     | 0.45              |
| 7:L:160:LYS:HA   | 7:L:163:ILE:HD12 | 1.98                     | 0.45              |
| 7:M:20:VAL:HA    | 7:M:75:PRO:HA    | 1.97                     | 0.45              |
| 7:l:129:SER:OG   | 7:l:130:ASP:N    | 2.49                     | 0.45              |
| 7:n:67:LYS:NZ    | 7:n:166:LEU:O    | 2.39                     | 0.45              |
| 7:x:10:ILE:HD12  | 7:x:68:GLY:HA2   | 1.99                     | 0.45              |
| 2:D:44:ILE:HB    | 2:D:89:ALA:HB3   | 1.99                     | 0.45              |
| 2:E:248:LYS:HB3  | 7:l:94:TYR:HD1   | 1.81                     | 0.45              |
| 4:I:158:LYS:NZ   | 9:V:31:G:OP2     | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:K:231:SER:O    | 6:K:235:TRP:N    | 2.50                     | 0.45              |
| 7:T:30:ILE:HD11  | 7:T:70:LEU:HB3   | 1.99                     | 0.45              |
| 7:t:16:ILE:HD13  | 7:t:141:VAL:HB   | 1.99                     | 0.45              |
| 7:t:31:THR:HG21  | 7:t:69:ILE:HG23  | 1.98                     | 0.45              |
| 7:w:144:LYS:HG3  | 7:w:145:ILE:HG13 | 1.98                     | 0.45              |
| 2:E:142:LYS:HD3  | 2:E:183:ILE:HG13 | 1.99                     | 0.45              |
| 2:F:100:GLU:HG3  | 2:F:160:LEU:HD22 | 1.97                     | 0.45              |
| 3:H:112:GLU:OE2  | 6:K:661:LYS:NZ   | 2.35                     | 0.45              |
| 2:E:185:ASN:HB2  | 2:E:280:ARG:HH12 | 1.81                     | 0.45              |
| 6:K:275:SER:HB3  | 6:K:278:VAL:HG23 | 1.99                     | 0.45              |
| 6:K:797:ILE:HD11 | 6:K:807:MET:HE3  | 1.98                     | 0.45              |
| 6:K:824:PHE:HB2  | 6:K:857:ARG:HH11 | 1.82                     | 0.45              |
| 6:K:1004:TYR:O   | 6:K:1007:ARG:NH1 | 2.50                     | 0.45              |
| 7:l:22:ILE:HG22  | 7:l:25:GLY:H     | 1.82                     | 0.45              |
| 7:q:22:ILE:HD12  | 7:q:74:THR:HB    | 1.97                     | 0.45              |
| 7:q:90:ALA:HB3   | 7:q:104:ASP:HA   | 1.99                     | 0.45              |
| 7:X:5:ARG:HB2    | 7:X:108:ILE:HG13 | 1.98                     | 0.45              |
| 7:x:5:ARG:HE     | 7:x:30:ILE:HG12  | 1.82                     | 0.45              |
| 7:x:48:ALA:O     | 7:x:56:LEU:HA    | 2.16                     | 0.45              |
| 2:E:20:VAL:HG13  | 2:E:267:GLY:HA2  | 1.99                     | 0.45              |
| 5:J:107:LYS:HG2  | 7:T:94:TYR:CD1   | 2.52                     | 0.45              |
| 6:K:164:GLU:HA   | 6:K:847:ALA:HA   | 1.99                     | 0.45              |
| 6:K:636:ARG:HH22 | 7:l:99:LYS:HG3   | 1.82                     | 0.45              |
| 6:K:789:VAL:HG22 | 6:K:794:GLY:HA3  | 1.99                     | 0.45              |
| 7:p:90:ALA:HB1   | 7:p:102:ILE:HB   | 1.98                     | 0.45              |
| 7:r:136:ASN:HA   | 7:r:139:LYS:HB3  | 1.98                     | 0.45              |
| 7:w:150:GLN:HG2  | 7:w:156:ILE:HG21 | 1.99                     | 0.45              |
| 7:X:61:ASP:OD1   | 7:X:63:CYS:N     | 2.50                     | 0.45              |
| 2:G:9:PRO:HG2    | 2:G:282:VAL:HB   | 1.98                     | 0.45              |
| 3:H:305:LYS:HB3  | 7:x:94:TYR:CD2   | 2.51                     | 0.45              |
| 5:J:74:VAL:O     | 5:J:82:SER:OG    | 2.31                     | 0.45              |
| 5:J:332:GLU:HG2  | 5:J:469:GLU:N    | 2.32                     | 0.45              |
| 1:A:63:SER:O     | 1:A:66:SER:OG    | 2.35                     | 0.44              |
| 2:G:7:ALA:HB2    | 2:G:243:LEU:HD23 | 1.98                     | 0.44              |
| 5:J:236:LEU:HD22 | 5:J:271:ILE:HG23 | 1.99                     | 0.44              |
| 5:J:332:GLU:OE2  | 5:J:468:LEU:HB3  | 2.16                     | 0.44              |
| 7:T:80:SER:OG    | 7:T:85:THR:OG1   | 2.25                     | 0.44              |
| 7:l:90:ALA:HA    | 7:l:93:LEU:HG    | 1.98                     | 0.44              |
| 7:p:124:LYS:N    | 7:p:171:ALA:O    | 2.41                     | 0.44              |
| 7:t:48:ALA:O     | 7:t:57:VAL:N     | 2.47                     | 0.44              |
| 9:V:18:U:O4      | 9:V:19:A:N6      | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:41:ILE:HG23  | 1:B:46:PHE:HA    | 2.00                     | 0.44              |
| 3:H:65:THR:HB    | 3:H:294:LYS:HD3  | 1.98                     | 0.44              |
| 5:J:129:ILE:HD12 | 5:J:137:LYS:HD3  | 2.00                     | 0.44              |
| 7:O:131:ASP:O    | 7:O:135:ASN:N    | 2.49                     | 0.44              |
| 7:Q:12:ILE:HD11  | 7:Q:128:ILE:HA   | 1.98                     | 0.44              |
| 7:m:148:ILE:HG13 | 7:m:152:GLU:HB3  | 1.98                     | 0.44              |
| 7:o:142:PHE:HE2  | 7:o:163:ILE:HD12 | 1.82                     | 0.44              |
| 1:C:14:PHE:HE2   | 1:C:151:LEU:HD12 | 1.81                     | 0.44              |
| 2:G:54:LYS:NZ    | 9:V:7:A:OP1      | 2.33                     | 0.44              |
| 3:H:131:ILE:HG23 | 3:H:166:VAL:HG21 | 1.99                     | 0.44              |
| 5:J:106:ASP:CA   | 5:J:109:ILE:HG13 | 2.45                     | 0.44              |
| 7:Q:30:ILE:HD11  | 7:Q:70:LEU:HD23  | 1.99                     | 0.44              |
| 7:n:16:ILE:HG12  | 7:n:141:VAL:HG21 | 1.99                     | 0.44              |
| 7:q:135:ASN:HA   | 7:q:138:ILE:HD12 | 1.97                     | 0.44              |
| 7:s:2:SER:OG     | 7:s:3:THR:N      | 2.49                     | 0.44              |
| 7:M:123:THR:HG22 | 7:M:172:LEU:HD23 | 1.99                     | 0.44              |
| 1:C:72:SER:OG    | 1:C:73:SER:N     | 2.51                     | 0.44              |
| 2:E:54:LYS:NZ    | 9:V:19:A:OP1     | 2.43                     | 0.44              |
| 2:E:139:LEU:HD22 | 2:E:282:VAL:HG11 | 2.00                     | 0.44              |
| 2:F:115:TYR:HD1  | 2:F:147:LEU:HD23 | 1.82                     | 0.44              |
| 4:I:120:THR:OG1  | 4:I:122:THR:O    | 2.36                     | 0.44              |
| 4:I:211:TYR:HE2  | 9:V:38:C:H41     | 1.66                     | 0.44              |
| 4:I:249:LYS:HB3  | 7:P:94:TYR:HD1   | 1.82                     | 0.44              |
| 5:J:360:ILE:HG22 | 5:J:361:ILE:HG13 | 1.99                     | 0.44              |
| 5:J:361:ILE:CD1  | 5:J:467:ILE:HD13 | 2.41                     | 0.44              |
| 7:M:131:ASP:HA   | 7:M:134:VAL:HG22 | 1.98                     | 0.44              |
| 7:N:42:LEU:HA    | 7:N:95:LEU:HA    | 2.00                     | 0.44              |
| 7:O:153:LYS:HD3  | 7:O:156:ILE:HA   | 2.00                     | 0.44              |
| 7:S:5:ARG:HD3    | 7:S:72:ALA:HA    | 1.98                     | 0.44              |
| 7:r:56:LEU:HD12  | 7:r:110:ILE:HG23 | 1.99                     | 0.44              |
| 7:X:67:LYS:NZ    | 7:X:166:LEU:O    | 2.43                     | 0.44              |
| 7:x:30:ILE:HB    | 7:x:70:LEU:HB2   | 1.99                     | 0.44              |
| 5:J:12:ALA:HB2   | 5:J:255:LEU:HD23 | 2.00                     | 0.44              |
| 6:K:179:ASP:OD1  | 6:K:256:ARG:NH2  | 2.43                     | 0.44              |
| 7:L:56:LEU:HD12  | 7:L:110:ILE:HG23 | 1.99                     | 0.44              |
| 7:O:55:ARG:HB2   | 7:O:113:SER:HB2  | 2.00                     | 0.44              |
| 7:X:6:GLU:HG3    | 7:X:71:VAL:O     | 2.17                     | 0.44              |
| 7:x:11:PRO:HA    | 7:x:169:TYR:CE1  | 2.52                     | 0.44              |
| 7:x:22:ILE:HD13  | 7:x:74:THR:HG23  | 1.99                     | 0.44              |
| 2:G:94:ILE:HG21  | 2:G:202:ILE:HG23 | 1.99                     | 0.44              |
| 6:K:656:ASP:OD2  | 6:K:663:THR:OG1  | 2.35                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:Q:44:ILE:HG23  | 7:q:60:LEU:HD22  | 1.99                     | 0.44              |
| 7:l:71:VAL:HG11  | 7:l:145:ILE:HG21 | 2.00                     | 0.44              |
| 7:w:4:GLN:HG2    | 7:w:109:TYR:HE2  | 1.83                     | 0.44              |
| 7:w:21:LYS:HB3   | 7:w:77:GLN:HE22  | 1.82                     | 0.44              |
| 1:B:138:ARG:HD3  | 2:F:27:GLU:HB2   | 2.00                     | 0.44              |
| 2:G:114:THR:HG22 | 2:G:198:GLY:HA3  | 2.00                     | 0.44              |
| 3:H:288:ARG:NH2  | 3:H:292:TYR:OH   | 2.50                     | 0.44              |
| 5:J:261:LYS:HE3  | 5:J:263:TYR:HE1  | 1.82                     | 0.44              |
| 7:P:124:LYS:N    | 7:P:171:ALA:O    | 2.43                     | 0.44              |
| 1:A:11:LEU:HD11  | 1:B:123:ILE:HG22 | 2.00                     | 0.44              |
| 1:A:95:LEU:HD23  | 1:A:98:LEU:HD12  | 2.00                     | 0.44              |
| 2:D:37:ASP:OD1   | 2:D:40:GLY:N     | 2.50                     | 0.44              |
| 2:F:13:HIS:CE1   | 2:F:280:ARG:HG3  | 2.53                     | 0.44              |
| 5:J:43:ARG:HB3   | 5:J:47:ARG:HH12  | 1.82                     | 0.44              |
| 5:J:469:GLU:H    | 5:J:469:GLU:HG3  | 1.54                     | 0.44              |
| 6:K:716:LEU:H    | 6:K:716:LEU:HG   | 1.63                     | 0.44              |
| 6:K:886:GLU:O    | 6:K:902:LYS:NZ   | 2.44                     | 0.44              |
| 7:M:96:ILE:HD12  | 7:M:166:LEU:HD11 | 2.00                     | 0.44              |
| 7:P:22:ILE:HD12  | 7:P:74:THR:H     | 1.83                     | 0.44              |
| 7:W:146:TYR:HB3  | 7:W:148:ILE:HD12 | 2.00                     | 0.44              |
| 7:m:138:ILE:HG23 | 7:m:142:PHE:HB2  | 2.00                     | 0.44              |
| 7:X:20:VAL:HG12  | 7:X:21:LYS:N     | 2.33                     | 0.44              |
| 7:x:31:THR:HG22  | 7:x:70:LEU:O     | 2.17                     | 0.44              |
| 6:K:14:LYS:HZ1   | 6:K:192:LEU:HD12 | 1.82                     | 0.43              |
| 7:Q:62:PRO:HA    | 7:q:45:THR:HG21  | 2.00                     | 0.43              |
| 7:l:84:LEU:HB2   | 7:l:110:ILE:HB   | 1.98                     | 0.43              |
| 7:n:80:SER:HA    | 7:n:83:PHE:HB2   | 2.00                     | 0.43              |
| 7:o:138:ILE:HA   | 7:o:142:PHE:HB2  | 2.00                     | 0.43              |
| 7:p:134:VAL:HA   | 7:p:137:ILE:HG22 | 1.99                     | 0.43              |
| 7:w:74:THR:HG23  | 7:w:77:GLN:HE21  | 1.83                     | 0.43              |
| 3:H:45:MET:HE1   | 3:H:197:LEU:HD21 | 2.00                     | 0.43              |
| 5:J:305:THR:O    | 5:J:305:THR:OG1  | 2.30                     | 0.43              |
| 7:O:43:VAL:HB    | 7:O:94:TYR:CD2   | 2.53                     | 0.43              |
| 7:P:82:ASP:OD1   | 7:P:82:ASP:N     | 2.48                     | 0.43              |
| 7:P:95:LEU:HD12  | 7:P:98:LYS:HE2   | 2.00                     | 0.43              |
| 7:p:142:PHE:HB3  | 7:p:149:THR:HG21 | 1.99                     | 0.43              |
| 7:s:132:THR:HA   | 7:s:135:ASN:HD22 | 1.82                     | 0.43              |
| 7:s:139:LYS:NZ   | 7:s:140:GLU:OE2  | 2.46                     | 0.43              |
| 1:B:23:HIS:CD2   | 1:B:25:GLY:H     | 2.36                     | 0.43              |
| 6:K:889:ARG:HG2  | 6:K:902:LYS:HG2  | 2.00                     | 0.43              |
| 7:R:159:VAL:HA   | 7:R:162:ASP:HB2  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:T:42:LEU:HD13  | 7:T:93:LEU:HD22  | 2.00                     | 0.43              |
| 7:n:156:ILE:HA   | 7:n:159:VAL:HG12 | 2.00                     | 0.43              |
| 7:o:46:GLY:N     | 7:o:64:ASP:O     | 2.41                     | 0.43              |
| 7:t:121:MET:HG3  | 7:t:172:LEU:HD12 | 2.00                     | 0.43              |
| 9:V:45:A:H2'     | 9:V:46:A:C8      | 2.53                     | 0.43              |
| 1:A:107:LYS:HE2  | 7:R:92:LYS:HA    | 2.00                     | 0.43              |
| 7:M:163:ILE:HA   | 7:M:167:PHE:HD2  | 1.83                     | 0.43              |
| 7:o:31:THR:HG21  | 7:o:69:ILE:HB    | 1.99                     | 0.43              |
| 2:F:158:SER:OG   | 2:F:159:ASP:N    | 2.50                     | 0.43              |
| 3:H:8:PRO:HB3    | 3:H:12:LEU:HD11  | 2.00                     | 0.43              |
| 3:H:39:PRO:HA    | 3:H:42:ILE:HD12  | 2.01                     | 0.43              |
| 3:H:159:TYR:HB3  | 3:H:160:LEU:H    | 1.71                     | 0.43              |
| 6:K:650:ASP:HB2  | 6:K:881:LEU:HD21 | 1.99                     | 0.43              |
| 7:W:6:GLU:HG2    | 7:W:109:TYR:HB2  | 1.99                     | 0.43              |
| 7:m:156:ILE:HG23 | 7:m:160:LYS:HE2  | 2.00                     | 0.43              |
| 7:s:43:VAL:HG22  | 7:s:67:LYS:HB3   | 2.00                     | 0.43              |
| 7:t:76:GLN:HB2   | 7:t:79:GLN:HB2   | 2.00                     | 0.43              |
| 4:I:190:THR:HG23 | 4:I:241:TYR:HE1  | 1.84                     | 0.43              |
| 6:K:656:ASP:HB2  | 6:K:661:LYS:HB2  | 2.01                     | 0.43              |
| 7:P:41:VAL:HG21  | 7:P:166:LEU:HD21 | 2.00                     | 0.43              |
| 8:U:4:U:O4       | 8:U:5:A:N6       | 2.51                     | 0.43              |
| 7:X:50:ASP:HB2   | 7:X:55:ARG:H     | 1.83                     | 0.43              |
| 2:E:17:HIS:O     | 2:E:275:GLY:N    | 2.49                     | 0.43              |
| 2:E:216:ARG:HH22 | 9:V:25:C:H4'     | 1.84                     | 0.43              |
| 2:F:102:ASP:N    | 2:F:102:ASP:OD1  | 2.51                     | 0.43              |
| 2:G:49:LEU:HD11  | 2:G:89:ALA:HB2   | 2.00                     | 0.43              |
| 3:H:219:ILE:HD11 | 3:H:300:LEU:HD21 | 2.00                     | 0.43              |
| 3:H:305:LYS:HD3  | 7:x:94:TYR:CZ    | 2.53                     | 0.43              |
| 5:J:140:ILE:HD13 | 5:J:140:ILE:HA   | 1.87                     | 0.43              |
| 5:J:288:LYS:HA   | 5:J:291:ILE:HD12 | 2.00                     | 0.43              |
| 6:K:145:LEU:O    | 6:K:148:GLN:NE2  | 2.48                     | 0.43              |
| 6:K:585:GLU:O    | 6:K:610:ASN:ND2  | 2.46                     | 0.43              |
| 7:R:64:ASP:HA    | 7:R:170:TYR:CD2  | 2.54                     | 0.43              |
| 7:W:169:TYR:HE2  | 7:W:171:ALA:HB2  | 1.82                     | 0.43              |
| 7:t:84:LEU:N     | 7:t:110:ILE:O    | 2.50                     | 0.43              |
| 7:X:123:THR:OG1  | 7:X:124:LYS:N    | 2.51                     | 0.43              |
| 5:J:14:TYR:CE1   | 5:J:204:GLN:HB3  | 2.53                     | 0.43              |
| 7:L:6:GLU:HB3    | 7:L:109:TYR:HD2  | 1.84                     | 0.43              |
| 7:M:5:ARG:HD3    | 7:M:72:ALA:HA    | 2.00                     | 0.43              |
| 7:m:124:LYS:N    | 7:m:171:ALA:O    | 2.49                     | 0.43              |
| 7:q:31:THR:HG21  | 7:q:69:ILE:HG23  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:r:13:THR:HG21  | 7:r:51:GLU:HB3   | 2.00                     | 0.43              |
| 7:w:169:TYR:HE2  | 7:w:171:ALA:HB2  | 1.84                     | 0.43              |
| 7:X:76:GLN:HE21  | 7:X:78:ALA:HB3   | 1.83                     | 0.43              |
| 3:H:236:TYR:HB3  | 3:H:273:ILE:HD13 | 2.01                     | 0.43              |
| 5:J:2:GLU:HB3    | 5:J:216:LYS:H    | 1.83                     | 0.43              |
| 6:K:815:ASP:OD1  | 6:K:815:ASP:N    | 2.51                     | 0.43              |
| 7:N:124:LYS:HD2  | 7:N:125:PRO:HD2  | 2.00                     | 0.43              |
| 7:P:131:ASP:N    | 7:P:131:ASP:OD1  | 2.52                     | 0.43              |
| 7:x:44:ILE:HG12  | 7:x:66:VAL:O     | 2.19                     | 0.43              |
| 7:x:169:TYR:O    | 7:x:170:TYR:HD1  | 2.02                     | 0.43              |
| 2:E:66:ASP:OD1   | 2:E:66:ASP:N     | 2.50                     | 0.43              |
| 7:N:22:ILE:HD12  | 7:N:74:THR:H     | 1.83                     | 0.43              |
| 7:T:92:LYS:NZ    | 7:t:121:MET:C    | 2.70                     | 0.43              |
| 7:W:162:ASP:OD1  | 7:W:163:ILE:N    | 2.51                     | 0.43              |
| 7:m:89:PRO:HA    | 7:m:105:ASP:H    | 1.83                     | 0.43              |
| 7:X:41:VAL:O     | 7:X:96:ILE:N     | 2.49                     | 0.43              |
| 1:C:68:ILE:HG12  | 1:C:110:ILE:HD12 | 2.00                     | 0.42              |
| 2:D:146:ILE:HG23 | 2:D:154:ILE:HD11 | 2.01                     | 0.42              |
| 2:E:12:ILE:HG23  | 2:E:277:VAL:HG13 | 1.99                     | 0.42              |
| 2:E:63:ASP:OD1   | 2:E:63:ASP:N     | 2.52                     | 0.42              |
| 2:F:146:ILE:HG23 | 2:F:154:ILE:HD11 | 2.01                     | 0.42              |
| 6:K:341:GLU:O    | 6:K:345:GLU:N    | 2.52                     | 0.42              |
| 7:L:92:LYS:HB3   | 7:l:61:ASP:HB2   | 2.01                     | 0.42              |
| 7:N:137:ILE:HA   | 7:N:140:GLU:HB2  | 2.00                     | 0.42              |
| 7:T:86:LEU:HB2   | 7:t:121:MET:HE1  | 2.01                     | 0.42              |
| 7:T:92:LYS:HE2   | 7:t:122:LYS:HA   | 2.00                     | 0.42              |
| 1:B:5:GLU:HB2    | 1:B:101:ARG:HH12 | 1.84                     | 0.42              |
| 2:D:137:SER:O    | 2:D:141:ASN:N    | 2.52                     | 0.42              |
| 2:F:117:LEU:HD23 | 2:F:120:LYS:HD3  | 2.01                     | 0.42              |
| 2:G:47:SER:OG    | 9:V:9:U:OP1      | 2.29                     | 0.42              |
| 2:G:248:LYS:HG3  | 7:N:94:TYR:HD1   | 1.85                     | 0.42              |
| 7:W:90:ALA:HB2   | 7:W:106:LEU:HD22 | 2.01                     | 0.42              |
| 7:X:58:PRO:HG3   | 7:X:112:TYR:HE1  | 1.84                     | 0.42              |
| 7:x:102:ILE:HG22 | 7:x:103:SER:H    | 1.84                     | 0.42              |
| 7:x:130:ASP:O    | 7:x:133:ILE:N    | 2.45                     | 0.42              |
| 5:J:107:LYS:CD   | 7:T:94:TYR:HA    | 2.48                     | 0.42              |
| 7:L:9:PHE:HD2    | 7:L:11:PRO:HD2   | 1.83                     | 0.42              |
| 7:O:84:LEU:HB2   | 7:O:110:ILE:HB   | 2.01                     | 0.42              |
| 7:S:20:VAL:HB    | 7:S:144:LYS:HE2  | 1.99                     | 0.42              |
| 7:n:81:ASN:OD1   | 7:n:81:ASN:N     | 2.52                     | 0.42              |
| 7:o:57:VAL:HG21  | 7:o:172:LEU:HD11 | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:o:163:ILE:HA   | 7:o:167:PHE:CD2  | 2.55                     | 0.42              |
| 1:B:99:ILE:HD12  | 1:B:106:GLN:HA   | 2.02                     | 0.42              |
| 2:F:42:PRO:HD2   | 2:F:91:LEU:HD22  | 2.01                     | 0.42              |
| 7:M:120:SER:HA   | 7:m:87:LYS:HB3   | 2.01                     | 0.42              |
| 7:o:6:GLU:N      | 7:o:71:VAL:O     | 2.44                     | 0.42              |
| 7:w:30:ILE:HB    | 7:w:70:LEU:HB3   | 2.02                     | 0.42              |
| 7:X:123:THR:OG1  | 7:X:171:ALA:O    | 2.29                     | 0.42              |
| 7:x:28:ASP:O     | 7:x:72:ALA:HB2   | 2.19                     | 0.42              |
| 1:B:35:ARG:HH22  | 8:U:29:C:P       | 2.42                     | 0.42              |
| 2:D:115:TYR:CZ   | 2:D:150:GLU:HA   | 2.54                     | 0.42              |
| 7:L:138:ILE:HA   | 7:L:142:PHE:HB2  | 2.01                     | 0.42              |
| 7:O:134:VAL:HA   | 7:O:137:ILE:HB   | 2.01                     | 0.42              |
| 7:t:9:PHE:HE2    | 7:t:11:PRO:HB3   | 1.83                     | 0.42              |
| 7:w:22:ILE:HG22  | 7:w:24:ILE:H     | 1.83                     | 0.42              |
| 7:w:31:THR:HG21  | 7:w:69:ILE:HG23  | 2.01                     | 0.42              |
| 7:X:31:THR:CG2   | 7:X:69:ILE:HG23  | 2.49                     | 0.42              |
| 1:C:35:ARG:NH2   | 8:U:17:C:OP2     | 2.41                     | 0.42              |
| 2:D:180:ILE:HG12 | 2:D:183:ILE:HD12 | 2.02                     | 0.42              |
| 2:F:259:ARG:HG3  | 7:M:94:TYR:CE1   | 2.52                     | 0.42              |
| 2:F:284:ASP:HA   | 7:M:97:ARG:HD3   | 2.02                     | 0.42              |
| 5:J:172:VAL:HG13 | 5:J:192:LEU:HD13 | 2.02                     | 0.42              |
| 6:K:244:GLU:HG3  | 6:K:321:ARG:HE   | 1.84                     | 0.42              |
| 6:K:658:LEU:HD21 | 6:K:774:ILE:HG21 | 2.01                     | 0.42              |
| 7:l:30:ILE:HD11  | 7:l:106:LEU:HD13 | 2.02                     | 0.42              |
| 7:m:121:MET:HG2  | 7:m:172:LEU:HD21 | 2.02                     | 0.42              |
| 7:p:5:ARG:NH2    | 7:p:28:ASP:OD1   | 2.53                     | 0.42              |
| 7:X:106:LEU:HD23 | 7:X:108:ILE:HD11 | 2.01                     | 0.42              |
| 7:x:155:LYS:HG2  | 7:x:158:LYS:HB2  | 2.01                     | 0.42              |
| 3:H:73:GLY:HA3   | 3:H:299:THR:HG21 | 2.02                     | 0.42              |
| 5:J:106:ASP:H    | 5:J:109:ILE:HG13 | 1.84                     | 0.42              |
| 6:K:198:ALA:HB2  | 6:K:397:GLU:HG2  | 2.02                     | 0.42              |
| 6:K:213:PHE:CG   | 6:K:386:LEU:HD21 | 2.54                     | 0.42              |
| 7:M:59:THR:OG1   | 7:M:60:LEU:N     | 2.53                     | 0.42              |
| 7:S:149:THR:HG22 | 7:S:153:LYS:HE3  | 2.02                     | 0.42              |
| 7:w:102:ILE:HG21 | 7:w:106:LEU:HD11 | 2.01                     | 0.42              |
| 7:X:43:VAL:HG22  | 7:X:67:LYS:HG2   | 2.01                     | 0.42              |
| 7:X:79:GLN:HG2   | 7:X:83:PHE:CD2   | 2.55                     | 0.42              |
| 4:I:171:GLU:N    | 7:P:165:GLU:OE2  | 2.53                     | 0.42              |
| 6:K:656:ASP:HB2  | 6:K:661:LYS:HD2  | 2.02                     | 0.42              |
| 7:W:117:ALA:O    | 7:w:87:LYS:NZ    | 2.53                     | 0.42              |
| 7:l:146:TYR:HA   | 7:l:148:ILE:HG22 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:s:144:LYS:HG3  | 7:s:145:ILE:HG12 | 2.02                     | 0.42              |
| 7:x:42:LEU:HA    | 7:x:95:LEU:HG    | 2.02                     | 0.42              |
| 2:G:32:LEU:HD12  | 2:G:229:GLU:HG2  | 2.01                     | 0.42              |
| 3:H:75:PHE:O     | 3:H:169:VAL:N    | 2.50                     | 0.42              |
| 5:J:441:SER:OG   | 5:J:442:ASN:N    | 2.53                     | 0.42              |
| 5:J:467:ILE:O    | 5:J:467:ILE:HG22 | 2.19                     | 0.42              |
| 6:K:703:ASP:HA   | 6:K:706:LYS:HG2  | 2.00                     | 0.42              |
| 7:L:31:THR:HG1   | 7:L:70:LEU:H     | 1.61                     | 0.42              |
| 7:o:162:ASP:HB2  | 7:o:166:LEU:HD12 | 2.02                     | 0.42              |
| 7:x:45:THR:OG1   | 7:x:62:PRO:O     | 2.38                     | 0.42              |
| 7:x:158:LYS:HA   | 7:x:161:GLU:HB2  | 2.01                     | 0.42              |
| 2:D:63:ASP:OD2   | 7:O:170:TYR:OH   | 2.29                     | 0.42              |
| 3:H:61:LEU:HD13  | 3:H:292:TYR:CE1  | 2.55                     | 0.42              |
| 5:J:336:ILE:HD12 | 5:J:444:SER:HB3  | 2.02                     | 0.42              |
| 6:K:478:LYS:NZ   | 6:K:507:PRO:HB2  | 2.34                     | 0.42              |
| 7:N:153:LYS:HE2  | 7:N:153:LYS:HB3  | 1.92                     | 0.42              |
| 7:q:137:ILE:HA   | 7:q:140:GLU:HG2  | 2.01                     | 0.42              |
| 7:r:7:TYR:HA     | 7:r:70:LEU:HD23  | 2.01                     | 0.42              |
| 1:A:40:GLU:OE2   | 2:E:210:ARG:NH2  | 2.52                     | 0.41              |
| 1:C:116:GLU:HB2  | 4:I:38:GLU:HG3   | 2.02                     | 0.41              |
| 6:K:535:ASP:HA   | 6:K:542:ILE:HD11 | 2.01                     | 0.41              |
| 7:O:22:ILE:HD11  | 7:O:74:THR:HG22  | 2.02                     | 0.41              |
| 7:O:33:ILE:HG12  | 7:O:38:ILE:HG12  | 2.01                     | 0.41              |
| 7:n:138:ILE:HA   | 7:n:142:PHE:HB2  | 2.02                     | 0.41              |
| 7:p:43:VAL:HB    | 7:p:94:TYR:HD2   | 1.84                     | 0.41              |
| 8:U:16:C:O2      | 9:V:33:G:N2      | 2.47                     | 0.41              |
| 7:x:52:LYS:O     | 7:x:52:LYS:HG3   | 2.19                     | 0.41              |
| 2:D:95:PRO:O     | 2:D:205:SER:OG   | 2.35                     | 0.41              |
| 2:F:142:LYS:HD3  | 2:F:181:PRO:HG2  | 2.01                     | 0.41              |
| 3:H:121:LEU:HA   | 3:H:125:LYS:HB2  | 2.01                     | 0.41              |
| 5:J:107:LYS:CG   | 7:T:94:TYR:HA    | 2.48                     | 0.41              |
| 6:K:923:ARG:HD3  | 6:K:923:ARG:HA   | 1.90                     | 0.41              |
| 7:P:42:LEU:HD22  | 7:P:70:LEU:HD11  | 2.01                     | 0.41              |
| 7:T:44:ILE:HG23  | 7:t:60:LEU:CD1   | 2.51                     | 0.41              |
| 7:X:49:VAL:HG21  | 7:X:169:TYR:HE2  | 1.85                     | 0.41              |
| 7:X:162:ASP:OD1  | 7:X:163:ILE:HG13 | 2.19                     | 0.41              |
| 2:F:6:PHE:HE1    | 2:F:250:SER:HB3  | 1.85                     | 0.41              |
| 2:G:125:LEU:HB3  | 2:G:140:LYS:HE2  | 2.02                     | 0.41              |
| 4:I:133:GLY:O    | 4:I:137:PHE:N    | 2.50                     | 0.41              |
| 6:K:262:ALA:HB3  | 6:K:291:PHE:HE2  | 1.85                     | 0.41              |
| 7:P:78:ALA:H     | 7:P:79:GLN:HG2   | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:R:28:ASP:OD1   | 7:R:28:ASP:N     | 2.53                     | 0.41              |
| 7:o:55:ARG:HB2   | 7:o:113:SER:HB2  | 2.01                     | 0.41              |
| 7:o:137:ILE:HG22 | 7:o:141:VAL:HG12 | 2.01                     | 0.41              |
| 7:w:62:PRO:N     | 7:w:63:CYS:H     | 2.17                     | 0.41              |
| 7:x:39:HIS:HA    | 7:x:97:ARG:HG3   | 2.02                     | 0.41              |
| 7:x:87:LYS:HA    | 7:x:107:LYS:HA   | 2.02                     | 0.41              |
| 1:B:103:ILE:HG22 | 1:B:129:LEU:HD13 | 2.03                     | 0.41              |
| 2:D:66:ASP:OD1   | 2:D:66:ASP:N     | 2.50                     | 0.41              |
| 4:I:155:SER:OG   | 9:V:33:G:OP1     | 2.34                     | 0.41              |
| 4:I:176:GLU:HG2  | 4:I:183:ARG:HH12 | 1.85                     | 0.41              |
| 4:I:242:TYR:HE2  | 4:I:245:GLU:HA   | 1.86                     | 0.41              |
| 6:K:744:VAL:HG13 | 6:K:747:GLU:HB2  | 2.03                     | 0.41              |
| 7:N:120:SER:HA   | 7:n:87:LYS:HG3   | 2.02                     | 0.41              |
| 7:R:124:LYS:N    | 7:R:171:ALA:O    | 2.45                     | 0.41              |
| 7:S:136:ASN:O    | 7:S:140:GLU:N    | 2.38                     | 0.41              |
| 7:o:58:PRO:HG2   | 7:o:115:PRO:HG3  | 2.01                     | 0.41              |
| 7:s:88:LEU:HD22  | 7:s:92:LYS:HD3   | 2.02                     | 0.41              |
| 7:X:135:ASN:HA   | 7:X:160:LYS:NZ   | 2.35                     | 0.41              |
| 1:A:14:PHE:HE2   | 1:A:151:LEU:HD12 | 1.85                     | 0.41              |
| 1:C:107:LYS:HE2  | 1:C:107:LYS:HB2  | 1.82                     | 0.41              |
| 1:C:141:LEU:HD23 | 1:C:141:LEU:HA   | 1.90                     | 0.41              |
| 2:E:57:LEU:HD21  | 2:E:261:LEU:HD13 | 2.03                     | 0.41              |
| 6:K:832:LEU:HB3  | 6:K:833:GLY:H    | 1.78                     | 0.41              |
| 6:K:890:TYR:CZ   | 6:K:918:PRO:HB3  | 2.55                     | 0.41              |
| 7:M:157:GLU:HA   | 7:M:160:LYS:HB3  | 2.03                     | 0.41              |
| 7:T:84:LEU:HB3   | 7:T:86:LEU:HD22  | 2.01                     | 0.41              |
| 7:X:158:LYS:O    | 7:X:161:GLU:HG3  | 2.21                     | 0.41              |
| 7:x:17:THR:HG23  | 7:x:18:ILE:N     | 2.35                     | 0.41              |
| 1:C:110:ILE:O    | 1:C:114:ARG:N    | 2.54                     | 0.41              |
| 4:I:271:TYR:HD1  | 4:I:271:TYR:HA   | 1.73                     | 0.41              |
| 6:K:134:LEU:HA   | 6:K:137:VAL:HG22 | 2.03                     | 0.41              |
| 6:K:233:LEU:HD23 | 6:K:531:LEU:HD11 | 2.03                     | 0.41              |
| 7:O:20:VAL:HG22  | 7:O:22:ILE:H     | 1.86                     | 0.41              |
| 7:S:124:LYS:HE3  | 7:S:125:PRO:HD2  | 2.02                     | 0.41              |
| 7:q:47:TYR:HB3   | 7:q:56:LEU:HD22  | 2.03                     | 0.41              |
| 7:s:6:GLU:HG3    | 7:s:71:VAL:HG23  | 2.02                     | 0.41              |
| 7:x:70:LEU:HD13  | 7:x:95:LEU:HD21  | 2.02                     | 0.41              |
| 2:D:205:SER:O    | 4:I:146:TYR:OH   | 2.36                     | 0.41              |
| 4:I:160:ILE:HG21 | 4:I:263:LEU:HD12 | 2.03                     | 0.41              |
| 5:J:371:LEU:HB3  | 5:J:378:ARG:HE   | 1.85                     | 0.41              |
| 6:K:444:LEU:HD23 | 6:K:449:LYS:HB2  | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:X:5:ARG:HH11   | 7:X:72:ALA:HB2   | 1.86                     | 0.41              |
| 7:x:84:LEU:HG    | 7:x:112:TYR:CG   | 2.55                     | 0.41              |
| 7:x:149:THR:C    | 7:x:151:LYS:H    | 2.29                     | 0.41              |
| 2:D:215:ASP:O    | 2:D:219:LYS:N    | 2.47                     | 0.41              |
| 6:K:183:ALA:HB1  | 6:K:768:PRO:HB2  | 2.03                     | 0.41              |
| 6:K:335:PHE:O    | 6:K:339:VAL:N    | 2.40                     | 0.41              |
| 7:L:67:LYS:HD2   | 7:L:168:SER:H    | 1.85                     | 0.41              |
| 7:M:43:VAL:HB    | 7:M:94:TYR:CD2   | 2.56                     | 0.41              |
| 7:S:43:VAL:HG12  | 7:S:67:LYS:HG2   | 2.02                     | 0.41              |
| 7:W:24:ILE:HG13  | 7:W:25:GLY:H     | 1.86                     | 0.41              |
| 7:m:19:ASP:HB3   | 7:m:75:PRO:HA    | 2.03                     | 0.41              |
| 7:q:67:LYS:HD3   | 7:q:166:LEU:HD23 | 2.01                     | 0.41              |
| 7:t:119:ASN:HB3  | 7:t:174:GLN:HG2  | 2.03                     | 0.41              |
| 1:A:5:GLU:O      | 1:A:101:ARG:NH1  | 2.54                     | 0.41              |
| 2:D:157:ASP:OD1  | 2:D:157:ASP:N    | 2.53                     | 0.41              |
| 2:F:63:ASP:OD1   | 2:F:63:ASP:N     | 2.52                     | 0.41              |
| 2:G:41:TYR:CG    | 2:G:117:LEU:HD21 | 2.56                     | 0.41              |
| 2:G:66:ASP:OD1   | 2:G:66:ASP:N     | 2.54                     | 0.41              |
| 3:H:174:ASN:OD1  | 3:H:175:ASP:N    | 2.53                     | 0.41              |
| 4:I:168:LYS:O    | 7:P:67:LYS:NZ    | 2.46                     | 0.41              |
| 5:J:332:GLU:HB2  | 5:J:468:LEU:HD11 | 1.94                     | 0.41              |
| 6:K:533:LEU:HD13 | 6:K:533:LEU:HA   | 1.92                     | 0.41              |
| 6:K:711:CYS:HA   | 6:K:714:GLU:HB3  | 2.02                     | 0.41              |
| 7:L:131:ASP:HA   | 7:L:134:VAL:HG22 | 2.02                     | 0.41              |
| 7:M:42:LEU:HD22  | 7:M:70:LEU:HD11  | 2.02                     | 0.41              |
| 7:O:131:ASP:HB2  | 7:O:160:LYS:HD2  | 2.02                     | 0.41              |
| 7:R:128:ILE:HG13 | 7:R:164:LYS:HA   | 2.01                     | 0.41              |
| 7:W:21:LYS:HD3   | 7:W:77:GLN:HB2   | 2.03                     | 0.41              |
| 7:m:93:LEU:HD23  | 7:m:93:LEU:HA    | 1.88                     | 0.41              |
| 7:X:4:GLN:CB     | 7:X:107:LYS:HB3  | 2.51                     | 0.41              |
| 7:X:70:LEU:HD13  | 7:X:108:ILE:HG21 | 2.02                     | 0.41              |
| 7:x:86:LEU:HD21  | 7:x:88:LEU:HG    | 2.02                     | 0.41              |
| 1:A:7:TYR:HD2    | 1:B:47:ILE:HG22  | 1.86                     | 0.41              |
| 2:G:10:PHE:HB3   | 2:G:281:TRP:CE3  | 2.56                     | 0.41              |
| 3:H:247:LEU:HD12 | 3:H:258:GLU:HB2  | 2.03                     | 0.41              |
| 4:I:210:HIS:NE2  | 4:I:222:PRO:HB3  | 2.36                     | 0.41              |
| 5:J:463:TYR:C    | 5:J:463:TYR:CD1  | 2.98                     | 0.41              |
| 6:K:20:HIS:CE1   | 6:K:184:THR:HG21 | 2.56                     | 0.41              |
| 6:K:655:GLY:O    | 6:K:659:GLU:N    | 2.53                     | 0.41              |
| 7:M:79:GLN:NE2   | 7:M:81:ASN:OD1   | 2.54                     | 0.41              |
| 7:P:84:LEU:HB3   | 7:P:110:ILE:HG13 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:Q:60:LEU:HD13  | 7:q:44:ILE:HG12   | 2.02                     | 0.41              |
| 7:S:45:THR:HG21  | 7:s:62:PRO:HB3    | 2.03                     | 0.41              |
| 7:W:32:ASN:HB2   | 7:W:39:HIS:HB2    | 2.03                     | 0.41              |
| 7:l:8:VAL:HG21   | 7:l:141:VAL:HG21  | 2.02                     | 0.41              |
| 7:p:56:LEU:HD21  | 7:p:66:VAL:HG11   | 2.03                     | 0.41              |
| 7:x:34:ASP:O     | 7:x:36:ARG:HG2    | 2.21                     | 0.41              |
| 7:x:130:ASP:O    | 7:x:133:ILE:HG22  | 2.20                     | 0.41              |
| 1:C:35:ARG:NE    | 1:C:149:GLU:OE2   | 2.54                     | 0.40              |
| 2:D:280:ARG:HA   | 2:D:280:ARG:HD3   | 1.93                     | 0.40              |
| 2:F:110:VAL:HG23 | 2:F:189:PRO:HG2   | 2.03                     | 0.40              |
| 3:H:76:ILE:HG23  | 3:H:166:VAL:HG13  | 2.03                     | 0.40              |
| 4:I:210:HIS:CE1  | 9:V:38:C:H2'      | 2.57                     | 0.40              |
| 5:J:6:MET:SD     | 5:J:8:LEU:HD11    | 2.62                     | 0.40              |
| 6:K:314:LEU:HB3  | 6:K:316:LEU:HG    | 2.02                     | 0.40              |
| 6:K:959:LEU:HD12 | 6:K:1026:VAL:HG13 | 2.03                     | 0.40              |
| 7:N:159:VAL:HA   | 7:N:162:ASP:HB2   | 2.03                     | 0.40              |
| 7:w:30:ILE:HG22  | 7:w:40:ASN:HB3    | 2.02                     | 0.40              |
| 7:x:9:PHE:CD1    | 7:x:11:PRO:HD3    | 2.50                     | 0.40              |
| 7:x:102:ILE:H    | 7:x:102:ILE:HD12  | 1.85                     | 0.40              |
| 2:F:144:ASP:O    | 2:F:148:ALA:N     | 2.54                     | 0.40              |
| 6:K:478:LYS:HG2  | 6:K:508:GLY:HA3   | 2.01                     | 0.40              |
| 7:n:35:GLU:O     | 7:n:158:LYS:NZ    | 2.41                     | 0.40              |
| 7:n:84:LEU:HB3   | 7:n:110:ILE:HB    | 2.03                     | 0.40              |
| 7:x:124:LYS:O    | 7:x:170:TYR:HA    | 2.20                     | 0.40              |
| 7:x:156:ILE:O    | 7:x:160:LYS:HG3   | 2.22                     | 0.40              |
| 1:B:68:ILE:HA    | 1:B:71:PHE:HD2    | 1.86                     | 0.40              |
| 2:D:139:LEU:HD23 | 2:D:139:LEU:HA    | 1.95                     | 0.40              |
| 2:G:166:ASN:HD21 | 2:G:205:SER:HB2   | 1.86                     | 0.40              |
| 5:J:148:ILE:O    | 5:J:153:LYS:NZ    | 2.54                     | 0.40              |
| 7:T:88:LEU:HD22  | 7:T:93:LEU:HD11   | 2.03                     | 0.40              |
| 7:n:141:VAL:O    | 7:n:145:ILE:N     | 2.41                     | 0.40              |
| 7:p:123:THR:HA   | 7:p:172:LEU:HA    | 2.04                     | 0.40              |
| 7:w:67:LYS:HG3   | 7:w:168:SER:H     | 1.86                     | 0.40              |
| 2:E:10:PHE:HB3   | 2:E:281:TRP:CE3   | 2.57                     | 0.40              |
| 2:G:63:ASP:OD1   | 2:G:63:ASP:N      | 2.50                     | 0.40              |
| 5:J:470:LYS:HE3  | 7:W:94:TYR:HD1    | 1.85                     | 0.40              |
| 6:K:73:ASP:OD1   | 6:K:88:TYR:OH     | 2.31                     | 0.40              |
| 6:K:148:GLN:HA   | 6:K:247:PRO:HG3   | 2.02                     | 0.40              |
| 6:K:207:THR:HA   | 6:K:388:ILE:HA    | 2.04                     | 0.40              |
| 6:K:922:LYS:O    | 6:K:923:ARG:NH2   | 2.55                     | 0.40              |
| 7:N:6:GLU:N      | 7:N:71:VAL:O      | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:N:48:ALA:O     | 7:N:57:VAL:N     | 2.55                     | 0.40              |
| 7:T:121:MET:SD   | 7:T:121:MET:N    | 2.95                     | 0.40              |
| 7:m:33:ILE:HG12  | 7:m:159:VAL:HG21 | 2.03                     | 0.40              |
| 7:m:40:ASN:OD1   | 7:m:99:LYS:N     | 2.55                     | 0.40              |
| 7:m:102:ILE:HG22 | 7:m:103:SER:H    | 1.86                     | 0.40              |
| 7:o:79:GLN:HB3   | 7:o:80:SER:H     | 1.76                     | 0.40              |
| 7:r:89:PRO:HA    | 7:r:105:ASP:H    | 1.86                     | 0.40              |
| 7:s:93:LEU:HB3   | 7:s:95:LEU:HG    | 2.03                     | 0.40              |
| 7:w:127:SER:OG   | 7:w:128:ILE:N    | 2.54                     | 0.40              |
| 7:X:143:ASP:CG   | 7:X:149:THR:HB   | 2.46                     | 0.40              |
| 1:A:6:ASP:OD1    | 1:A:101:ARG:NH1  | 2.42                     | 0.40              |
| 1:A:120:LEU:HD23 | 1:A:120:LEU:HA   | 1.95                     | 0.40              |
| 2:F:17:HIS:CD2   | 2:F:233:PRO:HA   | 2.56                     | 0.40              |
| 5:J:14:TYR:H     | 5:J:204:GLN:HA   | 1.86                     | 0.40              |
| 7:N:22:ILE:HB    | 7:N:73:GLY:HA2   | 2.04                     | 0.40              |
| 7:S:5:ARG:HG3    | 7:S:106:LEU:HD11 | 2.04                     | 0.40              |
| 7:S:56:LEU:HD22  | 7:S:66:VAL:HG11  | 2.04                     | 0.40              |
| 7:p:96:ILE:HG22  | 7:p:97:ARG:HG3   | 2.04                     | 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   | A     | 151/155 (97%) | 145 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | B     | 152/155 (98%) | 143 (94%) | 8 (5%)  | 1 (1%)   | 18          | 52  |
| 1   | C     | 152/155 (98%) | 146 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 2   | D     | 283/286 (99%) | 257 (91%) | 26 (9%) | 0        | 100         | 100 |
| 2   | E     | 283/286 (99%) | 261 (92%) | 22 (8%) | 0        | 100         | 100 |
| 2   | F     | 283/286 (99%) | 258 (91%) | 25 (9%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 2   | G     | 283/286 (99%)   | 255 (90%)  | 28 (10%)  | 0        | 100         | 100 |
| 3   | H     | 310/313 (99%)   | 280 (90%)  | 30 (10%)  | 0        | 100         | 100 |
| 4   | I     | 282/296 (95%)   | 263 (93%)  | 19 (7%)   | 0        | 100         | 100 |
| 5   | J     | 473/476 (99%)   | 429 (91%)  | 43 (9%)   | 1 (0%)   | 43          | 74  |
| 6   | K     | 1005/1037 (97%) | 891 (89%)  | 113 (11%) | 1 (0%)   | 48          | 79  |
| 7   | L     | 171/174 (98%)   | 142 (83%)  | 28 (16%)  | 1 (1%)   | 21          | 55  |
| 7   | M     | 171/174 (98%)   | 147 (86%)  | 24 (14%)  | 0        | 100         | 100 |
| 7   | N     | 171/174 (98%)   | 149 (87%)  | 21 (12%)  | 1 (1%)   | 21          | 55  |
| 7   | O     | 171/174 (98%)   | 137 (80%)  | 34 (20%)  | 0        | 100         | 100 |
| 7   | P     | 171/174 (98%)   | 143 (84%)  | 28 (16%)  | 0        | 100         | 100 |
| 7   | Q     | 171/174 (98%)   | 139 (81%)  | 32 (19%)  | 0        | 100         | 100 |
| 7   | R     | 171/174 (98%)   | 143 (84%)  | 28 (16%)  | 0        | 100         | 100 |
| 7   | S     | 171/174 (98%)   | 146 (85%)  | 24 (14%)  | 1 (1%)   | 21          | 55  |
| 7   | T     | 171/174 (98%)   | 138 (81%)  | 31 (18%)  | 2 (1%)   | 10          | 42  |
| 7   | W     | 171/174 (98%)   | 141 (82%)  | 29 (17%)  | 1 (1%)   | 21          | 55  |
| 7   | X     | 171/174 (98%)   | 139 (81%)  | 31 (18%)  | 1 (1%)   | 21          | 55  |
| 7   | l     | 171/174 (98%)   | 139 (81%)  | 30 (18%)  | 2 (1%)   | 10          | 42  |
| 7   | m     | 171/174 (98%)   | 140 (82%)  | 29 (17%)  | 2 (1%)   | 10          | 42  |
| 7   | n     | 171/174 (98%)   | 141 (82%)  | 30 (18%)  | 0        | 100         | 100 |
| 7   | o     | 171/174 (98%)   | 143 (84%)  | 28 (16%)  | 0        | 100         | 100 |
| 7   | p     | 171/174 (98%)   | 146 (85%)  | 24 (14%)  | 1 (1%)   | 21          | 55  |
| 7   | q     | 171/174 (98%)   | 148 (86%)  | 23 (14%)  | 0        | 100         | 100 |
| 7   | r     | 171/174 (98%)   | 139 (81%)  | 31 (18%)  | 1 (1%)   | 21          | 55  |
| 7   | s     | 171/174 (98%)   | 149 (87%)  | 22 (13%)  | 0        | 100         | 100 |
| 7   | t     | 171/174 (98%)   | 145 (85%)  | 25 (15%)  | 1 (1%)   | 21          | 55  |
| 7   | w     | 171/174 (98%)   | 142 (83%)  | 28 (16%)  | 1 (1%)   | 21          | 55  |
| 7   | x     | 171/174 (98%)   | 129 (75%)  | 41 (24%)  | 1 (1%)   | 21          | 55  |
| All | All   | 7419/7559 (98%) | 6453 (87%) | 947 (13%) | 19 (0%)  | 37          | 66  |

All (19) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | K     | 482 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | J     | 364 | LYS  |
| 7   | N     | 131 | ASP  |
| 7   | T     | 131 | ASP  |
| 7   | W     | 131 | ASP  |
| 7   | l     | 51  | GLU  |
| 7   | r     | 131 | ASP  |
| 7   | x     | 51  | GLU  |
| 7   | l     | 75  | PRO  |
| 7   | m     | 75  | PRO  |
| 7   | L     | 131 | ASP  |
| 7   | p     | 131 | ASP  |
| 7   | X     | 35  | GLU  |
| 7   | m     | 105 | ASP  |
| 7   | w     | 76  | GLN  |
| 1   | B     | 74  | ASP  |
| 7   | S     | 75  | PRO  |
| 7   | T     | 75  | PRO  |
| 7   | t     | 62  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 134/136 (98%)  | 134 (100%) | 0        | 100         | 100 |
| 1   | B     | 135/136 (99%)  | 135 (100%) | 0        | 100         | 100 |
| 1   | C     | 135/136 (99%)  | 135 (100%) | 0        | 100         | 100 |
| 2   | D     | 252/253 (100%) | 249 (99%)  | 3 (1%)   | 63          | 73  |
| 2   | E     | 252/253 (100%) | 252 (100%) | 0        | 100         | 100 |
| 2   | F     | 252/253 (100%) | 252 (100%) | 0        | 100         | 100 |
| 2   | G     | 251/253 (99%)  | 250 (100%) | 1 (0%)   | 84          | 82  |
| 3   | H     | 279/280 (100%) | 278 (100%) | 1 (0%)   | 84          | 82  |
| 4   | I     | 255/266 (96%)  | 255 (100%) | 0        | 100         | 100 |
| 5   | J     | 442/445 (99%)  | 430 (97%)  | 12 (3%)  | 39          | 62  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 6   | K     | 921/949 (97%)   | 910 (99%)  | 11 (1%)  | 63          | 73  |
| 7   | L     | 159/160 (99%)   | 158 (99%)  | 1 (1%)   | 78          | 80  |
| 7   | M     | 159/160 (99%)   | 158 (99%)  | 1 (1%)   | 78          | 80  |
| 7   | N     | 159/160 (99%)   | 159 (100%) | 0        | 100         | 100 |
| 7   | O     | 159/160 (99%)   | 158 (99%)  | 1 (1%)   | 78          | 80  |
| 7   | P     | 159/160 (99%)   | 156 (98%)  | 3 (2%)   | 50          | 68  |
| 7   | Q     | 159/160 (99%)   | 158 (99%)  | 1 (1%)   | 78          | 80  |
| 7   | R     | 159/160 (99%)   | 159 (100%) | 0        | 100         | 100 |
| 7   | S     | 159/160 (99%)   | 159 (100%) | 0        | 100         | 100 |
| 7   | T     | 159/160 (99%)   | 153 (96%)  | 6 (4%)   | 29          | 56  |
| 7   | W     | 159/160 (99%)   | 159 (100%) | 0        | 100         | 100 |
| 7   | X     | 159/160 (99%)   | 159 (100%) | 0        | 100         | 100 |
| 7   | l     | 159/160 (99%)   | 159 (100%) | 0        | 100         | 100 |
| 7   | m     | 159/160 (99%)   | 156 (98%)  | 3 (2%)   | 50          | 68  |
| 7   | n     | 159/160 (99%)   | 158 (99%)  | 1 (1%)   | 78          | 80  |
| 7   | o     | 159/160 (99%)   | 159 (100%) | 0        | 100         | 100 |
| 7   | p     | 159/160 (99%)   | 158 (99%)  | 1 (1%)   | 78          | 80  |
| 7   | q     | 159/160 (99%)   | 159 (100%) | 0        | 100         | 100 |
| 7   | r     | 159/160 (99%)   | 159 (100%) | 0        | 100         | 100 |
| 7   | s     | 159/160 (99%)   | 158 (99%)  | 1 (1%)   | 78          | 80  |
| 7   | t     | 159/160 (99%)   | 158 (99%)  | 1 (1%)   | 78          | 80  |
| 7   | w     | 159/160 (99%)   | 158 (99%)  | 1 (1%)   | 78          | 80  |
| 7   | x     | 159/160 (99%)   | 159 (100%) | 0        | 100         | 100 |
| All | All   | 6806/6880 (99%) | 6757 (99%) | 49 (1%)  | 73          | 78  |

All (49) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 120 | LYS  |
| 2   | D     | 152 | LYS  |
| 2   | D     | 277 | VAL  |
| 2   | G     | 203 | ASN  |
| 3   | H     | 68  | LEU  |
| 5   | J     | 107 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | J     | 108 | VAL  |
| 5   | J     | 109 | ILE  |
| 5   | J     | 111 | CYS  |
| 5   | J     | 113 | ARG  |
| 5   | J     | 138 | ILE  |
| 5   | J     | 140 | ILE  |
| 5   | J     | 461 | ILE  |
| 5   | J     | 465 | ARG  |
| 5   | J     | 468 | LEU  |
| 5   | J     | 469 | GLU  |
| 5   | J     | 471 | LEU  |
| 6   | K     | 384 | THR  |
| 6   | K     | 478 | LYS  |
| 6   | K     | 479 | GLU  |
| 6   | K     | 480 | ASP  |
| 6   | K     | 481 | GLU  |
| 6   | K     | 483 | GLU  |
| 6   | K     | 716 | LEU  |
| 6   | K     | 774 | ILE  |
| 6   | K     | 933 | ASN  |
| 6   | K     | 943 | LEU  |
| 6   | K     | 995 | VAL  |
| 7   | L     | 33  | ILE  |
| 7   | M     | 20  | VAL  |
| 7   | O     | 86  | LEU  |
| 7   | P     | 8   | VAL  |
| 7   | P     | 101 | ASN  |
| 7   | P     | 102 | ILE  |
| 7   | Q     | 86  | LEU  |
| 7   | T     | 41  | VAL  |
| 7   | T     | 42  | LEU  |
| 7   | T     | 43  | VAL  |
| 7   | T     | 60  | LEU  |
| 7   | T     | 92  | LYS  |
| 7   | T     | 93  | LEU  |
| 7   | m     | 8   | VAL  |
| 7   | m     | 33  | ILE  |
| 7   | m     | 86  | LEU  |
| 7   | n     | 8   | VAL  |
| 7   | p     | 106 | LEU  |
| 7   | s     | 86  | LEU  |
| 7   | t     | 60  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | w     | 64  | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 84  | ASN  |
| 1   | B     | 19  | ASN  |
| 1   | B     | 23  | HIS  |
| 1   | B     | 111 | GLN  |
| 1   | B     | 128 | ASN  |
| 1   | C     | 19  | ASN  |
| 1   | C     | 128 | ASN  |
| 2   | D     | 13  | HIS  |
| 2   | D     | 17  | HIS  |
| 2   | D     | 133 | ASN  |
| 2   | E     | 13  | HIS  |
| 2   | E     | 19  | HIS  |
| 2   | E     | 260 | ASN  |
| 2   | F     | 17  | HIS  |
| 2   | F     | 77  | ASN  |
| 2   | F     | 130 | GLN  |
| 2   | F     | 141 | ASN  |
| 2   | F     | 166 | ASN  |
| 2   | F     | 185 | ASN  |
| 2   | F     | 260 | ASN  |
| 2   | G     | 19  | HIS  |
| 2   | G     | 77  | ASN  |
| 2   | G     | 141 | ASN  |
| 2   | G     | 203 | ASN  |
| 3   | H     | 66  | ASN  |
| 3   | H     | 182 | ASN  |
| 3   | H     | 253 | ASN  |
| 4   | I     | 21  | ASN  |
| 4   | I     | 34  | ASN  |
| 4   | I     | 74  | ASN  |
| 4   | I     | 212 | ASN  |
| 5   | J     | 126 | ASN  |
| 5   | J     | 145 | ASN  |
| 5   | J     | 220 | HIS  |
| 5   | J     | 277 | ASN  |
| 5   | J     | 285 | ASN  |
| 6   | K     | 64  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | K     | 71   | ASN  |
| 6   | K     | 172  | ASN  |
| 6   | K     | 299  | ASN  |
| 6   | K     | 452  | GLN  |
| 6   | K     | 503  | ASN  |
| 6   | K     | 544  | ASN  |
| 6   | K     | 635  | HIS  |
| 6   | K     | 695  | ASN  |
| 6   | K     | 738  | ASN  |
| 6   | K     | 771  | HIS  |
| 6   | K     | 846  | ASN  |
| 6   | K     | 911  | GLN  |
| 6   | K     | 967  | HIS  |
| 6   | K     | 1024 | ASN  |
| 7   | L     | 14   | ASN  |
| 7   | L     | 135  | ASN  |
| 7   | L     | 150  | GLN  |
| 7   | M     | 40   | ASN  |
| 7   | M     | 76   | GLN  |
| 7   | M     | 77   | GLN  |
| 7   | M     | 174  | GLN  |
| 7   | N     | 14   | ASN  |
| 7   | N     | 32   | ASN  |
| 7   | N     | 40   | ASN  |
| 7   | N     | 135  | ASN  |
| 7   | O     | 40   | ASN  |
| 7   | O     | 53   | ASN  |
| 7   | P     | 14   | ASN  |
| 7   | P     | 101  | ASN  |
| 7   | Q     | 135  | ASN  |
| 7   | R     | 32   | ASN  |
| 7   | R     | 147  | ASN  |
| 7   | S     | 32   | ASN  |
| 7   | S     | 39   | HIS  |
| 7   | S     | 136  | ASN  |
| 7   | T     | 53   | ASN  |
| 7   | T     | 91   | ASN  |
| 7   | T     | 101  | ASN  |
| 7   | T     | 150  | GLN  |
| 7   | W     | 14   | ASN  |
| 7   | W     | 135  | ASN  |
| 7   | l     | 40   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | l     | 53  | ASN  |
| 7   | l     | 79  | GLN  |
| 7   | l     | 136 | ASN  |
| 7   | m     | 39  | HIS  |
| 7   | n     | 174 | GLN  |
| 7   | o     | 4   | GLN  |
| 7   | o     | 39  | HIS  |
| 7   | o     | 40  | ASN  |
| 7   | o     | 101 | ASN  |
| 7   | p     | 14  | ASN  |
| 7   | p     | 147 | ASN  |
| 7   | q     | 14  | ASN  |
| 7   | r     | 76  | GLN  |
| 7   | r     | 77  | GLN  |
| 7   | r     | 135 | ASN  |
| 7   | r     | 147 | ASN  |
| 7   | s     | 91  | ASN  |
| 7   | t     | 4   | GLN  |
| 7   | t     | 40  | ASN  |
| 7   | t     | 135 | ASN  |
| 7   | t     | 150 | GLN  |
| 7   | w     | 79  | GLN  |
| 7   | w     | 135 | ASN  |
| 7   | X     | 29  | HIS  |
| 7   | X     | 39  | HIS  |
| 7   | X     | 40  | ASN  |
| 7   | X     | 76  | GLN  |
| 7   | X     | 77  | GLN  |
| 7   | x     | 32  | ASN  |
| 7   | x     | 136 | ASN  |
| 7   | x     | 147 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 8   | U     | 41/46 (89%) | 15 (36%)          | 2 (4%)          |
| 9   | V     | 47/51 (92%) | 12 (25%)          | 0               |
| All | All   | 88/97 (90%) | 27 (30%)          | 2 (2%)          |

All (27) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | U     | 3   | U    |
| 8   | U     | 5   | A    |
| 8   | U     | 6   | A    |
| 8   | U     | 7   | G    |
| 8   | U     | 12  | G    |
| 8   | U     | 18  | C    |
| 8   | U     | 24  | G    |
| 8   | U     | 30  | U    |
| 8   | U     | 33  | G    |
| 8   | U     | 36  | U    |
| 8   | U     | 39  | A    |
| 8   | U     | 40  | A    |
| 8   | U     | 41  | A    |
| 8   | U     | 42  | A    |
| 8   | U     | 43  | A    |
| 9   | V     | 2   | U    |
| 9   | V     | 3   | U    |
| 9   | V     | 8   | G    |
| 9   | V     | 9   | U    |
| 9   | V     | 12  | A    |
| 9   | V     | 14  | A    |
| 9   | V     | 16  | C    |
| 9   | V     | 20  | G    |
| 9   | V     | 22  | U    |
| 9   | V     | 26  | C    |
| 9   | V     | 34  | A    |
| 9   | V     | 39  | A    |

All (2) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | U     | 5   | A    |
| 8   | U     | 42  | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

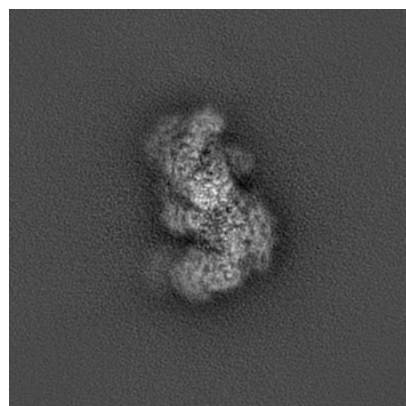
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10209. These allow visual inspection of the internal detail of the map and identification of artifacts.

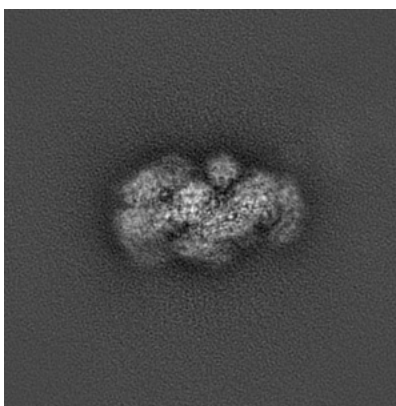
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

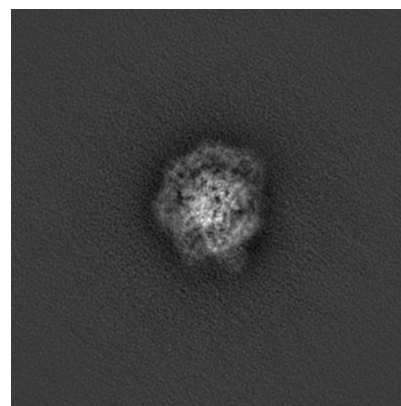
#### 6.1.1 Primary map



X

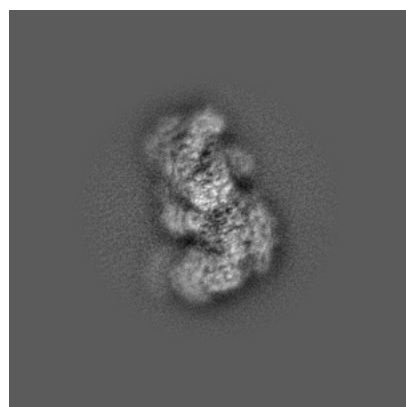


Y

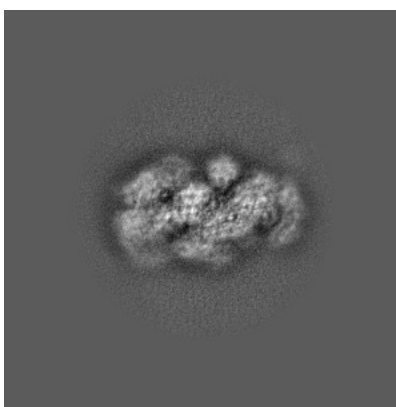


Z

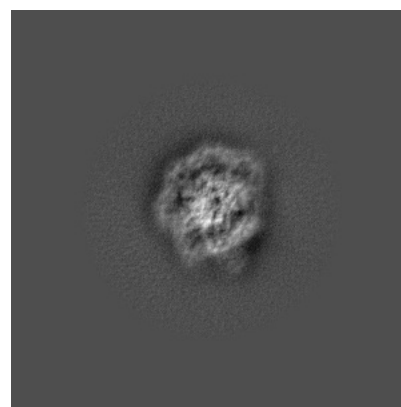
#### 6.1.2 Raw map



X



Y

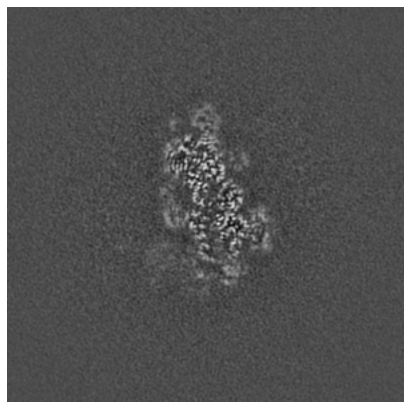


Z

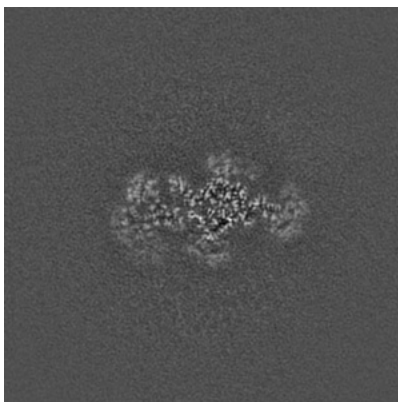
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

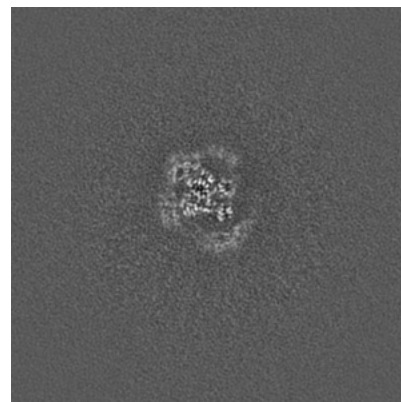
### 6.2.1 Primary map



X Index: 240

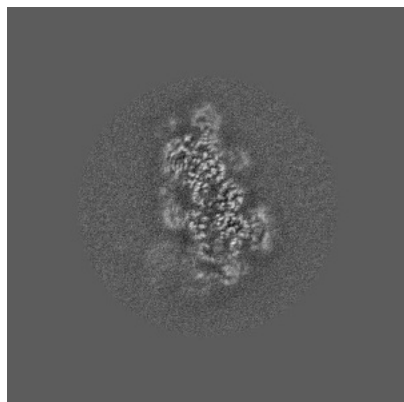


Y Index: 240

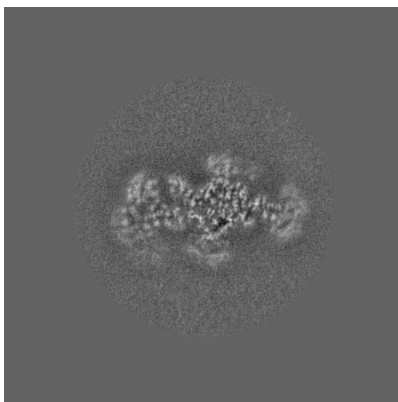


Z Index: 240

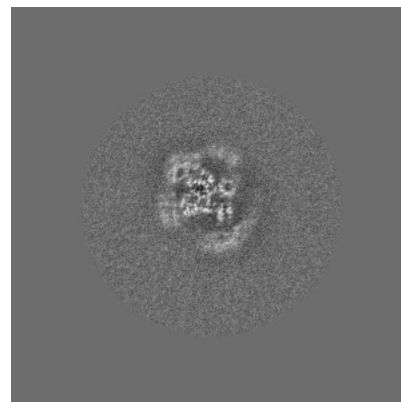
### 6.2.2 Raw map



X Index: 240



Y Index: 240

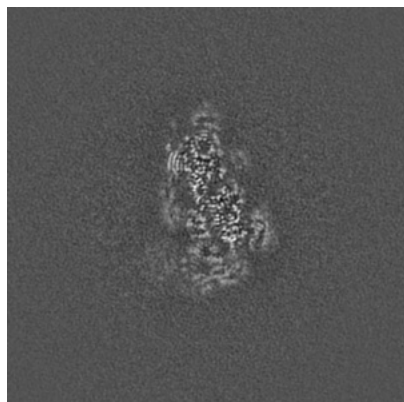


Z Index: 240

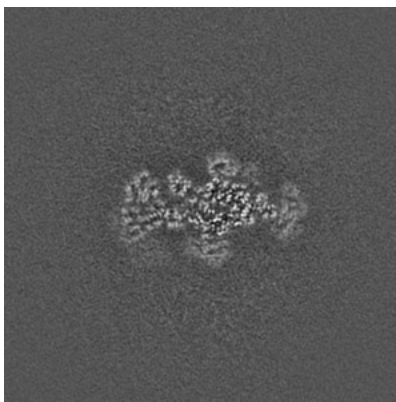
The images above show central slices of the map in three orthogonal directions.

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

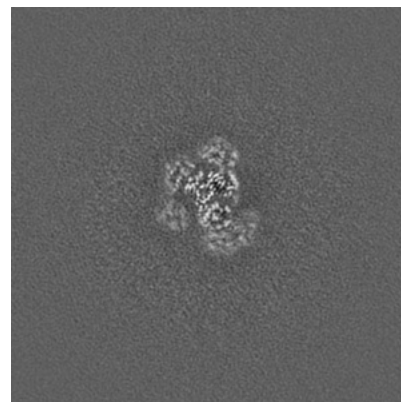
### 6.3.1 Primary map



X Index: 237

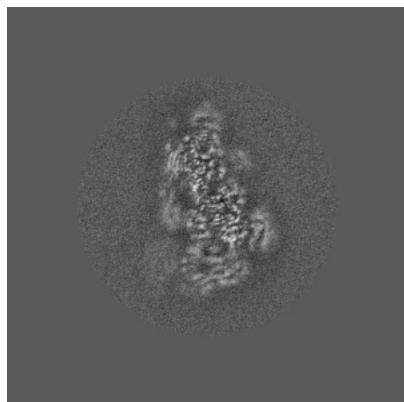


Y Index: 243

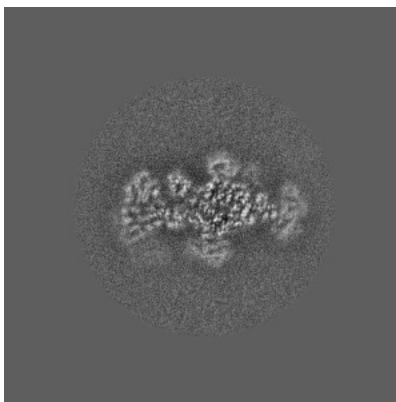


Z Index: 225

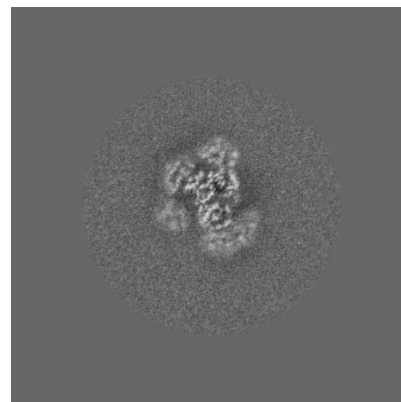
### 6.3.2 Raw map



X Index: 237



Y Index: 243

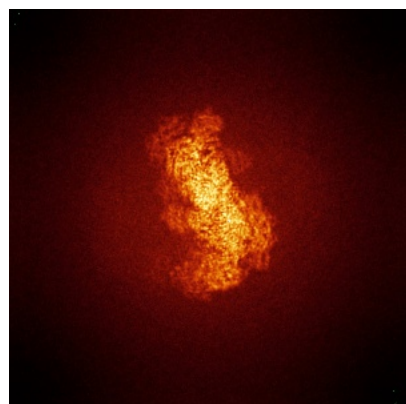


Z Index: 225

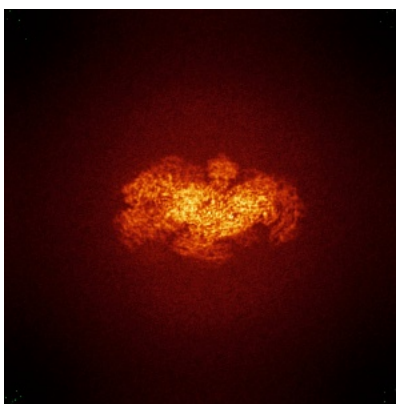
The images above show the largest variance slices of the map in three orthogonal directions.

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

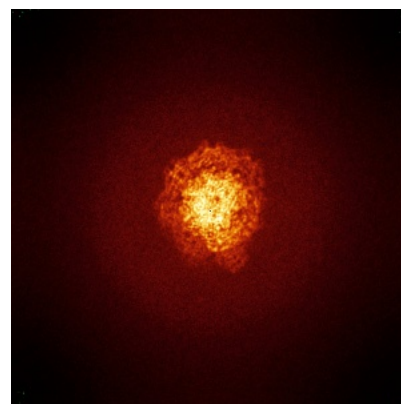
### 6.4.1 Primary map



X

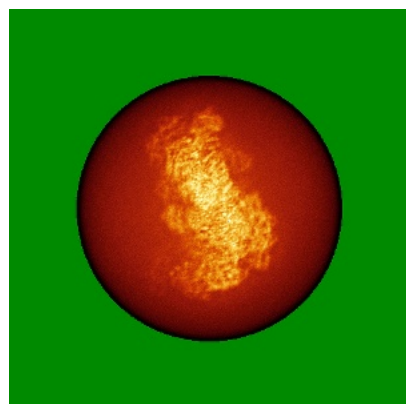


Y

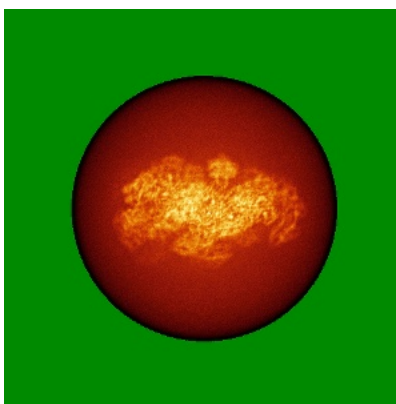


Z

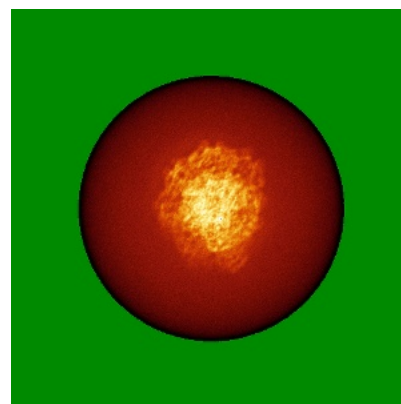
### 6.4.2 Raw map



X



Y

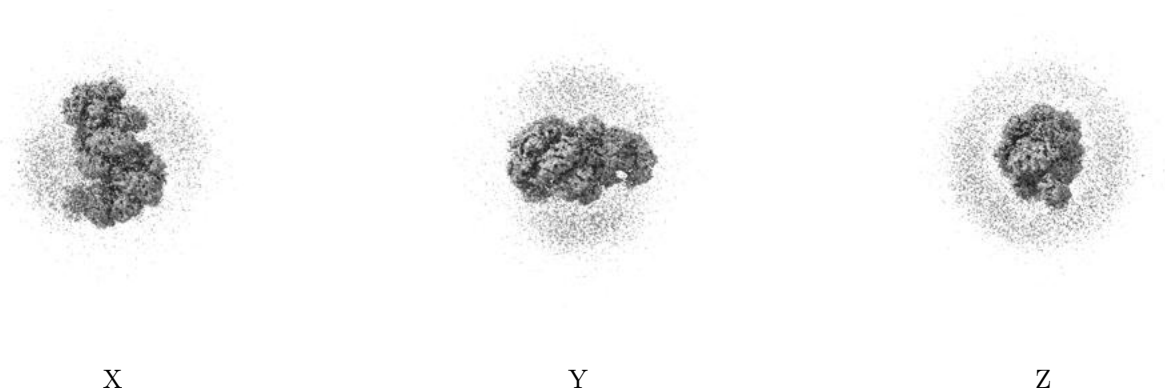


Z

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

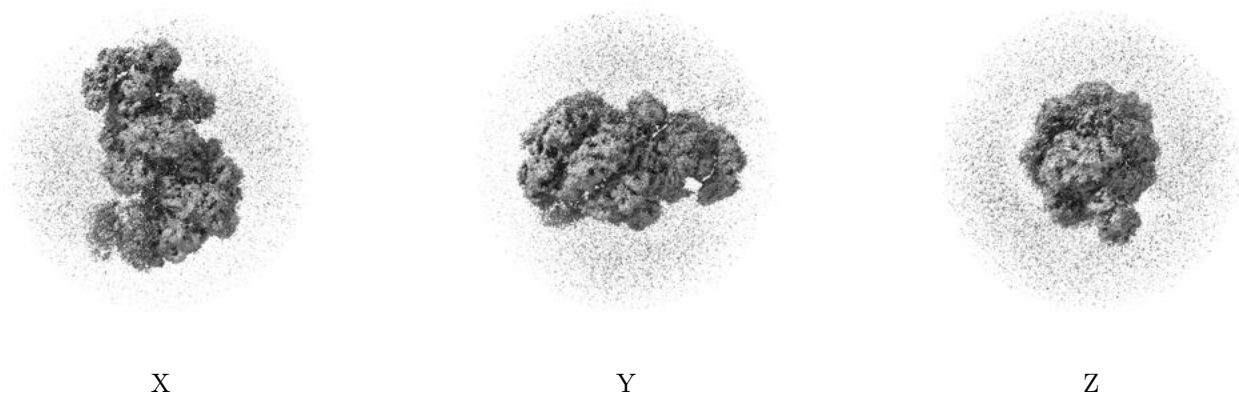
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

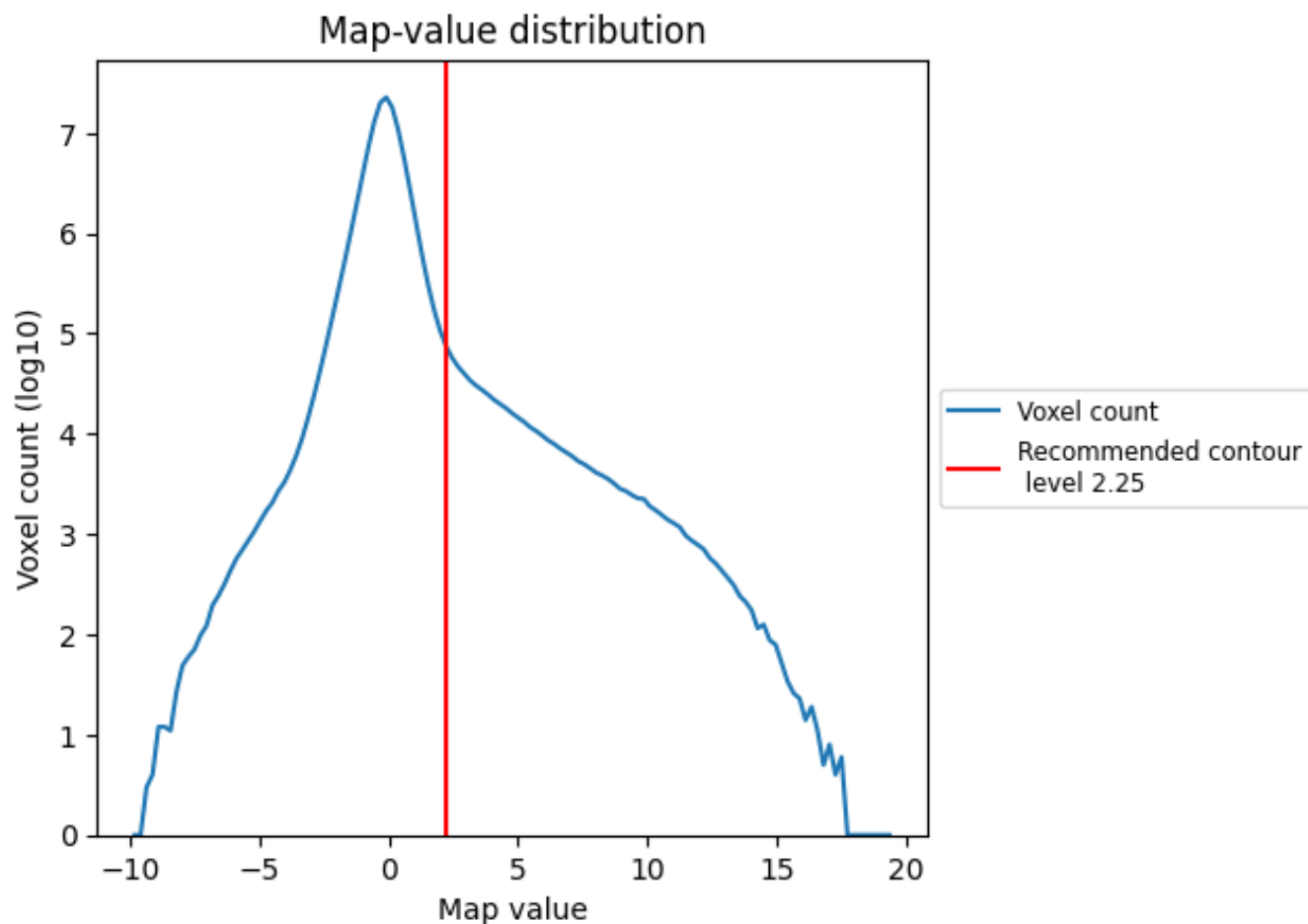
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

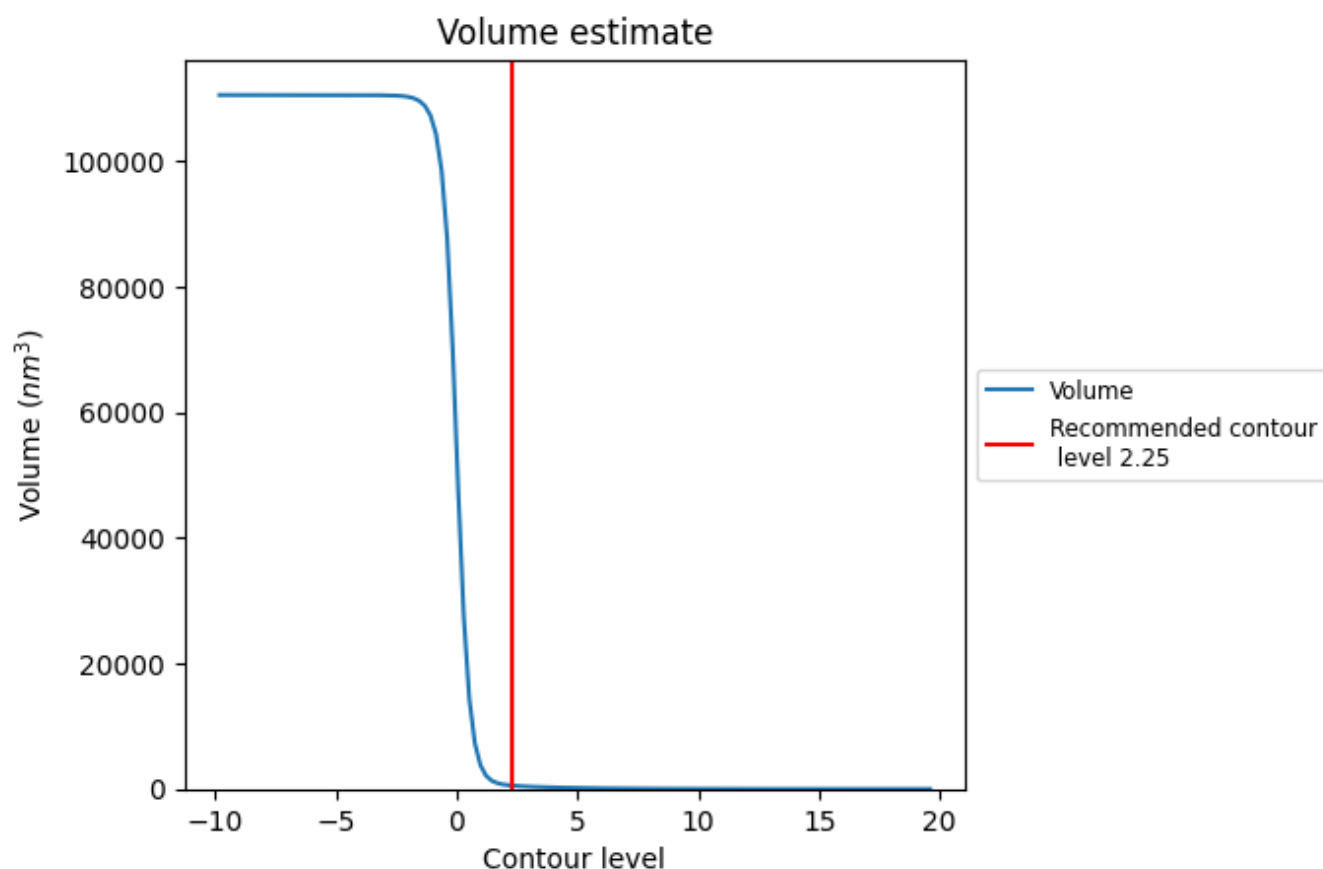
This section contains the results of statistical analysis of the map.

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



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

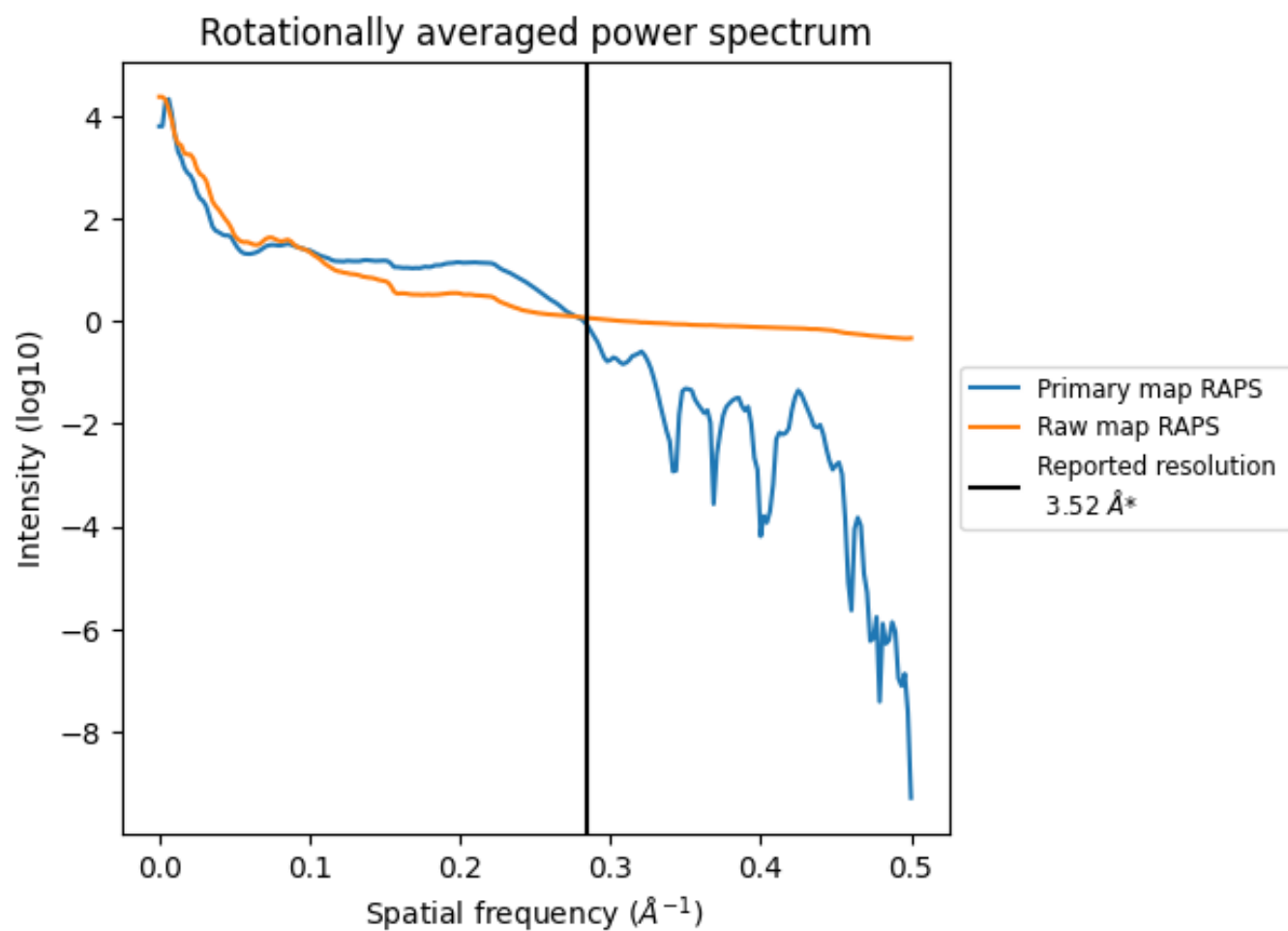
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 561  $\text{nm}^3$ ; this corresponds to an approximate mass of 506 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 ⓘ

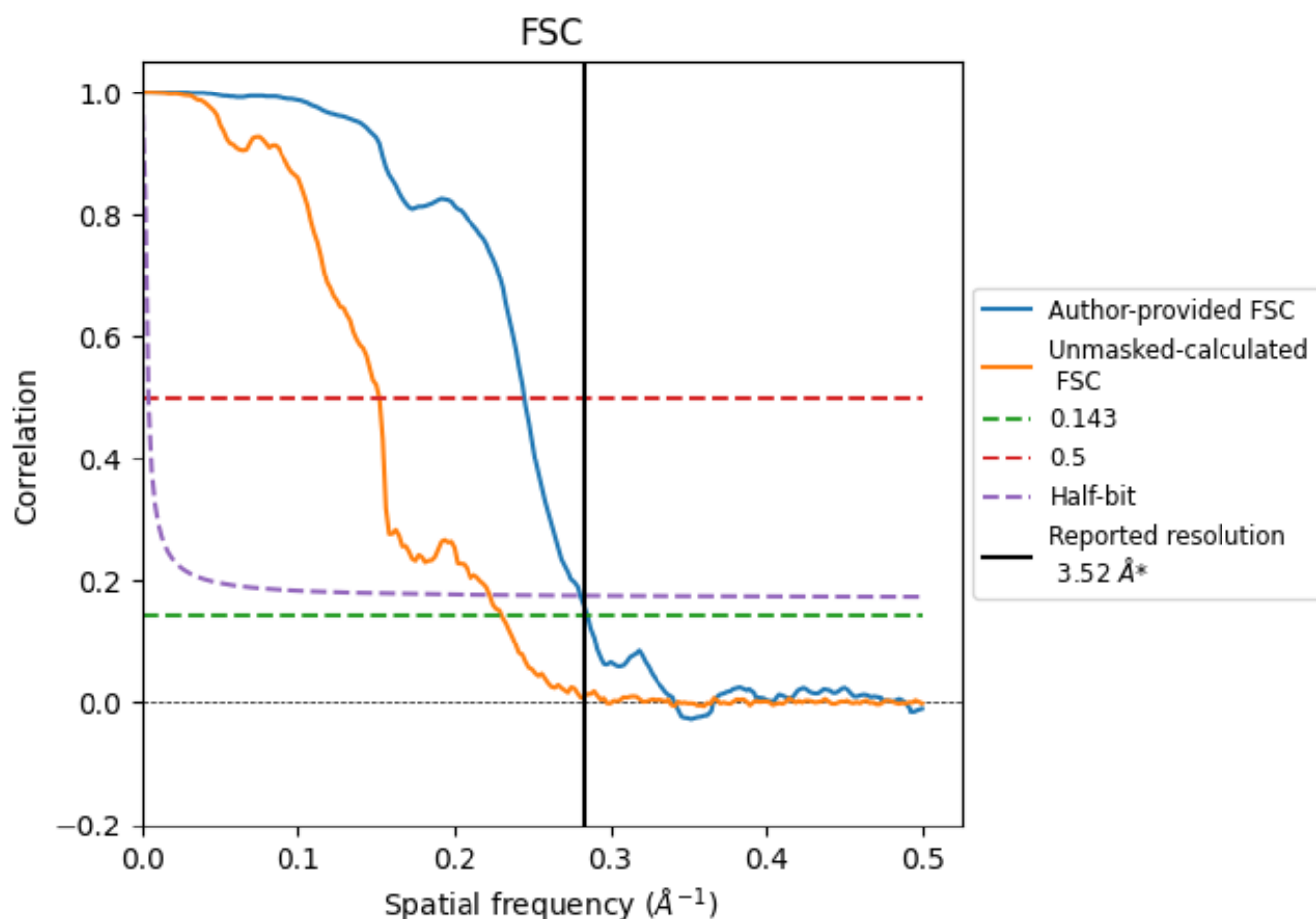


\*Reported resolution corresponds to spatial frequency of 0.284 Å<sup>-1</sup>

## 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 0.284  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

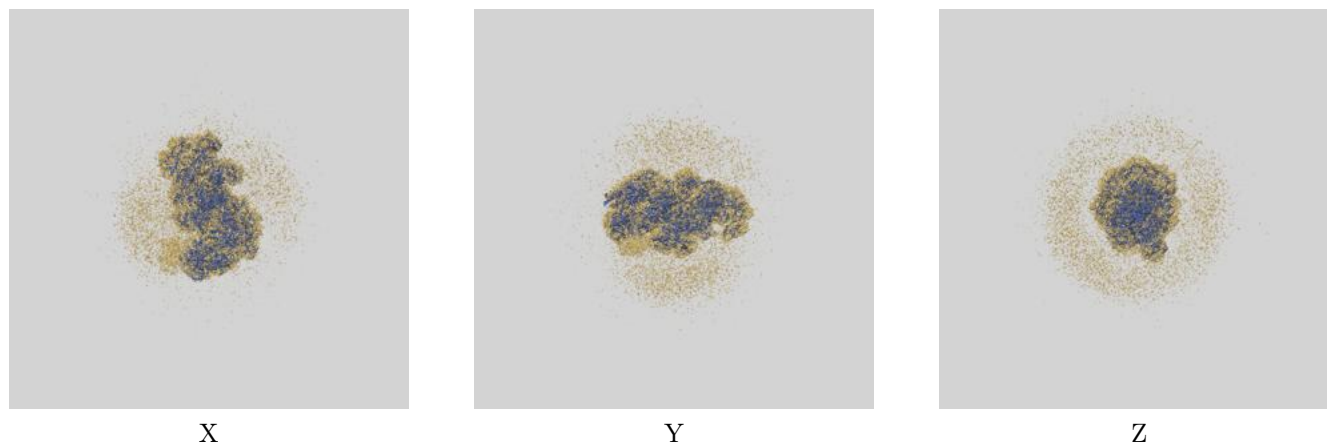
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.52                               | -    | -        |
| Author-provided FSC curve | 3.51                               | 4.08 | 3.56     |
| Unmasked-calculated*      | 4.33                               | 6.58 | 4.49     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.33 differs from the reported value 3.52 by more than 10 %

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

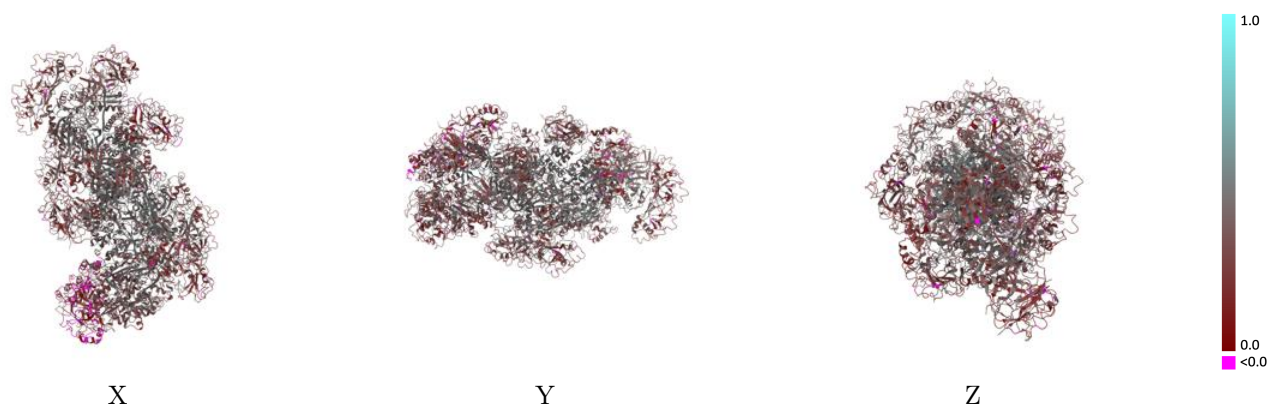
This section contains information regarding the fit between EMDB map EMD-10209 and PDB model 6SIC. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



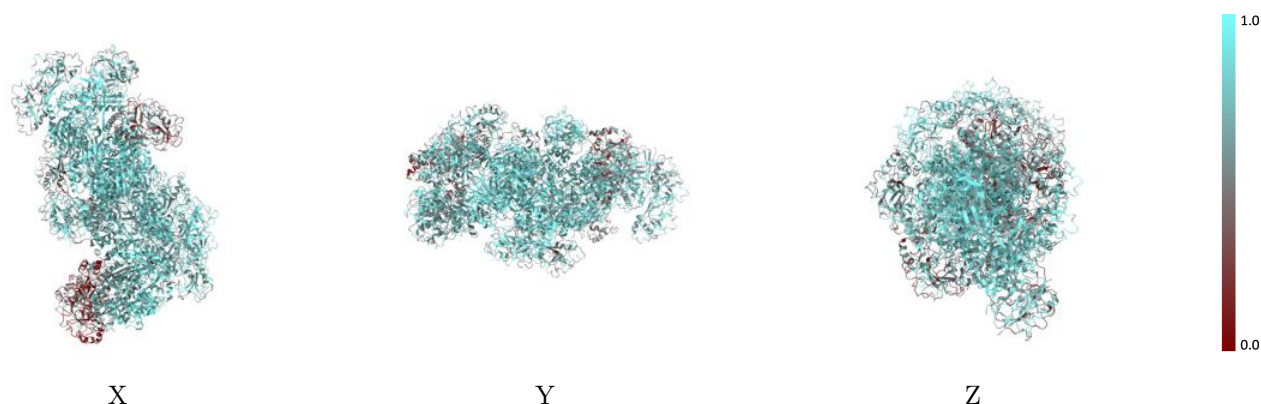
The images above show the 3D surface view of the map at the recommended contour level 2.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



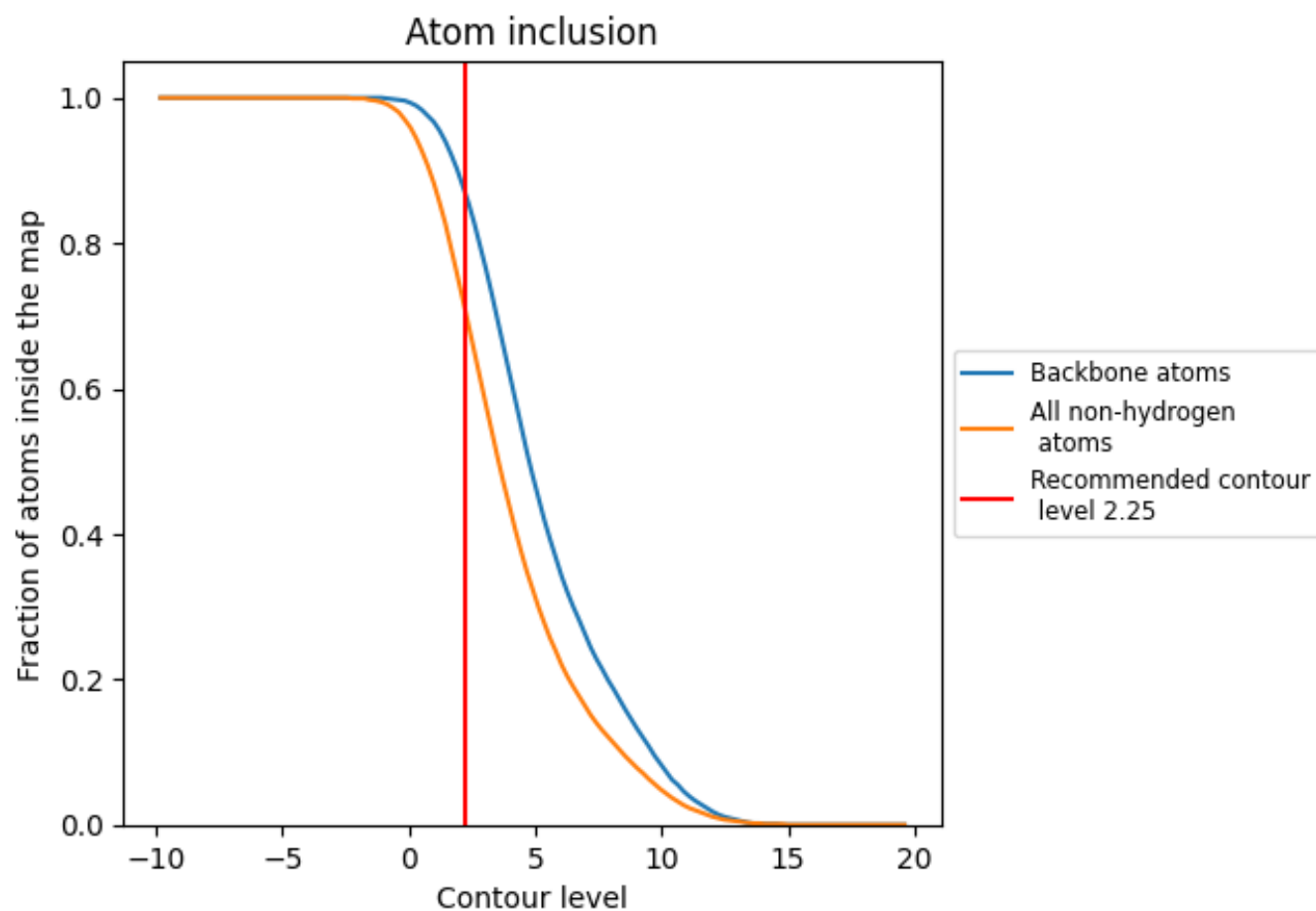
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.25) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7050   |  0.3430   |
| A     |  0.8220   |  0.4420   |
| B     |  0.8250   |  0.4160   |
| C     |  0.8370   |  0.4370   |
| D     |  0.8350   |  0.4440   |
| E     |  0.8320   |  0.4490   |
| F     |  0.8270   |  0.4450   |
| G     |  0.8280   |  0.4250   |
| H     |  0.7870   |  0.3750   |
| I     |  0.8450   |  0.4350   |
| J     |  0.8230   |  0.4020   |
| K     |  0.6680   |  0.3130   |
| L     |  0.7640   |  0.3470   |
| M     |  0.7950   |  0.3300   |
| N     |  0.6450  |  0.2730  |
| O     |  0.5980 |  0.3070 |
| P     |  0.5390 |  0.3050 |
| Q     |  0.6340 |  0.2990 |
| R     |  0.7920 |  0.3140 |
| S     |  0.4440 |  0.2810 |
| T     |  0.7010 |  0.2940 |
| U     |  0.9560 |  0.4680 |
| V     |  0.9720 |  0.4820 |
| W     |  0.6380 |  0.3010 |
| X     |  0.2160 |  0.1150 |
| l     |  0.7700 |  0.3440 |
| m     |  0.8010 |  0.3520 |
| n     |  0.6250 |  0.2640 |
| o     |  0.6370 |  0.3050 |
| p     |  0.5530 |  0.2970 |
| q     |  0.7030 |  0.2940 |
| r     |  0.7800 |  0.3170 |
| s     |  0.4050 |  0.2770 |
| t     |  0.6730 |  0.2870 |
| w     |  0.6000 |  0.2790 |
| x     |  0.1760 |  0.1090 |

