



## Full wwPDB EM Validation Report ⓘ

Aug 9, 2026 – 05:40 PM JST

PDB ID : 9WE7 / pdb\_00009we7  
EMDB ID : EMD-65914  
Title : Cryo-EM structure of RNF170-Erlin1-Erlin2  
Authors : Qian, H.W.; Jia, X.X.  
Deposited on : 2025-08-19  
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

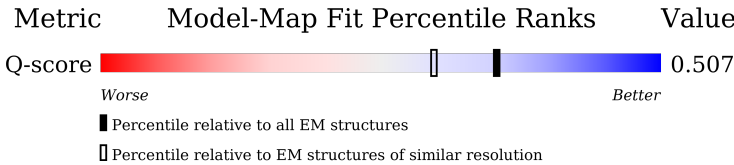
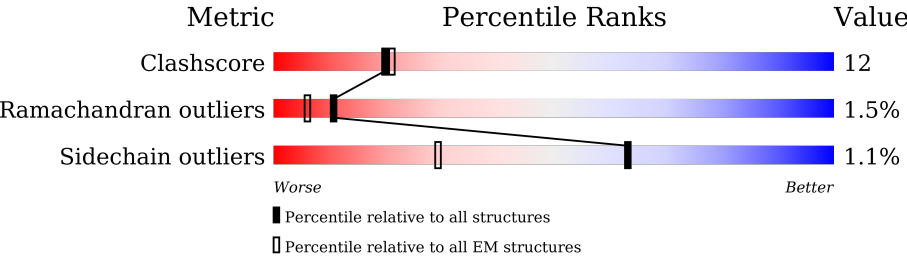
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.05 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.



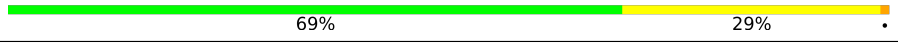
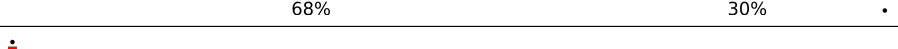
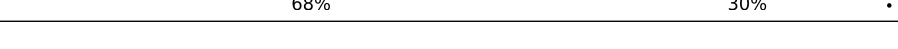
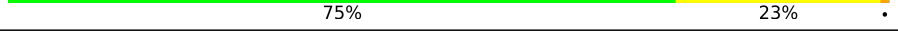
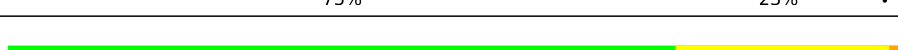
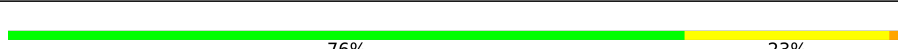
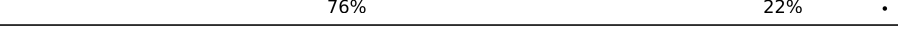
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 13971 ( 2.55 - 3.55 )                                    |

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     | 278    |                  |
| 1   | C     | 278    |                  |
| 1   | E     | 278    |                  |
| 1   | G     | 278    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | I     | 278    |    |
| 1   | K     | 278    |    |
| 1   | M     | 278    |    |
| 1   | O     | 278    |    |
| 1   | Q     | 278    |    |
| 1   | S     | 278    |    |
| 1   | U     | 278    |    |
| 1   | W     | 278    |    |
| 1   | Y     | 278    |    |
| 2   | B     | 277    |   |
| 2   | D     | 277    |  |
| 2   | F     | 277    |  |
| 2   | H     | 277    |  |
| 2   | J     | 277    |  |
| 2   | L     | 277    |  |
| 2   | N     | 277    |  |
| 2   | P     | 277    |  |
| 2   | R     | 277    |  |
| 2   | T     | 277    |  |
| 2   | V     | 277    |  |
| 2   | X     | 277    |  |
| 2   | Z     | 277    |  |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 57407 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 Erlin-1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 278      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2219  | 1416 | 378 | 417 | 8 |         |       |
| 1   | C     | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2207  | 1407 | 377 | 415 | 8 |         |       |
| 1   | E     | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2207  | 1407 | 377 | 415 | 8 |         |       |
| 1   | G     | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2207  | 1407 | 377 | 415 | 8 |         |       |
| 1   | I     | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2207  | 1407 | 377 | 415 | 8 |         |       |
| 1   | K     | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2207  | 1407 | 377 | 415 | 8 |         |       |
| 1   | M     | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2207  | 1407 | 377 | 415 | 8 |         |       |
| 1   | O     | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2207  | 1407 | 377 | 415 | 8 |         |       |
| 1   | Q     | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2207  | 1407 | 377 | 415 | 8 |         |       |
| 1   | S     | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2207  | 1407 | 377 | 415 | 8 |         |       |
| 1   | U     | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2207  | 1407 | 377 | 415 | 8 |         |       |
| 1   | W     | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2207  | 1407 | 377 | 415 | 8 |         |       |
| 1   | Y     | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2207  | 1407 | 377 | 415 | 8 |         |       |

- Molecule 2 is a protein called Erlin-2.

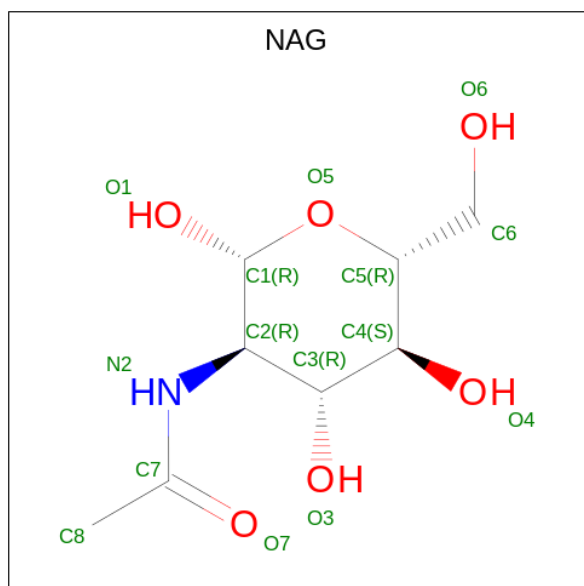
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2180  | 1390 | 361 | 419 | 10 |         |       |
| 2   | D     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2180  | 1390 | 361 | 419 | 10 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | F     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2180  | 1390 | 361 | 419 | 10 |         |       |
| 2   | H     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2180  | 1390 | 361 | 419 | 10 |         |       |
| 2   | J     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2180  | 1390 | 361 | 419 | 10 |         |       |
| 2   | L     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2180  | 1390 | 361 | 419 | 10 |         |       |
| 2   | N     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2180  | 1390 | 361 | 419 | 10 |         |       |
| 2   | P     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2180  | 1390 | 361 | 419 | 10 |         |       |
| 2   | R     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2180  | 1390 | 361 | 419 | 10 |         |       |
| 2   | T     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2180  | 1390 | 361 | 419 | 10 |         |       |
| 2   | V     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2180  | 1390 | 361 | 419 | 10 |         |       |
| 2   | X     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2180  | 1390 | 361 | 419 | 10 |         |       |
| 2   | Z     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2180  | 1390 | 361 | 419 | 10 |         |       |

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 3   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | D     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | E     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | F     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | G     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | H     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | I     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | J     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | K     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | L     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | M     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | N     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | O     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | P     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | Q     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | R     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | S     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | T     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | U     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | V     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

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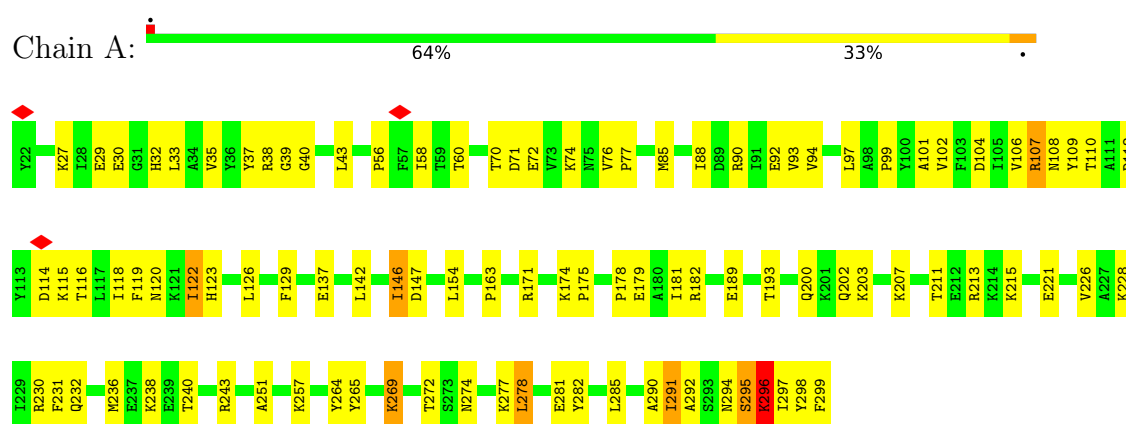
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| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 3   | W     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | X     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | Y     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 3   | Z     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

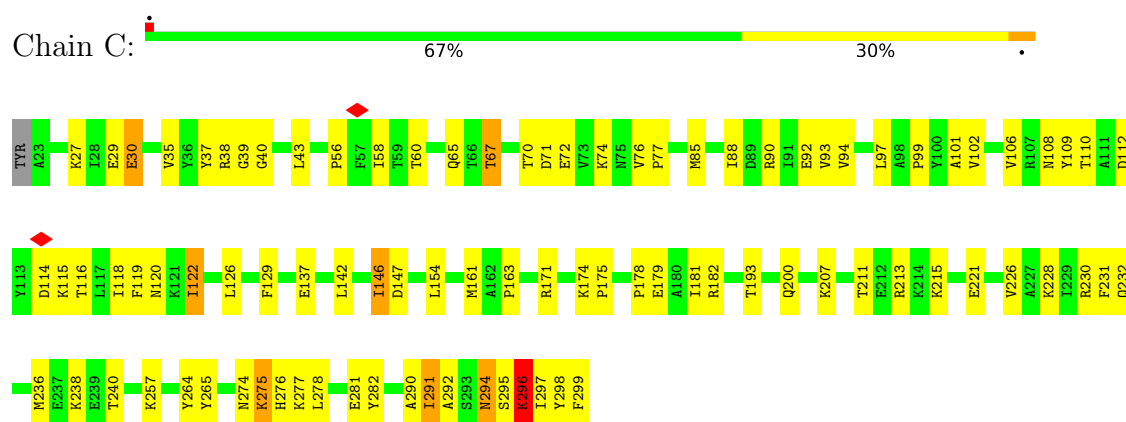
### 3 Residue-property plots

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

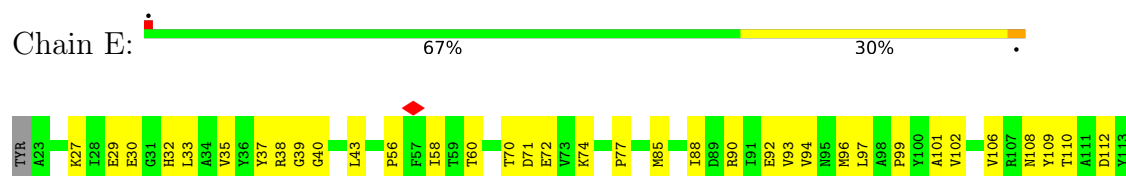
#### • Molecule 1: Erlin-1

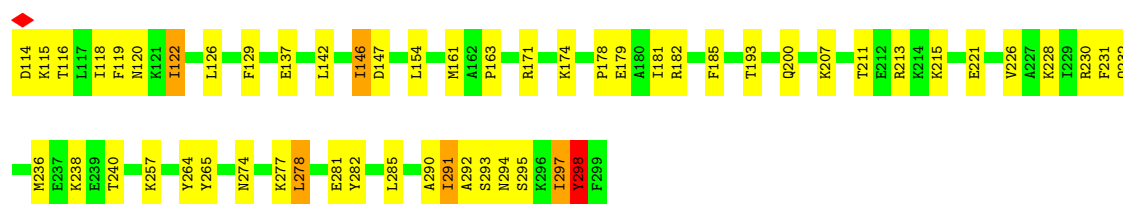


#### • Molecule 1: Erlin-1

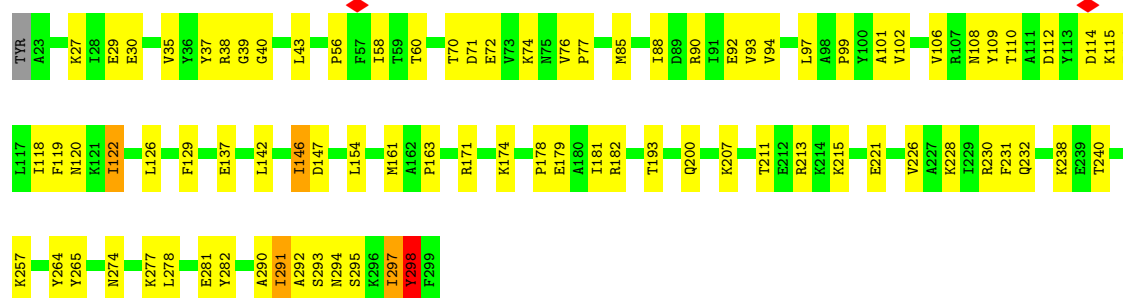


#### • Molecule 1: Erlin-1

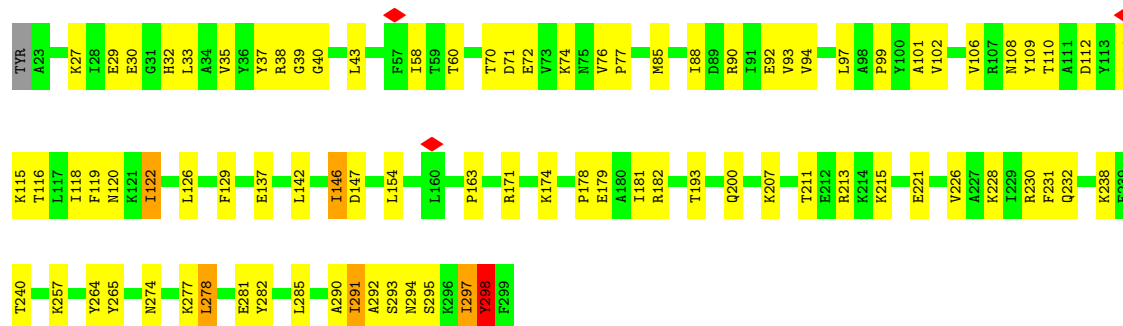




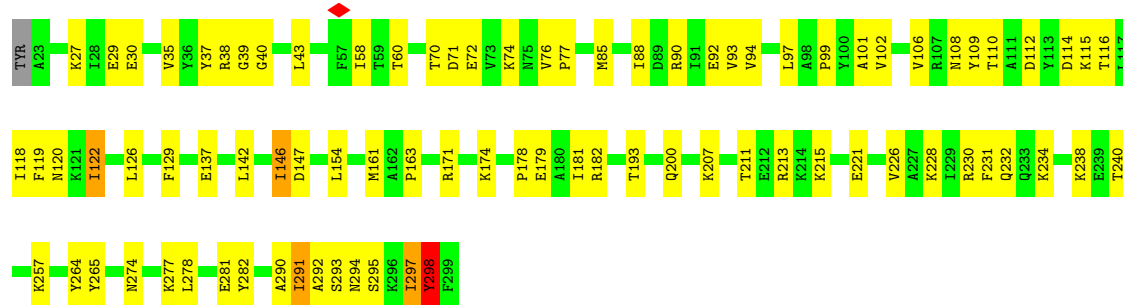
• Molecule 1: Erlin-1



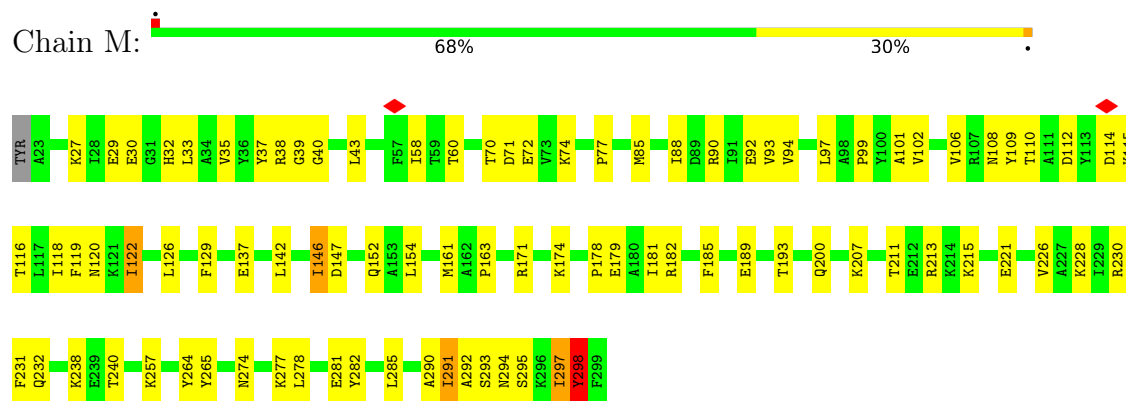
• Molecule 1: Erlin-1



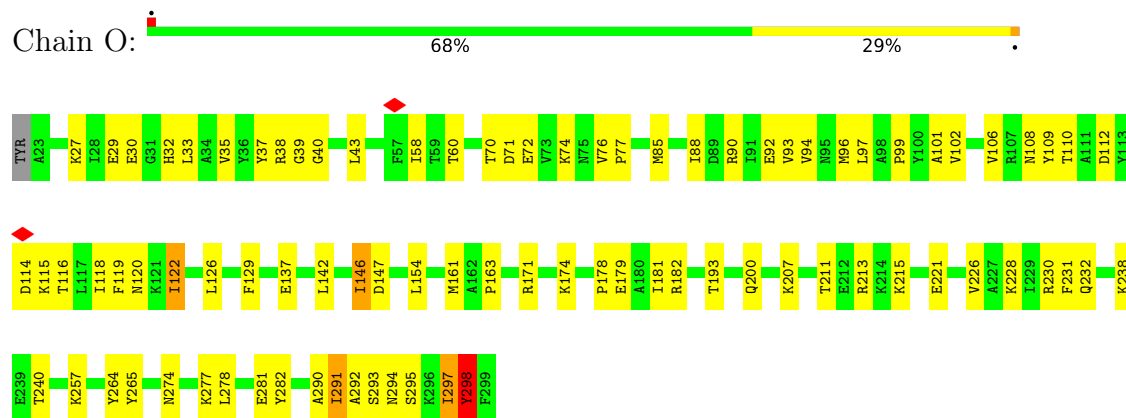
• Molecule 1: Erlin-1



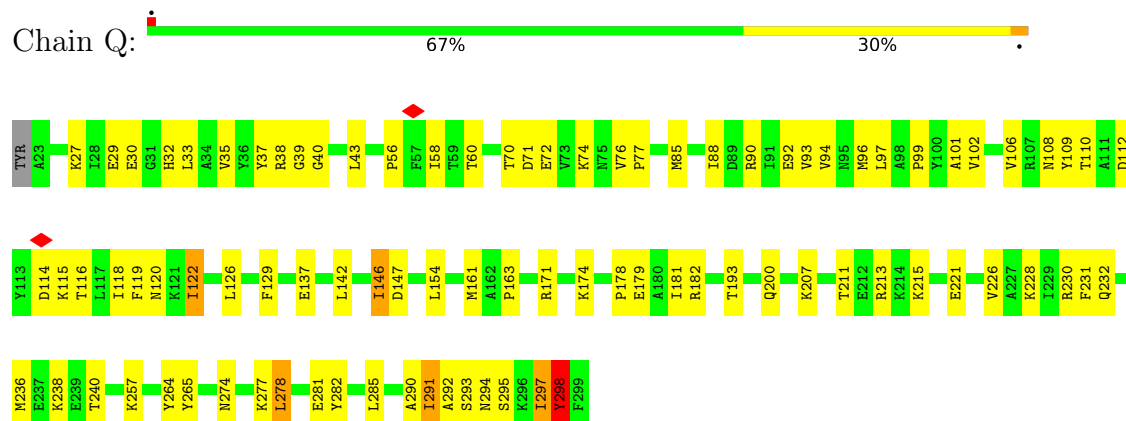
• Molecule 1: Erlin-1



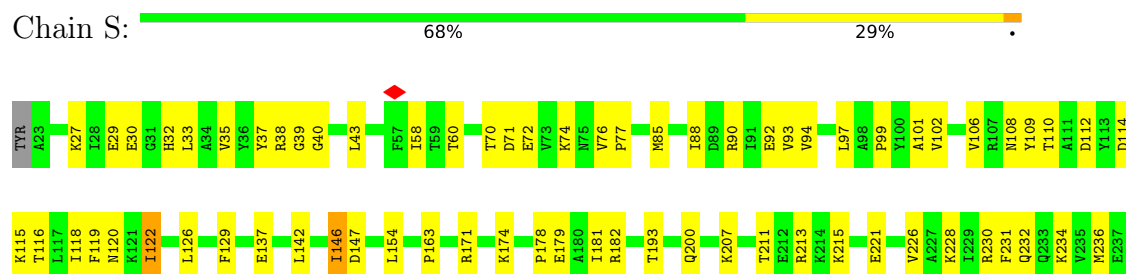
• Molecule 1: Erlin-1



• Molecule 1: Erlin-1

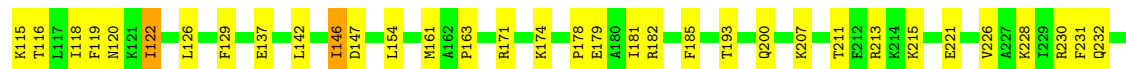


• Molecule 1: Erlin-1





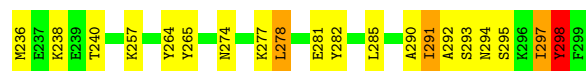
• Molecule 1: Erlin-1



• Molecule 1: Erlin-1

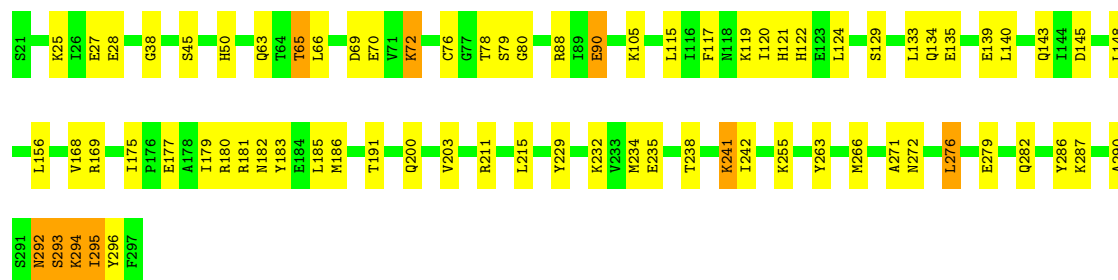


• Molecule 1: Erlin-1



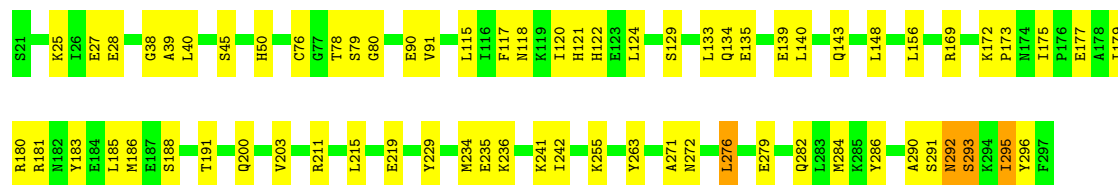
• Molecule 2: Erlin-2





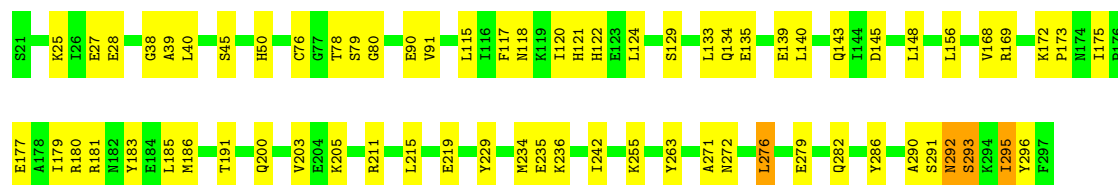
- Molecule 2: Erlin-2

Chain D: 75% 23% .



- Molecule 2: Erlin-2

Chain F: 75% 23% .



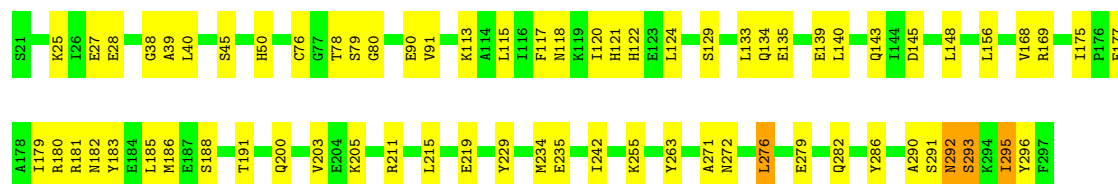
- Molecule 2: Erlin-2

Chain H: 75% 23% .



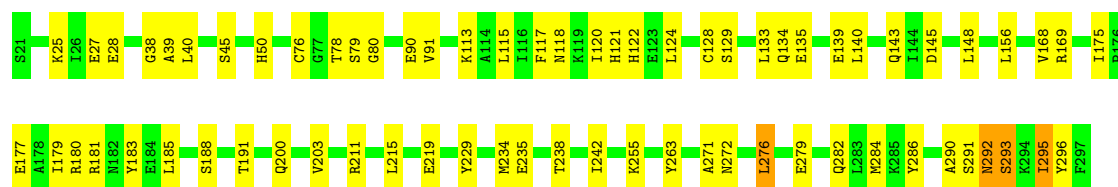
- Molecule 2: Erlin-2

Chain J: 75% 23% .



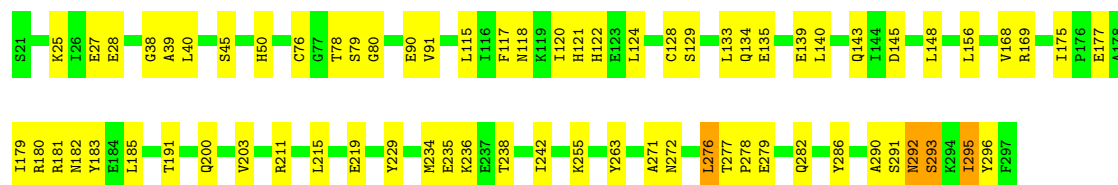
- Molecule 2: Erlin-2

Chain L:  75% 23% .



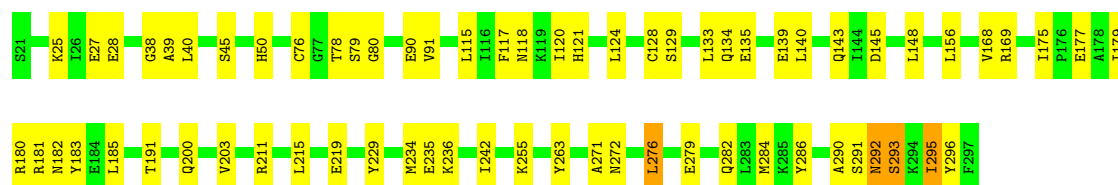
• Molecule 2: Erlin-2

Chain N:  75% 24% .



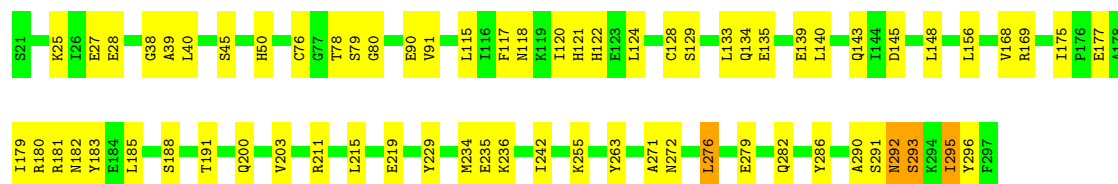
• Molecule 2: Erlin-2

Chain P:  76% 23% .



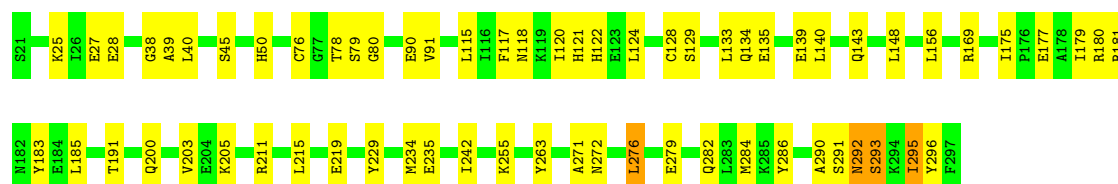
• Molecule 2: Erlin-2

Chain R:  75% 23% .



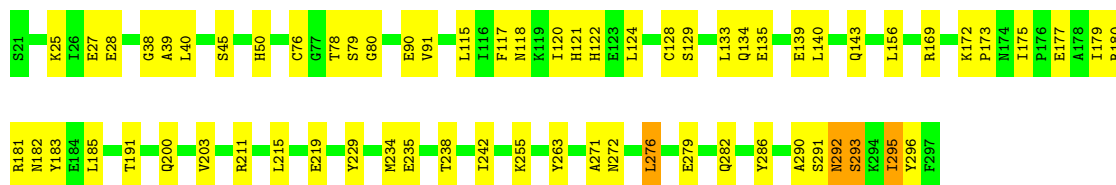
• Molecule 2: Erlin-2

Chain T:  77% 22% .



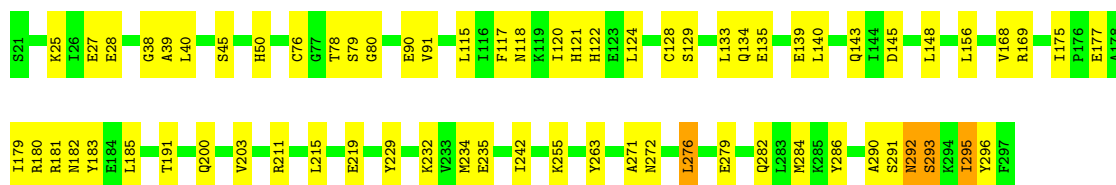
• Molecule 2: Erlin-2

Chain V:  76% 22%



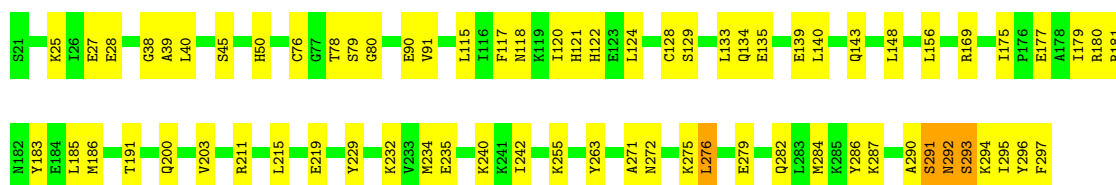
• Molecule 2: Erlin-2

Chain X:  75% 23%



• Molecule 2: Erlin-2

Chain Z:  74% 24%



## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, Not provided |           |
| Number of particles used             | 106695              | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF   | Depositor |
| CTF correction method                | NONE                | Depositor |
| Microscope                           | FEI POLARA 300      | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                  | Depositor |
| Minimum defocus (nm)                 | 1500                | Depositor |
| Maximum defocus (nm)                 | 1700                | Depositor |
| Magnification                        | Not provided        |           |
| Image detector                       | GATAN K3 (6k x 4k)  | Depositor |
| Maximum map value                    | 1.233               | Depositor |
| Minimum map value                    | -0.589              | Depositor |
| Average map value                    | 0.005               | Depositor |
| Map value standard deviation         | 0.044               | Depositor |
| Recommended contour level            | 0.133               | Depositor |
| Map size ( $\text{\AA}$ )            | 385.2, 385.2, 385.2 | wwPDB     |
| Map dimensions                       | 360, 360, 360       | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0    | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.07, 1.07, 1.07    | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.44         | 1/2258 (0.0%)  | 0.86        | 7/3047 (0.2%)    |
| 1   | C     | 0.33         | 0/2245         | 0.81        | 6/3029 (0.2%)    |
| 1   | E     | 0.31         | 0/2245         | 0.81        | 4/3029 (0.1%)    |
| 1   | G     | 0.31         | 0/2245         | 0.81        | 6/3029 (0.2%)    |
| 1   | I     | 0.31         | 0/2245         | 0.81        | 6/3029 (0.2%)    |
| 1   | K     | 0.31         | 0/2245         | 0.81        | 6/3029 (0.2%)    |
| 1   | M     | 0.31         | 0/2245         | 0.81        | 5/3029 (0.2%)    |
| 1   | O     | 0.31         | 0/2245         | 0.81        | 6/3029 (0.2%)    |
| 1   | Q     | 0.31         | 0/2245         | 0.81        | 6/3029 (0.2%)    |
| 1   | S     | 0.31         | 0/2245         | 0.81        | 6/3029 (0.2%)    |
| 1   | U     | 0.32         | 0/2245         | 0.81        | 6/3029 (0.2%)    |
| 1   | W     | 0.31         | 0/2245         | 0.81        | 7/3029 (0.2%)    |
| 1   | Y     | 0.31         | 0/2245         | 0.81        | 6/3029 (0.2%)    |
| 2   | B     | 0.41         | 1/2214 (0.0%)  | 0.71        | 2/2989 (0.1%)    |
| 2   | D     | 0.27         | 0/2214         | 0.71        | 4/2989 (0.1%)    |
| 2   | F     | 0.27         | 0/2214         | 0.71        | 4/2989 (0.1%)    |
| 2   | H     | 0.27         | 0/2214         | 0.71        | 4/2989 (0.1%)    |
| 2   | J     | 0.27         | 0/2214         | 0.71        | 4/2989 (0.1%)    |
| 2   | L     | 0.27         | 0/2214         | 0.71        | 4/2989 (0.1%)    |
| 2   | N     | 0.27         | 0/2214         | 0.71        | 4/2989 (0.1%)    |
| 2   | P     | 0.27         | 0/2214         | 0.71        | 4/2989 (0.1%)    |
| 2   | R     | 0.27         | 0/2214         | 0.71        | 4/2989 (0.1%)    |
| 2   | T     | 0.27         | 0/2214         | 0.71        | 4/2989 (0.1%)    |
| 2   | V     | 0.27         | 0/2214         | 0.71        | 4/2989 (0.1%)    |
| 2   | X     | 0.27         | 0/2214         | 0.71        | 4/2989 (0.1%)    |
| 2   | Z     | 0.33         | 0/2214         | 0.72        | 4/2989 (0.1%)    |
| All | All   | 0.31         | 2/57980 (0.0%) | 0.77        | 127/78252 (0.2%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 296 | LYS  | C-O   | 6.24  | 1.31        | 1.24     |
| 2   | B     | 90  | GLU  | CA-C  | -5.25 | 1.46        | 1.52     |

All (127) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 295 | SER  | N-CA-C | 12.66 | 128.12      | 107.73   |
| 1   | K     | 146 | ILE  | N-CA-C | -8.75 | 102.02      | 110.42   |
| 1   | Q     | 146 | ILE  | N-CA-C | -8.73 | 102.04      | 110.42   |
| 1   | G     | 146 | ILE  | N-CA-C | -8.70 | 102.06      | 110.42   |
| 1   | U     | 146 | ILE  | N-CA-C | -8.70 | 102.06      | 110.42   |
| 1   | Y     | 146 | ILE  | N-CA-C | -8.70 | 102.06      | 110.42   |
| 1   | O     | 146 | ILE  | N-CA-C | -8.70 | 102.07      | 110.42   |
| 1   | I     | 146 | ILE  | N-CA-C | -8.70 | 102.07      | 110.42   |
| 1   | C     | 146 | ILE  | N-CA-C | -8.69 | 102.08      | 110.42   |
| 1   | W     | 146 | ILE  | N-CA-C | -8.68 | 102.08      | 110.42   |
| 1   | E     | 146 | ILE  | N-CA-C | -8.68 | 102.09      | 110.42   |
| 1   | S     | 146 | ILE  | N-CA-C | -8.64 | 102.13      | 110.42   |
| 1   | M     | 146 | ILE  | N-CA-C | -8.62 | 102.15      | 110.42   |
| 1   | A     | 146 | ILE  | N-CA-C | -8.62 | 102.15      | 110.42   |
| 1   | A     | 296 | LYS  | N-CA-C | 8.52  | 128.96      | 110.80   |
| 2   | V     | 117 | PHE  | N-CA-C | 7.15  | 118.72      | 111.07   |
| 2   | T     | 117 | PHE  | N-CA-C | 7.12  | 118.68      | 111.07   |
| 2   | H     | 117 | PHE  | N-CA-C | 7.10  | 118.67      | 111.07   |
| 2   | P     | 117 | PHE  | N-CA-C | 7.10  | 118.66      | 111.07   |
| 2   | X     | 117 | PHE  | N-CA-C | 7.08  | 118.64      | 111.07   |
| 2   | R     | 117 | PHE  | N-CA-C | 7.06  | 118.62      | 111.07   |
| 2   | J     | 117 | PHE  | N-CA-C | 7.05  | 118.61      | 111.07   |
| 2   | Z     | 117 | PHE  | N-CA-C | 7.04  | 118.61      | 111.07   |
| 2   | D     | 117 | PHE  | N-CA-C | 7.04  | 118.60      | 111.07   |
| 2   | L     | 117 | PHE  | N-CA-C | 7.03  | 118.59      | 111.07   |
| 2   | F     | 117 | PHE  | N-CA-C | 7.02  | 118.58      | 111.07   |
| 2   | N     | 117 | PHE  | N-CA-C | 7.02  | 118.58      | 111.07   |
| 2   | Z     | 291 | SER  | N-CA-C | -6.85 | 104.65      | 112.87   |
| 2   | B     | 72  | LYS  | N-CA-C | 6.54  | 119.84      | 109.50   |
| 1   | K     | 76  | VAL  | CA-C-N | -5.96 | 113.82      | 120.14   |
| 1   | K     | 76  | VAL  | C-N-CA | -5.96 | 113.82      | 120.14   |
| 1   | U     | 76  | VAL  | CA-C-N | -5.52 | 114.29      | 120.14   |
| 1   | U     | 76  | VAL  | C-N-CA | -5.52 | 114.29      | 120.14   |
| 1   | C     | 296 | LYS  | N-CA-C | 5.52  | 122.55      | 110.80   |
| 1   | O     | 76  | VAL  | CA-C-N | -5.52 | 114.29      | 120.14   |
| 1   | O     | 76  | VAL  | C-N-CA | -5.52 | 114.29      | 120.14   |
| 1   | W     | 76  | VAL  | CA-C-N | -5.47 | 114.34      | 120.14   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | W     | 76  | VAL  | C-N-CA   | -5.47 | 114.34      | 120.14   |
| 2   | B     | 276 | LEU  | CA-CB-CG | -5.40 | 97.39       | 116.30   |
| 2   | N     | 276 | LEU  | CA-CB-CG | -5.40 | 97.39       | 116.30   |
| 2   | V     | 276 | LEU  | CA-CB-CG | -5.40 | 97.39       | 116.30   |
| 2   | F     | 276 | LEU  | CA-CB-CG | -5.40 | 97.40       | 116.30   |
| 2   | R     | 276 | LEU  | CA-CB-CG | -5.39 | 97.43       | 116.30   |
| 2   | L     | 276 | LEU  | CA-CB-CG | -5.39 | 97.43       | 116.30   |
| 2   | T     | 276 | LEU  | CA-CB-CG | -5.39 | 97.44       | 116.30   |
| 2   | D     | 276 | LEU  | CA-CB-CG | -5.38 | 97.46       | 116.30   |
| 2   | H     | 276 | LEU  | CA-CB-CG | -5.38 | 97.45       | 116.30   |
| 2   | J     | 276 | LEU  | CA-CB-CG | -5.38 | 97.46       | 116.30   |
| 2   | X     | 276 | LEU  | CA-CB-CG | -5.38 | 97.47       | 116.30   |
| 2   | Z     | 276 | LEU  | CA-CB-CG | -5.38 | 97.48       | 116.30   |
| 2   | P     | 276 | LEU  | CA-CB-CG | -5.38 | 97.48       | 116.30   |
| 1   | C     | 76  | VAL  | CA-C-N   | -5.32 | 114.50      | 120.14   |
| 1   | C     | 76  | VAL  | C-N-CA   | -5.32 | 114.50      | 120.14   |
| 1   | Q     | 163 | PRO  | CA-N-CD  | -5.31 | 104.57      | 112.00   |
| 1   | E     | 163 | PRO  | CA-N-CD  | -5.30 | 104.57      | 112.00   |
| 1   | M     | 163 | PRO  | CA-N-CD  | -5.30 | 104.57      | 112.00   |
| 1   | O     | 163 | PRO  | CA-N-CD  | -5.30 | 104.58      | 112.00   |
| 1   | A     | 163 | PRO  | CA-N-CD  | -5.28 | 104.61      | 112.00   |
| 1   | G     | 163 | PRO  | CA-N-CD  | -5.28 | 104.61      | 112.00   |
| 1   | W     | 163 | PRO  | CA-N-CD  | -5.27 | 104.62      | 112.00   |
| 1   | G     | 76  | VAL  | CA-C-N   | -5.27 | 114.56      | 120.14   |
| 1   | G     | 76  | VAL  | C-N-CA   | -5.27 | 114.56      | 120.14   |
| 1   | K     | 163 | PRO  | CA-N-CD  | -5.27 | 104.62      | 112.00   |
| 1   | U     | 163 | PRO  | CA-N-CD  | -5.27 | 104.62      | 112.00   |
| 1   | K     | 298 | TYR  | N-CA-C   | 5.27  | 122.02      | 110.80   |
| 1   | I     | 163 | PRO  | CA-N-CD  | -5.26 | 104.63      | 112.00   |
| 1   | S     | 298 | TYR  | N-CA-C   | 5.25  | 121.99      | 110.80   |
| 1   | Y     | 163 | PRO  | CA-N-CD  | -5.25 | 104.65      | 112.00   |
| 1   | M     | 298 | TYR  | N-CA-C   | 5.25  | 121.98      | 110.80   |
| 1   | O     | 298 | TYR  | N-CA-C   | 5.25  | 121.97      | 110.80   |
| 1   | C     | 163 | PRO  | CA-N-CD  | -5.24 | 104.66      | 112.00   |
| 1   | I     | 298 | TYR  | N-CA-C   | 5.24  | 121.97      | 110.80   |
| 1   | U     | 298 | TYR  | N-CA-C   | 5.24  | 121.97      | 110.80   |
| 1   | Q     | 298 | TYR  | N-CA-C   | 5.24  | 121.96      | 110.80   |
| 1   | Y     | 298 | TYR  | N-CA-C   | 5.24  | 121.96      | 110.80   |
| 1   | S     | 163 | PRO  | CA-N-CD  | -5.23 | 104.67      | 112.00   |
| 1   | G     | 298 | TYR  | N-CA-C   | 5.23  | 121.94      | 110.80   |
| 1   | E     | 298 | TYR  | N-CA-C   | 5.21  | 121.90      | 110.80   |
| 1   | W     | 298 | TYR  | N-CA-C   | 5.19  | 121.86      | 110.80   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | Y     | 76  | VAL  | CA-C-N  | -5.18 | 114.65      | 120.14   |
| 1   | Y     | 76  | VAL  | C-N-CA  | -5.18 | 114.65      | 120.14   |
| 2   | Z     | 294 | LYS  | N-CA-C  | 5.17  | 115.07      | 108.24   |
| 1   | K     | 122 | ILE  | N-CA-C  | 5.16  | 115.78      | 110.36   |
| 1   | A     | 76  | VAL  | CA-C-N  | -5.15 | 114.68      | 120.14   |
| 1   | A     | 76  | VAL  | C-N-CA  | -5.15 | 114.68      | 120.14   |
| 1   | W     | 122 | ILE  | N-CA-C  | 5.14  | 115.76      | 110.36   |
| 1   | A     | 122 | ILE  | N-CA-C  | 5.14  | 115.76      | 110.36   |
| 1   | G     | 122 | ILE  | N-CA-C  | 5.13  | 115.75      | 110.36   |
| 1   | S     | 122 | ILE  | N-CA-C  | 5.13  | 115.75      | 110.36   |
| 1   | I     | 122 | ILE  | N-CA-C  | 5.13  | 115.74      | 110.36   |
| 1   | Q     | 76  | VAL  | CA-C-N  | -5.13 | 114.70      | 120.14   |
| 1   | Q     | 76  | VAL  | C-N-CA  | -5.13 | 114.70      | 120.14   |
| 1   | Q     | 122 | ILE  | N-CA-C  | 5.12  | 115.73      | 110.36   |
| 1   | W     | 152 | GLN  | N-CA-C  | 5.11  | 116.85      | 111.28   |
| 1   | C     | 122 | ILE  | N-CA-C  | 5.10  | 115.71      | 110.36   |
| 1   | O     | 122 | ILE  | N-CA-C  | 5.10  | 115.71      | 110.36   |
| 1   | Y     | 122 | ILE  | N-CA-C  | 5.10  | 115.71      | 110.36   |
| 1   | I     | 76  | VAL  | CA-C-N  | -5.09 | 114.74      | 120.14   |
| 1   | I     | 76  | VAL  | C-N-CA  | -5.09 | 114.74      | 120.14   |
| 1   | U     | 122 | ILE  | N-CA-C  | 5.09  | 115.71      | 110.36   |
| 2   | N     | 296 | TYR  | N-CA-C  | 5.08  | 121.63      | 110.80   |
| 1   | S     | 76  | VAL  | CA-C-N  | -5.07 | 114.77      | 120.14   |
| 1   | S     | 76  | VAL  | C-N-CA  | -5.07 | 114.77      | 120.14   |
| 2   | F     | 295 | ILE  | CB-CA-C | -5.07 | 102.98      | 111.29   |
| 2   | X     | 295 | ILE  | CB-CA-C | -5.07 | 102.98      | 111.29   |
| 2   | R     | 296 | TYR  | N-CA-C  | 5.07  | 121.59      | 110.80   |
| 2   | V     | 295 | ILE  | CB-CA-C | -5.07 | 102.98      | 111.29   |
| 2   | X     | 296 | TYR  | N-CA-C  | 5.06  | 121.58      | 110.80   |
| 2   | D     | 296 | TYR  | N-CA-C  | 5.06  | 121.58      | 110.80   |
| 2   | J     | 296 | TYR  | N-CA-C  | 5.06  | 121.57      | 110.80   |
| 2   | N     | 295 | ILE  | CB-CA-C | -5.06 | 103.00      | 111.29   |
| 2   | J     | 295 | ILE  | CB-CA-C | -5.05 | 103.01      | 111.29   |
| 2   | L     | 296 | TYR  | N-CA-C  | 5.05  | 121.55      | 110.80   |
| 2   | F     | 296 | TYR  | N-CA-C  | 5.05  | 121.55      | 110.80   |
| 2   | L     | 295 | ILE  | CB-CA-C | -5.05 | 103.02      | 111.29   |
| 2   | R     | 295 | ILE  | CB-CA-C | -5.05 | 103.01      | 111.29   |
| 2   | H     | 296 | TYR  | N-CA-C  | 5.04  | 121.54      | 110.80   |
| 1   | M     | 152 | GLN  | N-CA-C  | 5.04  | 116.86      | 111.36   |
| 2   | P     | 295 | ILE  | CB-CA-C | -5.04 | 103.02      | 111.29   |
| 1   | M     | 122 | ILE  | N-CA-C  | 5.04  | 115.65      | 110.36   |
| 1   | E     | 122 | ILE  | N-CA-C  | 5.03  | 115.64      | 110.36   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | T     | 295 | ILE  | CB-CA-C | -5.03 | 103.04      | 111.29   |
| 2   | T     | 296 | TYR  | N-CA-C  | 5.03  | 121.52      | 110.80   |
| 2   | P     | 296 | TYR  | N-CA-C  | 5.03  | 121.51      | 110.80   |
| 2   | H     | 295 | ILE  | CB-CA-C | -5.03 | 103.05      | 111.29   |
| 2   | V     | 296 | TYR  | N-CA-C  | 5.02  | 121.50      | 110.80   |
| 2   | D     | 295 | ILE  | CB-CA-C | -5.02 | 103.06      | 111.29   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2219  | 0        | 2245     | 88      | 0            |
| 1   | C     | 2207  | 0        | 2236     | 84      | 0            |
| 1   | E     | 2207  | 0        | 2236     | 81      | 0            |
| 1   | G     | 2207  | 0        | 2236     | 76      | 0            |
| 1   | I     | 2207  | 0        | 2236     | 79      | 0            |
| 1   | K     | 2207  | 0        | 2236     | 79      | 0            |
| 1   | M     | 2207  | 0        | 2236     | 78      | 0            |
| 1   | O     | 2207  | 0        | 2236     | 78      | 0            |
| 1   | Q     | 2207  | 0        | 2236     | 83      | 0            |
| 1   | S     | 2207  | 0        | 2236     | 77      | 0            |
| 1   | U     | 2207  | 0        | 2236     | 77      | 0            |
| 1   | W     | 2207  | 0        | 2236     | 80      | 0            |
| 1   | Y     | 2207  | 0        | 2236     | 80      | 0            |
| 2   | B     | 2180  | 0        | 2209     | 66      | 0            |
| 2   | D     | 2180  | 0        | 2209     | 63      | 0            |
| 2   | F     | 2180  | 0        | 2209     | 59      | 0            |
| 2   | H     | 2180  | 0        | 2209     | 62      | 0            |
| 2   | J     | 2180  | 0        | 2209     | 60      | 0            |
| 2   | L     | 2180  | 0        | 2209     | 61      | 0            |
| 2   | N     | 2180  | 0        | 2209     | 60      | 0            |
| 2   | P     | 2180  | 0        | 2209     | 58      | 0            |
| 2   | R     | 2180  | 0        | 2209     | 59      | 0            |
| 2   | T     | 2180  | 0        | 2209     | 58      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | V     | 2180  | 0        | 2209     | 57      | 0            |
| 2   | X     | 2180  | 0        | 2209     | 61      | 0            |
| 2   | Z     | 2180  | 0        | 2209     | 67      | 0            |
| 3   | A     | 14    | 0        | 13       | 1       | 0            |
| 3   | B     | 14    | 0        | 13       | 0       | 0            |
| 3   | C     | 14    | 0        | 13       | 1       | 0            |
| 3   | D     | 14    | 0        | 13       | 0       | 0            |
| 3   | E     | 14    | 0        | 13       | 1       | 0            |
| 3   | F     | 14    | 0        | 13       | 0       | 0            |
| 3   | G     | 14    | 0        | 13       | 1       | 0            |
| 3   | H     | 14    | 0        | 13       | 0       | 0            |
| 3   | I     | 14    | 0        | 13       | 1       | 0            |
| 3   | J     | 14    | 0        | 13       | 0       | 0            |
| 3   | K     | 14    | 0        | 13       | 1       | 0            |
| 3   | L     | 14    | 0        | 13       | 0       | 0            |
| 3   | M     | 14    | 0        | 13       | 1       | 0            |
| 3   | N     | 14    | 0        | 13       | 0       | 0            |
| 3   | O     | 14    | 0        | 13       | 1       | 0            |
| 3   | P     | 14    | 0        | 13       | 0       | 0            |
| 3   | Q     | 14    | 0        | 13       | 1       | 0            |
| 3   | R     | 14    | 0        | 13       | 0       | 0            |
| 3   | S     | 14    | 0        | 13       | 1       | 0            |
| 3   | T     | 14    | 0        | 13       | 0       | 0            |
| 3   | U     | 14    | 0        | 13       | 1       | 0            |
| 3   | V     | 14    | 0        | 13       | 0       | 0            |
| 3   | W     | 14    | 0        | 13       | 1       | 0            |
| 3   | X     | 14    | 0        | 13       | 0       | 0            |
| 3   | Y     | 14    | 0        | 13       | 1       | 0            |
| 3   | Z     | 14    | 0        | 13       | 0       | 0            |
| All | All   | 57407 | 0        | 58132    | 1434    | 0            |

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

All (1434) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 2:X:135:GLU:HG2 | 2:X:140:LEU:HG | 1.58                     | 0.86              |
| 2:V:135:GLU:HG2 | 2:V:140:LEU:HG | 1.57                     | 0.86              |
| 1:A:174:LYS:NZ  | 2:Z:129:SER:OG | 2.09                     | 0.86              |
| 2:Z:135:GLU:HG2 | 2:Z:140:LEU:HG | 1.58                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:133:LEU:HD21 | 2:N:175:ILE:HD11 | 1.57                     | 0.86              |
| 2:R:133:LEU:HD21 | 2:R:175:ILE:HD11 | 1.57                     | 0.86              |
| 2:R:135:GLU:HG2  | 2:R:140:LEU:HG   | 1.58                     | 0.86              |
| 2:T:135:GLU:HG2  | 2:T:140:LEU:HG   | 1.58                     | 0.86              |
| 2:F:133:LEU:HD21 | 2:F:175:ILE:HD11 | 1.57                     | 0.86              |
| 2:Z:133:LEU:HD21 | 2:Z:175:ILE:HD11 | 1.57                     | 0.85              |
| 2:T:133:LEU:HD21 | 2:T:175:ILE:HD11 | 1.57                     | 0.85              |
| 2:L:133:LEU:HD21 | 2:L:175:ILE:HD11 | 1.57                     | 0.85              |
| 2:P:133:LEU:HD21 | 2:P:175:ILE:HD11 | 1.57                     | 0.85              |
| 2:P:135:GLU:HG2  | 2:P:140:LEU:HG   | 1.58                     | 0.85              |
| 2:B:135:GLU:HG2  | 2:B:140:LEU:HG   | 1.58                     | 0.85              |
| 2:D:129:SER:OG   | 1:E:174:LYS:NZ   | 2.10                     | 0.85              |
| 2:B:133:LEU:HD21 | 2:B:175:ILE:HD11 | 1.57                     | 0.85              |
| 2:D:133:LEU:HD21 | 2:D:175:ILE:HD11 | 1.57                     | 0.85              |
| 2:N:135:GLU:HG2  | 2:N:140:LEU:HG   | 1.57                     | 0.85              |
| 2:L:129:SER:OG   | 1:M:174:LYS:NZ   | 2.10                     | 0.84              |
| 2:D:135:GLU:HG2  | 2:D:140:LEU:HG   | 1.58                     | 0.84              |
| 2:V:133:LEU:HD21 | 2:V:175:ILE:HD11 | 1.57                     | 0.84              |
| 2:F:135:GLU:HG2  | 2:F:140:LEU:HG   | 1.58                     | 0.84              |
| 2:J:133:LEU:HD21 | 2:J:175:ILE:HD11 | 1.57                     | 0.84              |
| 2:T:129:SER:OG   | 1:U:174:LYS:NZ   | 2.10                     | 0.84              |
| 2:L:135:GLU:HG2  | 2:L:140:LEU:HG   | 1.58                     | 0.84              |
| 2:P:129:SER:OG   | 1:Q:174:LYS:NZ   | 2.11                     | 0.84              |
| 2:H:135:GLU:HG2  | 2:H:140:LEU:HG   | 1.58                     | 0.83              |
| 2:H:133:LEU:HD21 | 2:H:175:ILE:HD11 | 1.57                     | 0.83              |
| 2:J:135:GLU:HG2  | 2:J:140:LEU:HG   | 1.58                     | 0.83              |
| 2:X:133:LEU:HD21 | 2:X:175:ILE:HD11 | 1.57                     | 0.83              |
| 2:H:129:SER:OG   | 1:I:174:LYS:NZ   | 2.11                     | 0.83              |
| 2:J:129:SER:OG   | 1:K:174:LYS:NZ   | 2.12                     | 0.83              |
| 2:F:129:SER:OG   | 1:G:174:LYS:NZ   | 2.12                     | 0.83              |
| 2:R:129:SER:OG   | 1:S:174:LYS:NZ   | 2.12                     | 0.82              |
| 2:N:129:SER:OG   | 1:O:174:LYS:NZ   | 2.12                     | 0.82              |
| 2:V:129:SER:OG   | 1:W:174:LYS:NZ   | 2.12                     | 0.82              |
| 2:X:129:SER:OG   | 1:Y:174:LYS:NZ   | 2.13                     | 0.82              |
| 2:B:129:SER:OG   | 1:C:174:LYS:NZ   | 2.12                     | 0.82              |
| 2:H:177:GLU:OE2  | 2:H:180:ARG:NH2  | 2.16                     | 0.78              |
| 2:P:177:GLU:OE2  | 2:P:180:ARG:NH2  | 2.17                     | 0.78              |
| 2:L:177:GLU:OE2  | 2:L:180:ARG:NH2  | 2.17                     | 0.78              |
| 2:F:177:GLU:OE2  | 2:F:180:ARG:NH2  | 2.17                     | 0.76              |
| 2:N:177:GLU:OE2  | 2:N:180:ARG:NH2  | 2.16                     | 0.75              |
| 2:J:177:GLU:OE2  | 2:J:180:ARG:NH2  | 2.17                     | 0.75              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:X:177:GLU:OE2 | 2:X:180:ARG:NH2  | 2.17                     | 0.75              |
| 2:R:177:GLU:OE2 | 2:R:180:ARG:NH2  | 2.17                     | 0.75              |
| 2:B:177:GLU:OE2 | 2:B:180:ARG:NH2  | 2.17                     | 0.74              |
| 2:Z:177:GLU:OE2 | 2:Z:180:ARG:NH2  | 2.17                     | 0.74              |
| 2:V:177:GLU:OE2 | 2:V:180:ARG:NH2  | 2.17                     | 0.74              |
| 2:T:177:GLU:OE2 | 2:T:180:ARG:NH2  | 2.17                     | 0.73              |
| 2:D:177:GLU:OE2 | 2:D:180:ARG:NH2  | 2.17                     | 0.73              |
| 1:I:93:VAL:HG21 | 1:I:122:ILE:HD11 | 1.71                     | 0.72              |
| 1:K:93:VAL:HG21 | 1:K:122:ILE:HD11 | 1.71                     | 0.72              |
| 1:O:93:VAL:HG21 | 1:O:122:ILE:HD11 | 1.71                     | 0.72              |
| 1:M:93:VAL:HG21 | 1:M:122:ILE:HD11 | 1.71                     | 0.72              |
| 1:Y:179:GLU:OE2 | 1:Y:182:ARG:NH2  | 2.23                     | 0.72              |
| 1:G:93:VAL:HG21 | 1:G:122:ILE:HD11 | 1.71                     | 0.72              |
| 1:W:93:VAL:HG21 | 1:W:122:ILE:HD11 | 1.71                     | 0.72              |
| 1:A:93:VAL:HG21 | 1:A:122:ILE:HD11 | 1.71                     | 0.72              |
| 1:S:179:GLU:OE2 | 1:S:182:ARG:NH2  | 2.23                     | 0.72              |
| 1:U:179:GLU:OE2 | 1:U:182:ARG:NH2  | 2.23                     | 0.72              |
| 1:Y:93:VAL:HG21 | 1:Y:122:ILE:HD11 | 1.71                     | 0.72              |
| 1:Q:93:VAL:HG21 | 1:Q:122:ILE:HD11 | 1.71                     | 0.71              |
| 1:E:179:GLU:OE2 | 1:E:182:ARG:NH2  | 2.23                     | 0.71              |
| 1:C:179:GLU:OE2 | 1:C:182:ARG:NH2  | 2.23                     | 0.71              |
| 1:E:93:VAL:HG21 | 1:E:122:ILE:HD11 | 1.71                     | 0.71              |
| 1:E:238:LYS:HG2 | 2:F:242:ILE:HG23 | 1.72                     | 0.71              |
| 1:A:179:GLU:OE2 | 1:A:182:ARG:NH2  | 2.23                     | 0.71              |
| 1:C:93:VAL:HG21 | 1:C:122:ILE:HD11 | 1.71                     | 0.71              |
| 1:O:179:GLU:OE2 | 1:O:182:ARG:NH2  | 2.23                     | 0.71              |
| 1:Q:238:LYS:HG2 | 2:R:242:ILE:HG23 | 1.72                     | 0.71              |
| 1:W:179:GLU:OE2 | 1:W:182:ARG:NH2  | 2.23                     | 0.71              |
| 1:G:92:GLU:HG3  | 1:G:171:ARG:HB2  | 1.73                     | 0.71              |
| 1:O:92:GLU:HG3  | 1:O:171:ARG:HB2  | 1.73                     | 0.71              |
| 1:S:93:VAL:HG21 | 1:S:122:ILE:HD11 | 1.71                     | 0.71              |
| 1:U:93:VAL:HG21 | 1:U:122:ILE:HD11 | 1.71                     | 0.71              |
| 1:K:92:GLU:HG3  | 1:K:171:ARG:HB2  | 1.73                     | 0.71              |
| 1:S:238:LYS:HG2 | 2:T:242:ILE:HG23 | 1.72                     | 0.71              |
| 1:A:238:LYS:HG2 | 2:B:242:ILE:HG23 | 1.72                     | 0.71              |
| 1:U:238:LYS:HG2 | 2:V:242:ILE:HG23 | 1.72                     | 0.71              |
| 1:C:238:LYS:HG2 | 2:D:242:ILE:HG23 | 1.72                     | 0.71              |
| 1:I:92:GLU:HG3  | 1:I:171:ARG:HB2  | 1.73                     | 0.71              |
| 1:I:179:GLU:OE2 | 1:I:182:ARG:NH2  | 2.23                     | 0.71              |
| 1:M:238:LYS:HG2 | 2:N:242:ILE:HG23 | 1.72                     | 0.71              |
| 1:G:238:LYS:HG2 | 2:H:242:ILE:HG23 | 1.72                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:92:GLU:HG3   | 1:M:171:ARG:HB2  | 1.73                     | 0.71              |
| 1:O:238:LYS:HG2  | 2:P:242:ILE:HG23 | 1.72                     | 0.70              |
| 1:I:238:LYS:HG2  | 2:J:242:ILE:HG23 | 1.72                     | 0.70              |
| 1:Q:92:GLU:HG3   | 1:Q:171:ARG:HB2  | 1.73                     | 0.70              |
| 1:C:92:GLU:HG3   | 1:C:171:ARG:HB2  | 1.73                     | 0.70              |
| 1:Q:179:GLU:OE2  | 1:Q:182:ARG:NH2  | 2.23                     | 0.70              |
| 1:S:92:GLU:HG3   | 1:S:171:ARG:HB2  | 1.73                     | 0.70              |
| 1:M:179:GLU:OE2  | 1:M:182:ARG:NH2  | 2.23                     | 0.70              |
| 1:E:92:GLU:HG3   | 1:E:171:ARG:HB2  | 1.73                     | 0.70              |
| 1:Y:238:LYS:HG2  | 2:Z:242:ILE:HG23 | 1.72                     | 0.70              |
| 1:W:238:LYS:HG2  | 2:X:242:ILE:HG23 | 1.72                     | 0.70              |
| 1:K:179:GLU:OE2  | 1:K:182:ARG:NH2  | 2.23                     | 0.70              |
| 1:U:92:GLU:HG3   | 1:U:171:ARG:HB2  | 1.73                     | 0.70              |
| 1:A:92:GLU:HG3   | 1:A:171:ARG:HB2  | 1.73                     | 0.70              |
| 1:G:179:GLU:OE2  | 1:G:182:ARG:NH2  | 2.23                     | 0.70              |
| 1:K:238:LYS:HG2  | 2:L:242:ILE:HG23 | 1.72                     | 0.69              |
| 1:W:92:GLU:HG3   | 1:W:171:ARG:HB2  | 1.73                     | 0.69              |
| 1:Y:92:GLU:HG3   | 1:Y:171:ARG:HB2  | 1.73                     | 0.69              |
| 2:B:229:TYR:HD2  | 1:C:240:THR:HG21 | 1.59                     | 0.68              |
| 1:S:92:GLU:OE2   | 1:S:171:ARG:NE   | 2.15                     | 0.68              |
| 2:V:229:TYR:HD2  | 1:W:240:THR:HG21 | 1.59                     | 0.68              |
| 1:C:65:GLN:HE21  | 1:C:67:THR:HG22  | 1.59                     | 0.68              |
| 1:C:292:ALA:C    | 1:C:294:ASN:H    | 1.99                     | 0.68              |
| 1:G:92:GLU:OE2   | 1:G:171:ARG:NE   | 2.15                     | 0.68              |
| 1:I:92:GLU:OE2   | 1:I:171:ARG:NE   | 2.16                     | 0.68              |
| 2:R:229:TYR:HD2  | 1:S:240:THR:HG21 | 1.59                     | 0.68              |
| 1:E:92:GLU:OE2   | 1:E:171:ARG:NE   | 2.16                     | 0.68              |
| 2:N:229:TYR:HD2  | 1:O:240:THR:HG21 | 1.59                     | 0.68              |
| 1:Q:122:ILE:HG13 | 1:Q:154:LEU:HD21 | 1.76                     | 0.68              |
| 1:S:122:ILE:HG13 | 1:S:154:LEU:HD21 | 1.76                     | 0.68              |
| 1:A:122:ILE:HG13 | 1:A:154:LEU:HD21 | 1.76                     | 0.67              |
| 1:C:92:GLU:OE2   | 1:C:171:ARG:NE   | 2.16                     | 0.67              |
| 1:M:92:GLU:OE2   | 1:M:171:ARG:NE   | 2.16                     | 0.67              |
| 1:C:122:ILE:HG13 | 1:C:154:LEU:HD21 | 1.76                     | 0.67              |
| 2:T:291:SER:O    | 2:T:292:ASN:HB2  | 1.95                     | 0.67              |
| 1:A:92:GLU:OE2   | 1:A:171:ARG:NE   | 2.15                     | 0.67              |
| 1:A:240:THR:HG21 | 2:Z:229:TYR:HD2  | 1.60                     | 0.67              |
| 2:P:291:SER:O    | 2:P:292:ASN:HB2  | 1.95                     | 0.67              |
| 2:F:229:TYR:HD2  | 1:G:240:THR:HG21 | 1.58                     | 0.67              |
| 2:J:291:SER:O    | 2:J:292:ASN:HB2  | 1.95                     | 0.67              |
| 1:O:122:ILE:HG13 | 1:O:154:LEU:HD21 | 1.76                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:122:ILE:HG13 | 1:E:154:LEU:HD21 | 1.76                     | 0.67              |
| 2:J:229:TYR:HD2  | 1:K:240:THR:HG21 | 1.59                     | 0.67              |
| 1:U:122:ILE:HG13 | 1:U:154:LEU:HD21 | 1.76                     | 0.67              |
| 1:I:181:ILE:HG23 | 2:J:191:THR:HG21 | 1.77                     | 0.67              |
| 2:N:291:SER:O    | 2:N:292:ASN:HB2  | 1.95                     | 0.67              |
| 2:L:179:ILE:HG23 | 1:M:193:THR:HG21 | 1.77                     | 0.67              |
| 1:W:92:GLU:OE2   | 1:W:171:ARG:NE   | 2.16                     | 0.67              |
| 1:G:122:ILE:HG13 | 1:G:154:LEU:HD21 | 1.76                     | 0.67              |
| 1:S:181:ILE:HG23 | 2:T:191:THR:HG21 | 1.77                     | 0.67              |
| 1:E:181:ILE:HG23 | 2:F:191:THR:HG21 | 1.77                     | 0.67              |
| 2:V:291:SER:O    | 2:V:292:ASN:HB2  | 1.95                     | 0.67              |
| 1:W:181:ILE:HG23 | 2:X:191:THR:HG21 | 1.77                     | 0.67              |
| 1:Y:122:ILE:HG13 | 1:Y:154:LEU:HD21 | 1.76                     | 0.67              |
| 1:A:181:ILE:HG23 | 2:B:191:THR:HG21 | 1.77                     | 0.66              |
| 1:A:298:TYR:O    | 1:A:299:PHE:C    | 2.37                     | 0.66              |
| 2:L:229:TYR:HD2  | 1:M:240:THR:HG21 | 1.60                     | 0.66              |
| 1:M:181:ILE:HG23 | 2:N:191:THR:HG21 | 1.77                     | 0.66              |
| 1:I:122:ILE:HG13 | 1:I:154:LEU:HD21 | 1.76                     | 0.66              |
| 2:P:229:TYR:HD2  | 1:Q:240:THR:HG21 | 1.60                     | 0.66              |
| 2:X:179:ILE:HG23 | 1:Y:193:THR:HG21 | 1.76                     | 0.66              |
| 1:W:122:ILE:HG13 | 1:W:154:LEU:HD21 | 1.76                     | 0.66              |
| 2:L:291:SER:O    | 2:L:292:ASN:HB2  | 1.95                     | 0.66              |
| 2:D:179:ILE:HG23 | 1:E:193:THR:HG21 | 1.77                     | 0.66              |
| 2:D:229:TYR:HD2  | 1:E:240:THR:HG21 | 1.60                     | 0.66              |
| 2:D:291:SER:O    | 2:D:292:ASN:HB2  | 1.95                     | 0.66              |
| 2:F:291:SER:O    | 2:F:292:ASN:HB2  | 1.95                     | 0.66              |
| 2:H:179:ILE:HG23 | 1:I:193:THR:HG21 | 1.77                     | 0.66              |
| 2:H:291:SER:O    | 2:H:292:ASN:HB2  | 1.95                     | 0.66              |
| 1:K:122:ILE:HG13 | 1:K:154:LEU:HD21 | 1.76                     | 0.66              |
| 1:M:122:ILE:HG13 | 1:M:154:LEU:HD21 | 1.76                     | 0.66              |
| 2:X:229:TYR:HD2  | 1:Y:240:THR:HG21 | 1.61                     | 0.66              |
| 2:X:291:SER:O    | 2:X:292:ASN:HB2  | 1.95                     | 0.66              |
| 1:Y:92:GLU:OE2   | 1:Y:171:ARG:NE   | 2.16                     | 0.66              |
| 1:Y:181:ILE:HG23 | 2:Z:191:THR:HG21 | 1.77                     | 0.66              |
| 2:B:179:ILE:HG23 | 1:C:193:THR:HG21 | 1.78                     | 0.66              |
| 2:B:200:GLN:HE21 | 1:C:211:THR:HG22 | 1.60                     | 0.66              |
| 1:C:298:TYR:O    | 1:C:299:PHE:C    | 2.38                     | 0.66              |
| 2:F:179:ILE:HG23 | 1:G:193:THR:HG21 | 1.78                     | 0.66              |
| 1:O:181:ILE:HG23 | 2:P:191:THR:HG21 | 1.77                     | 0.66              |
| 2:H:229:TYR:HD2  | 1:I:240:THR:HG21 | 1.60                     | 0.66              |
| 1:O:88:ILE:HD12  | 1:O:126:LEU:HD21 | 1.78                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:179:ILE:HG23 | 1:Q:193:THR:HG21 | 1.78                     | 0.66              |
| 1:K:88:ILE:HD12  | 1:K:126:LEU:HD21 | 1.78                     | 0.65              |
| 2:N:179:ILE:HG23 | 1:O:193:THR:HG21 | 1.78                     | 0.65              |
| 2:R:179:ILE:HG23 | 1:S:193:THR:HG21 | 1.78                     | 0.65              |
| 2:T:229:TYR:HD2  | 1:U:240:THR:HG21 | 1.60                     | 0.65              |
| 1:C:181:ILE:HG23 | 2:D:191:THR:HG21 | 1.77                     | 0.65              |
| 1:Q:181:ILE:HG23 | 2:R:191:THR:HG21 | 1.77                     | 0.65              |
| 2:R:291:SER:O    | 2:R:292:ASN:HB2  | 1.95                     | 0.65              |
| 1:S:88:ILE:HD12  | 1:S:126:LEU:HD21 | 1.78                     | 0.65              |
| 2:V:179:ILE:HG23 | 1:W:193:THR:HG21 | 1.78                     | 0.65              |
| 1:A:193:THR:HG21 | 2:Z:179:ILE:HG23 | 1.78                     | 0.65              |
| 1:G:181:ILE:HG23 | 2:H:191:THR:HG21 | 1.77                     | 0.65              |
| 2:J:179:ILE:HG23 | 1:K:193:THR:HG21 | 1.78                     | 0.65              |
| 1:M:88:ILE:HD12  | 1:M:126:LEU:HD21 | 1.78                     | 0.65              |
| 1:U:181:ILE:HG23 | 2:V:191:THR:HG21 | 1.77                     | 0.65              |
| 1:I:88:ILE:HD12  | 1:I:126:LEU:HD21 | 1.78                     | 0.65              |
| 1:Q:88:ILE:HD12  | 1:Q:126:LEU:HD21 | 1.78                     | 0.65              |
| 1:K:181:ILE:HG23 | 2:L:191:THR:HG21 | 1.77                     | 0.65              |
| 1:E:109:TYR:O    | 1:E:110:THR:OG1  | 2.15                     | 0.65              |
| 1:G:109:TYR:O    | 1:G:110:THR:OG1  | 2.15                     | 0.65              |
| 2:T:179:ILE:HG23 | 1:U:193:THR:HG21 | 1.77                     | 0.65              |
| 1:G:88:ILE:HD12  | 1:G:126:LEU:HD21 | 1.78                     | 0.64              |
| 1:Q:115:LYS:HD3  | 1:Q:119:PHE:HD2  | 1.63                     | 0.64              |
| 1:U:88:ILE:HD12  | 1:U:126:LEU:HD21 | 1.79                     | 0.64              |
| 1:G:115:LYS:HD3  | 1:G:119:PHE:HD2  | 1.63                     | 0.64              |
| 1:M:109:TYR:O    | 1:M:110:THR:OG1  | 2.15                     | 0.64              |
| 1:W:88:ILE:HD12  | 1:W:126:LEU:HD21 | 1.78                     | 0.64              |
| 1:E:115:LYS:HD3  | 1:E:119:PHE:HD2  | 1.63                     | 0.64              |
| 2:D:276:LEU:HD13 | 1:E:281:GLU:HB2  | 1.80                     | 0.64              |
| 1:U:109:TYR:O    | 1:U:110:THR:OG1  | 2.15                     | 0.64              |
| 1:Y:115:LYS:HD3  | 1:Y:119:PHE:HD2  | 1.63                     | 0.64              |
| 1:E:88:ILE:HD12  | 1:E:126:LEU:HD21 | 1.78                     | 0.64              |
| 1:W:115:LYS:HD3  | 1:W:119:PHE:HD2  | 1.63                     | 0.64              |
| 1:A:281:GLU:HB2  | 2:Z:276:LEU:HD13 | 1.80                     | 0.64              |
| 1:K:115:LYS:HD3  | 1:K:119:PHE:HD2  | 1.63                     | 0.64              |
| 1:K:274:ASN:O    | 1:K:278:LEU:HD13 | 1.98                     | 0.64              |
| 1:S:109:TYR:O    | 1:S:110:THR:OG1  | 2.15                     | 0.64              |
| 1:M:115:LYS:HD3  | 1:M:119:PHE:HD2  | 1.62                     | 0.64              |
| 1:Q:274:ASN:O    | 1:Q:278:LEU:HD13 | 1.98                     | 0.64              |
| 1:S:274:ASN:O    | 1:S:278:LEU:HD13 | 1.98                     | 0.64              |
| 1:W:109:TYR:O    | 1:W:110:THR:OG1  | 2.15                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:109:TYR:O    | 1:A:110:THR:OG1  | 2.15                     | 0.64              |
| 1:S:115:LYS:HD3  | 1:S:119:PHE:HD2  | 1.63                     | 0.64              |
| 1:C:88:ILE:HD12  | 1:C:126:LEU:HD21 | 1.78                     | 0.63              |
| 1:I:109:TYR:O    | 1:I:110:THR:OG1  | 2.15                     | 0.63              |
| 1:U:274:ASN:O    | 1:U:278:LEU:HD13 | 1.98                     | 0.63              |
| 1:A:88:ILE:HD12  | 1:A:126:LEU:HD21 | 1.78                     | 0.63              |
| 1:C:115:LYS:HD3  | 1:C:119:PHE:HD2  | 1.63                     | 0.63              |
| 1:Q:109:TYR:O    | 1:Q:110:THR:OG1  | 2.15                     | 0.63              |
| 1:Y:88:ILE:HD12  | 1:Y:126:LEU:HD21 | 1.78                     | 0.63              |
| 1:C:274:ASN:O    | 1:C:278:LEU:HD13 | 1.98                     | 0.63              |
| 1:G:274:ASN:O    | 1:G:278:LEU:HD13 | 1.98                     | 0.63              |
| 1:Y:109:TYR:O    | 1:Y:110:THR:OG1  | 2.15                     | 0.63              |
| 1:I:274:ASN:O    | 1:I:278:LEU:HD13 | 1.99                     | 0.63              |
| 1:M:274:ASN:O    | 1:M:278:LEU:HD13 | 1.98                     | 0.63              |
| 1:O:115:LYS:HD3  | 1:O:119:PHE:HD2  | 1.63                     | 0.63              |
| 1:A:115:LYS:HD3  | 1:A:119:PHE:HD2  | 1.63                     | 0.63              |
| 1:A:274:ASN:O    | 1:A:278:LEU:HD13 | 1.98                     | 0.63              |
| 1:O:274:ASN:O    | 1:O:278:LEU:HD13 | 1.98                     | 0.63              |
| 1:Q:92:GLU:OE2   | 1:Q:171:ARG:NE   | 2.16                     | 0.63              |
| 1:E:274:ASN:O    | 1:E:278:LEU:HD13 | 1.98                     | 0.63              |
| 1:W:274:ASN:O    | 1:W:278:LEU:HD13 | 1.98                     | 0.63              |
| 2:H:276:LEU:HD13 | 1:I:281:GLU:HB2  | 1.80                     | 0.62              |
| 1:O:109:TYR:O    | 1:O:110:THR:OG1  | 2.15                     | 0.62              |
| 2:P:276:LEU:HD13 | 1:Q:281:GLU:HB2  | 1.79                     | 0.62              |
| 1:C:109:TYR:O    | 1:C:110:THR:OG1  | 2.15                     | 0.62              |
| 1:K:92:GLU:OE2   | 1:K:171:ARG:NE   | 2.15                     | 0.62              |
| 2:T:276:LEU:HD13 | 1:U:281:GLU:HB2  | 1.80                     | 0.62              |
| 1:U:115:LYS:HD3  | 1:U:119:PHE:HD2  | 1.63                     | 0.62              |
| 2:X:276:LEU:HD13 | 1:Y:281:GLU:HB2  | 1.81                     | 0.62              |
| 2:B:286:TYR:O    | 2:B:290:ALA:HB2  | 2.00                     | 0.62              |
| 1:Y:274:ASN:O    | 1:Y:278:LEU:HD13 | 1.98                     | 0.62              |
| 1:I:115:LYS:HD3  | 1:I:119:PHE:HD2  | 1.63                     | 0.62              |
| 2:L:276:LEU:HD13 | 1:M:281:GLU:HB2  | 1.80                     | 0.62              |
| 1:U:92:GLU:OE2   | 1:U:171:ARG:NE   | 2.16                     | 0.62              |
| 1:C:120:ASN:HB3  | 2:D:169:ARG:NH1  | 2.15                     | 0.61              |
| 1:K:120:ASN:HB3  | 2:L:169:ARG:NH1  | 2.16                     | 0.61              |
| 1:M:120:ASN:HB3  | 2:N:169:ARG:NH1  | 2.16                     | 0.61              |
| 1:Y:120:ASN:HB3  | 2:Z:169:ARG:NH1  | 2.16                     | 0.61              |
| 2:Z:90:GLU:HG3   | 2:Z:169:ARG:HB2  | 1.83                     | 0.61              |
| 1:I:120:ASN:HB3  | 2:J:169:ARG:NH1  | 2.16                     | 0.61              |
| 1:K:109:TYR:O    | 1:K:110:THR:OG1  | 2.15                     | 0.61              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:O:120:ASN:HB3  | 2:P:169:ARG:NH1 | 2.16                     | 0.61              |
| 1:Q:120:ASN:HB3  | 2:R:169:ARG:NH1 | 2.16                     | 0.61              |
| 2:R:90:GLU:HG3   | 2:R:169:ARG:HB2 | 1.83                     | 0.61              |
| 2:T:90:GLU:HG3   | 2:T:169:ARG:HB2 | 1.83                     | 0.61              |
| 2:V:90:GLU:HG3   | 2:V:169:ARG:HB2 | 1.83                     | 0.61              |
| 2:X:90:GLU:HG3   | 2:X:169:ARG:HB2 | 1.83                     | 0.61              |
| 2:D:90:GLU:HG3   | 2:D:169:ARG:HB2 | 1.83                     | 0.61              |
| 1:G:120:ASN:HB3  | 2:H:169:ARG:NH1 | 2.16                     | 0.61              |
| 1:S:120:ASN:HB3  | 2:T:169:ARG:NH1 | 2.16                     | 0.61              |
| 2:P:90:GLU:HG3   | 2:P:169:ARG:HB2 | 1.83                     | 0.61              |
| 1:U:120:ASN:HB3  | 2:V:169:ARG:NH1 | 2.15                     | 0.61              |
| 1:W:120:ASN:HB3  | 2:X:169:ARG:NH1 | 2.16                     | 0.61              |
| 2:F:90:GLU:HG3   | 2:F:169:ARG:HB2 | 1.83                     | 0.60              |
| 2:B:276:LEU:HD13 | 1:C:281:GLU:HB2 | 1.84                     | 0.60              |
| 1:C:290:ALA:C    | 1:C:292:ALA:H   | 2.10                     | 0.60              |
| 1:E:290:ALA:C    | 1:E:292:ALA:H   | 2.10                     | 0.60              |
| 1:G:290:ALA:C    | 1:G:292:ALA:H   | 2.10                     | 0.60              |
| 1:A:290:ALA:C    | 1:A:292:ALA:H   | 2.10                     | 0.60              |
| 1:E:120:ASN:HB3  | 2:F:169:ARG:NH1 | 2.16                     | 0.60              |
| 1:A:265:TYR:CE2  | 2:Z:255:LYS:HG3 | 2.37                     | 0.60              |
| 1:I:290:ALA:C    | 1:I:292:ALA:H   | 2.09                     | 0.60              |
| 1:A:120:ASN:HB3  | 2:B:169:ARG:NH1 | 2.16                     | 0.60              |
| 2:N:90:GLU:HG3   | 2:N:169:ARG:HB2 | 1.83                     | 0.60              |
| 1:O:92:GLU:OE2   | 1:O:171:ARG:NE  | 2.16                     | 0.60              |
| 1:Y:290:ALA:C    | 1:Y:292:ALA:H   | 2.09                     | 0.60              |
| 1:K:290:ALA:C    | 1:K:292:ALA:H   | 2.10                     | 0.60              |
| 1:W:290:ALA:C    | 1:W:292:ALA:H   | 2.10                     | 0.60              |
| 1:A:251:ALA:HB2  | 2:Z:240:LYS:HG3 | 1.84                     | 0.59              |
| 2:H:90:GLU:HG3   | 2:H:169:ARG:HB2 | 1.83                     | 0.59              |
| 1:M:290:ALA:C    | 1:M:292:ALA:H   | 2.10                     | 0.59              |
| 2:V:255:LYS:HG3  | 1:W:265:TYR:CE2 | 2.37                     | 0.59              |
| 1:A:292:ALA:C    | 1:A:294:ASN:H   | 2.09                     | 0.59              |
| 2:F:276:LEU:HD13 | 1:G:281:GLU:HB2 | 1.84                     | 0.59              |
| 1:G:27:LYS:NZ    | 1:G:29:GLU:OE1  | 2.35                     | 0.59              |
| 1:Q:290:ALA:C    | 1:Q:292:ALA:H   | 2.09                     | 0.59              |
| 1:U:290:ALA:C    | 1:U:292:ALA:H   | 2.10                     | 0.59              |
| 1:W:27:LYS:NZ    | 1:W:29:GLU:OE1  | 2.35                     | 0.59              |
| 1:I:27:LYS:NZ    | 1:I:29:GLU:OE1  | 2.35                     | 0.59              |
| 1:O:290:ALA:C    | 1:O:292:ALA:H   | 2.10                     | 0.59              |
| 1:Q:27:LYS:NZ    | 1:Q:29:GLU:OE1  | 2.35                     | 0.59              |
| 1:E:27:LYS:NZ    | 1:E:29:GLU:OE1  | 2.35                     | 0.59              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:S:27:LYS:NZ    | 1:S:29:GLU:OE1  | 2.35                     | 0.59              |
| 2:V:276:LEU:HD13 | 1:W:281:GLU:HB2 | 1.84                     | 0.59              |
| 2:F:255:LYS:HG3  | 1:G:265:TYR:CE2 | 2.37                     | 0.59              |
| 2:L:90:GLU:HG3   | 2:L:169:ARG:HB2 | 1.83                     | 0.59              |
| 2:B:255:LYS:HG3  | 1:C:265:TYR:CE2 | 2.37                     | 0.59              |
| 1:K:27:LYS:NZ    | 1:K:29:GLU:OE1  | 2.35                     | 0.59              |
| 2:P:255:LYS:HG3  | 1:Q:265:TYR:CE2 | 2.37                     | 0.59              |
| 1:S:290:ALA:C    | 1:S:292:ALA:H   | 2.10                     | 0.59              |
| 2:X:255:LYS:HG3  | 1:Y:265:TYR:CE2 | 2.38                     | 0.59              |
| 1:Y:27:LYS:NZ    | 1:Y:29:GLU:OE1  | 2.35                     | 0.59              |
| 2:J:255:LYS:HG3  | 1:K:265:TYR:CE2 | 2.37                     | 0.59              |
| 2:N:255:LYS:HG3  | 1:O:265:TYR:CE2 | 2.37                     | 0.59              |
| 2:R:255:LYS:HG3  | 1:S:265:TYR:CE2 | 2.37                     | 0.59              |
| 2:V:134:GLN:OE1  | 2:V:183:TYR:OH  | 2.21                     | 0.59              |
| 1:U:27:LYS:NZ    | 1:U:29:GLU:OE1  | 2.35                     | 0.59              |
| 2:P:134:GLN:OE1  | 2:P:183:TYR:OH  | 2.21                     | 0.59              |
| 2:X:134:GLN:OE1  | 2:X:183:TYR:OH  | 2.21                     | 0.59              |
| 1:C:27:LYS:NZ    | 1:C:29:GLU:OE1  | 2.35                     | 0.58              |
| 2:F:229:TYR:HD2  | 1:G:240:THR:CG2 | 2.16                     | 0.58              |
| 2:J:276:LEU:HD13 | 1:K:281:GLU:HB2 | 1.84                     | 0.58              |
| 2:N:229:TYR:HD2  | 1:O:240:THR:CG2 | 2.16                     | 0.58              |
| 2:J:90:GLU:HG3   | 2:J:169:ARG:HB2 | 1.83                     | 0.58              |
| 1:M:27:LYS:NZ    | 1:M:29:GLU:OE1  | 2.35                     | 0.58              |
| 1:O:27:LYS:NZ    | 1:O:29:GLU:OE1  | 2.35                     | 0.58              |
| 1:A:27:LYS:NZ    | 1:A:29:GLU:OE1  | 2.35                     | 0.58              |
| 2:Z:134:GLN:OE1  | 2:Z:183:TYR:OH  | 2.21                     | 0.58              |
| 2:B:229:TYR:HD2  | 1:C:240:THR:CG2 | 2.16                     | 0.58              |
| 1:C:292:ALA:C    | 1:C:294:ASN:N   | 2.62                     | 0.58              |
| 2:J:229:TYR:HD2  | 1:K:240:THR:CG2 | 2.16                     | 0.58              |
| 2:N:276:LEU:HD13 | 1:O:281:GLU:HB2 | 1.84                     | 0.58              |
| 2:R:229:TYR:HD2  | 1:S:240:THR:CG2 | 2.16                     | 0.58              |
| 2:R:276:LEU:HD13 | 1:S:281:GLU:HB2 | 1.84                     | 0.58              |
| 2:X:38:GLY:O     | 1:Y:30:GLU:N    | 2.36                     | 0.58              |
| 2:B:134:GLN:OE1  | 2:B:183:TYR:OH  | 2.21                     | 0.58              |
| 2:D:255:LYS:HG3  | 1:E:265:TYR:CE2 | 2.39                     | 0.58              |
| 2:V:229:TYR:HD2  | 1:W:240:THR:CG2 | 2.16                     | 0.58              |
| 2:D:134:GLN:OE1  | 2:D:183:TYR:OH  | 2.21                     | 0.58              |
| 2:H:255:LYS:HG3  | 1:I:265:TYR:CE2 | 2.38                     | 0.58              |
| 2:F:134:GLN:OE1  | 2:F:183:TYR:OH  | 2.21                     | 0.57              |
| 2:H:134:GLN:OE1  | 2:H:183:TYR:OH  | 2.21                     | 0.57              |
| 2:J:134:GLN:OE1  | 2:J:183:TYR:OH  | 2.21                     | 0.57              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:T:38:GLY:O    | 1:U:30:GLU:N     | 2.36                     | 0.57              |
| 2:D:38:GLY:O    | 1:E:30:GLU:N     | 2.36                     | 0.57              |
| 2:L:255:LYS:HG3 | 1:M:265:TYR:CE2  | 2.39                     | 0.57              |
| 2:Z:291:SER:O   | 2:Z:292:ASN:C    | 2.47                     | 0.57              |
| 2:L:134:GLN:OE1 | 2:L:183:TYR:OH   | 2.21                     | 0.57              |
| 1:K:71:ASP:HB3  | 1:K:119:PHE:HZ   | 1.70                     | 0.57              |
| 1:O:71:ASP:HB3  | 1:O:119:PHE:HZ   | 1.70                     | 0.57              |
| 2:L:38:GLY:O    | 1:M:30:GLU:N     | 2.36                     | 0.57              |
| 1:M:71:ASP:HB3  | 1:M:119:PHE:HZ   | 1.70                     | 0.57              |
| 1:G:71:ASP:HB3  | 1:G:119:PHE:HZ   | 1.70                     | 0.57              |
| 2:H:129:SER:HG  | 1:I:174:LYS:NZ   | 2.02                     | 0.57              |
| 1:Q:71:ASP:HB3  | 1:Q:119:PHE:HZ   | 1.70                     | 0.57              |
| 2:T:255:LYS:HG3 | 1:U:265:TYR:CE2  | 2.39                     | 0.57              |
| 1:I:71:ASP:HB3  | 1:I:119:PHE:HZ   | 1.70                     | 0.57              |
| 1:O:257:LYS:HG3 | 2:P:263:TYR:CE2  | 2.40                     | 0.57              |
| 1:K:257:LYS:HG3 | 2:L:263:TYR:CE2  | 2.40                     | 0.57              |
| 2:N:134:GLN:OE1 | 2:N:183:TYR:OH   | 2.21                     | 0.56              |
| 1:S:257:LYS:HG3 | 2:T:263:TYR:CE2  | 2.40                     | 0.56              |
| 1:C:207:LYS:O   | 1:C:211:THR:HG23 | 2.05                     | 0.56              |
| 1:S:71:ASP:HB3  | 1:S:119:PHE:HZ   | 1.70                     | 0.56              |
| 1:A:207:LYS:O   | 1:A:211:THR:HG23 | 2.05                     | 0.56              |
| 1:A:294:ASN:O   | 1:A:295:SER:HB2  | 2.05                     | 0.56              |
| 2:B:292:ASN:O   | 2:B:293:SER:HB3  | 2.04                     | 0.56              |
| 1:E:207:LYS:O   | 1:E:211:THR:HG23 | 2.06                     | 0.56              |
| 2:R:134:GLN:OE1 | 2:R:183:TYR:OH   | 2.21                     | 0.56              |
| 2:T:134:GLN:OE1 | 2:T:183:TYR:OH   | 2.21                     | 0.56              |
| 2:Z:290:ALA:C   | 2:Z:292:ASN:H    | 2.12                     | 0.56              |
| 2:T:291:SER:O   | 2:T:292:ASN:CB   | 2.54                     | 0.56              |
| 1:W:114:ASP:OD1 | 1:W:118:ILE:HD12 | 2.06                     | 0.56              |
| 2:H:291:SER:O   | 2:H:292:ASN:CB   | 2.54                     | 0.56              |
| 1:I:114:ASP:OD1 | 1:I:118:ILE:HD12 | 2.06                     | 0.56              |
| 2:L:291:SER:O   | 2:L:292:ASN:CB   | 2.54                     | 0.56              |
| 1:M:257:LYS:HG3 | 2:N:263:TYR:CE2  | 2.40                     | 0.56              |
| 1:E:114:ASP:OD1 | 1:E:118:ILE:HD12 | 2.06                     | 0.56              |
| 1:U:71:ASP:HB3  | 1:U:119:PHE:HZ   | 1.70                     | 0.56              |
| 2:X:291:SER:O   | 2:X:292:ASN:CB   | 2.54                     | 0.56              |
| 1:C:114:ASP:OD1 | 1:C:118:ILE:HD12 | 2.06                     | 0.56              |
| 1:G:207:LYS:O   | 1:G:211:THR:HG23 | 2.06                     | 0.56              |
| 1:G:257:LYS:HG3 | 2:H:263:TYR:CE2  | 2.40                     | 0.56              |
| 1:K:114:ASP:OD1 | 1:K:118:ILE:HD12 | 2.06                     | 0.56              |
| 1:K:207:LYS:O   | 1:K:211:THR:HG23 | 2.06                     | 0.56              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:P:291:SER:O   | 2:P:292:ASN:CB   | 2.54                     | 0.56              |
| 1:Q:257:LYS:HG3 | 2:R:263:TYR:CE2  | 2.40                     | 0.56              |
| 2:D:291:SER:O   | 2:D:292:ASN:CB   | 2.54                     | 0.55              |
| 1:O:114:ASP:OD1 | 1:O:118:ILE:HD12 | 2.06                     | 0.55              |
| 1:S:114:ASP:OD1 | 1:S:118:ILE:HD12 | 2.06                     | 0.55              |
| 1:U:257:LYS:HG3 | 2:V:263:TYR:CE2  | 2.40                     | 0.55              |
| 1:W:257:LYS:HG3 | 2:X:263:TYR:CE2  | 2.40                     | 0.55              |
| 1:C:257:LYS:HG3 | 2:D:263:TYR:CE2  | 2.40                     | 0.55              |
| 1:E:40:GLY:O    | 2:F:28:GLU:N     | 2.37                     | 0.55              |
| 1:G:114:ASP:OD1 | 1:G:118:ILE:HD12 | 2.06                     | 0.55              |
| 1:I:257:LYS:HG3 | 2:J:263:TYR:CE2  | 2.40                     | 0.55              |
| 1:Q:207:LYS:O   | 1:Q:211:THR:HG23 | 2.06                     | 0.55              |
| 1:U:207:LYS:O   | 1:U:211:THR:HG23 | 2.06                     | 0.55              |
| 1:Y:257:LYS:HG3 | 2:Z:263:TYR:CE2  | 2.40                     | 0.55              |
| 1:E:71:ASP:HB3  | 1:E:119:PHE:HZ   | 1.70                     | 0.55              |
| 1:I:207:LYS:O   | 1:I:211:THR:HG23 | 2.06                     | 0.55              |
| 1:Y:71:ASP:HB3  | 1:Y:119:PHE:HZ   | 1.70                     | 0.55              |
| 1:A:257:LYS:HG3 | 2:B:263:TYR:CE2  | 2.40                     | 0.55              |
| 2:B:115:LEU:HB3 | 2:B:156:LEU:HD21 | 1.89                     | 0.55              |
| 2:D:115:LEU:HB3 | 2:D:156:LEU:HD21 | 1.89                     | 0.55              |
| 1:E:257:LYS:HG3 | 2:F:263:TYR:CE2  | 2.40                     | 0.55              |
| 2:F:291:SER:O   | 2:F:292:ASN:CB   | 2.54                     | 0.55              |
| 2:J:115:LEU:HB3 | 2:J:156:LEU:HD21 | 1.89                     | 0.55              |
| 2:L:115:LEU:HB3 | 2:L:156:LEU:HD21 | 1.89                     | 0.55              |
| 1:M:207:LYS:O   | 1:M:211:THR:HG23 | 2.06                     | 0.55              |
| 2:P:115:LEU:HB3 | 2:P:156:LEU:HD21 | 1.89                     | 0.55              |
| 2:R:115:LEU:HB3 | 2:R:156:LEU:HD21 | 1.89                     | 0.55              |
| 1:W:71:ASP:HB3  | 1:W:119:PHE:HZ   | 1.70                     | 0.55              |
| 1:W:207:LYS:O   | 1:W:211:THR:HG23 | 2.06                     | 0.55              |
| 2:Z:115:LEU:HB3 | 2:Z:156:LEU:HD21 | 1.89                     | 0.55              |
| 2:F:115:LEU:HB3 | 2:F:156:LEU:HD21 | 1.89                     | 0.55              |
| 2:N:115:LEU:HB3 | 2:N:156:LEU:HD21 | 1.89                     | 0.55              |
| 1:Y:114:ASP:OD1 | 1:Y:118:ILE:HD12 | 2.06                     | 0.55              |
| 1:A:240:THR:CG2 | 2:Z:229:TYR:HD2  | 2.18                     | 0.55              |
| 2:H:115:LEU:HB3 | 2:H:156:LEU:HD21 | 1.89                     | 0.55              |
| 1:M:114:ASP:OD1 | 1:M:118:ILE:HD12 | 2.06                     | 0.55              |
| 1:S:207:LYS:O   | 1:S:211:THR:HG23 | 2.05                     | 0.55              |
| 1:A:114:ASP:OD1 | 1:A:118:ILE:HD12 | 2.06                     | 0.55              |
| 2:J:291:SER:O   | 2:J:292:ASN:CB   | 2.54                     | 0.55              |
| 2:V:291:SER:O   | 2:V:292:ASN:CB   | 2.54                     | 0.55              |
| 2:B:63:GLN:HE21 | 2:B:65:THR:HG22  | 1.71                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:N:118:ASN:O   | 2:N:121:HIS:ND1  | 2.37                     | 0.55              |
| 1:Q:114:ASP:OD1 | 1:Q:118:ILE:HD12 | 2.06                     | 0.55              |
| 1:Y:207:LYS:O   | 1:Y:211:THR:HG23 | 2.06                     | 0.55              |
| 2:T:115:LEU:HB3 | 2:T:156:LEU:HD21 | 1.89                     | 0.55              |
| 2:Z:287:LYS:O   | 2:Z:290:ALA:HB3  | 2.06                     | 0.55              |
| 2:P:38:GLY:O    | 1:Q:30:GLU:N     | 2.40                     | 0.55              |
| 2:X:115:LEU:HB3 | 2:X:156:LEU:HD21 | 1.89                     | 0.55              |
| 2:X:229:TYR:HD2 | 1:Y:240:THR:CG2  | 2.20                     | 0.55              |
| 2:N:291:SER:O   | 2:N:292:ASN:CB   | 2.54                     | 0.54              |
| 1:O:207:LYS:O   | 1:O:211:THR:HG23 | 2.06                     | 0.54              |
| 1:U:114:ASP:OD1 | 1:U:118:ILE:HD12 | 2.06                     | 0.54              |
| 2:Z:290:ALA:C   | 2:Z:292:ASN:N    | 2.59                     | 0.54              |
| 2:R:291:SER:O   | 2:R:292:ASN:CB   | 2.54                     | 0.54              |
| 2:V:115:LEU:HB3 | 2:V:156:LEU:HD21 | 1.89                     | 0.54              |
| 1:A:71:ASP:HB3  | 1:A:119:PHE:HZ   | 1.70                     | 0.54              |
| 1:A:30:GLU:N    | 2:Z:38:GLY:O     | 2.40                     | 0.54              |
| 2:D:229:TYR:HD2 | 1:E:240:THR:CG2  | 2.19                     | 0.54              |
| 1:G:40:GLY:O    | 2:H:28:GLU:N     | 2.37                     | 0.54              |
| 1:A:228:LYS:HZ3 | 2:B:234:MET:HE2  | 1.71                     | 0.54              |
| 2:D:118:ASN:O   | 2:D:121:HIS:ND1  | 2.37                     | 0.54              |
| 2:L:229:TYR:HD2 | 1:M:240:THR:CG2  | 2.20                     | 0.54              |
| 2:T:229:TYR:HD2 | 1:U:240:THR:CG2  | 2.19                     | 0.54              |
| 1:C:71:ASP:HB3  | 1:C:119:PHE:HZ   | 1.70                     | 0.54              |
| 1:I:290:ALA:C   | 1:I:292:ALA:N    | 2.66                     | 0.54              |
| 2:P:229:TYR:HD2 | 1:Q:240:THR:CG2  | 2.19                     | 0.54              |
| 1:G:290:ALA:C   | 1:G:292:ALA:N    | 2.66                     | 0.54              |
| 1:M:40:GLY:O    | 2:N:28:GLU:N     | 2.37                     | 0.54              |
| 2:H:229:TYR:HD2 | 1:I:240:THR:CG2  | 2.19                     | 0.54              |
| 1:K:290:ALA:C   | 1:K:292:ALA:N    | 2.66                     | 0.54              |
| 1:M:40:GLY:HA3  | 2:N:27:GLU:HA    | 1.90                     | 0.54              |
| 2:Z:118:ASN:O   | 2:Z:121:HIS:ND1  | 2.37                     | 0.54              |
| 1:G:40:GLY:HA3  | 2:H:27:GLU:HA    | 1.90                     | 0.53              |
| 1:M:290:ALA:C   | 1:M:292:ALA:N    | 2.66                     | 0.53              |
| 1:O:40:GLY:HA3  | 2:P:27:GLU:HA    | 1.91                     | 0.53              |
| 1:I:40:GLY:HA3  | 2:J:27:GLU:HA    | 1.90                     | 0.53              |
| 2:R:118:ASN:O   | 2:R:121:HIS:ND1  | 2.37                     | 0.53              |
| 1:K:40:GLY:HA3  | 2:L:27:GLU:HA    | 1.91                     | 0.53              |
| 1:O:290:ALA:C   | 1:O:292:ALA:N    | 2.66                     | 0.53              |
| 1:Q:40:GLY:HA3  | 2:R:27:GLU:HA    | 1.90                     | 0.53              |
| 1:Q:290:ALA:C   | 1:Q:292:ALA:N    | 2.66                     | 0.53              |
| 2:N:229:TYR:CD2 | 1:O:240:THR:HG21 | 2.43                     | 0.53              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:M:228:LYS:HZ3  | 2:N:234:MET:HE2 | 1.73                     | 0.53              |
| 1:S:40:GLY:HA3   | 2:T:27:GLU:HA   | 1.91                     | 0.53              |
| 1:E:40:GLY:HA3   | 2:F:27:GLU:HA   | 1.90                     | 0.53              |
| 2:H:118:ASN:O    | 2:H:121:HIS:ND1 | 2.37                     | 0.53              |
| 1:I:257:LYS:HG3  | 2:J:263:TYR:HE2 | 1.74                     | 0.53              |
| 1:M:257:LYS:HG3  | 2:N:263:TYR:HE2 | 1.74                     | 0.53              |
| 1:I:40:GLY:O     | 2:J:28:GLU:N    | 2.37                     | 0.53              |
| 1:O:257:LYS:HG3  | 2:P:263:TYR:HE2 | 1.74                     | 0.53              |
| 2:D:78:THR:O     | 2:D:80:GLY:N    | 2.40                     | 0.53              |
| 2:H:38:GLY:O     | 1:I:30:GLU:N    | 2.38                     | 0.53              |
| 1:I:228:LYS:NZ   | 2:J:234:MET:HE2 | 2.24                     | 0.53              |
| 1:U:40:GLY:HA3   | 2:V:27:GLU:HA   | 1.90                     | 0.53              |
| 2:V:118:ASN:O    | 2:V:121:HIS:ND1 | 2.37                     | 0.53              |
| 1:Y:257:LYS:HG3  | 2:Z:263:TYR:HE2 | 1.74                     | 0.53              |
| 1:C:40:GLY:HA3   | 2:D:27:GLU:HA   | 1.91                     | 0.53              |
| 2:N:140:LEU:HD13 | 2:N:143:GLN:OE1 | 2.09                     | 0.53              |
| 1:S:257:LYS:HG3  | 2:T:263:TYR:HE2 | 1.74                     | 0.53              |
| 2:T:140:LEU:HD13 | 2:T:143:GLN:OE1 | 2.09                     | 0.53              |
| 1:C:257:LYS:HG3  | 2:D:263:TYR:HE2 | 1.74                     | 0.52              |
| 1:G:257:LYS:HG3  | 2:H:263:TYR:HE2 | 1.74                     | 0.52              |
| 2:H:78:THR:O     | 2:H:80:GLY:N    | 2.40                     | 0.52              |
| 1:K:228:LYS:NZ   | 2:L:234:MET:HE2 | 2.24                     | 0.52              |
| 1:W:40:GLY:HA3   | 2:X:27:GLU:HA   | 1.90                     | 0.52              |
| 1:K:40:GLY:O     | 2:L:28:GLU:N    | 2.38                     | 0.52              |
| 1:Y:40:GLY:HA3   | 2:Z:27:GLU:HA   | 1.90                     | 0.52              |
| 2:Z:140:LEU:HD13 | 2:Z:143:GLN:OE1 | 2.09                     | 0.52              |
| 1:A:40:GLY:HA3   | 2:B:27:GLU:HA   | 1.90                     | 0.52              |
| 1:Y:228:LYS:NZ   | 2:Z:234:MET:HE2 | 2.24                     | 0.52              |
| 1:G:228:LYS:NZ   | 2:H:234:MET:HE2 | 2.25                     | 0.52              |
| 1:M:278:LEU:HD23 | 2:N:279:GLU:HB2 | 1.92                     | 0.52              |
| 2:X:140:LEU:HD13 | 2:X:143:GLN:OE1 | 2.09                     | 0.52              |
| 1:Q:228:LYS:NZ   | 2:R:234:MET:HE2 | 2.24                     | 0.52              |
| 2:R:140:LEU:HD13 | 2:R:143:GLN:OE1 | 2.10                     | 0.52              |
| 1:U:257:LYS:HG3  | 2:V:263:TYR:HE2 | 1.74                     | 0.52              |
| 1:K:278:LEU:HD23 | 2:L:279:GLU:HB2 | 1.92                     | 0.52              |
| 2:P:140:LEU:HD13 | 2:P:143:GLN:OE1 | 2.09                     | 0.52              |
| 1:A:257:LYS:HG3  | 2:B:263:TYR:HE2 | 1.74                     | 0.52              |
| 2:L:140:LEU:HD13 | 2:L:143:GLN:OE1 | 2.09                     | 0.52              |
| 2:J:140:LEU:HD13 | 2:J:143:GLN:OE1 | 2.09                     | 0.52              |
| 1:M:228:LYS:NZ   | 2:N:234:MET:HE2 | 2.24                     | 0.52              |
| 1:S:228:LYS:NZ   | 2:T:234:MET:HE2 | 2.24                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:278:LEU:HD23 | 2:T:279:GLU:HB2  | 1.91                     | 0.52              |
| 1:S:290:ALA:O    | 2:T:290:ALA:HB1  | 2.10                     | 0.52              |
| 1:U:290:ALA:O    | 2:V:290:ALA:HB1  | 2.10                     | 0.52              |
| 2:V:38:GLY:O     | 1:W:30:GLU:N     | 2.43                     | 0.52              |
| 1:W:228:LYS:NZ   | 2:X:234:MET:HE2  | 2.25                     | 0.52              |
| 2:F:78:THR:O     | 2:F:80:GLY:N     | 2.39                     | 0.52              |
| 1:G:228:LYS:HZ3  | 2:H:234:MET:HE2  | 1.74                     | 0.52              |
| 2:V:140:LEU:HD13 | 2:V:143:GLN:OE1  | 2.09                     | 0.52              |
| 2:D:140:LEU:HD13 | 2:D:143:GLN:OE1  | 2.09                     | 0.52              |
| 2:X:39:ALA:HA    | 1:Y:30:GLU:HG2   | 1.92                     | 0.52              |
| 1:A:228:LYS:NZ   | 2:B:234:MET:HE2  | 2.25                     | 0.51              |
| 1:A:278:LEU:HD23 | 2:B:279:GLU:HB2  | 1.92                     | 0.51              |
| 1:C:228:LYS:NZ   | 2:D:234:MET:HE2  | 2.24                     | 0.51              |
| 1:E:228:LYS:NZ   | 2:F:234:MET:HE2  | 2.24                     | 0.51              |
| 1:O:228:LYS:NZ   | 2:P:234:MET:HE2  | 2.25                     | 0.51              |
| 2:J:229:TYR:CD2  | 1:K:240:THR:HG21 | 2.43                     | 0.51              |
| 2:L:118:ASN:O    | 2:L:121:HIS:ND1  | 2.37                     | 0.51              |
| 1:O:231:PHE:CZ   | 2:P:235:GLU:HG2  | 2.46                     | 0.51              |
| 1:O:278:LEU:HD23 | 2:P:279:GLU:HB2  | 1.91                     | 0.51              |
| 1:G:221:GLU:HA   | 1:G:221:GLU:OE1  | 2.11                     | 0.51              |
| 2:H:140:LEU:HD13 | 2:H:143:GLN:OE1  | 2.10                     | 0.51              |
| 1:I:221:GLU:HA   | 1:I:221:GLU:OE1  | 2.11                     | 0.51              |
| 1:K:221:GLU:OE1  | 1:K:221:GLU:HA   | 2.11                     | 0.51              |
| 1:K:257:LYS:HG3  | 2:L:263:TYR:HE2  | 1.74                     | 0.51              |
| 1:K:290:ALA:O    | 2:L:290:ALA:HB1  | 2.10                     | 0.51              |
| 1:M:231:PHE:CZ   | 2:N:235:GLU:HG2  | 2.46                     | 0.51              |
| 1:Q:231:PHE:CZ   | 2:R:235:GLU:HG2  | 2.46                     | 0.51              |
| 2:R:38:GLY:O     | 1:S:30:GLU:N     | 2.43                     | 0.51              |
| 1:W:231:PHE:CZ   | 2:X:235:GLU:HG2  | 2.46                     | 0.51              |
| 1:Y:231:PHE:CZ   | 2:Z:235:GLU:HG2  | 2.46                     | 0.51              |
| 2:Z:78:THR:O     | 2:Z:80:GLY:N     | 2.40                     | 0.51              |
| 2:D:276:LEU:HD22 | 1:E:281:GLU:HB3  | 1.92                     | 0.51              |
| 1:E:231:PHE:CZ   | 2:F:235:GLU:HG2  | 2.46                     | 0.51              |
| 1:Q:278:LEU:HD23 | 2:R:279:GLU:HB2  | 1.91                     | 0.51              |
| 1:S:231:PHE:CZ   | 2:T:235:GLU:HG2  | 2.46                     | 0.51              |
| 2:T:276:LEU:HD22 | 1:U:281:GLU:HB3  | 1.93                     | 0.51              |
| 2:B:140:LEU:HD13 | 2:B:143:GLN:OE1  | 2.09                     | 0.51              |
| 1:C:278:LEU:HD23 | 2:D:279:GLU:HB2  | 1.92                     | 0.51              |
| 1:E:221:GLU:HA   | 1:E:221:GLU:OE1  | 2.11                     | 0.51              |
| 2:F:140:LEU:HD13 | 2:F:143:GLN:OE1  | 2.10                     | 0.51              |
| 1:G:231:PHE:CZ   | 2:H:235:GLU:HG2  | 2.46                     | 0.51              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:G:290:ALA:O    | 2:H:290:ALA:HB1 | 2.10                     | 0.51              |
| 1:U:231:PHE:CZ   | 2:V:235:GLU:HG2 | 2.45                     | 0.51              |
| 1:Y:108:ASN:HD22 | 3:Y:401:NAG:H83 | 1.76                     | 0.51              |
| 1:A:296:LYS:HA   | 2:Z:293:SER:HB3 | 1.92                     | 0.51              |
| 1:C:290:ALA:O    | 2:D:290:ALA:HB1 | 2.10                     | 0.51              |
| 1:E:257:LYS:HG3  | 2:F:263:TYR:HE2 | 1.74                     | 0.51              |
| 1:Q:290:ALA:O    | 2:R:290:ALA:HB1 | 2.10                     | 0.51              |
| 1:U:228:LYS:NZ   | 2:V:234:MET:HE2 | 2.24                     | 0.51              |
| 1:U:278:LEU:HD23 | 2:V:279:GLU:HB2 | 1.91                     | 0.51              |
| 1:Y:278:LEU:HD23 | 2:Z:279:GLU:HB2 | 1.92                     | 0.51              |
| 1:A:108:ASN:HD22 | 3:A:401:NAG:H83 | 1.76                     | 0.51              |
| 1:A:231:PHE:CZ   | 2:B:235:GLU:HG2 | 2.46                     | 0.51              |
| 1:A:292:ALA:C    | 1:A:294:ASN:N   | 2.68                     | 0.51              |
| 1:E:278:LEU:HD23 | 2:F:279:GLU:HB2 | 1.91                     | 0.51              |
| 2:F:38:GLY:O     | 1:G:30:GLU:N    | 2.43                     | 0.51              |
| 1:M:221:GLU:OE1  | 1:M:221:GLU:HA  | 2.11                     | 0.51              |
| 1:O:108:ASN:HD22 | 3:O:401:NAG:H83 | 1.76                     | 0.51              |
| 1:W:290:ALA:O    | 2:X:290:ALA:HB1 | 2.10                     | 0.51              |
| 1:C:221:GLU:OE1  | 1:C:221:GLU:HA  | 2.11                     | 0.51              |
| 2:L:78:THR:O     | 2:L:80:GLY:N    | 2.39                     | 0.51              |
| 1:W:278:LEU:HD23 | 2:X:279:GLU:HB2 | 1.91                     | 0.51              |
| 1:C:231:PHE:CZ   | 2:D:235:GLU:HG2 | 2.46                     | 0.51              |
| 1:G:278:LEU:HD23 | 2:H:279:GLU:HB2 | 1.92                     | 0.51              |
| 1:I:278:LEU:HD23 | 2:J:279:GLU:HB2 | 1.91                     | 0.51              |
| 2:P:276:LEU:HD22 | 1:Q:281:GLU:HB3 | 1.93                     | 0.51              |
| 1:Q:257:LYS:HG3  | 2:R:263:TYR:HE2 | 1.74                     | 0.51              |
| 1:S:108:ASN:HD22 | 3:S:401:NAG:H83 | 1.76                     | 0.51              |
| 2:B:78:THR:O     | 2:B:80:GLY:N    | 2.40                     | 0.51              |
| 1:E:290:ALA:O    | 2:F:290:ALA:HB1 | 2.10                     | 0.51              |
| 1:G:108:ASN:HD22 | 3:G:401:NAG:H83 | 1.76                     | 0.51              |
| 1:I:231:PHE:CZ   | 2:J:235:GLU:HG2 | 2.46                     | 0.51              |
| 1:K:97:LEU:HD11  | 1:K:101:ALA:O   | 2.12                     | 0.51              |
| 1:K:228:LYS:HZ3  | 2:L:234:MET:HE2 | 1.75                     | 0.51              |
| 1:K:231:PHE:CZ   | 2:L:235:GLU:HG2 | 2.46                     | 0.51              |
| 1:W:97:LEU:HD11  | 1:W:101:ALA:O   | 2.11                     | 0.51              |
| 1:A:290:ALA:C    | 1:A:292:ALA:N   | 2.66                     | 0.50              |
| 2:J:78:THR:O     | 2:J:80:GLY:N    | 2.40                     | 0.50              |
| 1:K:108:ASN:HD22 | 3:K:401:NAG:H83 | 1.76                     | 0.50              |
| 1:U:40:GLY:O     | 2:V:28:GLU:N    | 2.37                     | 0.50              |
| 1:I:108:ASN:HD22 | 3:I:401:NAG:H83 | 1.76                     | 0.50              |
| 1:I:290:ALA:O    | 2:J:290:ALA:HB1 | 2.10                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:290:ALA:O    | 2:N:290:ALA:HB1  | 2.10                     | 0.50              |
| 1:O:290:ALA:O    | 2:P:290:ALA:HB1  | 2.10                     | 0.50              |
| 1:Q:97:LEU:HD11  | 1:Q:101:ALA:O    | 2.12                     | 0.50              |
| 2:V:272:ASN:O    | 2:V:276:LEU:HG   | 2.12                     | 0.50              |
| 2:Z:272:ASN:O    | 2:Z:276:LEU:HG   | 2.12                     | 0.50              |
| 1:M:108:ASN:HD22 | 3:M:401:NAG:H83  | 1.76                     | 0.50              |
| 2:N:38:GLY:O     | 1:O:30:GLU:N     | 2.43                     | 0.50              |
| 2:N:39:ALA:HA    | 1:O:30:GLU:HG2   | 1.92                     | 0.50              |
| 2:T:272:ASN:O    | 2:T:276:LEU:HG   | 2.12                     | 0.50              |
| 2:V:39:ALA:HA    | 1:W:30:GLU:HG2   | 1.93                     | 0.50              |
| 2:X:272:ASN:O    | 2:X:276:LEU:HG   | 2.11                     | 0.50              |
| 1:Y:290:ALA:C    | 1:Y:292:ALA:N    | 2.66                     | 0.50              |
| 2:B:293:SER:OG   | 2:B:294:LYS:N    | 2.40                     | 0.50              |
| 2:H:272:ASN:O    | 2:H:276:LEU:HG   | 2.11                     | 0.50              |
| 1:I:228:LYS:HZ3  | 2:J:234:MET:HE2  | 1.76                     | 0.50              |
| 1:O:221:GLU:OE1  | 1:O:221:GLU:HA   | 2.11                     | 0.50              |
| 1:A:221:GLU:OE1  | 1:A:221:GLU:HA   | 2.11                     | 0.50              |
| 1:C:290:ALA:C    | 1:C:292:ALA:N    | 2.66                     | 0.50              |
| 2:D:272:ASN:O    | 2:D:276:LEU:HG   | 2.12                     | 0.50              |
| 1:E:108:ASN:HD22 | 3:E:401:NAG:H83  | 1.76                     | 0.50              |
| 2:F:39:ALA:HA    | 1:G:30:GLU:HG2   | 1.92                     | 0.50              |
| 1:G:97:LEU:HD11  | 1:G:101:ALA:O    | 2.11                     | 0.50              |
| 1:U:97:LEU:HD11  | 1:U:101:ALA:O    | 2.11                     | 0.50              |
| 2:B:290:ALA:C    | 2:B:292:ASN:H    | 2.20                     | 0.50              |
| 1:I:97:LEU:HD11  | 1:I:101:ALA:O    | 2.11                     | 0.50              |
| 1:M:97:LEU:HD11  | 1:M:101:ALA:O    | 2.11                     | 0.50              |
| 1:M:99:PRO:O     | 1:M:102:VAL:HG23 | 2.12                     | 0.50              |
| 1:A:97:LEU:HD11  | 1:A:101:ALA:O    | 2.12                     | 0.50              |
| 2:F:272:ASN:O    | 2:F:276:LEU:HG   | 2.12                     | 0.50              |
| 2:R:272:ASN:O    | 2:R:276:LEU:HG   | 2.12                     | 0.50              |
| 1:W:99:PRO:O     | 1:W:102:VAL:HG23 | 2.12                     | 0.50              |
| 1:W:108:ASN:HD22 | 3:W:401:NAG:H83  | 1.76                     | 0.50              |
| 1:A:281:GLU:HB3  | 2:Z:276:LEU:HD22 | 1.94                     | 0.50              |
| 1:E:97:LEU:HD11  | 1:E:101:ALA:O    | 2.11                     | 0.50              |
| 1:E:228:LYS:HZ3  | 2:F:234:MET:HE2  | 1.75                     | 0.50              |
| 2:J:272:ASN:O    | 2:J:276:LEU:HG   | 2.12                     | 0.50              |
| 2:R:39:ALA:HA    | 1:S:30:GLU:HG2   | 1.93                     | 0.50              |
| 1:S:97:LEU:HD11  | 1:S:101:ALA:O    | 2.12                     | 0.50              |
| 1:U:108:ASN:HD22 | 3:U:401:NAG:H83  | 1.76                     | 0.50              |
| 1:C:97:LEU:HD11  | 1:C:101:ALA:O    | 2.11                     | 0.50              |
| 1:C:108:ASN:HD22 | 3:C:401:NAG:H83  | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:39:ALA:HA    | 1:K:30:GLU:HG2   | 1.93                     | 0.50              |
| 1:M:72:GLU:OE1   | 1:M:74:LYS:HE3   | 2.12                     | 0.50              |
| 1:Y:221:GLU:OE1  | 1:Y:221:GLU:HA   | 2.11                     | 0.50              |
| 2:D:39:ALA:HA    | 1:E:30:GLU:HG2   | 1.94                     | 0.49              |
| 1:O:97:LEU:HD11  | 1:O:101:ALA:O    | 2.11                     | 0.49              |
| 2:P:118:ASN:O    | 2:P:121:HIS:ND1  | 2.37                     | 0.49              |
| 1:W:221:GLU:OE1  | 1:W:221:GLU:HA   | 2.11                     | 0.49              |
| 2:F:118:ASN:O    | 2:F:121:HIS:ND1  | 2.37                     | 0.49              |
| 1:A:72:GLU:OE1   | 1:A:74:LYS:HE3   | 2.13                     | 0.49              |
| 1:E:137:GLU:HB3  | 1:E:142:LEU:HD12 | 1.95                     | 0.49              |
| 1:G:72:GLU:OE1   | 1:G:74:LYS:HE3   | 2.13                     | 0.49              |
| 1:K:72:GLU:OE1   | 1:K:74:LYS:HE3   | 2.12                     | 0.49              |
| 2:L:272:ASN:O    | 2:L:276:LEU:HG   | 2.12                     | 0.49              |
| 1:S:221:GLU:HA   | 1:S:221:GLU:OE1  | 2.11                     | 0.49              |
| 2:X:91:VAL:HG21  | 2:X:120:ILE:HD11 | 1.95                     | 0.49              |
| 2:X:276:LEU:HD22 | 1:Y:281:GLU:HB3  | 1.94                     | 0.49              |
| 2:L:276:LEU:HD22 | 1:M:281:GLU:HB3  | 1.92                     | 0.49              |
| 1:Q:108:ASN:HD22 | 3:Q:401:NAG:H83  | 1.76                     | 0.49              |
| 1:U:221:GLU:HA   | 1:U:221:GLU:OE1  | 2.11                     | 0.49              |
| 1:Q:221:GLU:HA   | 1:Q:221:GLU:OE1  | 2.11                     | 0.49              |
| 1:W:290:ALA:C    | 1:W:292:ALA:N    | 2.66                     | 0.49              |
| 1:G:137:GLU:HB3  | 1:G:142:LEU:HD12 | 1.95                     | 0.49              |
| 2:H:276:LEU:HD22 | 1:I:281:GLU:HB3  | 1.94                     | 0.49              |
| 2:T:91:VAL:HG21  | 2:T:120:ILE:HD11 | 1.95                     | 0.49              |
| 1:Y:97:LEU:HD11  | 1:Y:101:ALA:O    | 2.12                     | 0.49              |
| 2:B:229:TYR:CD2  | 1:C:240:THR:HG21 | 2.43                     | 0.49              |
| 2:B:272:ASN:O    | 2:B:276:LEU:HG   | 2.12                     | 0.49              |
| 1:O:40:GLY:O     | 2:P:28:GLU:N     | 2.38                     | 0.49              |
| 2:P:272:ASN:O    | 2:P:276:LEU:HG   | 2.11                     | 0.49              |
| 1:Q:72:GLU:OE1   | 1:Q:74:LYS:HE3   | 2.13                     | 0.49              |
| 1:S:72:GLU:OE1   | 1:S:74:LYS:HE3   | 2.12                     | 0.49              |
| 1:U:99:PRO:O     | 1:U:102:VAL:HG23 | 2.13                     | 0.49              |
| 2:V:91:VAL:HG21  | 2:V:120:ILE:HD11 | 1.95                     | 0.49              |
| 1:C:72:GLU:OE1   | 1:C:74:LYS:HE3   | 2.13                     | 0.49              |
| 1:C:137:GLU:HB3  | 1:C:142:LEU:HD12 | 1.95                     | 0.49              |
| 1:E:72:GLU:OE1   | 1:E:74:LYS:HE3   | 2.12                     | 0.49              |
| 2:J:38:GLY:O     | 1:K:30:GLU:N     | 2.43                     | 0.49              |
| 2:J:118:ASN:O    | 2:J:121:HIS:ND1  | 2.37                     | 0.49              |
| 2:L:39:ALA:HA    | 1:M:30:GLU:HG2   | 1.94                     | 0.49              |
| 2:N:272:ASN:O    | 2:N:276:LEU:HG   | 2.12                     | 0.49              |
| 2:P:78:THR:O     | 2:P:80:GLY:N     | 2.40                     | 0.49              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:W:115:LYS:O   | 1:W:119:PHE:HB2  | 2.13                     | 0.49              |
| 2:X:78:THR:O    | 2:X:80:GLY:N     | 2.40                     | 0.49              |
| 2:D:91:VAL:HG21 | 2:D:120:ILE:HD11 | 1.95                     | 0.49              |
| 2:F:91:VAL:HG21 | 2:F:120:ILE:HD11 | 1.95                     | 0.49              |
| 1:G:115:LYS:O   | 1:G:119:PHE:HB2  | 2.13                     | 0.49              |
| 1:K:115:LYS:O   | 1:K:119:PHE:HB2  | 2.13                     | 0.49              |
| 1:Q:228:LYS:HZ3 | 2:R:234:MET:HE2  | 1.78                     | 0.49              |
| 1:W:257:LYS:HG3 | 2:X:263:TYR:HE2  | 1.74                     | 0.49              |
| 1:Y:72:GLU:OE1  | 1:Y:74:LYS:HE3   | 2.13                     | 0.49              |
| 2:Z:91:VAL:HG21 | 2:Z:120:ILE:HD11 | 1.95                     | 0.49              |
| 1:C:115:LYS:O   | 1:C:119:PHE:HB2  | 2.13                     | 0.49              |
| 1:U:72:GLU:OE1  | 1:U:74:LYS:HE3   | 2.12                     | 0.49              |
| 2:V:78:THR:O    | 2:V:80:GLY:N     | 2.39                     | 0.49              |
| 1:A:30:GLU:HG2  | 2:Z:39:ALA:HA    | 1.95                     | 0.48              |
| 1:A:40:GLY:O    | 2:B:28:GLU:N     | 2.37                     | 0.48              |
| 1:O:72:GLU:OE1  | 1:O:74:LYS:HE3   | 2.13                     | 0.48              |
| 2:R:91:VAL:HG21 | 2:R:120:ILE:HD11 | 1.95                     | 0.48              |
| 1:I:72:GLU:OE1  | 1:I:74:LYS:HE3   | 2.12                     | 0.48              |
| 1:M:115:LYS:O   | 1:M:119:PHE:HB2  | 2.13                     | 0.48              |
| 2:V:229:TYR:CD2 | 1:W:240:THR:HG21 | 2.43                     | 0.48              |
| 1:Y:115:LYS:O   | 1:Y:119:PHE:HB2  | 2.13                     | 0.48              |
| 1:A:269:LYS:O   | 1:A:272:THR:HG22 | 2.13                     | 0.48              |
| 1:I:99:PRO:O    | 1:I:102:VAL:HG23 | 2.13                     | 0.48              |
| 1:I:137:GLU:HB3 | 1:I:142:LEU:HD12 | 1.95                     | 0.48              |
| 1:Q:40:GLY:O    | 2:R:28:GLU:N     | 2.37                     | 0.48              |
| 1:Q:115:LYS:O   | 1:Q:119:PHE:HB2  | 2.13                     | 0.48              |
| 2:T:39:ALA:HA   | 1:U:30:GLU:HG2   | 1.94                     | 0.48              |
| 1:A:115:LYS:O   | 1:A:119:PHE:HB2  | 2.13                     | 0.48              |
| 1:C:294:ASN:ND2 | 2:D:290:ALA:O    | 2.47                     | 0.48              |
| 2:D:40:LEU:HD13 | 1:E:30:GLU:HG3   | 1.95                     | 0.48              |
| 1:G:200:GLN:HA  | 1:G:200:GLN:OE1  | 2.14                     | 0.48              |
| 2:H:39:ALA:HA   | 1:I:30:GLU:HG2   | 1.94                     | 0.48              |
| 2:P:91:VAL:HG21 | 2:P:120:ILE:HD11 | 1.95                     | 0.48              |
| 1:S:116:THR:O   | 1:S:120:ASN:HB2  | 2.14                     | 0.48              |
| 2:X:118:ASN:O   | 2:X:121:HIS:ND1  | 2.37                     | 0.48              |
| 2:B:76:CYS:SG   | 2:B:124:LEU:HG   | 2.54                     | 0.48              |
| 2:H:90:GLU:OE1  | 2:H:169:ARG:HD2  | 2.14                     | 0.48              |
| 1:K:200:GLN:OE1 | 1:K:200:GLN:HA   | 2.14                     | 0.48              |
| 1:O:116:THR:O   | 1:O:120:ASN:HB2  | 2.14                     | 0.48              |
| 2:P:39:ALA:HA   | 1:Q:30:GLU:HG2   | 1.95                     | 0.48              |
| 2:P:76:CYS:SG   | 2:P:124:LEU:HG   | 2.54                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:229:TYR:CD2  | 1:S:240:THR:HG21 | 2.43                     | 0.48              |
| 2:T:118:ASN:O    | 2:T:121:HIS:ND1  | 2.37                     | 0.48              |
| 2:Z:90:GLU:OE1   | 2:Z:169:ARG:HD2  | 2.14                     | 0.48              |
| 1:A:137:GLU:HB3  | 1:A:142:LEU:HD12 | 1.95                     | 0.48              |
| 1:A:296:LYS:H    | 2:Z:293:SER:HB3  | 1.78                     | 0.48              |
| 1:E:290:ALA:C    | 1:E:292:ALA:N    | 2.66                     | 0.48              |
| 2:H:91:VAL:HG21  | 2:H:120:ILE:HD11 | 1.95                     | 0.48              |
| 1:Q:116:THR:O    | 1:Q:120:ASN:HB2  | 2.14                     | 0.48              |
| 1:S:40:GLY:O     | 2:T:28:GLU:N     | 2.38                     | 0.48              |
| 1:S:115:LYS:O    | 1:S:119:PHE:HB2  | 2.13                     | 0.48              |
| 2:T:78:THR:O     | 2:T:80:GLY:N     | 2.40                     | 0.48              |
| 1:U:116:THR:O    | 1:U:120:ASN:HB2  | 2.14                     | 0.48              |
| 2:V:76:CYS:SG    | 2:V:124:LEU:HG   | 2.54                     | 0.48              |
| 1:W:72:GLU:OE1   | 1:W:74:LYS:HE3   | 2.13                     | 0.48              |
| 2:X:203:VAL:CG1  | 1:Y:215:LYS:HE2  | 2.44                     | 0.48              |
| 2:J:91:VAL:HG21  | 2:J:120:ILE:HD11 | 1.95                     | 0.48              |
| 1:M:213:ARG:HG2  | 1:M:213:ARG:HH11 | 1.79                     | 0.48              |
| 2:N:91:VAL:HG21  | 2:N:120:ILE:HD11 | 1.95                     | 0.48              |
| 1:O:213:ARG:HH11 | 1:O:213:ARG:HG2  | 1.79                     | 0.48              |
| 1:Q:200:GLN:HA   | 1:Q:200:GLN:OE1  | 2.14                     | 0.48              |
| 2:T:90:GLU:OE1   | 2:T:169:ARG:HD2  | 2.14                     | 0.48              |
| 2:V:90:GLU:OE1   | 2:V:169:ARG:HD2  | 2.14                     | 0.48              |
| 2:Z:286:TYR:O    | 2:Z:290:ALA:HB2  | 2.13                     | 0.48              |
| 2:B:290:ALA:C    | 2:B:292:ASN:N    | 2.71                     | 0.48              |
| 1:G:77:PRO:HB2   | 1:G:85:MET:HE3   | 1.96                     | 0.48              |
| 2:L:91:VAL:HG21  | 2:L:120:ILE:HD11 | 1.95                     | 0.48              |
| 2:T:203:VAL:CG1  | 1:U:215:LYS:HE2  | 2.44                     | 0.48              |
| 1:U:137:GLU:HB3  | 1:U:142:LEU:HD12 | 1.95                     | 0.48              |
| 1:Y:40:GLY:O     | 2:Z:28:GLU:N     | 2.37                     | 0.48              |
| 1:A:77:PRO:HB2   | 1:A:85:MET:HE3   | 1.96                     | 0.48              |
| 1:C:200:GLN:HA   | 1:C:200:GLN:OE1  | 2.14                     | 0.48              |
| 1:E:115:LYS:O    | 1:E:119:PHE:HB2  | 2.13                     | 0.48              |
| 2:L:76:CYS:SG    | 2:L:124:LEU:HG   | 2.54                     | 0.48              |
| 2:N:76:CYS:SG    | 2:N:124:LEU:HG   | 2.54                     | 0.48              |
| 1:O:137:GLU:HB3  | 1:O:142:LEU:HD12 | 1.95                     | 0.48              |
| 1:O:200:GLN:HA   | 1:O:200:GLN:OE1  | 2.14                     | 0.48              |
| 2:P:90:GLU:OE1   | 2:P:169:ARG:HD2  | 2.14                     | 0.48              |
| 1:S:99:PRO:O     | 1:S:102:VAL:HG23 | 2.14                     | 0.48              |
| 1:S:137:GLU:HB3  | 1:S:142:LEU:HD12 | 1.95                     | 0.48              |
| 1:W:40:GLY:O     | 2:X:28:GLU:N     | 2.37                     | 0.48              |
| 1:Y:116:THR:O    | 1:Y:120:ASN:HB2  | 2.14                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:Z:76:CYS:SG   | 2:Z:124:LEU:HG   | 2.54                     | 0.48              |
| 2:D:76:CYS:SG   | 2:D:124:LEU:HG   | 2.54                     | 0.48              |
| 1:I:77:PRO:HB2  | 1:I:85:MET:HE3   | 1.96                     | 0.48              |
| 1:I:115:LYS:O   | 1:I:119:PHE:HB2  | 2.13                     | 0.48              |
| 1:K:213:ARG:HG2 | 1:K:213:ARG:HH11 | 1.79                     | 0.48              |
| 1:M:116:THR:O   | 1:M:120:ASN:HB2  | 2.14                     | 0.48              |
| 1:M:137:GLU:HB3 | 1:M:142:LEU:HD12 | 1.95                     | 0.48              |
| 1:M:200:GLN:OE1 | 1:M:200:GLN:HA   | 2.14                     | 0.48              |
| 2:N:90:GLU:OE1  | 2:N:169:ARG:HD2  | 2.14                     | 0.48              |
| 1:Q:137:GLU:HB3 | 1:Q:142:LEU:HD12 | 1.95                     | 0.48              |
| 2:T:76:CYS:SG   | 2:T:124:LEU:HG   | 2.54                     | 0.48              |
| 1:U:161:MET:HE2 | 1:U:161:MET:HB3  | 1.80                     | 0.48              |
| 1:W:116:THR:O   | 1:W:120:ASN:HB2  | 2.14                     | 0.48              |
| 1:W:213:ARG:HG2 | 1:W:213:ARG:HH11 | 1.79                     | 0.48              |
| 1:Y:200:GLN:OE1 | 1:Y:200:GLN:HA   | 2.14                     | 0.48              |
| 1:A:200:GLN:OE1 | 1:A:200:GLN:HA   | 2.14                     | 0.47              |
| 1:K:161:MET:HE2 | 1:K:161:MET:HB3  | 1.80                     | 0.47              |
| 2:L:40:LEU:HD13 | 1:M:30:GLU:HG3   | 1.95                     | 0.47              |
| 2:R:76:CYS:SG   | 2:R:124:LEU:HG   | 2.54                     | 0.47              |
| 1:U:290:ALA:C   | 1:U:292:ALA:N    | 2.66                     | 0.47              |
| 2:F:90:GLU:OE1  | 2:F:169:ARG:HD2  | 2.14                     | 0.47              |
| 1:G:116:THR:O   | 1:G:120:ASN:HB2  | 2.14                     | 0.47              |
| 2:J:90:GLU:OE1  | 2:J:169:ARG:HD2  | 2.14                     | 0.47              |
| 1:K:137:GLU:HB3 | 1:K:142:LEU:HD12 | 1.95                     | 0.47              |
| 2:N:78:THR:O    | 2:N:80:GLY:N     | 2.39                     | 0.47              |
| 2:P:203:VAL:CG1 | 1:Q:215:LYS:HE2  | 2.44                     | 0.47              |
| 1:W:77:PRO:HB2  | 1:W:85:MET:HE3   | 1.96                     | 0.47              |
| 1:C:40:GLY:O    | 2:D:28:GLU:N     | 2.37                     | 0.47              |
| 1:C:77:PRO:HB2  | 1:C:85:MET:HE3   | 1.96                     | 0.47              |
| 1:I:200:GLN:OE1 | 1:I:200:GLN:HA   | 2.14                     | 0.47              |
| 1:K:116:THR:O   | 1:K:120:ASN:HB2  | 2.14                     | 0.47              |
| 1:U:115:LYS:O   | 1:U:119:PHE:HB2  | 2.13                     | 0.47              |
| 2:X:40:LEU:HD13 | 1:Y:30:GLU:HG3   | 1.95                     | 0.47              |
| 2:X:76:CYS:SG   | 2:X:124:LEU:HG   | 2.54                     | 0.47              |
| 1:Y:228:LYS:HZ3 | 2:Z:234:MET:HE2  | 1.79                     | 0.47              |
| 1:C:213:ARG:HG2 | 1:C:213:ARG:HH11 | 1.79                     | 0.47              |
| 1:E:116:THR:O   | 1:E:120:ASN:HB2  | 2.14                     | 0.47              |
| 2:F:76:CYS:SG   | 2:F:124:LEU:HG   | 2.54                     | 0.47              |
| 1:I:116:THR:O   | 1:I:120:ASN:HB2  | 2.14                     | 0.47              |
| 1:I:213:ARG:HG2 | 1:I:213:ARG:HH11 | 1.79                     | 0.47              |
| 2:L:203:VAL:CG1 | 1:M:215:LYS:HE2  | 2.44                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:115:LYS:O    | 1:O:119:PHE:HB2  | 2.13                     | 0.47              |
| 1:S:213:ARG:HG2  | 1:S:213:ARG:HH11 | 1.79                     | 0.47              |
| 1:W:200:GLN:OE1  | 1:W:200:GLN:HA   | 2.14                     | 0.47              |
| 2:D:203:VAL:CG1  | 1:E:215:LYS:HE2  | 2.44                     | 0.47              |
| 2:J:76:CYS:SG    | 2:J:124:LEU:HG   | 2.54                     | 0.47              |
| 2:L:90:GLU:OE1   | 2:L:169:ARG:HD2  | 2.14                     | 0.47              |
| 1:Q:213:ARG:HH11 | 1:Q:213:ARG:HG2  | 1.79                     | 0.47              |
| 1:U:200:GLN:OE1  | 1:U:200:GLN:HA   | 2.14                     | 0.47              |
| 2:X:90:GLU:OE1   | 2:X:169:ARG:HD2  | 2.14                     | 0.47              |
| 1:Y:213:ARG:HG2  | 1:Y:213:ARG:HH11 | 1.79                     | 0.47              |
| 1:C:116:THR:O    | 1:C:120:ASN:HB2  | 2.14                     | 0.47              |
| 1:W:137:GLU:HB3  | 1:W:142:LEU:HD12 | 1.95                     | 0.47              |
| 1:C:99:PRO:O     | 1:C:102:VAL:HG23 | 2.15                     | 0.47              |
| 2:D:90:GLU:OE1   | 2:D:169:ARG:HD2  | 2.14                     | 0.47              |
| 1:E:200:GLN:HA   | 1:E:200:GLN:OE1  | 2.14                     | 0.47              |
| 1:K:99:PRO:O     | 1:K:102:VAL:HG23 | 2.15                     | 0.47              |
| 2:P:229:TYR:CD2  | 1:Q:240:THR:HG21 | 2.46                     | 0.47              |
| 1:Q:77:PRO:HB2   | 1:Q:85:MET:HE3   | 1.97                     | 0.47              |
| 2:T:40:LEU:HD13  | 1:U:30:GLU:HG3   | 1.95                     | 0.47              |
| 1:A:116:THR:O    | 1:A:120:ASN:HB2  | 2.14                     | 0.47              |
| 2:F:229:TYR:CD2  | 1:G:240:THR:HG21 | 2.43                     | 0.47              |
| 1:G:213:ARG:HG2  | 1:G:213:ARG:HH11 | 1.79                     | 0.47              |
| 2:H:203:VAL:CG1  | 1:I:215:LYS:HE2  | 2.44                     | 0.47              |
| 1:Y:99:PRO:O     | 1:Y:102:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:90:ARG:NH2   | 1:A:92:GLU:OE1   | 2.48                     | 0.47              |
| 1:A:215:LYS:HE2  | 2:Z:203:VAL:CG1  | 2.45                     | 0.47              |
| 2:D:229:TYR:CD2  | 1:E:240:THR:HG21 | 2.46                     | 0.47              |
| 1:E:77:PRO:HB2   | 1:E:85:MET:HE3   | 1.96                     | 0.47              |
| 1:E:99:PRO:O     | 1:E:102:VAL:HG23 | 2.15                     | 0.47              |
| 2:P:276:LEU:HD23 | 2:P:276:LEU:HA   | 1.60                     | 0.47              |
| 1:Q:99:PRO:O     | 1:Q:102:VAL:HG23 | 2.15                     | 0.47              |
| 1:Y:137:GLU:HB3  | 1:Y:142:LEU:HD12 | 1.95                     | 0.47              |
| 1:A:240:THR:HG21 | 2:Z:229:TYR:CD2  | 2.45                     | 0.47              |
| 2:F:276:LEU:HD23 | 2:F:276:LEU:HA   | 1.60                     | 0.47              |
| 1:G:99:PRO:O     | 1:G:102:VAL:HG23 | 2.14                     | 0.47              |
| 1:K:90:ARG:NH2   | 1:K:92:GLU:OE1   | 2.48                     | 0.47              |
| 1:M:77:PRO:HB2   | 1:M:85:MET:HE3   | 1.96                     | 0.47              |
| 1:O:77:PRO:HB2   | 1:O:85:MET:HE3   | 1.97                     | 0.47              |
| 2:R:78:THR:O     | 2:R:80:GLY:N     | 2.40                     | 0.47              |
| 2:R:90:GLU:OE1   | 2:R:169:ARG:HD2  | 2.14                     | 0.47              |
| 1:S:200:GLN:HA   | 1:S:200:GLN:OE1  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:294:ASN:ND2  | 2:B:290:ALA:O    | 2.48                     | 0.46              |
| 1:G:90:ARG:NH2   | 1:G:92:GLU:OE1   | 2.48                     | 0.46              |
| 1:I:90:ARG:NH2   | 1:I:92:GLU:OE1   | 2.48                     | 0.46              |
| 1:U:213:ARG:HG2  | 1:U:213:ARG:HH11 | 1.79                     | 0.46              |
| 1:A:99:PRO:O     | 1:A:102:VAL:HG23 | 2.15                     | 0.46              |
| 1:A:213:ARG:HG2  | 1:A:213:ARG:HH11 | 1.79                     | 0.46              |
| 1:C:228:LYS:HZ2  | 2:D:234:MET:HE2  | 1.80                     | 0.46              |
| 1:O:90:ARG:NH2   | 1:O:92:GLU:OE1   | 2.48                     | 0.46              |
| 1:Q:90:ARG:NH2   | 1:Q:92:GLU:OE1   | 2.48                     | 0.46              |
| 1:U:77:PRO:HB2   | 1:U:85:MET:HE3   | 1.97                     | 0.46              |
| 1:E:90:ARG:NH2   | 1:E:92:GLU:OE1   | 2.48                     | 0.46              |
| 2:H:76:CYS:SG    | 2:H:124:LEU:HG   | 2.54                     | 0.46              |
| 2:H:235:GLU:O    | 2:H:238:THR:OG1  | 2.32                     | 0.46              |
| 1:U:228:LYS:HZ3  | 2:V:234:MET:HE2  | 1.80                     | 0.46              |
| 1:U:90:ARG:NH2   | 1:U:92:GLU:OE1   | 2.48                     | 0.46              |
| 2:X:229:TYR:CD2  | 1:Y:240:THR:HG21 | 2.46                     | 0.46              |
| 1:Y:90:ARG:NH2   | 1:Y:92:GLU:OE1   | 2.48                     | 0.46              |
| 2:B:69:ASP:HB3   | 2:B:117:PHE:CZ   | 2.49                     | 0.46              |
| 2:B:276:LEU:HD22 | 1:C:281:GLU:HB3  | 1.98                     | 0.46              |
| 1:E:213:ARG:HH11 | 1:E:213:ARG:HG2  | 1.79                     | 0.46              |
| 2:N:211:ARG:O    | 2:N:215:LEU:HD13 | 2.16                     | 0.46              |
| 2:R:276:LEU:HD22 | 1:S:281:GLU:HB3  | 1.98                     | 0.46              |
| 2:V:276:LEU:HD22 | 1:W:281:GLU:HB3  | 1.98                     | 0.46              |
| 1:W:90:ARG:NH2   | 1:W:92:GLU:OE1   | 2.48                     | 0.46              |
| 2:Z:211:ARG:O    | 2:Z:215:LEU:HD13 | 2.16                     | 0.46              |
| 2:B:65:THR:O     | 2:B:66:LEU:C     | 2.59                     | 0.46              |
| 2:B:287:LYS:O    | 2:B:290:ALA:HB3  | 2.16                     | 0.46              |
| 2:F:211:ARG:O    | 2:F:215:LEU:HD13 | 2.16                     | 0.46              |
| 1:M:90:ARG:NH2   | 1:M:92:GLU:OE1   | 2.48                     | 0.46              |
| 2:R:211:ARG:O    | 2:R:215:LEU:HD13 | 2.16                     | 0.46              |
| 1:Y:77:PRO:HB2   | 1:Y:85:MET:HE3   | 1.96                     | 0.46              |
| 1:S:77:PRO:HB2   | 1:S:85:MET:HE3   | 1.97                     | 0.46              |
| 1:S:90:ARG:NH2   | 1:S:92:GLU:OE1   | 2.48                     | 0.46              |
| 2:V:211:ARG:O    | 2:V:215:LEU:HD13 | 2.16                     | 0.46              |
| 2:L:200:GLN:HB2  | 1:M:211:THR:HG22 | 1.98                     | 0.46              |
| 1:C:90:ARG:NH2   | 1:C:92:GLU:OE1   | 2.48                     | 0.46              |
| 2:D:211:ARG:O    | 2:D:215:LEU:HD13 | 2.16                     | 0.46              |
| 2:L:78:THR:C     | 2:L:80:GLY:H     | 2.24                     | 0.46              |
| 2:L:211:ARG:O    | 2:L:215:LEU:HD13 | 2.16                     | 0.46              |
| 1:M:129:PHE:CE2  | 1:M:146:ILE:HG12 | 2.51                     | 0.46              |
| 1:O:129:PHE:CE2  | 1:O:146:ILE:HG12 | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:129:PHE:CE2  | 1:Q:146:ILE:HG12 | 2.51                     | 0.46              |
| 2:P:211:ARG:O    | 2:P:215:LEU:HD13 | 2.16                     | 0.46              |
| 1:A:129:PHE:CE2  | 1:A:146:ILE:HG12 | 2.51                     | 0.45              |
| 1:C:129:PHE:CE2  | 1:C:146:ILE:HG12 | 2.51                     | 0.45              |
| 2:F:276:LEU:HD22 | 1:G:281:GLU:HB3  | 1.98                     | 0.45              |
| 2:H:211:ARG:O    | 2:H:215:LEU:HD13 | 2.16                     | 0.45              |
| 1:S:129:PHE:CE2  | 1:S:146:ILE:HG12 | 2.51                     | 0.45              |
| 1:S:290:ALA:C    | 1:S:292:ALA:N    | 2.66                     | 0.45              |
| 1:U:129:PHE:CE2  | 1:U:146:ILE:HG12 | 2.51                     | 0.45              |
| 2:X:200:GLN:HB2  | 1:Y:211:THR:HG22 | 1.97                     | 0.45              |
| 2:Z:78:THR:C     | 2:Z:80:GLY:H     | 2.24                     | 0.45              |
| 2:F:78:THR:C     | 2:F:80:GLY:H     | 2.24                     | 0.45              |
| 1:I:38:ARG:HB2   | 1:I:43:LEU:HD21  | 1.99                     | 0.45              |
| 1:C:38:ARG:HB2   | 1:C:43:LEU:HD21  | 1.99                     | 0.45              |
| 2:H:78:THR:C     | 2:H:80:GLY:H     | 2.24                     | 0.45              |
| 1:K:112:ASP:N    | 1:K:112:ASP:OD1  | 2.50                     | 0.45              |
| 1:K:129:PHE:CE2  | 1:K:146:ILE:HG12 | 2.51                     | 0.45              |
| 1:M:38:ARG:HB2   | 1:M:43:LEU:HD21  | 1.99                     | 0.45              |
| 1:U:112:ASP:N    | 1:U:112:ASP:OD1  | 2.49                     | 0.45              |
| 1:C:112:ASP:OD1  | 1:C:112:ASP:N    | 2.50                     | 0.45              |
| 1:C:275:LYS:HB2  | 1:C:275:LYS:HE2  | 1.45                     | 0.45              |
| 2:D:186:MET:HB3  | 2:D:186:MET:HE3  | 1.81                     | 0.45              |
| 1:E:112:ASP:OD1  | 1:E:112:ASP:N    | 2.50                     | 0.45              |
| 2:H:282:GLN:HG2  | 2:H:286:TYR:CE2  | 2.52                     | 0.45              |
| 1:M:112:ASP:OD1  | 1:M:112:ASP:N    | 2.49                     | 0.45              |
| 1:M:297:ILE:O    | 1:M:298:TYR:CB   | 2.65                     | 0.45              |
| 1:O:38:ARG:HB2   | 1:O:43:LEU:HD21  | 1.99                     | 0.45              |
| 2:P:40:LEU:HD13  | 1:Q:30:GLU:HG3   | 1.98                     | 0.45              |
| 2:P:78:THR:C     | 2:P:80:GLY:H     | 2.24                     | 0.45              |
| 1:S:112:ASP:N    | 1:S:112:ASP:OD1  | 2.50                     | 0.45              |
| 1:W:112:ASP:OD1  | 1:W:112:ASP:N    | 2.50                     | 0.45              |
| 1:W:129:PHE:CE2  | 1:W:146:ILE:HG12 | 2.51                     | 0.45              |
| 1:Y:129:PHE:CE2  | 1:Y:146:ILE:HG12 | 2.51                     | 0.45              |
| 1:C:161:MET:HE2  | 1:C:161:MET:HB3  | 1.80                     | 0.45              |
| 1:E:129:PHE:CE2  | 1:E:146:ILE:HG12 | 2.51                     | 0.45              |
| 1:G:38:ARG:HB2   | 1:G:43:LEU:HD21  | 1.99                     | 0.45              |
| 2:J:188:SER:O    | 2:J:191:THR:OG1  | 2.34                     | 0.45              |
| 2:J:211:ARG:O    | 2:J:215:LEU:HD13 | 2.16                     | 0.45              |
| 2:J:282:GLN:HG2  | 2:J:286:TYR:CE2  | 2.52                     | 0.45              |
| 1:K:297:ILE:O    | 1:K:298:TYR:CB   | 2.65                     | 0.45              |
| 1:O:99:PRO:O     | 1:O:102:VAL:HG23 | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:282:GLN:HG2  | 2:R:286:TYR:CE2  | 2.52                     | 0.45              |
| 1:W:228:LYS:HZ3  | 2:X:234:MET:HE2  | 1.81                     | 0.45              |
| 2:X:122:HIS:NE2  | 1:Y:147:ASP:OD2  | 2.50                     | 0.45              |
| 2:B:266:MET:SD   | 1:C:276:HIS:ND1  | 2.90                     | 0.45              |
| 2:D:200:GLN:HB2  | 1:E:211:THR:HG22 | 1.98                     | 0.45              |
| 2:H:40:LEU:HD13  | 1:I:30:GLU:HG3   | 1.97                     | 0.45              |
| 1:I:112:ASP:N    | 1:I:112:ASP:OD1  | 2.49                     | 0.45              |
| 2:T:229:TYR:CD2  | 1:U:240:THR:HG21 | 2.46                     | 0.45              |
| 2:B:211:ARG:O    | 2:B:215:LEU:HD13 | 2.16                     | 0.45              |
| 2:L:235:GLU:O    | 2:L:238:THR:OG1  | 2.32                     | 0.45              |
| 2:N:276:LEU:HD22 | 1:O:281:GLU:HB3  | 1.98                     | 0.45              |
| 2:R:203:VAL:CG1  | 1:S:215:LYS:HE2  | 2.47                     | 0.45              |
| 1:U:115:LYS:HE2  | 1:U:115:LYS:HB2  | 1.85                     | 0.45              |
| 1:W:178:PRO:HG2  | 1:W:181:ILE:HD12 | 1.99                     | 0.45              |
| 1:Y:112:ASP:OD1  | 1:Y:112:ASP:N    | 2.50                     | 0.45              |
| 1:G:129:PHE:CE2  | 1:G:146:ILE:HG12 | 2.51                     | 0.45              |
| 1:I:297:ILE:O    | 1:I:298:TYR:CB   | 2.65                     | 0.45              |
| 2:L:282:GLN:HG2  | 2:L:286:TYR:CE2  | 2.52                     | 0.45              |
| 1:M:161:MET:HE2  | 1:M:161:MET:HB3  | 1.80                     | 0.45              |
| 2:N:282:GLN:HG2  | 2:N:286:TYR:CE2  | 2.52                     | 0.45              |
| 1:O:297:ILE:O    | 1:O:298:TYR:CB   | 2.65                     | 0.45              |
| 2:P:282:GLN:HG2  | 2:P:286:TYR:CE2  | 2.52                     | 0.45              |
| 1:Q:112:ASP:OD1  | 1:Q:112:ASP:N    | 2.50                     | 0.45              |
| 1:S:178:PRO:HG2  | 1:S:181:ILE:HD12 | 1.99                     | 0.45              |
| 2:T:211:ARG:O    | 2:T:215:LEU:HD13 | 2.16                     | 0.45              |
| 2:T:282:GLN:HG2  | 2:T:286:TYR:CE2  | 2.52                     | 0.45              |
| 2:B:282:GLN:HG2  | 2:B:286:TYR:CE2  | 2.52                     | 0.45              |
| 1:G:70:THR:OG1   | 1:G:94:VAL:HG22  | 2.17                     | 0.45              |
| 1:G:264:TYR:HD1  | 2:H:271:ALA:HB2  | 1.82                     | 0.45              |
| 1:G:290:ALA:HB1  | 2:H:290:ALA:CB   | 2.47                     | 0.45              |
| 2:N:203:VAL:CG1  | 1:O:215:LYS:HE2  | 2.47                     | 0.45              |
| 1:S:38:ARG:HB2   | 1:S:43:LEU:HD21  | 1.99                     | 0.45              |
| 1:U:297:ILE:O    | 1:U:298:TYR:CB   | 2.65                     | 0.45              |
| 2:X:211:ARG:O    | 2:X:215:LEU:HD13 | 2.16                     | 0.45              |
| 2:Z:292:ASN:O    | 2:Z:293:SER:HB2  | 2.16                     | 0.45              |
| 1:A:38:ARG:HB2   | 1:A:43:LEU:HD21  | 1.99                     | 0.45              |
| 1:A:112:ASP:OD1  | 1:A:112:ASP:N    | 2.50                     | 0.45              |
| 1:E:264:TYR:HD1  | 2:F:271:ALA:HB2  | 1.82                     | 0.45              |
| 1:E:290:ALA:HB1  | 2:F:290:ALA:CB   | 2.47                     | 0.45              |
| 2:H:276:LEU:HD23 | 2:H:276:LEU:HA   | 1.60                     | 0.45              |
| 1:I:70:THR:OG1   | 1:I:94:VAL:HG22  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:129:PHE:CE2  | 1:I:146:ILE:HG12 | 2.51                     | 0.45              |
| 1:I:290:ALA:HB1  | 2:J:290:ALA:CB   | 2.47                     | 0.45              |
| 1:O:112:ASP:OD1  | 1:O:112:ASP:N    | 2.50                     | 0.45              |
| 1:S:264:TYR:HD1  | 2:T:271:ALA:HB2  | 1.82                     | 0.45              |
| 2:T:200:GLN:HB2  | 1:U:211:THR:HG22 | 1.98                     | 0.45              |
| 2:V:203:VAL:CG1  | 1:W:215:LYS:HE2  | 2.47                     | 0.45              |
| 2:X:276:LEU:HA   | 2:X:276:LEU:HD23 | 1.60                     | 0.45              |
| 2:Z:282:GLN:HG2  | 2:Z:286:TYR:CE2  | 2.52                     | 0.45              |
| 2:D:276:LEU:HD23 | 2:D:276:LEU:HA   | 1.60                     | 0.44              |
| 2:F:282:GLN:HG2  | 2:F:286:TYR:CE2  | 2.52                     | 0.44              |
| 1:I:264:TYR:HD1  | 2:J:271:ALA:HB2  | 1.82                     | 0.44              |
| 1:K:264:TYR:HD1  | 2:L:271:ALA:HB2  | 1.82                     | 0.44              |
| 1:M:264:TYR:HD1  | 2:N:271:ALA:HB2  | 1.82                     | 0.44              |
| 1:C:295:SER:O    | 1:C:296:LYS:O    | 2.36                     | 0.44              |
| 1:E:38:ARG:HB2   | 1:E:43:LEU:HD21  | 1.99                     | 0.44              |
| 2:J:276:LEU:HD22 | 1:K:281:GLU:HB3  | 1.98                     | 0.44              |
| 1:K:77:PRO:HB2   | 1:K:85:MET:HE3   | 1.98                     | 0.44              |
| 1:U:38:ARG:HB2   | 1:U:43:LEU:HD21  | 1.99                     | 0.44              |
| 1:W:226:VAL:O    | 1:W:230:ARG:HD3  | 2.18                     | 0.44              |
| 1:W:290:ALA:HB1  | 2:X:290:ALA:CB   | 2.47                     | 0.44              |
| 1:A:211:THR:HG22 | 2:Z:200:GLN:HB2  | 1.98                     | 0.44              |
| 1:E:70:THR:OG1   | 1:E:94:VAL:HG22  | 2.17                     | 0.44              |
| 1:E:297:ILE:O    | 1:E:298:TYR:CB   | 2.65                     | 0.44              |
| 1:I:119:PHE:N    | 1:I:119:PHE:CD1  | 2.85                     | 0.44              |
| 2:N:200:GLN:HB2  | 1:O:211:THR:HG22 | 1.99                     | 0.44              |
| 1:Q:264:TYR:HD1  | 2:R:271:ALA:HB2  | 1.83                     | 0.44              |
| 1:S:297:ILE:O    | 1:S:298:TYR:CB   | 2.65                     | 0.44              |
| 1:W:297:ILE:O    | 1:W:298:TYR:CB   | 2.65                     | 0.44              |
| 1:A:30:GLU:HG3   | 2:Z:40:LEU:HD13  | 1.98                     | 0.44              |
| 2:B:70:GLU:HB2   | 2:B:90:GLU:HG2   | 1.99                     | 0.44              |
| 2:D:78:THR:C     | 2:D:80:GLY:H     | 2.24                     | 0.44              |
| 2:D:282:GLN:HG2  | 2:D:286:TYR:CE2  | 2.52                     | 0.44              |
| 2:F:203:VAL:CG1  | 1:G:215:LYS:HE2  | 2.47                     | 0.44              |
| 2:J:78:THR:C     | 2:J:80:GLY:H     | 2.24                     | 0.44              |
| 1:O:70:THR:OG1   | 1:O:94:VAL:HG22  | 2.17                     | 0.44              |
| 1:Q:297:ILE:O    | 1:Q:298:TYR:CB   | 2.65                     | 0.44              |
| 1:U:264:TYR:HD1  | 2:V:271:ALA:HB2  | 1.82                     | 0.44              |
| 1:U:290:ALA:HB1  | 2:V:290:ALA:CB   | 2.47                     | 0.44              |
| 1:C:264:TYR:HD1  | 2:D:271:ALA:HB2  | 1.82                     | 0.44              |
| 2:J:203:VAL:CG1  | 1:K:215:LYS:HE2  | 2.47                     | 0.44              |
| 1:O:178:PRO:HG2  | 1:O:181:ILE:HD12 | 1.99                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:O:264:TYR:HD1 | 2:P:271:ALA:HB2  | 1.82                     | 0.44              |
| 1:O:292:ALA:O   | 1:O:293:SER:HB2  | 2.18                     | 0.44              |
| 1:Q:292:ALA:O   | 1:Q:293:SER:HB2  | 2.18                     | 0.44              |
| 1:S:70:THR:OG1  | 1:S:94:VAL:HG22  | 2.17                     | 0.44              |
| 2:T:78:THR:C    | 2:T:80:GLY:H     | 2.24                     | 0.44              |
| 1:U:119:PHE:N   | 1:U:119:PHE:CD1  | 2.85                     | 0.44              |
| 1:W:264:TYR:HD1 | 2:X:271:ALA:HB2  | 1.82                     | 0.44              |
| 2:X:282:GLN:HG2 | 2:X:286:TYR:CE2  | 2.52                     | 0.44              |
| 1:Y:70:THR:OG1  | 1:Y:94:VAL:HG22  | 2.17                     | 0.44              |
| 1:A:178:PRO:HG2 | 1:A:181:ILE:HD12 | 1.99                     | 0.44              |
| 2:B:203:VAL:CG1 | 1:C:215:LYS:HE2  | 2.47                     | 0.44              |
| 1:C:290:ALA:HB1 | 2:D:290:ALA:CB   | 2.47                     | 0.44              |
| 1:G:112:ASP:N   | 1:G:112:ASP:OD1  | 2.50                     | 0.44              |
| 1:G:297:ILE:O   | 1:G:298:TYR:CB   | 2.65                     | 0.44              |
| 1:K:70:THR:OG1  | 1:K:94:VAL:HG22  | 2.17                     | 0.44              |
| 1:K:178:PRO:HG2 | 1:K:181:ILE:HD12 | 1.99                     | 0.44              |
| 1:S:226:VAL:O   | 1:S:230:ARG:HD3  | 2.18                     | 0.44              |
| 1:S:292:ALA:O   | 1:S:293:SER:HB2  | 2.18                     | 0.44              |
| 1:U:37:TYR:HB2  | 1:U:60:THR:OG1   | 2.18                     | 0.44              |
| 2:V:200:GLN:HB2 | 1:W:211:THR:HG22 | 1.99                     | 0.44              |
| 1:W:292:ALA:O   | 1:W:293:SER:HB2  | 2.18                     | 0.44              |
| 1:Y:292:ALA:O   | 1:Y:293:SER:HB2  | 2.18                     | 0.44              |
| 1:A:226:VAL:O   | 1:A:230:ARG:HD3  | 2.18                     | 0.44              |
| 2:F:200:GLN:HB2 | 1:G:211:THR:HG22 | 1.99                     | 0.44              |
| 2:H:200:GLN:HB2 | 1:I:211:THR:HG22 | 1.99                     | 0.44              |
| 1:K:37:TYR:HB2  | 1:K:60:THR:OG1   | 2.18                     | 0.44              |
| 1:K:290:ALA:HB1 | 2:L:290:ALA:CB   | 2.47                     | 0.44              |
| 1:U:292:ALA:O   | 1:U:293:SER:HB2  | 2.18                     | 0.44              |
| 1:W:38:ARG:HB2  | 1:W:43:LEU:HD21  | 1.99                     | 0.44              |
| 1:W:70:THR:OG1  | 1:W:94:VAL:HG22  | 2.17                     | 0.44              |
| 2:H:229:TYR:CD2 | 1:I:240:THR:HG21 | 2.46                     | 0.44              |
| 1:K:38:ARG:HB2  | 1:K:43:LEU:HD21  | 1.99                     | 0.44              |
| 1:M:292:ALA:O   | 1:M:293:SER:HB2  | 2.18                     | 0.44              |
| 1:Q:37:TYR:HB2  | 1:Q:60:THR:OG1   | 2.18                     | 0.44              |
| 1:Q:226:VAL:O   | 1:Q:230:ARG:HD3  | 2.18                     | 0.44              |
| 1:S:228:LYS:HZ3 | 2:T:234:MET:HE2  | 1.82                     | 0.44              |
| 1:U:226:VAL:O   | 1:U:230:ARG:HD3  | 2.18                     | 0.44              |
| 2:V:282:GLN:HG2 | 2:V:286:TYR:CE2  | 2.52                     | 0.44              |
| 1:W:213:ARG:HG2 | 1:W:213:ARG:NH1  | 2.33                     | 0.44              |
| 1:Y:264:TYR:HD1 | 2:Z:271:ALA:HB2  | 1.82                     | 0.44              |
| 1:A:70:THR:OG1  | 1:A:94:VAL:HG22  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:202:GLN:O    | 1:A:203:LYS:C    | 2.61                     | 0.44              |
| 1:C:37:TYR:HB2   | 1:C:60:THR:OG1   | 2.18                     | 0.44              |
| 1:E:119:PHE:N    | 1:E:119:PHE:CD1  | 2.85                     | 0.44              |
| 1:E:178:PRO:HG2  | 1:E:181:ILE:HD12 | 1.99                     | 0.44              |
| 1:I:37:TYR:HB2   | 1:I:60:THR:OG1   | 2.18                     | 0.44              |
| 1:K:292:ALA:O    | 1:K:293:SER:HB2  | 2.18                     | 0.44              |
| 1:M:37:TYR:HB2   | 1:M:60:THR:OG1   | 2.18                     | 0.44              |
| 1:Q:38:ARG:HB2   | 1:Q:43:LEU:HD21  | 1.99                     | 0.44              |
| 1:Q:290:ALA:HB1  | 2:R:290:ALA:CB   | 2.47                     | 0.44              |
| 1:S:290:ALA:HB1  | 2:T:290:ALA:CB   | 2.48                     | 0.44              |
| 1:Y:226:VAL:O    | 1:Y:230:ARG:HD3  | 2.18                     | 0.44              |
| 2:B:200:GLN:HB2  | 1:C:211:THR:HG22 | 1.99                     | 0.43              |
| 1:C:70:THR:OG1   | 1:C:94:VAL:HG22  | 2.17                     | 0.43              |
| 1:E:292:ALA:O    | 1:E:293:SER:HB2  | 2.18                     | 0.43              |
| 2:H:129:SER:HG   | 1:I:174:LYS:HZ2  | 1.57                     | 0.43              |
| 2:V:235:GLU:O    | 2:V:238:THR:OG1  | 2.32                     | 0.43              |
| 1:W:37:TYR:HB2   | 1:W:60:THR:OG1   | 2.18                     | 0.43              |
| 1:A:37:TYR:HB2   | 1:A:60:THR:OG1   | 2.18                     | 0.43              |
| 1:A:264:TYR:HD1  | 2:B:271:ALA:HB2  | 1.82                     | 0.43              |
| 1:C:178:PRO:HG2  | 1:C:181:ILE:HD12 | 1.99                     | 0.43              |
| 1:G:38:ARG:HG3   | 1:G:58:ILE:HG22  | 2.01                     | 0.43              |
| 1:I:178:PRO:HG2  | 1:I:181:ILE:HD12 | 1.99                     | 0.43              |
| 1:I:207:LYS:HB2  | 1:I:207:LYS:HE2  | 1.86                     | 0.43              |
| 1:M:178:PRO:HG2  | 1:M:181:ILE:HD12 | 1.99                     | 0.43              |
| 1:O:119:PHE:N    | 1:O:119:PHE:CD1  | 2.85                     | 0.43              |
| 2:P:200:GLN:HB2  | 1:Q:211:THR:HG22 | 1.98                     | 0.43              |
| 2:R:276:LEU:HD23 | 2:R:276:LEU:HA   | 1.60                     | 0.43              |
| 1:E:37:TYR:HB2   | 1:E:60:THR:OG1   | 2.18                     | 0.43              |
| 1:I:226:VAL:O    | 1:I:230:ARG:HD3  | 2.18                     | 0.43              |
| 2:J:200:GLN:HB2  | 1:K:211:THR:HG22 | 1.99                     | 0.43              |
| 1:O:37:TYR:HB2   | 1:O:60:THR:OG1   | 2.18                     | 0.43              |
| 1:O:213:ARG:HG2  | 1:O:213:ARG:NH1  | 2.33                     | 0.43              |
| 1:O:290:ALA:HB1  | 2:P:290:ALA:CB   | 2.47                     | 0.43              |
| 1:U:70:THR:OG1   | 1:U:94:VAL:HG22  | 2.17                     | 0.43              |
| 1:U:213:ARG:HG2  | 1:U:213:ARG:NH1  | 2.33                     | 0.43              |
| 1:Y:213:ARG:HG2  | 1:Y:213:ARG:NH1  | 2.33                     | 0.43              |
| 2:B:241:LYS:HE3  | 2:B:241:LYS:HB2  | 1.39                     | 0.43              |
| 1:C:294:ASN:O    | 1:C:295:SER:HB2  | 2.17                     | 0.43              |
| 1:K:35:VAL:HG21  | 1:K:106:VAL:HG11 | 2.01                     | 0.43              |
| 1:K:226:VAL:O    | 1:K:230:ARG:HD3  | 2.18                     | 0.43              |
| 1:M:35:VAL:HG21  | 1:M:106:VAL:HG11 | 2.01                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:M:70:THR:OG1  | 1:M:94:VAL:HG22  | 2.17                     | 0.43              |
| 2:N:40:LEU:HD13 | 1:O:30:GLU:HG3   | 2.00                     | 0.43              |
| 1:O:35:VAL:HG21 | 1:O:106:VAL:HG11 | 2.01                     | 0.43              |
| 2:X:78:THR:C    | 2:X:80:GLY:H     | 2.24                     | 0.43              |
| 1:Y:38:ARG:HB2  | 1:Y:43:LEU:HD21  | 1.99                     | 0.43              |
| 1:Y:297:ILE:O   | 1:Y:298:TYR:CB   | 2.65                     | 0.43              |
| 2:B:232:LYS:HB3 | 2:B:232:LYS:HE3  | 1.90                     | 0.43              |
| 1:G:178:PRO:HG2 | 1:G:181:ILE:HD12 | 1.99                     | 0.43              |
| 1:G:226:VAL:O   | 1:G:230:ARG:HD3  | 2.18                     | 0.43              |
| 1:I:35:VAL:HG21 | 1:I:106:VAL:HG11 | 2.01                     | 0.43              |
| 1:K:38:ARG:HG3  | 1:K:58:ILE:HG22  | 2.01                     | 0.43              |
| 1:O:115:LYS:HE2 | 1:O:115:LYS:HB2  | 1.85                     | 0.43              |
| 1:Q:38:ARG:HG3  | 1:Q:58:ILE:HG22  | 2.01                     | 0.43              |
| 1:C:226:VAL:O   | 1:C:230:ARG:HD3  | 2.18                     | 0.43              |
| 2:F:40:LEU:HD13 | 1:G:30:GLU:HG3   | 2.00                     | 0.43              |
| 1:M:213:ARG:HG2 | 1:M:213:ARG:NH1  | 2.33                     | 0.43              |
| 1:O:96:MET:HE2  | 1:O:96:MET:HB3   | 1.85                     | 0.43              |
| 1:O:115:LYS:HA  | 1:O:119:PHE:CD2  | 2.54                     | 0.43              |
| 1:Q:35:VAL:HG21 | 1:Q:106:VAL:HG11 | 2.01                     | 0.43              |
| 1:Q:115:LYS:HA  | 1:Q:119:PHE:CD2  | 2.54                     | 0.43              |
| 1:S:38:ARG:HG3  | 1:S:58:ILE:HG22  | 2.01                     | 0.43              |
| 1:S:115:LYS:HA  | 1:S:119:PHE:CD2  | 2.54                     | 0.43              |
| 2:T:122:HIS:NE2 | 1:U:147:ASP:OD2  | 2.52                     | 0.43              |
| 1:U:178:PRO:HG2 | 1:U:181:ILE:HD12 | 1.99                     | 0.43              |
| 1:W:38:ARG:HG3  | 1:W:58:ILE:HG22  | 2.01                     | 0.43              |
| 1:A:38:ARG:HG3  | 1:A:58:ILE:HG22  | 2.01                     | 0.43              |
| 2:B:295:ILE:O   | 2:B:296:TYR:C    | 2.58                     | 0.43              |
| 1:E:213:ARG:HG2 | 1:E:213:ARG:NH1  | 2.33                     | 0.43              |
| 1:I:292:ALA:O   | 1:I:293:SER:HB2  | 2.18                     | 0.43              |
| 1:Q:70:THR:OG1  | 1:Q:94:VAL:HG22  | 2.17                     | 0.43              |
| 2:R:200:GLN:HB2 | 1:S:211:THR:HG22 | 1.99                     | 0.43              |
| 1:U:115:LYS:HA  | 1:U:119:PHE:CD2  | 2.54                     | 0.43              |
| 1:W:115:LYS:HA  | 1:W:119:PHE:CD2  | 2.54                     | 0.43              |
| 2:B:186:MET:HE3 | 2:B:186:MET:HB3  | 1.81                     | 0.43              |
| 2:D:78:THR:HG21 | 2:D:133:LEU:HA   | 2.01                     | 0.43              |
| 1:G:35:VAL:HG21 | 1:G:106:VAL:HG11 | 2.01                     | 0.43              |
| 2:L:188:SER:O   | 2:L:191:THR:OG1  | 2.34                     | 0.43              |
| 1:M:38:ARG:HG3  | 1:M:58:ILE:HG22  | 2.01                     | 0.43              |
| 1:M:115:LYS:HA  | 1:M:119:PHE:CD2  | 2.54                     | 0.43              |
| 1:Q:178:PRO:HG2 | 1:Q:181:ILE:HD12 | 1.99                     | 0.43              |
| 1:A:119:PHE:N   | 1:A:119:PHE:CD1  | 2.85                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:213:ARG:HG2 | 1:A:213:ARG:NH1  | 2.33                     | 0.43              |
| 1:G:213:ARG:HG2 | 1:G:213:ARG:NH1  | 2.33                     | 0.43              |
| 2:J:45:SER:HB2  | 2:J:50:HIS:CD2   | 2.54                     | 0.43              |
| 1:M:226:VAL:O   | 1:M:230:ARG:HD3  | 2.18                     | 0.43              |
| 1:M:290:ALA:O   | 1:M:292:ALA:N    | 2.47                     | 0.43              |
| 1:M:290:ALA:HB1 | 2:N:290:ALA:CB   | 2.47                     | 0.43              |
| 1:O:38:ARG:HG3  | 1:O:58:ILE:HG22  | 2.01                     | 0.43              |
| 1:Q:213:ARG:HG2 | 1:Q:213:ARG:NH1  | 2.33                     | 0.43              |
| 2:R:40:LEU:HD13 | 1:S:30:GLU:HG3   | 2.00                     | 0.43              |
| 1:S:35:VAL:HG21 | 1:S:106:VAL:HG11 | 2.01                     | 0.43              |
| 2:V:78:THR:HG21 | 2:V:133:LEU:HA   | 2.01                     | 0.43              |
| 2:Z:296:TYR:O   | 2:Z:297:PHE:C    | 2.62                     | 0.43              |
| 1:A:207:LYS:HB2 | 1:A:207:LYS:HE2  | 1.86                     | 0.43              |
| 2:B:120:ILE:O   | 2:B:121:HIS:C    | 2.61                     | 0.43              |
| 1:C:38:ARG:HG3  | 1:C:58:ILE:HG22  | 2.01                     | 0.43              |
| 1:C:213:ARG:HG2 | 1:C:213:ARG:NH1  | 2.33                     | 0.43              |
| 2:D:172:LYS:HA  | 2:D:173:PRO:HD3  | 1.89                     | 0.43              |
| 2:H:45:SER:HB2  | 2:H:50:HIS:CD2   | 2.54                     | 0.43              |
| 1:S:37:TYR:HB2  | 1:S:60:THR:OG1   | 2.18                     | 0.43              |
| 2:V:45:SER:HB2  | 2:V:50:HIS:CD2   | 2.54                     | 0.43              |
| 2:X:78:THR:HG21 | 2:X:133:LEU:HA   | 2.01                     | 0.43              |
| 2:B:45:SER:HB2  | 2:B:50:HIS:CD2   | 2.54                     | 0.42              |
| 2:B:78:THR:HG21 | 2:B:133:LEU:HA   | 2.01                     | 0.42              |
| 2:D:122:HIS:NE2 | 1:E:147:ASP:OD2  | 2.52                     | 0.42              |
| 1:E:38:ARG:HG3  | 1:E:58:ILE:HG22  | 2.01                     | 0.42              |
| 2:J:40:LEU:HD13 | 1:K:30:GLU:HG3   | 2.00                     | 0.42              |
| 2:L:229:TYR:CD2 | 1:M:240:THR:HG21 | 2.46                     | 0.42              |
| 1:W:161:MET:HE2 | 1:W:161:MET:HB3  | 1.80                     | 0.42              |
| 1:Y:178:PRO:HG2 | 1:Y:181:ILE:HD12 | 1.99                     | 0.42              |
| 1:E:115:LYS:HA  | 1:E:119:PHE:CD2  | 2.54                     | 0.42              |
| 1:G:161:MET:HE2 | 1:G:161:MET:HB3  | 1.80                     | 0.42              |
| 1:I:38:ARG:HG3  | 1:I:58:ILE:HG22  | 2.01                     | 0.42              |
| 2:J:186:MET:HB3 | 2:J:186:MET:HE3  | 1.81                     | 0.42              |
| 1:K:115:LYS:HE2 | 1:K:115:LYS:HB2  | 1.85                     | 0.42              |
| 2:L:122:HIS:NE2 | 1:M:147:ASP:OD2  | 2.51                     | 0.42              |
| 2:N:78:THR:C    | 2:N:80:GLY:H     | 2.24                     | 0.42              |
| 1:U:38:ARG:HG3  | 1:U:58:ILE:HG22  | 2.01                     | 0.42              |
| 1:Y:37:TYR:HB2  | 1:Y:60:THR:OG1   | 2.18                     | 0.42              |
| 2:F:78:THR:HG21 | 2:F:133:LEU:HA   | 2.01                     | 0.42              |
| 1:G:115:LYS:HA  | 1:G:119:PHE:CD2  | 2.54                     | 0.42              |
| 2:P:45:SER:HB2  | 2:P:50:HIS:CD2   | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:213:ARG:HG2  | 1:S:213:ARG:NH1  | 2.34                     | 0.42              |
| 2:T:80:GLY:O     | 1:U:185:PHE:HD1  | 2.02                     | 0.42              |
| 2:V:40:LEU:HD13  | 1:W:30:GLU:HG3   | 2.00                     | 0.42              |
| 1:E:35:VAL:HG21  | 1:E:106:VAL:HG11 | 2.01                     | 0.42              |
| 2:F:124:LEU:HD13 | 2:F:148:LEU:HD21 | 2.02                     | 0.42              |
| 1:G:119:PHE:N    | 1:G:119:PHE:CD1  | 2.85                     | 0.42              |
| 1:O:226:VAL:O    | 1:O:230:ARG:HD3  | 2.18                     | 0.42              |
| 2:T:284:MET:HG3  | 1:U:285:LEU:HD11 | 2.02                     | 0.42              |
| 2:X:45:SER:HB2   | 2:X:50:HIS:CD2   | 2.54                     | 0.42              |
| 1:Y:115:LYS:HA   | 1:Y:119:PHE:CD2  | 2.54                     | 0.42              |
| 2:Z:276:LEU:HD23 | 2:Z:276:LEU:HA   | 1.60                     | 0.42              |
| 2:B:293:SER:O    | 2:B:294:LYS:O    | 2.37                     | 0.42              |
| 1:G:37:TYR:HB2   | 1:G:60:THR:OG1   | 2.18                     | 0.42              |
| 1:I:115:LYS:HB2  | 1:I:115:LYS:HE2  | 1.85                     | 0.42              |
| 1:I:213:ARG:HG2  | 1:I:213:ARG:NH1  | 2.33                     | 0.42              |
| 2:N:139:GLU:C    | 2:N:140:LEU:HD23 | 2.45                     | 0.42              |
| 1:U:35:VAL:HG21  | 1:U:106:VAL:HG11 | 2.01                     | 0.42              |
| 1:Y:35:VAL:HG21  | 1:Y:106:VAL:HG11 | 2.01                     | 0.42              |
| 1:Y:115:LYS:HB2  | 1:Y:115:LYS:HE2  | 1.85                     | 0.42              |
| 1:A:35:VAL:HG21  | 1:A:106:VAL:HG11 | 2.01                     | 0.42              |
| 1:C:35:VAL:HG21  | 1:C:106:VAL:HG11 | 2.01                     | 0.42              |
| 2:F:45:SER:HB2   | 2:F:50:HIS:CD2   | 2.54                     | 0.42              |
| 1:G:292:ALA:O    | 1:G:293:SER:HB2  | 2.18                     | 0.42              |
| 2:H:188:SER:O    | 2:H:191:THR:OG1  | 2.34                     | 0.42              |
| 2:J:113:LYS:HA   | 2:J:113:LYS:HD3  | 1.87                     | 0.42              |
| 2:J:205:LYS:HB2  | 2:J:205:LYS:HE2  | 1.93                     | 0.42              |
| 2:J:276:LEU:HA   | 2:J:276:LEU:HD23 | 1.60                     | 0.42              |
| 1:K:119:PHE:N    | 1:K:119:PHE:CD1  | 2.85                     | 0.42              |
| 2:L:139:GLU:C    | 2:L:140:LEU:HD23 | 2.45                     | 0.42              |
| 2:N:45:SER:HB2   | 2:N:50:HIS:CD2   | 2.54                     | 0.42              |
| 1:O:228:LYS:HZ3  | 2:P:234:MET:HE2  | 1.83                     | 0.42              |
| 2:P:78:THR:HG21  | 2:P:133:LEU:HA   | 2.01                     | 0.42              |
| 2:T:45:SER:HB2   | 2:T:50:HIS:CD2   | 2.54                     | 0.42              |
| 2:V:139:GLU:C    | 2:V:140:LEU:HD23 | 2.45                     | 0.42              |
| 1:W:35:VAL:HG21  | 1:W:106:VAL:HG11 | 2.01                     | 0.42              |
| 1:C:115:LYS:HA   | 1:C:119:PHE:CD2  | 2.54                     | 0.42              |
| 1:E:96:MET:HE2   | 1:E:96:MET:HB3   | 1.85                     | 0.42              |
| 2:F:122:HIS:NE2  | 1:G:147:ASP:OD2  | 2.53                     | 0.42              |
| 2:J:122:HIS:NE2  | 1:K:147:ASP:OD2  | 2.53                     | 0.42              |
| 1:K:115:LYS:HA   | 1:K:119:PHE:CD2  | 2.54                     | 0.42              |
| 2:N:122:HIS:NE2  | 1:O:147:ASP:OD2  | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:119:PHE:N    | 1:Q:119:PHE:CD1  | 2.85                     | 0.42              |
| 2:X:80:GLY:O     | 1:Y:185:PHE:HD1  | 2.02                     | 0.42              |
| 2:X:139:GLU:C    | 2:X:140:LEU:HD23 | 2.45                     | 0.42              |
| 2:Z:45:SER:HB2   | 2:Z:50:HIS:CD2   | 2.54                     | 0.42              |
| 2:D:124:LEU:HD13 | 2:D:148:LEU:HD21 | 2.02                     | 0.42              |
| 2:H:124:LEU:HD13 | 2:H:148:LEU:HD21 | 2.02                     | 0.42              |
| 2:L:284:MET:HG3  | 1:M:285:LEU:HD11 | 2.02                     | 0.42              |
| 2:N:78:THR:HG21  | 2:N:133:LEU:HA   | 2.01                     | 0.42              |
| 2:N:124:LEU:HD13 | 2:N:148:LEU:HD21 | 2.02                     | 0.42              |
| 2:Z:78:THR:HG21  | 2:Z:133:LEU:HA   | 2.01                     | 0.42              |
| 2:B:182:ASN:ND2  | 1:C:193:THR:OG1  | 2.53                     | 0.42              |
| 2:D:80:GLY:O     | 1:E:185:PHE:HD1  | 2.02                     | 0.42              |
| 2:D:284:MET:HG3  | 1:E:285:LEU:HD11 | 2.02                     | 0.42              |
| 1:E:226:VAL:O    | 1:E:230:ARG:HD3  | 2.18                     | 0.42              |
| 2:F:139:GLU:C    | 2:F:140:LEU:HD23 | 2.45                     | 0.42              |
| 2:J:182:ASN:ND2  | 1:K:193:THR:OG1  | 2.53                     | 0.42              |
| 2:L:45:SER:HB2   | 2:L:50:HIS:CD2   | 2.54                     | 0.42              |
| 2:L:80:GLY:O     | 1:M:185:PHE:HD1  | 2.02                     | 0.42              |
| 2:N:182:ASN:ND2  | 1:O:193:THR:OG1  | 2.53                     | 0.42              |
| 1:Q:207:LYS:HB2  | 1:Q:207:LYS:HE2  | 1.86                     | 0.42              |
| 2:X:182:ASN:ND2  | 1:Y:193:THR:OG1  | 2.53                     | 0.42              |
| 1:A:39:GLY:O     | 2:B:25:LYS:HB2   | 2.20                     | 0.42              |
| 2:B:122:HIS:NE2  | 1:C:147:ASP:OD2  | 2.53                     | 0.42              |
| 2:D:236:LYS:HB2  | 2:D:236:LYS:HE2  | 1.91                     | 0.42              |
| 2:H:122:HIS:NE2  | 1:I:147:ASP:OD2  | 2.53                     | 0.42              |
| 1:K:213:ARG:HG2  | 1:K:213:ARG:NH1  | 2.33                     | 0.42              |
| 2:L:78:THR:HG21  | 2:L:133:LEU:HA   | 2.01                     | 0.42              |
| 2:R:45:SER:HB2   | 2:R:50:HIS:CD2   | 2.54                     | 0.42              |
| 1:W:115:LYS:HE2  | 1:W:115:LYS:HB2  | 1.84                     | 0.42              |
| 1:W:119:PHE:N    | 1:W:119:PHE:CD1  | 2.85                     | 0.42              |
| 2:Z:124:LEU:HD13 | 2:Z:148:LEU:HD21 | 2.02                     | 0.42              |
| 1:A:115:LYS:HA   | 1:A:119:PHE:CD2  | 2.54                     | 0.41              |
| 2:D:45:SER:HB2   | 2:D:50:HIS:CD2   | 2.54                     | 0.41              |
| 2:H:215:LEU:O    | 2:H:219:GLU:HG3  | 2.20                     | 0.41              |
| 1:I:115:LYS:HA   | 1:I:119:PHE:CD2  | 2.54                     | 0.41              |
| 2:J:78:THR:HG21  | 2:J:133:LEU:HA   | 2.01                     | 0.41              |
| 2:J:139:GLU:C    | 2:J:140:LEU:HD23 | 2.45                     | 0.41              |
| 2:J:215:LEU:O    | 2:J:219:GLU:HG3  | 2.20                     | 0.41              |
| 2:L:124:LEU:HD13 | 2:L:148:LEU:HD21 | 2.02                     | 0.41              |
| 1:O:290:ALA:O    | 1:O:292:ALA:N    | 2.47                     | 0.41              |
| 2:P:139:GLU:C    | 2:P:140:LEU:HD23 | 2.45                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:122:HIS:NE2  | 1:S:147:ASP:OD2  | 2.53                     | 0.41              |
| 2:B:78:THR:C     | 2:B:80:GLY:H     | 2.24                     | 0.41              |
| 1:C:129:PHE:HE2  | 1:C:146:ILE:HG12 | 1.85                     | 0.41              |
| 1:C:207:LYS:HE2  | 1:C:207:LYS:HB2  | 1.86                     | 0.41              |
| 2:D:139:GLU:C    | 2:D:140:LEU:HD23 | 2.45                     | 0.41              |
| 2:F:181:ARG:O    | 2:F:185:LEU:HD13 | 2.21                     | 0.41              |
| 1:M:32:HIS:O     | 1:M:33:LEU:C     | 2.64                     | 0.41              |
| 1:Q:37:TYR:HB2   | 1:Q:60:THR:HG1   | 1.86                     | 0.41              |
| 2:R:78:THR:HG21  | 2:R:133:LEU:HA   | 2.01                     | 0.41              |
| 2:R:139:GLU:C    | 2:R:140:LEU:HD23 | 2.45                     | 0.41              |
| 1:S:39:GLY:O     | 2:T:25:LYS:HB2   | 2.20                     | 0.41              |
| 2:V:122:HIS:NE2  | 1:W:147:ASP:OD2  | 2.53                     | 0.41              |
| 1:W:129:PHE:HE2  | 1:W:146:ILE:HG12 | 1.85                     | 0.41              |
| 2:X:124:LEU:HD13 | 2:X:148:LEU:HD21 | 2.02                     | 0.41              |
| 1:Y:39:GLY:O     | 2:Z:25:LYS:HB2   | 2.20                     | 0.41              |
| 2:Z:139:GLU:C    | 2:Z:140:LEU:HD23 | 2.45                     | 0.41              |
| 2:Z:232:LYS:HB3  | 2:Z:232:LYS:HE3  | 1.90                     | 0.41              |
| 1:A:37:TYR:HB2   | 1:A:60:THR:HG1   | 1.86                     | 0.41              |
| 2:B:235:GLU:O    | 2:B:238:THR:OG1  | 2.32                     | 0.41              |
| 2:B:292:ASN:O    | 2:B:293:SER:CB   | 2.68                     | 0.41              |
| 2:L:215:LEU:O    | 2:L:219:GLU:HG3  | 2.20                     | 0.41              |
| 2:R:236:LYS:HB2  | 2:R:236:LYS:HE2  | 1.91                     | 0.41              |
| 2:F:215:LEU:O    | 2:F:219:GLU:HG3  | 2.20                     | 0.41              |
| 1:G:129:PHE:HE2  | 1:G:146:ILE:HG12 | 1.85                     | 0.41              |
| 2:H:139:GLU:C    | 2:H:140:LEU:HD23 | 2.45                     | 0.41              |
| 1:K:129:PHE:HE2  | 1:K:146:ILE:HG12 | 1.86                     | 0.41              |
| 2:P:284:MET:HG3  | 1:Q:285:LEU:HD11 | 2.03                     | 0.41              |
| 1:Q:39:GLY:O     | 2:R:25:LYS:HB2   | 2.20                     | 0.41              |
| 2:R:78:THR:HA    | 2:R:128:CYS:O    | 2.21                     | 0.41              |
| 2:V:78:THR:C     | 2:V:80:GLY:H     | 2.24                     | 0.41              |
| 1:Y:38:ARG:HG3   | 1:Y:58:ILE:HG22  | 2.01                     | 0.41              |
| 1:Y:161:MET:HE2  | 1:Y:161:MET:HB3  | 1.80                     | 0.41              |
| 2:B:38:GLY:O     | 1:C:30:GLU:N     | 2.54                     | 0.41              |
| 2:B:181:ARG:O    | 2:B:185:LEU:HD13 | 2.21                     | 0.41              |
| 1:I:32:HIS:O     | 1:I:33:LEU:C     | 2.64                     | 0.41              |
| 1:K:39:GLY:O     | 2:L:25:LYS:HB2   | 2.20                     | 0.41              |
| 1:M:39:GLY:O     | 2:N:25:LYS:HB2   | 2.20                     | 0.41              |
| 2:N:277:THR:HA   | 2:N:278:PRO:HD3  | 1.97                     | 0.41              |
| 1:O:39:GLY:O     | 2:P:25:LYS:HB2   | 2.20                     | 0.41              |
| 2:T:205:LYS:HB2  | 2:T:205:LYS:HE2  | 1.93                     | 0.41              |
| 1:U:32:HIS:O     | 1:U:33:LEU:C     | 2.64                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:39:GLY:O     | 2:V:25:LYS:HB2   | 2.20                     | 0.41              |
| 2:V:182:ASN:ND2  | 1:W:193:THR:OG1  | 2.53                     | 0.41              |
| 2:V:276:LEU:HA   | 2:V:276:LEU:HD23 | 1.60                     | 0.41              |
| 1:W:277:LYS:HE2  | 1:W:282:TYR:CZ   | 2.56                     | 0.41              |
| 1:A:129:PHE:HE2  | 1:A:146:ILE:HG12 | 1.85                     | 0.41              |
| 1:C:236:MET:HE2  | 1:C:236:MET:HB3  | 1.97                     | 0.41              |
| 2:F:186:MET:HB3  | 2:F:186:MET:HE3  | 1.82                     | 0.41              |
| 1:G:39:GLY:O     | 2:H:25:LYS:HB2   | 2.20                     | 0.41              |
| 1:I:39:GLY:O     | 2:J:25:LYS:HB2   | 2.20                     | 0.41              |
| 1:Q:32:HIS:O     | 1:Q:33:LEU:C     | 2.64                     | 0.41              |
| 1:S:234:LYS:HB3  | 1:S:234:LYS:HE3  | 1.94                     | 0.41              |
| 2:T:124:LEU:HD13 | 2:T:148:LEU:HD21 | 2.02                     | 0.41              |
| 2:T:139:GLU:C    | 2:T:140:LEU:HD23 | 2.45                     | 0.41              |
| 1:C:174:LYS:HA   | 1:C:175:PRO:HD3  | 1.95                     | 0.41              |
| 2:F:236:LYS:HB2  | 2:F:236:LYS:HE2  | 1.90                     | 0.41              |
| 2:J:181:ARG:O    | 2:J:185:LEU:HD13 | 2.21                     | 0.41              |
| 1:O:161:MET:HE2  | 1:O:161:MET:HB3  | 1.81                     | 0.41              |
| 2:P:215:LEU:O    | 2:P:219:GLU:HG3  | 2.21                     | 0.41              |
| 1:S:129:PHE:HE2  | 1:S:146:ILE:HG12 | 1.86                     | 0.41              |
| 1:U:277:LYS:HE2  | 1:U:282:TYR:CZ   | 2.56                     | 0.41              |
| 2:V:172:LYS:HA   | 2:V:173:PRO:HD3  | 1.89                     | 0.41              |
| 2:X:284:MET:HG3  | 1:Y:285:LEU:HD11 | 2.03                     | 0.41              |
| 1:Y:119:PHE:N    | 1:Y:119:PHE:CD1  | 2.85                     | 0.41              |
| 1:A:174:LYS:HA   | 1:A:175:PRO:HD3  | 1.95                     | 0.41              |
| 1:A:236:MET:HE2  | 1:A:236:MET:HB3  | 1.97                     | 0.41              |
| 2:B:124:LEU:HD13 | 2:B:148:LEU:HD21 | 2.02                     | 0.41              |
| 2:B:139:GLU:C    | 2:B:140:LEU:HD23 | 2.45                     | 0.41              |
| 2:D:181:ARG:O    | 2:D:185:LEU:HD13 | 2.21                     | 0.41              |
| 1:E:39:GLY:O     | 2:F:25:LYS:HB2   | 2.20                     | 0.41              |
| 1:E:56:PRO:C     | 1:E:58:ILE:H     | 2.29                     | 0.41              |
| 1:E:277:LYS:HE2  | 1:E:282:TYR:CZ   | 2.56                     | 0.41              |
| 2:H:78:THR:HG21  | 2:H:133:LEU:HA   | 2.01                     | 0.41              |
| 1:M:129:PHE:HE2  | 1:M:146:ILE:HG12 | 1.85                     | 0.41              |
| 2:N:276:LEU:HD23 | 2:N:276:LEU:HA   | 1.60                     | 0.41              |
| 1:Q:129:PHE:HE2  | 1:Q:146:ILE:HG12 | 1.85                     | 0.41              |
| 2:R:188:SER:O    | 2:R:191:THR:OG1  | 2.34                     | 0.41              |
| 2:T:78:THR:HA    | 2:T:128:CYS:O    | 2.21                     | 0.41              |
| 2:T:78:THR:HG21  | 2:T:133:LEU:HA   | 2.01                     | 0.41              |
| 1:W:32:HIS:O     | 1:W:33:LEU:C     | 2.64                     | 0.41              |
| 1:A:56:PRO:C     | 1:A:58:ILE:H     | 2.29                     | 0.41              |
| 2:D:133:LEU:HD11 | 2:D:175:ILE:HG13 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:172:LYS:HA   | 2:F:173:PRO:HD3  | 1.89                     | 0.41              |
| 2:H:181:ARG:O    | 2:H:185:LEU:HD13 | 2.21                     | 0.41              |
| 1:I:72:GLU:OE1   | 1:I:74:LYS:HG2   | 2.21                     | 0.41              |
| 1:I:129:PHE:HE2  | 1:I:146:ILE:HG12 | 1.85                     | 0.41              |
| 2:J:124:LEU:HD13 | 2:J:148:LEU:HD21 | 2.02                     | 0.41              |
| 1:K:37:TYR:HB2   | 1:K:60:THR:HG1   | 1.86                     | 0.41              |
| 2:L:181:ARG:O    | 2:L:185:LEU:HD13 | 2.21                     | 0.41              |
| 2:N:145:ASP:HB2  | 2:N:168:VAL:O    | 2.21                     | 0.41              |
| 2:N:215:LEU:O    | 2:N:219:GLU:HG3  | 2.21                     | 0.41              |
| 2:N:235:GLU:O    | 2:N:238:THR:OG1  | 2.32                     | 0.41              |
| 2:P:236:LYS:HB2  | 2:P:236:LYS:HE2  | 1.91                     | 0.41              |
| 1:Q:161:MET:HE2  | 1:Q:161:MET:HB3  | 1.80                     | 0.41              |
| 2:R:124:LEU:HD13 | 2:R:148:LEU:HD21 | 2.02                     | 0.41              |
| 2:R:145:ASP:HB2  | 2:R:168:VAL:O    | 2.21                     | 0.41              |
| 2:R:182:ASN:ND2  | 1:S:193:THR:OG1  | 2.53                     | 0.41              |
| 1:S:277:LYS:HE2  | 1:S:282:TYR:CZ   | 2.56                     | 0.41              |
| 2:T:215:LEU:O    | 2:T:219:GLU:HG3  | 2.21                     | 0.41              |
| 2:V:215:LEU:O    | 2:V:219:GLU:HG3  | 2.20                     | 0.41              |
| 2:X:78:THR:HA    | 2:X:128:CYS:O    | 2.21                     | 0.41              |
| 2:X:133:LEU:HD11 | 2:X:175:ILE:HG13 | 2.03                     | 0.41              |
| 2:X:215:LEU:O    | 2:X:219:GLU:HG3  | 2.20                     | 0.41              |
| 1:Y:147:ASP:OD1  | 1:Y:147:ASP:C    | 2.64                     | 0.41              |
| 1:Y:277:LYS:HE2  | 1:Y:282:TYR:CZ   | 2.56                     | 0.41              |
| 1:A:147:ASP:OD2  | 2:Z:122:HIS:NE2  | 2.54                     | 0.41              |
| 2:B:133:LEU:HD11 | 2:B:175:ILE:HG13 | 2.03                     | 0.41              |
| 1:C:39:GLY:O     | 2:D:25:LYS:HB2   | 2.20                     | 0.41              |
| 1:C:277:LYS:HE2  | 1:C:282:TYR:CZ   | 2.56                     | 0.41              |
| 2:D:215:LEU:O    | 2:D:219:GLU:HG3  | 2.20                     | 0.41              |
| 1:E:32:HIS:O     | 1:E:33:LEU:C     | 2.64                     | 0.41              |
| 1:E:72:GLU:OE1   | 1:E:74:LYS:HG2   | 2.21                     | 0.41              |
| 1:K:207:LYS:HE2  | 1:K:207:LYS:HB2  | 1.86                     | 0.41              |
| 1:K:277:LYS:HE2  | 1:K:282:TYR:CZ   | 2.56                     | 0.41              |
| 1:M:72:GLU:OE1   | 1:M:74:LYS:HG2   | 2.21                     | 0.41              |
| 1:O:72:GLU:OE1   | 1:O:74:LYS:HG2   | 2.21                     | 0.41              |
| 2:P:78:THR:HA    | 2:P:128:CYS:O    | 2.21                     | 0.41              |
| 2:P:181:ARG:O    | 2:P:185:LEU:HD13 | 2.21                     | 0.41              |
| 1:Q:236:MET:HE2  | 1:Q:236:MET:HB3  | 1.97                     | 0.41              |
| 2:R:181:ARG:O    | 2:R:185:LEU:HD13 | 2.21                     | 0.41              |
| 2:R:215:LEU:O    | 2:R:219:GLU:HG3  | 2.20                     | 0.41              |
| 1:S:32:HIS:O     | 1:S:33:LEU:C     | 2.64                     | 0.41              |
| 2:V:78:THR:HA    | 2:V:128:CYS:O    | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:147:ASP:OD1  | 1:W:147:ASP:C    | 2.64                     | 0.41              |
| 2:Z:181:ARG:O    | 2:Z:185:LEU:HD13 | 2.21                     | 0.41              |
| 1:A:147:ASP:OD1  | 1:A:147:ASP:C    | 2.64                     | 0.40              |
| 1:A:277:LYS:HE2  | 1:A:282:TYR:CZ   | 2.56                     | 0.40              |
| 1:A:285:LEU:HD11 | 2:Z:284:MET:HG3  | 2.03                     | 0.40              |
| 1:C:147:ASP:OD1  | 1:C:147:ASP:C    | 2.64                     | 0.40              |
| 2:H:145:ASP:HB2  | 2:H:168:VAL:O    | 2.21                     | 0.40              |
| 2:L:276:LEU:HA   | 2:L:276:LEU:HD23 | 1.60                     | 0.40              |
| 2:N:78:THR:HA    | 2:N:128:CYS:O    | 2.21                     | 0.40              |
| 1:Q:96:MET:HE2   | 1:Q:96:MET:HB3   | 1.85                     | 0.40              |
| 1:Q:277:LYS:HE2  | 1:Q:282:TYR:CZ   | 2.56                     | 0.40              |
| 2:T:181:ARG:O    | 2:T:185:LEU:HD13 | 2.21                     | 0.40              |
| 1:W:275:LYS:HB2  | 1:W:275:LYS:HE2  | 1.91                     | 0.40              |
| 2:Z:78:THR:HA    | 2:Z:128:CYS:O    | 2.21                     | 0.40              |
| 1:A:32:HIS:O     | 1:A:33:LEU:C     | 2.64                     | 0.40              |
| 2:D:188:SER:O    | 2:D:191:THR:OG1  | 2.34                     | 0.40              |
| 1:E:161:MET:HE2  | 1:E:161:MET:HB3  | 1.80                     | 0.40              |
| 2:F:145:ASP:HB2  | 2:F:168:VAL:O    | 2.21                     | 0.40              |
| 2:F:205:LYS:HB2  | 2:F:205:LYS:HE2  | 1.93                     | 0.40              |
| 1:G:56:PRO:C     | 1:G:58:ILE:H     | 2.29                     | 0.40              |
| 1:G:277:LYS:HE2  | 1:G:282:TYR:CZ   | 2.56                     | 0.40              |
| 2:H:275:LYS:HE3  | 2:H:275:LYS:HB2  | 1.87                     | 0.40              |
| 2:J:145:ASP:HB2  | 2:J:168:VAL:O    | 2.21                     | 0.40              |
| 2:L:145:ASP:HB2  | 2:L:168:VAL:O    | 2.21                     | 0.40              |
| 2:P:124:LEU:HD13 | 2:P:148:LEU:HD21 | 2.02                     | 0.40              |
| 1:S:72:GLU:OE1   | 1:S:74:LYS:HG2   | 2.21                     | 0.40              |
| 1:U:147:ASP:OD1  | 1:U:147:ASP:C    | 2.65                     | 0.40              |
| 1:W:37:TYR:HB2   | 1:W:60:THR:HG1   | 1.86                     | 0.40              |
| 1:W:56:PRO:C     | 1:W:58:ILE:H     | 2.29                     | 0.40              |
| 2:Z:215:LEU:O    | 2:Z:219:GLU:HG3  | 2.20                     | 0.40              |
| 2:B:145:ASP:HB2  | 2:B:168:VAL:O    | 2.21                     | 0.40              |
| 1:C:56:PRO:C     | 1:C:58:ILE:H     | 2.29                     | 0.40              |
| 2:D:241:LYS:HE2  | 2:D:241:LYS:HB2  | 1.99                     | 0.40              |
| 1:E:236:MET:HE2  | 1:E:236:MET:HB3  | 1.97                     | 0.40              |
| 1:G:37:TYR:HB2   | 1:G:60:THR:HG1   | 1.86                     | 0.40              |
| 2:H:284:MET:HG3  | 1:I:285:LEU:HD11 | 2.03                     | 0.40              |
| 1:I:277:LYS:HE2  | 1:I:282:TYR:CZ   | 2.56                     | 0.40              |
| 2:P:182:ASN:ND2  | 1:Q:193:THR:OG1  | 2.54                     | 0.40              |
| 1:Q:72:GLU:OE1   | 1:Q:74:LYS:HG2   | 2.21                     | 0.40              |
| 2:R:78:THR:C     | 2:R:80:GLY:H     | 2.24                     | 0.40              |
| 1:S:147:ASP:OD1  | 1:S:147:ASP:C    | 2.64                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:276:LEU:HD23 | 2:T:276:LEU:HA   | 1.60                     | 0.40              |
| 2:V:181:ARG:O    | 2:V:185:LEU:HD13 | 2.21                     | 0.40              |
| 1:W:39:GLY:O     | 2:X:25:LYS:HB2   | 2.20                     | 0.40              |
| 2:Z:275:LYS:HE3  | 2:Z:275:LYS:HB2  | 1.87                     | 0.40              |
| 2:Z:296:TYR:C    | 2:Z:297:PHE:O    | 2.62                     | 0.40              |
| 1:E:129:PHE:HE2  | 1:E:146:ILE:HG12 | 1.85                     | 0.40              |
| 1:G:72:GLU:OE1   | 1:G:74:LYS:HG2   | 2.21                     | 0.40              |
| 2:H:236:LYS:HB2  | 2:H:236:LYS:HE2  | 1.90                     | 0.40              |
| 1:K:72:GLU:OE1   | 1:K:74:LYS:HG2   | 2.21                     | 0.40              |
| 2:L:113:LYS:HA   | 2:L:113:LYS:HD3  | 1.87                     | 0.40              |
| 2:N:181:ARG:O    | 2:N:185:LEU:HD13 | 2.21                     | 0.40              |
| 2:N:236:LYS:HB2  | 2:N:236:LYS:HE2  | 1.90                     | 0.40              |
| 1:O:277:LYS:HE2  | 1:O:282:TYR:CZ   | 2.56                     | 0.40              |
| 1:Q:56:PRO:C     | 1:Q:58:ILE:H     | 2.29                     | 0.40              |
| 1:S:236:MET:HE2  | 1:S:236:MET:HB3  | 1.97                     | 0.40              |
| 2:X:232:LYS:HB3  | 2:X:232:LYS:HE3  | 1.90                     | 0.40              |
| 1:Y:189:GLU:O    | 1:Y:193:THR:HG23 | 2.22                     | 0.40              |
| 1:Y:236:MET:HE2  | 1:Y:236:MET:HB3  | 1.97                     | 0.40              |
| 2:Z:296:TYR:O    | 2:Z:297:PHE:O    | 2.39                     | 0.40              |
| 1:A:104:ASP:O    | 1:A:107:ARG:HG2  | 2.21                     | 0.40              |
| 1:A:189:GLU:O    | 1:A:193:THR:HG23 | 2.22                     | 0.40              |
| 1:E:147:ASP:OD1  | 1:E:147:ASP:C    | 2.64                     | 0.40              |
| 1:K:234:LYS:HB3  | 1:K:234:LYS:HE3  | 1.94                     | 0.40              |
| 2:L:78:THR:HA    | 2:L:128:CYS:O    | 2.21                     | 0.40              |
| 1:M:189:GLU:O    | 1:M:193:THR:HG23 | 2.21                     | 0.40              |
| 1:M:277:LYS:HE2  | 1:M:282:TYR:CZ   | 2.56                     | 0.40              |
| 1:O:32:HIS:O     | 1:O:33:LEU:C     | 2.64                     | 0.40              |
| 2:P:145:ASP:HB2  | 2:P:168:VAL:O    | 2.21                     | 0.40              |
| 1:Q:147:ASP:OD1  | 1:Q:147:ASP:C    | 2.64                     | 0.40              |
| 1:Q:290:ALA:O    | 1:Q:292:ALA:N    | 2.47                     | 0.40              |
| 2:X:145:ASP:HB2  | 2:X:168:VAL:O    | 2.21                     | 0.40              |
| 2:X:181:ARG:O    | 2:X:185:LEU:HD13 | 2.21                     | 0.40              |
| 1:Y:129:PHE:HE2  | 1:Y:146:ILE:HG12 | 1.85                     | 0.40              |
| 1:Y:174:LYS:HA   | 1:Y:175:PRO:HD3  | 1.95                     | 0.40              |
| 1:Y:207:LYS:HB2  | 1:Y:207:LYS:HE2  | 1.86                     | 0.40              |
| 2:Z:186:MET:HE3  | 2:Z:186:MET:HB3  | 1.82                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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     | 276/278 (99%) | 261 (95%) | 12 (4%) | 3 (1%)   | 11          | 34 |
| 1   | C     | 275/278 (99%) | 261 (95%) | 10 (4%) | 4 (2%)   | 8           | 28 |
| 1   | E     | 275/278 (99%) | 261 (95%) | 10 (4%) | 4 (2%)   | 8           | 28 |
| 1   | G     | 275/278 (99%) | 261 (95%) | 10 (4%) | 4 (2%)   | 8           | 28 |
| 1   | I     | 275/278 (99%) | 261 (95%) | 10 (4%) | 4 (2%)   | 8           | 28 |
| 1   | K     | 275/278 (99%) | 261 (95%) | 10 (4%) | 4 (2%)   | 8           | 28 |
| 1   | M     | 275/278 (99%) | 261 (95%) | 10 (4%) | 4 (2%)   | 8           | 28 |
| 1   | O     | 275/278 (99%) | 261 (95%) | 10 (4%) | 4 (2%)   | 8           | 28 |
| 1   | Q     | 275/278 (99%) | 261 (95%) | 10 (4%) | 4 (2%)   | 8           | 28 |
| 1   | S     | 275/278 (99%) | 261 (95%) | 10 (4%) | 4 (2%)   | 8           | 28 |
| 1   | U     | 275/278 (99%) | 261 (95%) | 10 (4%) | 4 (2%)   | 8           | 28 |
| 1   | W     | 275/278 (99%) | 261 (95%) | 10 (4%) | 4 (2%)   | 8           | 28 |
| 1   | Y     | 275/278 (99%) | 261 (95%) | 10 (4%) | 4 (2%)   | 8           | 28 |
| 2   | B     | 275/277 (99%) | 258 (94%) | 12 (4%) | 5 (2%)   | 6           | 24 |
| 2   | D     | 275/277 (99%) | 263 (96%) | 8 (3%)  | 4 (2%)   | 8           | 28 |
| 2   | F     | 275/277 (99%) | 263 (96%) | 8 (3%)  | 4 (2%)   | 8           | 28 |
| 2   | H     | 275/277 (99%) | 263 (96%) | 8 (3%)  | 4 (2%)   | 8           | 28 |
| 2   | J     | 275/277 (99%) | 263 (96%) | 8 (3%)  | 4 (2%)   | 8           | 28 |
| 2   | L     | 275/277 (99%) | 263 (96%) | 8 (3%)  | 4 (2%)   | 8           | 28 |
| 2   | N     | 275/277 (99%) | 263 (96%) | 8 (3%)  | 4 (2%)   | 8           | 28 |
| 2   | P     | 275/277 (99%) | 263 (96%) | 8 (3%)  | 4 (2%)   | 8           | 28 |
| 2   | R     | 275/277 (99%) | 263 (96%) | 8 (3%)  | 4 (2%)   | 8           | 28 |
| 2   | T     | 275/277 (99%) | 263 (96%) | 8 (3%)  | 4 (2%)   | 8           | 28 |
| 2   | V     | 275/277 (99%) | 263 (96%) | 8 (3%)  | 4 (2%)   | 8           | 28 |
| 2   | X     | 275/277 (99%) | 263 (96%) | 8 (3%)  | 4 (2%)   | 8           | 28 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 2   | Z     | 275/277 (99%)   | 262 (95%)  | 9 (3%)   | 4 (2%)   | 8           | 28 |
| All | All   | 7151/7215 (99%) | 6806 (95%) | 241 (3%) | 104 (2%) | 11          | 28 |

All (104) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 297 | ILE  |
| 2   | B     | 292 | ASN  |
| 2   | B     | 294 | LYS  |
| 1   | C     | 296 | LYS  |
| 1   | C     | 297 | ILE  |
| 2   | D     | 293 | SER  |
| 2   | D     | 295 | ILE  |
| 2   | F     | 293 | SER  |
| 2   | F     | 295 | ILE  |
| 2   | H     | 293 | SER  |
| 2   | H     | 295 | ILE  |
| 2   | J     | 293 | SER  |
| 2   | J     | 295 | ILE  |
| 2   | L     | 293 | SER  |
| 2   | L     | 295 | ILE  |
| 2   | N     | 293 | SER  |
| 2   | N     | 295 | ILE  |
| 2   | P     | 293 | SER  |
| 2   | P     | 295 | ILE  |
| 2   | R     | 293 | SER  |
| 2   | R     | 295 | ILE  |
| 2   | T     | 293 | SER  |
| 2   | T     | 295 | ILE  |
| 2   | V     | 293 | SER  |
| 2   | V     | 295 | ILE  |
| 2   | X     | 293 | SER  |
| 2   | X     | 295 | ILE  |
| 1   | A     | 291 | ILE  |
| 2   | B     | 79  | SER  |
| 1   | C     | 291 | ILE  |
| 2   | D     | 79  | SER  |
| 2   | D     | 292 | ASN  |
| 1   | E     | 291 | ILE  |
| 1   | E     | 297 | ILE  |
| 2   | F     | 79  | SER  |
| 2   | F     | 292 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 291 | ILE  |
| 1   | G     | 297 | ILE  |
| 2   | H     | 79  | SER  |
| 2   | H     | 292 | ASN  |
| 1   | I     | 291 | ILE  |
| 1   | I     | 297 | ILE  |
| 2   | J     | 79  | SER  |
| 2   | J     | 292 | ASN  |
| 1   | K     | 291 | ILE  |
| 1   | K     | 297 | ILE  |
| 2   | L     | 79  | SER  |
| 2   | L     | 292 | ASN  |
| 1   | M     | 291 | ILE  |
| 1   | M     | 297 | ILE  |
| 2   | N     | 79  | SER  |
| 2   | N     | 292 | ASN  |
| 1   | O     | 291 | ILE  |
| 1   | O     | 297 | ILE  |
| 2   | P     | 79  | SER  |
| 2   | P     | 292 | ASN  |
| 1   | Q     | 291 | ILE  |
| 1   | Q     | 297 | ILE  |
| 2   | R     | 79  | SER  |
| 2   | R     | 292 | ASN  |
| 1   | S     | 291 | ILE  |
| 1   | S     | 297 | ILE  |
| 2   | T     | 79  | SER  |
| 2   | T     | 292 | ASN  |
| 1   | U     | 291 | ILE  |
| 1   | U     | 297 | ILE  |
| 2   | V     | 79  | SER  |
| 2   | V     | 292 | ASN  |
| 1   | W     | 291 | ILE  |
| 1   | W     | 297 | ILE  |
| 2   | X     | 79  | SER  |
| 2   | X     | 292 | ASN  |
| 1   | Y     | 291 | ILE  |
| 1   | Y     | 297 | ILE  |
| 2   | Z     | 79  | SER  |
| 2   | Z     | 292 | ASN  |
| 2   | Z     | 293 | SER  |
| 2   | B     | 293 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 295 | SER  |
| 1   | E     | 298 | TYR  |
| 1   | G     | 295 | SER  |
| 1   | G     | 298 | TYR  |
| 1   | I     | 295 | SER  |
| 1   | I     | 298 | TYR  |
| 1   | K     | 295 | SER  |
| 1   | K     | 298 | TYR  |
| 1   | M     | 295 | SER  |
| 1   | M     | 298 | TYR  |
| 1   | O     | 295 | SER  |
| 1   | O     | 298 | TYR  |
| 1   | Q     | 295 | SER  |
| 1   | Q     | 298 | TYR  |
| 1   | S     | 295 | SER  |
| 1   | S     | 298 | TYR  |
| 1   | U     | 295 | SER  |
| 1   | U     | 298 | TYR  |
| 1   | W     | 295 | SER  |
| 1   | W     | 298 | TYR  |
| 1   | Y     | 295 | SER  |
| 1   | Y     | 298 | TYR  |
| 1   | A     | 296 | LYS  |
| 2   | B     | 295 | ILE  |
| 1   | C     | 294 | ASN  |
| 2   | Z     | 295 | ILE  |

### 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     | 235/239 (98%) | 228 (97%) | 7 (3%)   | 36          | 62 |
| 1   | C     | 234/239 (98%) | 229 (98%) | 5 (2%)   | 47          | 68 |
| 1   | E     | 234/239 (98%) | 230 (98%) | 4 (2%)   | 53          | 71 |
| 1   | G     | 234/239 (98%) | 231 (99%) | 3 (1%)   | 61          | 74 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | I     | 234/239 (98%)   | 230 (98%)  | 4 (2%)   | 53          | 71  |
| 1   | K     | 234/239 (98%)   | 231 (99%)  | 3 (1%)   | 61          | 74  |
| 1   | M     | 234/239 (98%)   | 231 (99%)  | 3 (1%)   | 61          | 74  |
| 1   | O     | 234/239 (98%)   | 231 (99%)  | 3 (1%)   | 61          | 74  |
| 1   | Q     | 234/239 (98%)   | 230 (98%)  | 4 (2%)   | 53          | 71  |
| 1   | S     | 234/239 (98%)   | 230 (98%)  | 4 (2%)   | 53          | 71  |
| 1   | U     | 234/239 (98%)   | 230 (98%)  | 4 (2%)   | 53          | 71  |
| 1   | W     | 234/239 (98%)   | 231 (99%)  | 3 (1%)   | 61          | 74  |
| 1   | Y     | 234/239 (98%)   | 230 (98%)  | 4 (2%)   | 53          | 71  |
| 2   | B     | 235/239 (98%)   | 229 (97%)  | 6 (3%)   | 40          | 65  |
| 2   | D     | 235/239 (98%)   | 234 (100%) | 1 (0%)   | 84          | 84  |
| 2   | F     | 235/239 (98%)   | 234 (100%) | 1 (0%)   | 84          | 84  |
| 2   | H     | 235/239 (98%)   | 234 (100%) | 1 (0%)   | 84          | 84  |
| 2   | J     | 235/239 (98%)   | 234 (100%) | 1 (0%)   | 84          | 84  |
| 2   | L     | 235/239 (98%)   | 234 (100%) | 1 (0%)   | 84          | 84  |
| 2   | N     | 235/239 (98%)   | 234 (100%) | 1 (0%)   | 84          | 84  |
| 2   | P     | 235/239 (98%)   | 234 (100%) | 1 (0%)   | 84          | 84  |
| 2   | R     | 235/239 (98%)   | 234 (100%) | 1 (0%)   | 84          | 84  |
| 2   | T     | 235/239 (98%)   | 234 (100%) | 1 (0%)   | 84          | 84  |
| 2   | V     | 235/239 (98%)   | 234 (100%) | 1 (0%)   | 84          | 84  |
| 2   | X     | 235/239 (98%)   | 234 (100%) | 1 (0%)   | 84          | 84  |
| 2   | Z     | 235/239 (98%)   | 235 (100%) | 0        | 100         | 100 |
| All | All   | 6098/6214 (98%) | 6030 (99%) | 68 (1%)  | 63          | 76  |

All (68) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 107 | ARG  |
| 1   | A     | 123 | HIS  |
| 1   | A     | 232 | GLN  |
| 1   | A     | 243 | ARG  |
| 1   | A     | 269 | LYS  |
| 1   | A     | 278 | LEU  |
| 1   | A     | 291 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 65  | THR  |
| 2   | B     | 72  | LYS  |
| 2   | B     | 88  | ARG  |
| 2   | B     | 105 | LYS  |
| 2   | B     | 119 | LYS  |
| 2   | B     | 241 | LYS  |
| 1   | C     | 30  | GLU  |
| 1   | C     | 67  | THR  |
| 1   | C     | 232 | GLN  |
| 1   | C     | 275 | LYS  |
| 1   | C     | 291 | ILE  |
| 2   | D     | 293 | SER  |
| 1   | E     | 232 | GLN  |
| 1   | E     | 278 | LEU  |
| 1   | E     | 291 | ILE  |
| 1   | E     | 294 | ASN  |
| 2   | F     | 293 | SER  |
| 1   | G     | 232 | GLN  |
| 1   | G     | 291 | ILE  |
| 1   | G     | 294 | ASN  |
| 2   | H     | 293 | SER  |
| 1   | I     | 232 | GLN  |
| 1   | I     | 278 | LEU  |
| 1   | I     | 291 | ILE  |
| 1   | I     | 294 | ASN  |
| 2   | J     | 293 | SER  |
| 1   | K     | 232 | GLN  |
| 1   | K     | 291 | ILE  |
| 1   | K     | 294 | ASN  |
| 2   | L     | 293 | SER  |
| 1   | M     | 232 | GLN  |
| 1   | M     | 291 | ILE  |
| 1   | M     | 294 | ASN  |
| 2   | N     | 293 | SER  |
| 1   | O     | 232 | GLN  |
| 1   | O     | 291 | ILE  |
| 1   | O     | 294 | ASN  |
| 2   | P     | 293 | SER  |
| 1   | Q     | 232 | GLN  |
| 1   | Q     | 278 | LEU  |
| 1   | Q     | 291 | ILE  |
| 1   | Q     | 294 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R     | 293 | SER  |
| 1   | S     | 232 | GLN  |
| 1   | S     | 278 | LEU  |
| 1   | S     | 291 | ILE  |
| 1   | S     | 294 | ASN  |
| 2   | T     | 293 | SER  |
| 1   | U     | 232 | GLN  |
| 1   | U     | 278 | LEU  |
| 1   | U     | 291 | ILE  |
| 1   | U     | 294 | ASN  |
| 2   | V     | 293 | SER  |
| 1   | W     | 232 | GLN  |
| 1   | W     | 291 | ILE  |
| 1   | W     | 294 | ASN  |
| 2   | X     | 293 | SER  |
| 1   | Y     | 232 | GLN  |
| 1   | Y     | 278 | LEU  |
| 1   | Y     | 291 | ILE  |
| 1   | Y     | 294 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 123 | HIS  |
| 1   | A     | 128 | GLN  |
| 2   | B     | 63  | GLN  |
| 2   | B     | 200 | GLN  |
| 1   | C     | 52  | HIS  |
| 1   | C     | 65  | GLN  |
| 1   | C     | 202 | GLN  |
| 2   | D     | 292 | ASN  |
| 1   | E     | 52  | HIS  |
| 1   | E     | 202 | GLN  |
| 2   | F     | 292 | ASN  |
| 1   | G     | 202 | GLN  |
| 2   | H     | 63  | GLN  |
| 2   | H     | 292 | ASN  |
| 1   | I     | 202 | GLN  |
| 2   | J     | 143 | GLN  |
| 2   | J     | 292 | ASN  |
| 1   | K     | 52  | HIS  |
| 1   | K     | 202 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 143 | GLN  |
| 2   | L     | 292 | ASN  |
| 1   | M     | 52  | HIS  |
| 1   | M     | 202 | GLN  |
| 2   | N     | 143 | GLN  |
| 2   | N     | 292 | ASN  |
| 1   | O     | 52  | HIS  |
| 1   | O     | 136 | GLN  |
| 1   | O     | 202 | GLN  |
| 2   | P     | 292 | ASN  |
| 1   | Q     | 52  | HIS  |
| 1   | Q     | 75  | ASN  |
| 1   | Q     | 202 | GLN  |
| 2   | R     | 143 | GLN  |
| 2   | R     | 292 | ASN  |
| 1   | S     | 202 | GLN  |
| 2   | T     | 143 | GLN  |
| 2   | T     | 292 | ASN  |
| 1   | U     | 75  | ASN  |
| 1   | U     | 202 | GLN  |
| 2   | V     | 63  | GLN  |
| 2   | V     | 292 | ASN  |
| 1   | W     | 52  | HIS  |
| 1   | W     | 202 | GLN  |
| 2   | X     | 292 | ASN  |
| 1   | Y     | 75  | ASN  |
| 1   | Y     | 202 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

26 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | NAG  | E     | 401 | 1    | 14,14,15     | 0.49 | 0        | 17,19,21    | 0.46 | 0        |
| 3   | NAG  | L     | 401 | 2    | 14,14,15     | 0.73 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 3   | NAG  | Y     | 401 | 1    | 14,14,15     | 0.50 | 0        | 17,19,21    | 0.45 | 0        |
| 3   | NAG  | M     | 401 | 1    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.46 | 0        |
| 3   | NAG  | W     | 401 | 1    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.46 | 0        |
| 3   | NAG  | N     | 401 | 2    | 14,14,15     | 0.73 | 1 (7%)   | 17,19,21    | 0.79 | 1 (5%)   |
| 3   | NAG  | K     | 401 | 1    | 14,14,15     | 0.46 | 0        | 17,19,21    | 0.45 | 0        |
| 3   | NAG  | R     | 401 | 2    | 14,14,15     | 0.70 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 3   | NAG  | G     | 401 | 1    | 14,14,15     | 0.47 | 0        | 17,19,21    | 0.45 | 0        |
| 3   | NAG  | B     | 401 | 2    | 14,14,15     | 0.73 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 3   | NAG  | S     | 401 | 1    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.45 | 0        |
| 3   | NAG  | Z     | 401 | 2    | 14,14,15     | 0.72 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 3   | NAG  | T     | 401 | 2    | 14,14,15     | 0.72 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 3   | NAG  | J     | 401 | 2    | 14,14,15     | 0.73 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 3   | NAG  | A     | 401 | 1    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.46 | 0        |
| 3   | NAG  | V     | 401 | 2    | 14,14,15     | 0.75 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 3   | NAG  | H     | 401 | 2    | 14,14,15     | 0.71 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 3   | NAG  | U     | 401 | 1    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.46 | 0        |
| 3   | NAG  | X     | 401 | 2    | 14,14,15     | 0.72 | 1 (7%)   | 17,19,21    | 0.79 | 1 (5%)   |
| 3   | NAG  | I     | 401 | 1    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.45 | 0        |
| 3   | NAG  | O     | 401 | 1    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.46 | 0        |
| 3   | NAG  | P     | 401 | 2    | 14,14,15     | 0.73 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 3   | NAG  | F     | 401 | 2    | 14,14,15     | 0.74 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 3   | NAG  | C     | 401 | 1    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.45 | 0        |
| 3   | NAG  | D     | 401 | 2    | 14,14,15     | 0.72 | 1 (7%)   | 17,19,21    | 0.80 | 1 (5%)   |
| 3   | NAG  | Q     | 401 | 1    | 14,14,15     | 0.50 | 0        | 17,19,21    | 0.45 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | NAG  | E     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | L     | 401 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | Y     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | M     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | W     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | N     | 401 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | K     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | R     | 401 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | G     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 401 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | S     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | Z     | 401 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | T     | 401 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | J     | 401 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | V     | 401 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | H     | 401 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | U     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | X     | 401 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | I     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | O     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | P     | 401 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | F     | 401 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | D     | 401 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | Q     | 401 | 1    | -       | 4/6/23/26 | 0/1/1/1 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | V     | 401 | NAG  | O5-C1 | -2.50 | 1.39        | 1.43     |
| 3   | F     | 401 | NAG  | O5-C1 | -2.47 | 1.39        | 1.43     |
| 3   | P     | 401 | NAG  | O5-C1 | -2.43 | 1.39        | 1.43     |
| 3   | L     | 401 | NAG  | O5-C1 | -2.42 | 1.39        | 1.43     |
| 3   | B     | 401 | NAG  | O5-C1 | -2.41 | 1.39        | 1.43     |
| 3   | T     | 401 | NAG  | O5-C1 | -2.40 | 1.39        | 1.43     |
| 3   | X     | 401 | NAG  | O5-C1 | -2.40 | 1.39        | 1.43     |
| 3   | J     | 401 | NAG  | O5-C1 | -2.39 | 1.39        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | D     | 401 | NAG  | O5-C1 | -2.39 | 1.39        | 1.43     |
| 3   | N     | 401 | NAG  | O5-C1 | -2.39 | 1.39        | 1.43     |
| 3   | Z     | 401 | NAG  | O5-C1 | -2.37 | 1.39        | 1.43     |
| 3   | H     | 401 | NAG  | O5-C1 | -2.37 | 1.39        | 1.43     |
| 3   | R     | 401 | NAG  | O5-C1 | -2.31 | 1.40        | 1.43     |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | Z     | 401 | NAG  | C3-C4-C5 | 2.54 | 114.78      | 110.24   |
| 3   | B     | 401 | NAG  | C3-C4-C5 | 2.53 | 114.75      | 110.24   |
| 3   | V     | 401 | NAG  | C3-C4-C5 | 2.52 | 114.73      | 110.24   |
| 3   | F     | 401 | NAG  | C3-C4-C5 | 2.51 | 114.72      | 110.24   |
| 3   | N     | 401 | NAG  | C3-C4-C5 | 2.51 | 114.72      | 110.24   |
| 3   | D     | 401 | NAG  | C3-C4-C5 | 2.51 | 114.72      | 110.24   |
| 3   | J     | 401 | NAG  | C3-C4-C5 | 2.50 | 114.70      | 110.24   |
| 3   | T     | 401 | NAG  | C3-C4-C5 | 2.50 | 114.70      | 110.24   |
| 3   | P     | 401 | NAG  | C3-C4-C5 | 2.49 | 114.69      | 110.24   |
| 3   | R     | 401 | NAG  | C3-C4-C5 | 2.49 | 114.69      | 110.24   |
| 3   | L     | 401 | NAG  | C3-C4-C5 | 2.48 | 114.67      | 110.24   |
| 3   | H     | 401 | NAG  | C3-C4-C5 | 2.48 | 114.67      | 110.24   |
| 3   | X     | 401 | NAG  | C3-C4-C5 | 2.48 | 114.66      | 110.24   |

There are no chirality outliers.

All (52) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | A     | 401 | NAG  | C4-C5-C6-O6 |
| 3   | C     | 401 | NAG  | C4-C5-C6-O6 |
| 3   | E     | 401 | NAG  | C4-C5-C6-O6 |
| 3   | G     | 401 | NAG  | C4-C5-C6-O6 |
| 3   | I     | 401 | NAG  | C4-C5-C6-O6 |
| 3   | K     | 401 | NAG  | C4-C5-C6-O6 |
| 3   | M     | 401 | NAG  | C4-C5-C6-O6 |
| 3   | O     | 401 | NAG  | C4-C5-C6-O6 |
| 3   | Q     | 401 | NAG  | C4-C5-C6-O6 |
| 3   | S     | 401 | NAG  | C4-C5-C6-O6 |
| 3   | U     | 401 | NAG  | C4-C5-C6-O6 |
| 3   | W     | 401 | NAG  | C4-C5-C6-O6 |
| 3   | Y     | 401 | NAG  | C4-C5-C6-O6 |
| 3   | A     | 401 | NAG  | C8-C7-N2-C2 |
| 3   | A     | 401 | NAG  | O7-C7-N2-C2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | C     | 401 | NAG  | C8-C7-N2-C2 |
| 3   | C     | 401 | NAG  | O7-C7-N2-C2 |
| 3   | E     | 401 | NAG  | C8-C7-N2-C2 |
| 3   | E     | 401 | NAG  | O7-C7-N2-C2 |
| 3   | G     | 401 | NAG  | C8-C7-N2-C2 |
| 3   | G     | 401 | NAG  | O7-C7-N2-C2 |
| 3   | I     | 401 | NAG  | C8-C7-N2-C2 |
| 3   | I     | 401 | NAG  | O7-C7-N2-C2 |
| 3   | K     | 401 | NAG  | C8-C7-N2-C2 |
| 3   | K     | 401 | NAG  | O7-C7-N2-C2 |
| 3   | M     | 401 | NAG  | C8-C7-N2-C2 |
| 3   | M     | 401 | NAG  | O7-C7-N2-C2 |
| 3   | O     | 401 | NAG  | C8-C7-N2-C2 |
| 3   | O     | 401 | NAG  | O7-C7-N2-C2 |
| 3   | Q     | 401 | NAG  | C8-C7-N2-C2 |
| 3   | Q     | 401 | NAG  | O7-C7-N2-C2 |
| 3   | S     | 401 | NAG  | C8-C7-N2-C2 |
| 3   | S     | 401 | NAG  | O7-C7-N2-C2 |
| 3   | U     | 401 | NAG  | C8-C7-N2-C2 |
| 3   | U     | 401 | NAG  | O7-C7-N2-C2 |
| 3   | W     | 401 | NAG  | C8-C7-N2-C2 |
| 3   | W     | 401 | NAG  | O7-C7-N2-C2 |
| 3   | Y     | 401 | NAG  | C8-C7-N2-C2 |
| 3   | Y     | 401 | NAG  | O7-C7-N2-C2 |
| 3   | A     | 401 | NAG  | O5-C5-C6-O6 |
| 3   | C     | 401 | NAG  | O5-C5-C6-O6 |
| 3   | E     | 401 | NAG  | O5-C5-C6-O6 |
| 3   | I     | 401 | NAG  | O5-C5-C6-O6 |
| 3   | K     | 401 | NAG  | O5-C5-C6-O6 |
| 3   | M     | 401 | NAG  | O5-C5-C6-O6 |
| 3   | O     | 401 | NAG  | O5-C5-C6-O6 |
| 3   | Q     | 401 | NAG  | O5-C5-C6-O6 |
| 3   | S     | 401 | NAG  | O5-C5-C6-O6 |
| 3   | U     | 401 | NAG  | O5-C5-C6-O6 |
| 3   | W     | 401 | NAG  | O5-C5-C6-O6 |
| 3   | Y     | 401 | NAG  | O5-C5-C6-O6 |
| 3   | G     | 401 | NAG  | O5-C5-C6-O6 |

There are no ring outliers.

13 monomers are involved in 13 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | E     | 401 | NAG  | 1       | 0            |
| 3   | Y     | 401 | NAG  | 1       | 0            |
| 3   | M     | 401 | NAG  | 1       | 0            |
| 3   | W     | 401 | NAG  | 1       | 0            |
| 3   | K     | 401 | NAG  | 1       | 0            |
| 3   | G     | 401 | NAG  | 1       | 0            |
| 3   | S     | 401 | NAG  | 1       | 0            |
| 3   | A     | 401 | NAG  | 1       | 0            |
| 3   | U     | 401 | NAG  | 1       | 0            |
| 3   | I     | 401 | NAG  | 1       | 0            |
| 3   | O     | 401 | NAG  | 1       | 0            |
| 3   | C     | 401 | NAG  | 1       | 0            |
| 3   | Q     | 401 | NAG  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

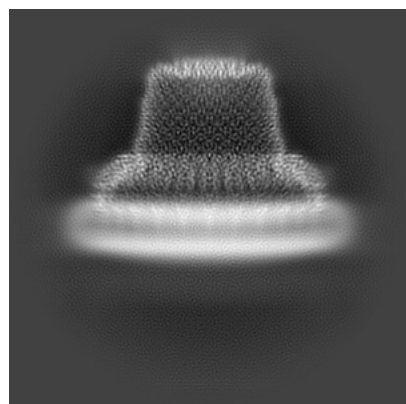
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65914. These allow visual inspection of the internal detail of the map and identification of artifacts.

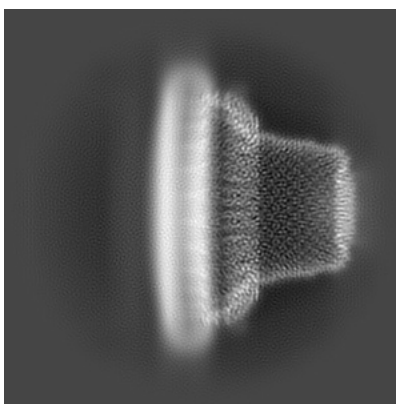
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

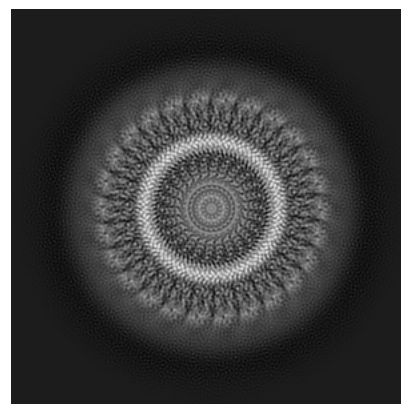
#### 6.1.1 Primary map



X

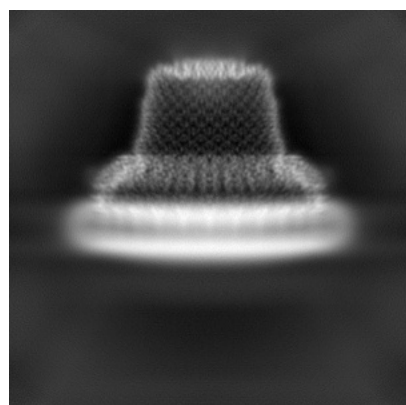


Y

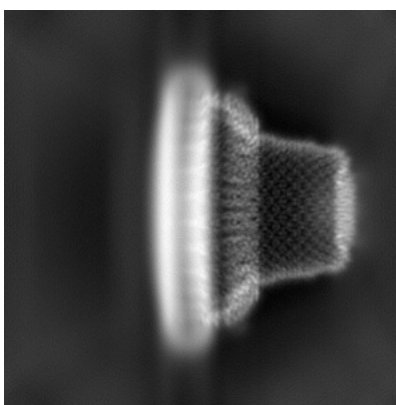


Z

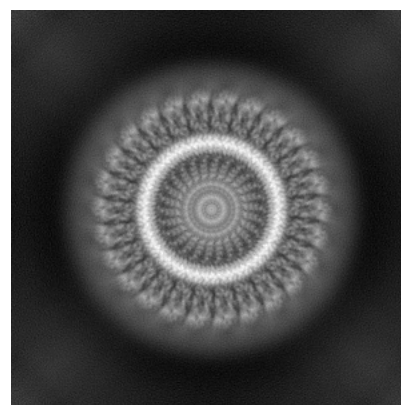
#### 6.1.2 Raw map



X



Y

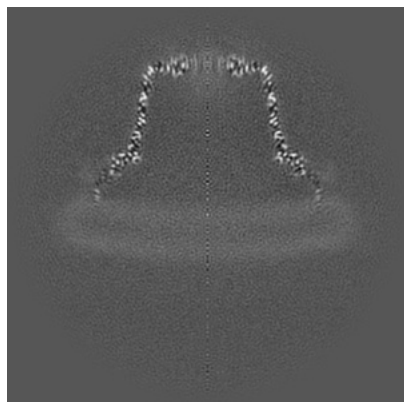


Z

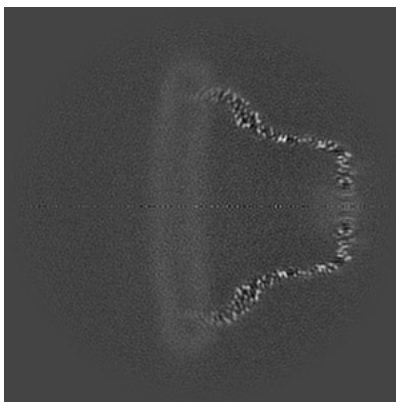
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

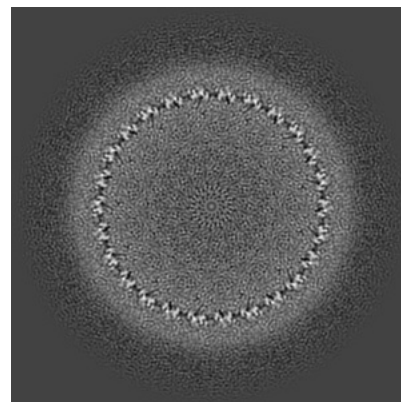
### 6.2.1 Primary map



X Index: 180

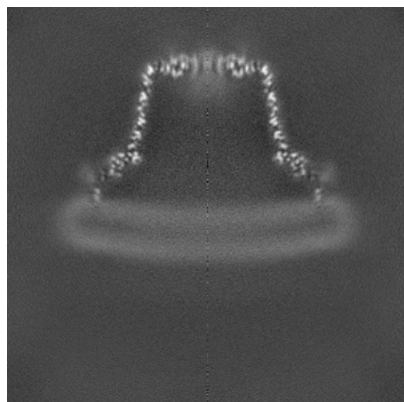


Y Index: 180

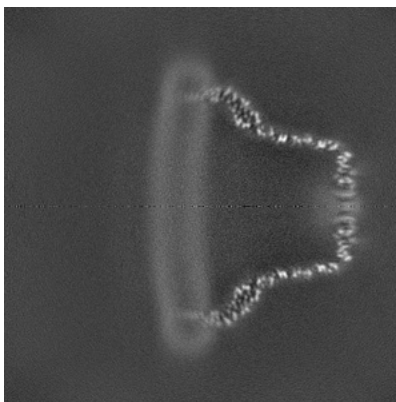


Z Index: 180

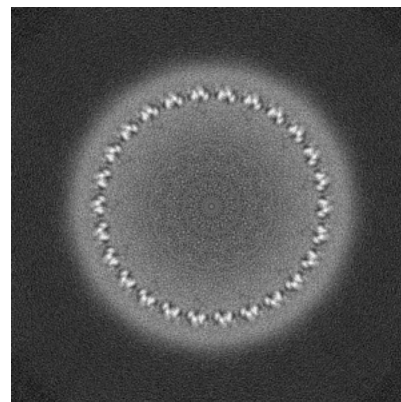
### 6.2.2 Raw map



X Index: 180



Y Index: 180

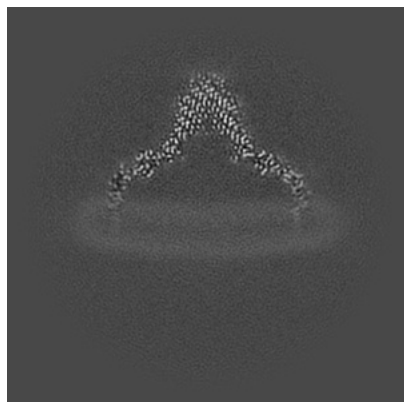


Z Index: 180

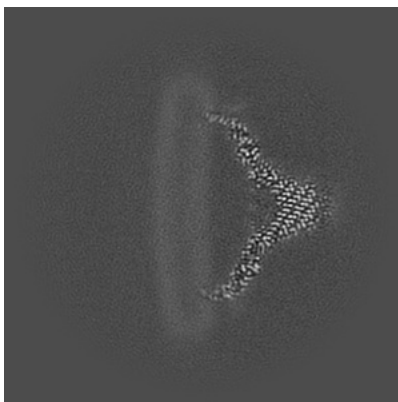
The images above show central slices of the map in three orthogonal directions.

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

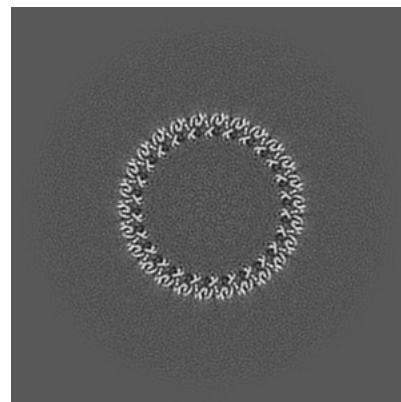
### 6.3.1 Primary map



X Index: 123

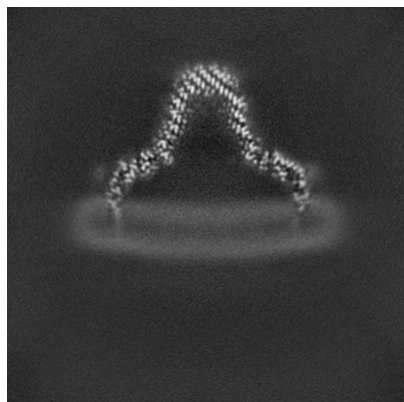


Y Index: 121

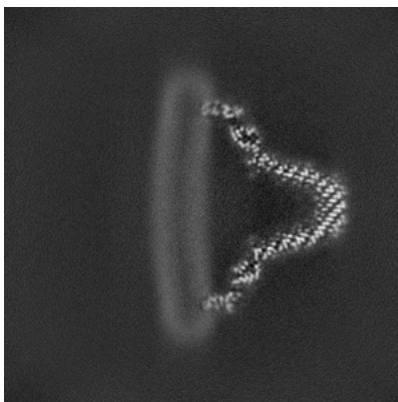


Z Index: 227

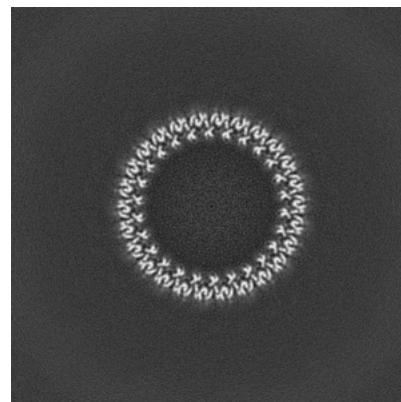
### 6.3.2 Raw map



X Index: 127



Y Index: 128

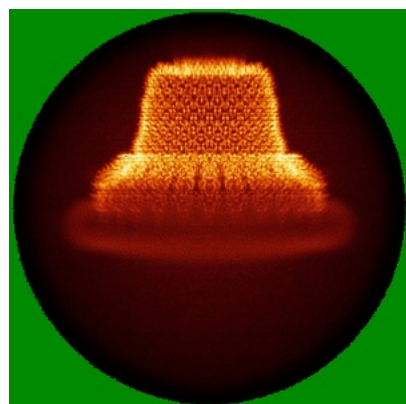


Z Index: 227

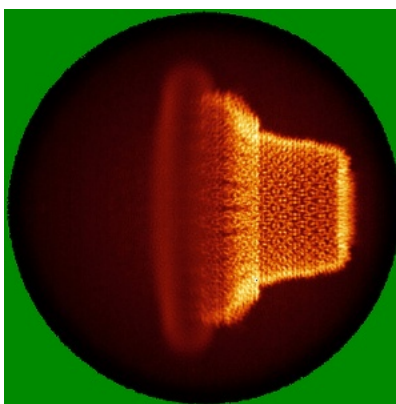
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X

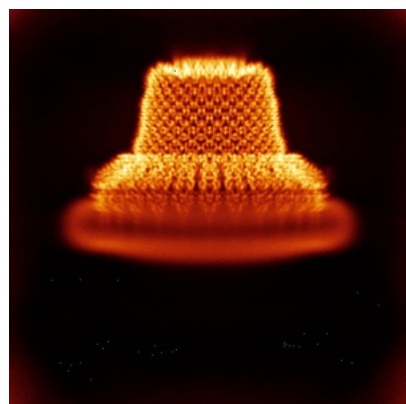


Y

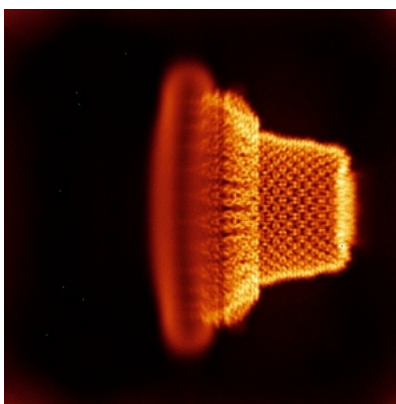


Z

### 6.4.2 Raw map



X



Y

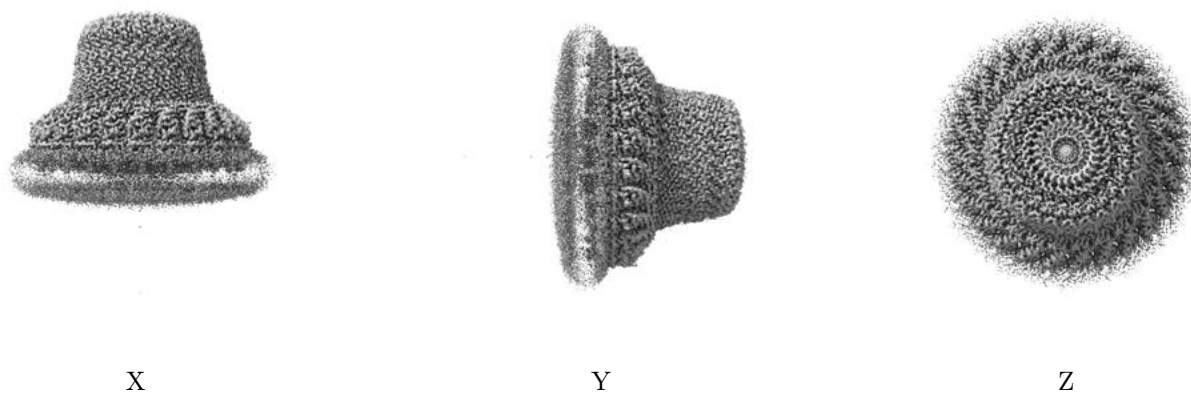


Z

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.

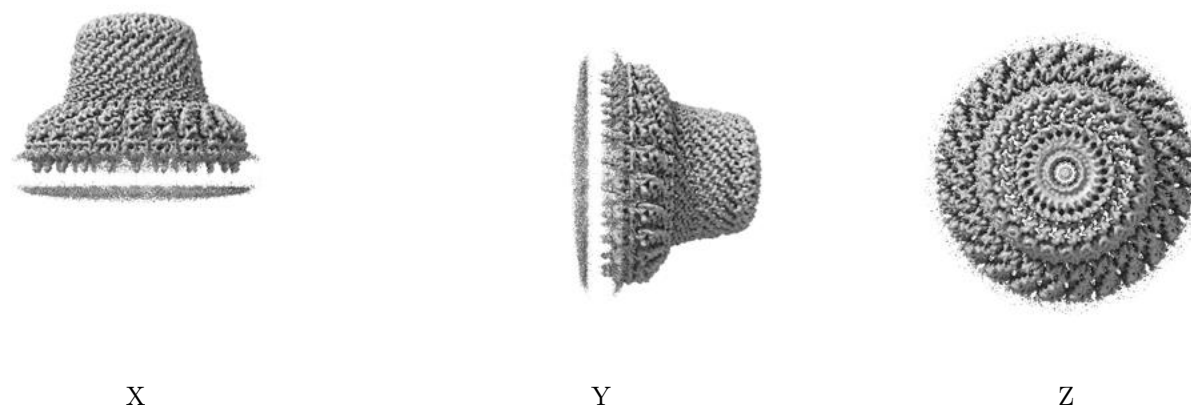
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.133. 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.

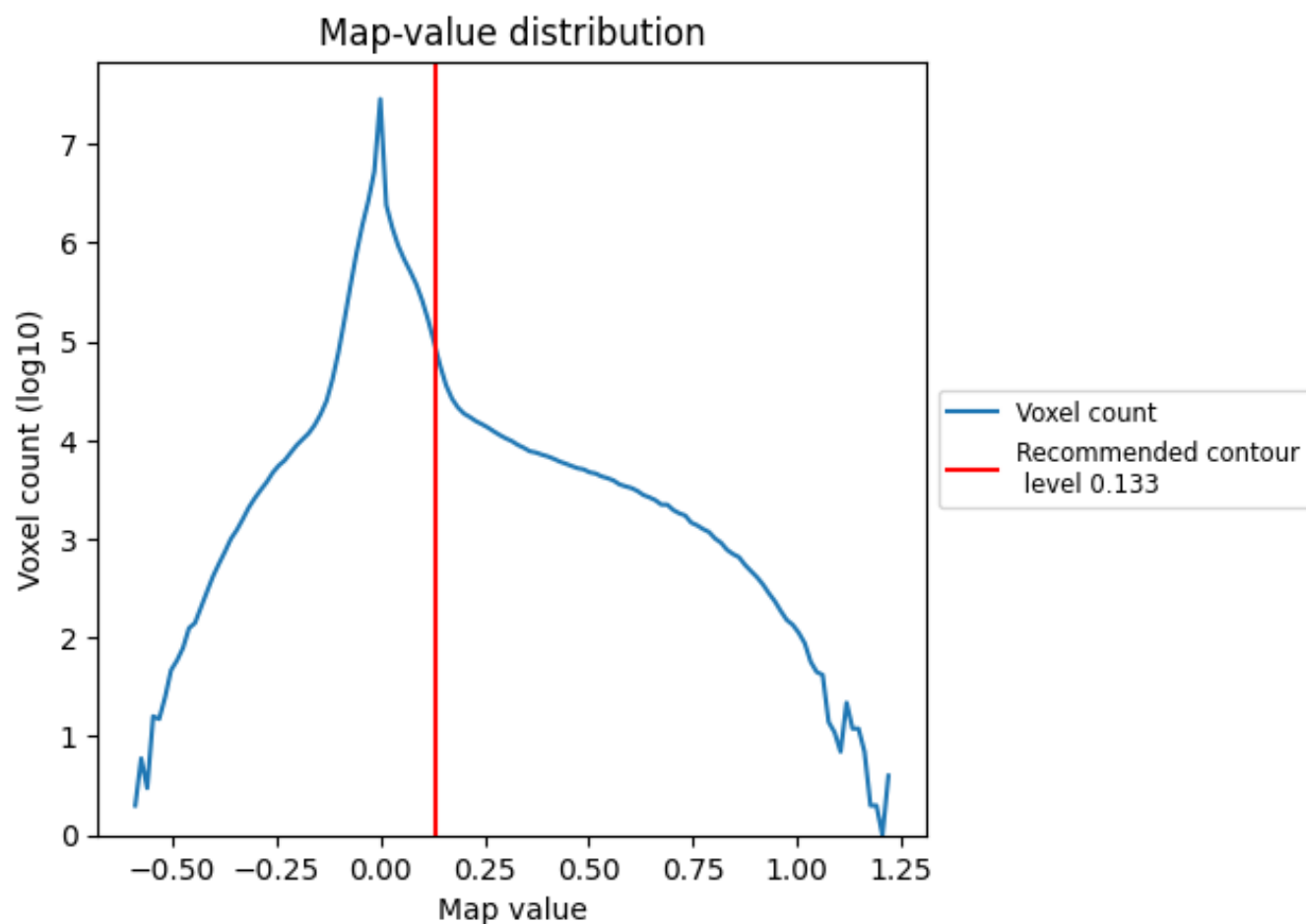
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

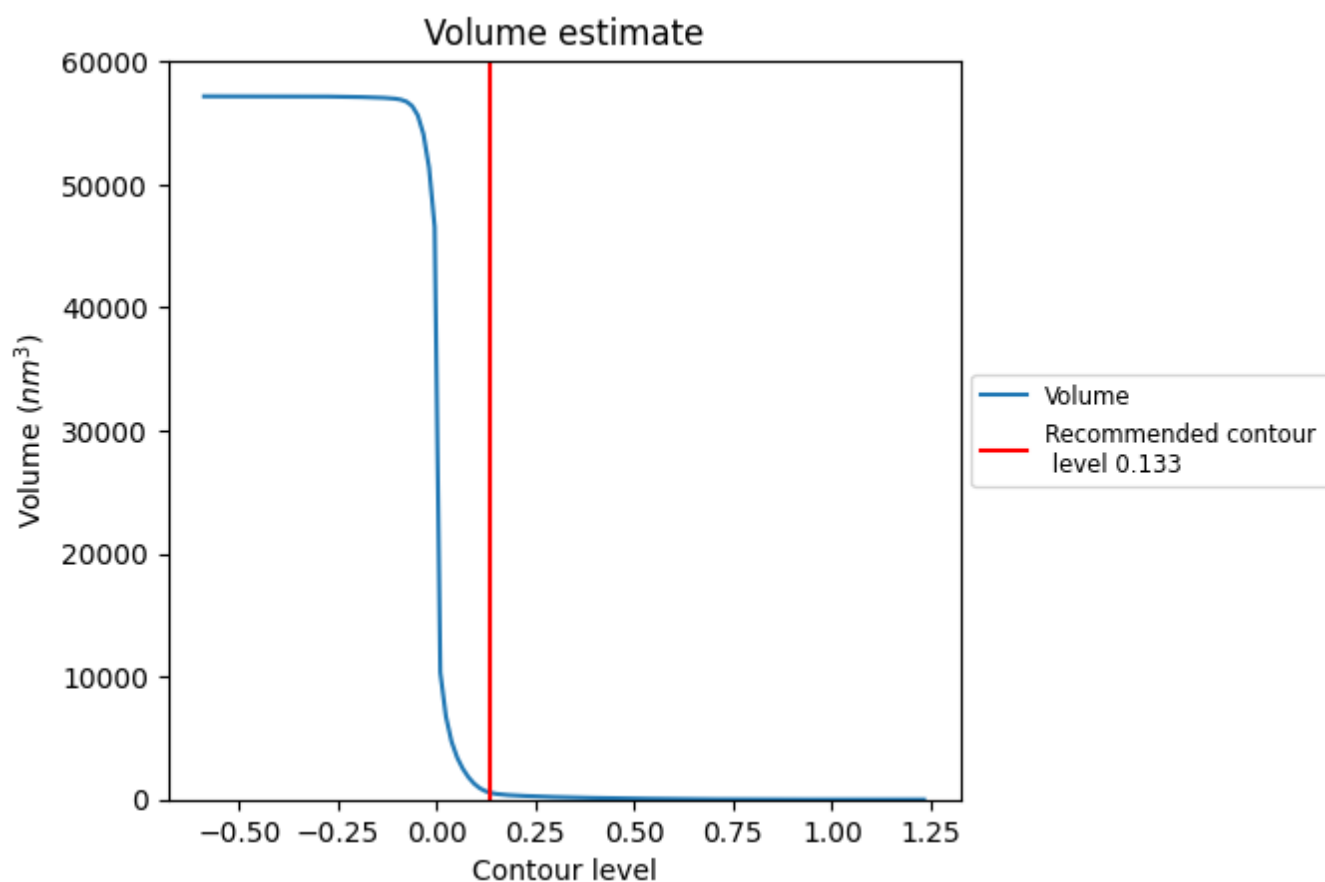
This section contains the results of statistical analysis of the map.

### 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.

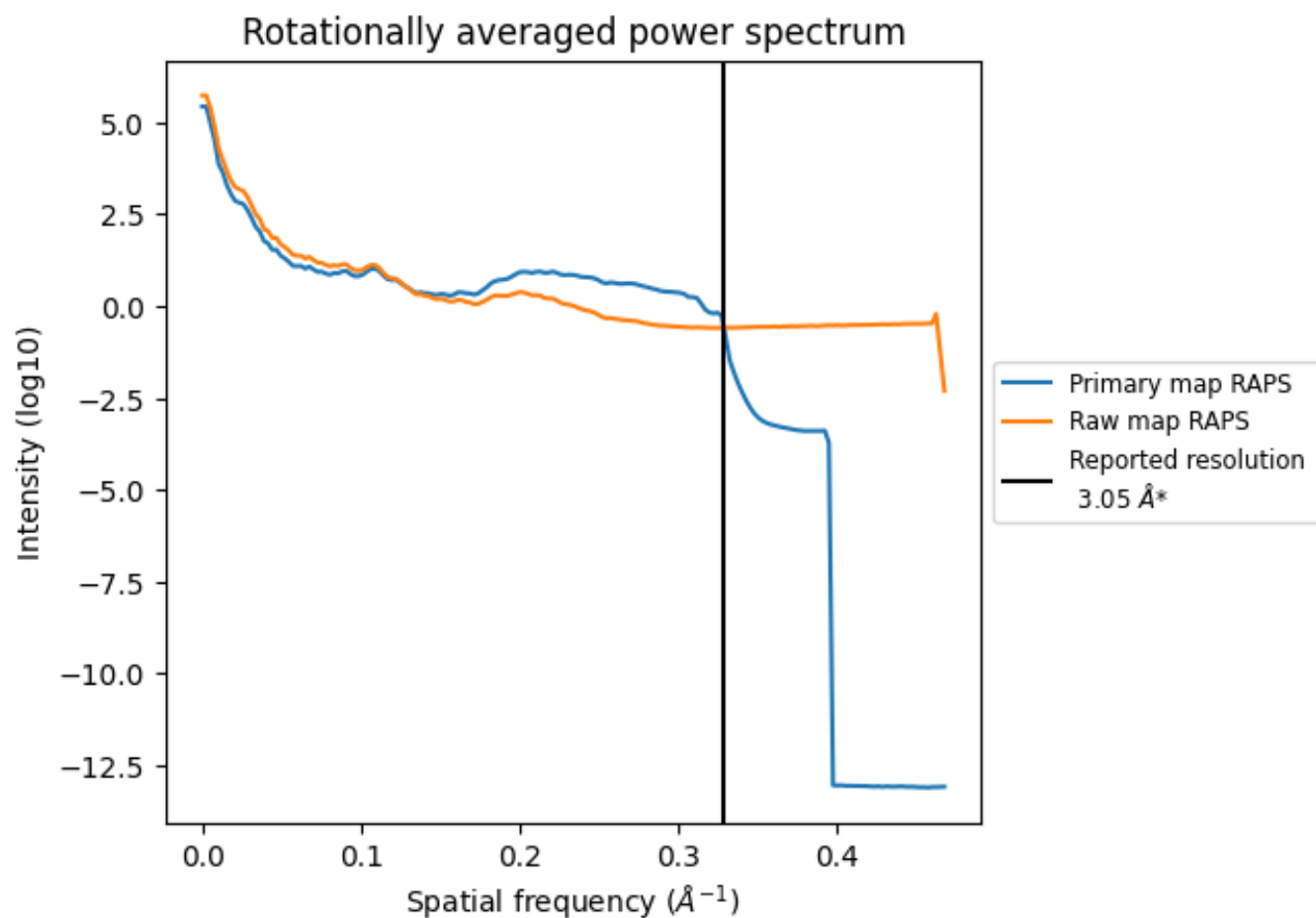
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 582 nm<sup>3</sup>; this corresponds to an approximate mass of 525 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 ⓘ

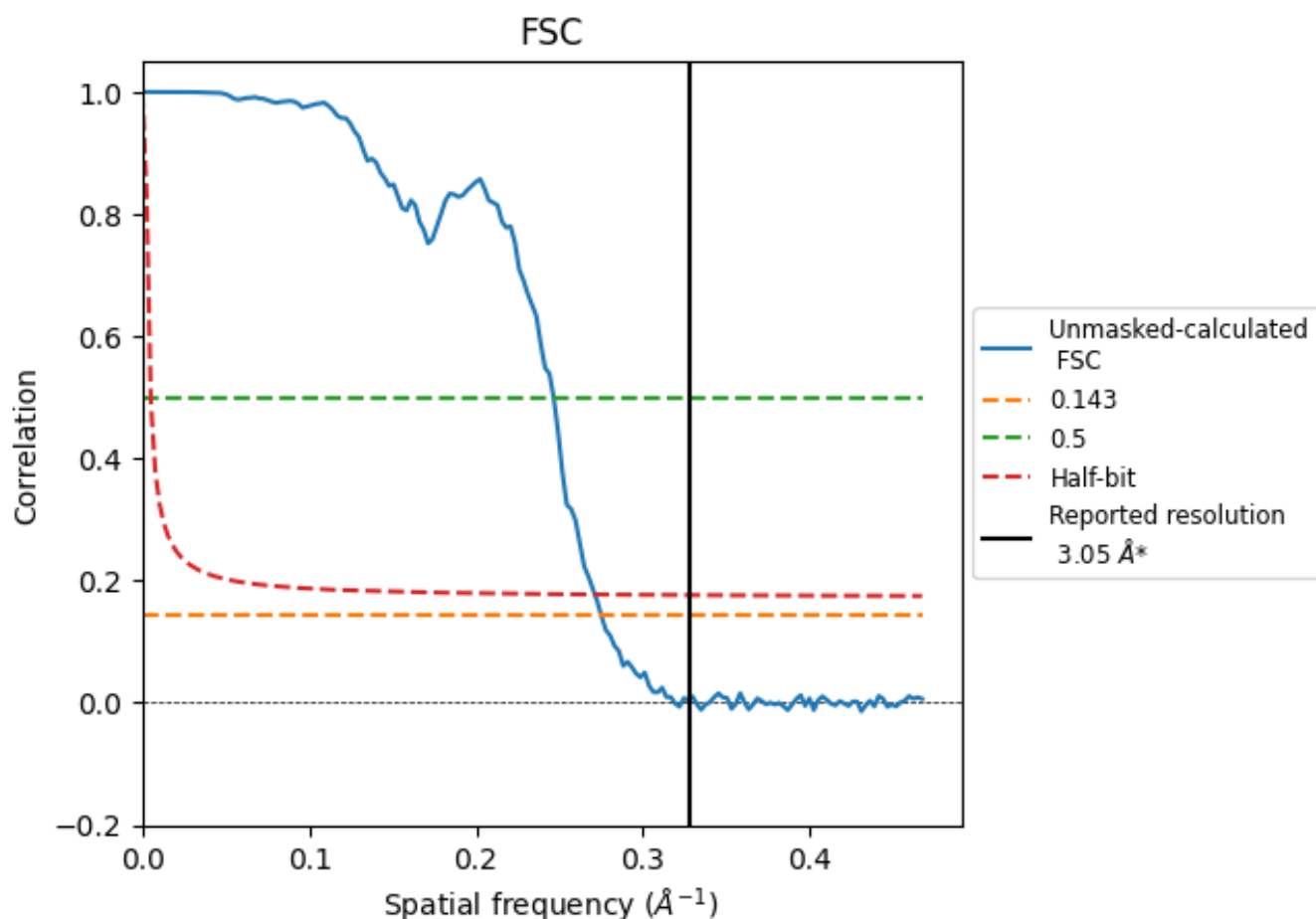


\*Reported resolution corresponds to spatial frequency of 0.328 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.05                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.64                               | 4.06 | 3.69     |

\*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 3.64 differs from the reported value 3.05 by more than 10 %

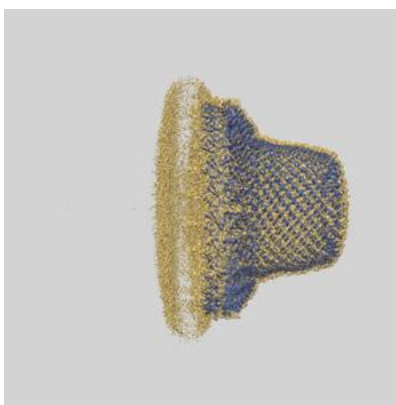
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65914 and PDB model 9WE7. Per-residue inclusion information can be found in section [3](#) on page [8](#).

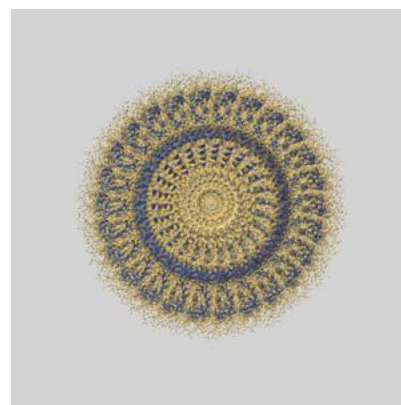
### 9.1 Map-model overlay [i](#)



X



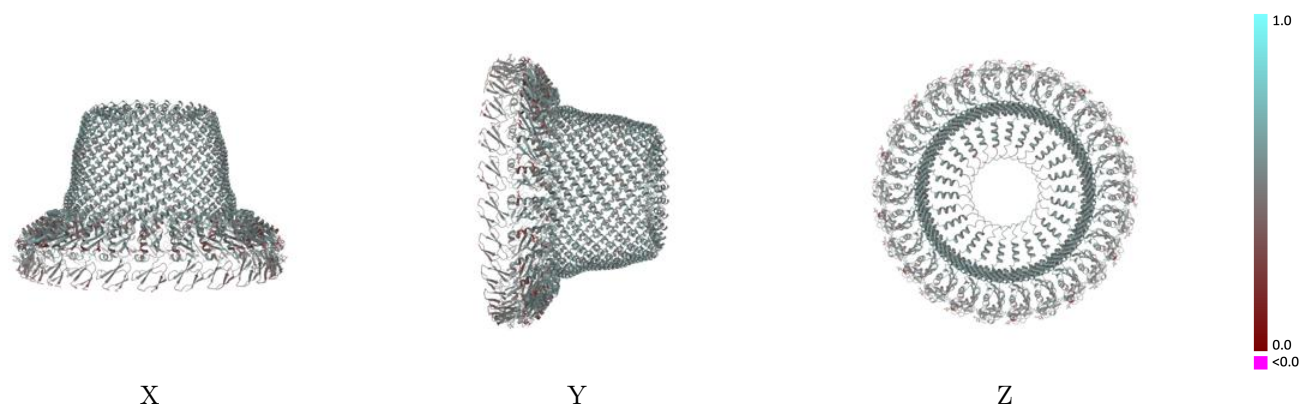
Y



Z

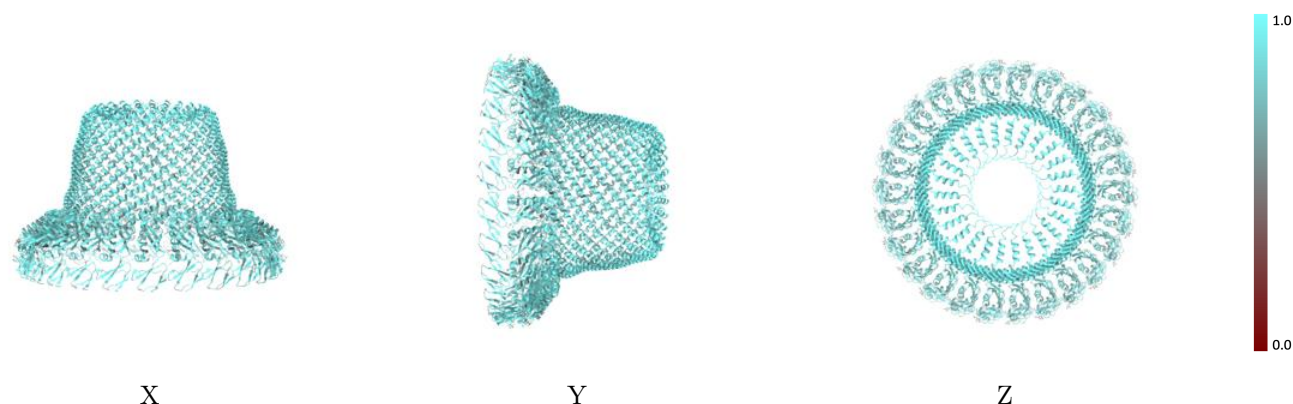
The images above show the 3D surface view of the map at the recommended contour level 0.133 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



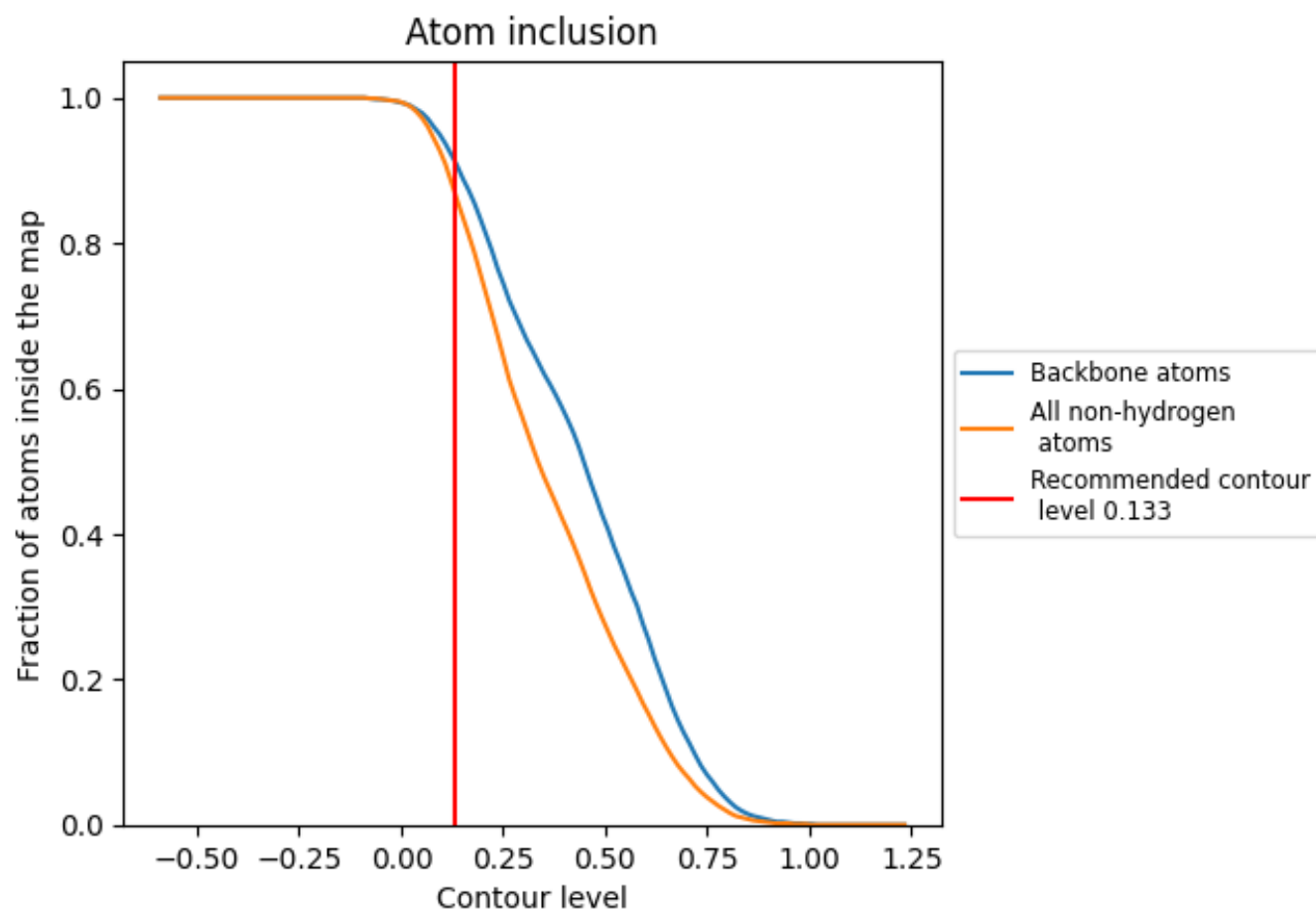
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.133).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.133) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8660   |  0.5070   |
| A     |  0.8610   |  0.5040   |
| B     |  0.8720   |  0.5170   |
| C     |  0.8640   |  0.5060   |
| D     |  0.8680   |  0.5110   |
| E     |  0.8610   |  0.5040   |
| F     |  0.8690   |  0.5100   |
| G     |  0.8610   |  0.5040   |
| H     |  0.8710   |  0.5090   |
| I     |  0.8600   |  0.5020   |
| J     |  0.8710   |  0.5090   |
| K     |  0.8620   |  0.5010   |
| L     |  0.8720   |  0.5100   |
| M     |  0.8610   |  0.5030   |
| N     |  0.8720  |  0.5080  |
| O     |  0.8560 |  0.5010 |
| P     |  0.8720 |  0.5090 |
| Q     |  0.8620 |  0.5020 |
| R     |  0.8690 |  0.5100 |
| S     |  0.8610 |  0.5020 |
| T     |  0.8710 |  0.5120 |
| U     |  0.8630 |  0.5040 |
| V     |  0.8730 |  0.5110 |
| W     |  0.8610 |  0.5050 |
| X     |  0.8690 |  0.5130 |
| Y     |  0.8620 |  0.5050 |
| Z     |  0.8730 |  0.5150 |

